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Abstract

A least-squares shape analysis program is described which is used at the Karlsruhe Nuclear Research Center for the extraction of resonance parameters from high-resolution capture data. The FORTRAN program was written for light to medium-weight or near-magic target nuclei whose cross sections are characterized on one hand by broad s-wave levels with negligible Doppler broadening but pronounced multi-level interference, on the other hand by narrow p-, d- ... wave resonances with negligible multi-level interference but pronounced Doppler broadening. Accordingly the Reich-Moore multi-level formalism without Doppler broadening is used for s-wave levels, and a single-level description with Doppler broadening for p-, d- ... wave levels. Calculated capture yields are resolution broadened. Multiple-collision events are simulated by Monte Carlo techniques. Up to five different time-of-flight capture data sets can be fitted simultaneously for samples containing up to ten isotopes. Input and output examples are given and a FORTRAN list is appended.

FANAC - Ein Multiniveau-Formanalysen-Programm zur Resonanzparameter-Bestimmung aus Neutroneneinfangdaten für leichte und mittelschwere Kerne

Zusammenfassung

Ein nach der Methode der kleinsten Quadrate arbeitendes Formanalysenprogramm wird beschrieben, welches am Kernforschungszentrum Karlsruhe zur Bestimmung von Resonanzparametern aus Neutroneneinfangdaten hoher Auflösung verwendet wird. Dieses FORTRAN-Programm wurde für leichte bis mittelschwere oder fastmagische Kerne geschrieben, deren keV-Querschnitte charakterisiert sind einerseits durch breite s-Wellen-Resonanzen mit starker Multiniveau-Interferenz bei vernachlässigbarer Doppler-Verbreiterung, andererseits durch sehr schmale p-, d- ... Wellen-Resonanzen mit vernachlässigbarer Multiniveau-Interferenz bei starker Doppler-Verbreiterung. Dementsprechend dient der Reich-Moore-Vielniveau-Formalismus ohne Doppler-Verbreiterung zur Beschreibung der s-Wellen-Resonanzen, während die p-, d- ... Wellen-Resonanzen durch Einniveau-Formeln mit Doppler-Verbreiterung beschrieben sind. Die gerechneten Einfangausbeuten werden auflösungsverbreitert. Vielfachstöße werden mit Hilfe der Monte-Carlo-Methode simuliert. An Einfangdaten von bis zu fünf verschiedenen Flugzeitmessungen kann gleichzeitig angepaßt werden für Proben bestehend aus bis zu zehn verschiedenen Isotopen. Ein- und Ausgabebeispiele sowie eine FORTRAN-Liste sind beigefügt.

Table of content

1. Main Characteristics of the Code

In the present report a computer program is described which was developped for shape analysis of data on neutron capture by structural materials. The program, FANAC, extracts resonance parameters from high-resolution capture yields measured with the time-of-flight method and calculates neutron capture cross sections corrected for experimental effects such as self-shielding, multiple scattering, instrumental resolution and detector efficiency. It permits determination of up to 20 cross section parameters by simultaneously fitting calculated capture yield curves to experimental data from up to 5 time-of-flight measurements that may differ with respect to sample thickness, flight path or other experimental characteristics. The measured and calculated capture yield data and the resulting cross sections are plotted with a general-purpose plotting subroutine in use at Karlsruhe (subroutine PLOTA, Ref. 1).

The methods employed are similar to those of the programs FANAL (for shape analysis of transmission data, Ref. 2) and TACASI (for single-level analysis of transmission areas, capture areas and self-indication ratios, Ref. 4). The main advantage over the area analysis code TACASI consists in the possibility to treat many resonances simultaneously, the more reliable interpretation of incompletely resolved multiplets and the multi-level cross section formalism which allows a better description of multiple scattering. FANAC fits obtained between 6 and 165 keV for various iron and nickel isotopes are shown e.g. in Ref. 3 .

Normally one derives neutron resonance capture cross sections from capture yield data, measured with the time-of-flight method by detection of the prompt gamma radiation that is emitted after each capture event. The count rate observed in a narrow flight time interval with neutron flux ϕ, after dead-time and background correction, can be written as

$$c = \phi \; y \; \varepsilon \qquad (1)$$

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where y, called the capture yield, is the probability that an incoming neutron is captured, and ε is the detector efficiency. The data reduction consists of stripping off ϕ and ε to get y and then to extract from y the capture cross section. For thin samples $y \approx n\sigma_\gamma$, where n is the sample thickness in atoms/b and σ_γ the radiative-capture cross section. The flux ϕ can be measured with a reference sample having a sufficiently well known yield (e.g. gold); the efficiency (or efficiency ratio in case of a relative measurement) is determined by the detector characteristics.

In practice one measures the resolution-broadened capture yield

$$\bar{y}(E) = \int r(E,E')y(E')dE', \qquad (2)$$

where $r(E,E')dE'$ is the probability that capture events induced by neutrons with energies E' in dE' are registered as if the energy were E.

A further complication arises especially for light- and medium weight nuclei from the fact that their scattering cross sections are very much larger than their capture cross sections. As a consequence self-shielding and multiple-scattering corrections are quite important for practical sample thicknesses and y cannot be taken as simply $n\sigma_\gamma$, but must be calculated as a more complicated functional of the total and capture cross sections.

Strictly speaking, the cross sections are Doppler-broadened by the thermal motion of the sample atoms. For light and medium-weight nuclides, however, Doppler broadening of typical s-wave resonances can be neglected. For the narrow p-, d- ... wave levels, on the other hand, Doppler broadening is important. Consequently, the FANAC program treats instrumental resolution according to Eq. (2) but neglects Doppler broadening for s-wave levels. It is therefore applicable only to resonance data where

the Doppler width $\Delta = \sqrt{4EkT/A}$ is much smaller than the width of the typical s-wave resonances. Narrow p-, d- ... wave levels are Doppler broadened.

The s-wave cross sections are parametrized with an R-matrix multi-level formula, whereas multi-level interference effects are neglected for narrow (p-, d-wave)levels. The program starts by calculating cross sections and capture yields from approximate values of the parameters. These starting values are then improved by application of the least-squares method (cf. e.g. Ref. 4,5). In order to make this method applicable the problem is linearized by Taylor expansion with respect to the cross section 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 number of iterations reaches a prescribed limit or until the sum of squared deviations, χ^2_k, differs by less than a given small fraction ε from that of the preceding step, χ^2_{k-1},

$$\left| \frac{\chi^2_k - \chi^2_{k-1}}{\chi^2_k} \right| < \varepsilon, \qquad (3)$$

where

$$\chi^2_k = \sum_i \left(\frac{\eta_i - \bar{y}_i^{(k)}}{\delta\eta_i} \right)^2; \qquad (4)$$

η_i: i-th measured capture yield,

$\delta\eta_i$: uncertainty of η_i,

$\bar{y}_i^{(k)}$: i-th calculated capture yield computed from parameters of k-th iteration.

The parameters to which χ^2 is most sensitive are

- resonance energies E_o;
- radiation widths Γ_γ and neutron widths Γ_n of strongly scattering (typically s-wave) levels with $\Gamma_n >> \Gamma_\gamma$;
- the capture peak area parameter $g_J\Gamma_n\Gamma_\gamma/\Gamma$ for narrow (typically p-, d- or f-wave) levels with unknown $g_J\Gamma_n$. If $g_J\Gamma_n$ is known one can get $g_J\Gamma_\gamma$.

2. Formulae

2.1 Cross sections for l = 0

In order to explain the approximations employed in FANAC the relevant cross section formalism is briefly reviewed in this section.

The total and reaction cross sections for a single nuclide and l = 0 (s-wave interactions) can be written as

$$\sigma_{To} = 2\pi\lambda\!\!\!^{-2}_n \sum_J g_J \,(1-\mathrm{Re}\; U^J_{nn}), \tag{5}$$

$$\sigma_{xo} = \pi\lambda\!\!\!^{-2}_n \sum_J g_J \,|\delta_{nx}-U^J_{nx}|^2 \tag{6}$$

where $2\pi\lambda\!\!\!^{-}_n$ is the neutron wave length in the center-of-mass system, δ_{nx} the Kronecker symbol and $g_J = (1/2)(2J+1)/(2I+1)$ the spin factor, with J and I the compound and target spin quantum numbers, respectively. The subscripts of the collision matrix elements U^J_{nn} and U^J_{nx} refer to reaction channels (n: elastic

scattering, x: arbitrary reaction). For l = 0 the spin sum consists of only one or two terms ($|I-1/2| \leq J \leq I+1/2$). According to R-matrix theory (Ref. 6) one can write

$$U^J_{cc'} = \Omega_c[(1-iK)^{-1}(1+iK)]_{cc'}\Omega_{c'} \qquad (7)$$

with

$$K_{cc'} = \frac{1}{2}\sum_\lambda \frac{\Gamma^{1/2}_{\lambda c}\Gamma^{1/2}_{\lambda c'}}{E_\lambda - E} , \qquad (8)$$

$$\Omega_c = e^{-ik_c a_c} , \qquad (9)$$

where a_c is the R-matrix channel radius and the level sum in Eq. (8) runs over all (∞) s-wave levels with spin J. The partial-width amplitudes

$$\Gamma^{1/2}_{\lambda c} = (2k_c a_c)^{1/2}\gamma_{\lambda c} \qquad (10)$$

are real quantities and vary with energy as $k_c^{1/2}$, where $k_c^2 = 1/\lambda\!\!\!^{-2}_c = 2m_c(E-E_c)/\hbar^2$ (m_c: reduced mass, E_c: reaction threshold, $\gamma_{\lambda c}$: energy-independent reduced width amplitude). The $\Gamma^{1/2}_{\lambda c}$ are to be understood as having the sign of $\gamma_{\lambda c}$.

In practice the level sum in Eq. (8) must be restricted to a finite number of resonances, typically those in a given energy interval. The levels outside this interval (distant levels) give rise to a K-matrix component, K^o say, that is smooth inside the interval. We assume that direct reactions are negligible. In this case K^o is diagonal and one can account for the distant levels omitted in Eq. (8) by using, instead of Eqs. (9) and (10),

$$\Omega_c = \exp[-i(k_c a_c - \text{arc tan } K^o_{cc})] \tag{11}$$

$$\Gamma^{1/2}_{\lambda c} = (2k_c a_c)^{1/2} \frac{\gamma_{\lambda c}}{|1-iK^o_{cc}|} \tag{12}$$

with

$$K^o_{cc} = k_c a_c \sum_\lambda{}' \frac{\gamma^2_{\lambda c}}{E_\lambda - E} \quad , \tag{13}$$

the prime indicating that the sum contains only terms from outside the interval ΔE (Ref. 6). Although the $\gamma_{\lambda c}$ and E_λ outside ΔE are mostly unknown one can estimate K^o_{cc} by means of level-statistical theory:

Introducing the optical-model pole strength, $s_c = \langle \gamma^2_{\lambda c} \rangle_\lambda / D_c$ (D_c: mean level spacing), one can replace the sum by an integration,

$$\sum_\lambda{}' \frac{\gamma^2_{\lambda c}}{E_\lambda - E} \approx P \int_{-\infty}^{\infty} dE' \frac{s_c(E')}{E'-E} - P \int_{\bar{E}-\Delta E/2}^{\bar{E}+\Delta E/2} dE' \frac{s_c(E')}{E'-E} \quad , \tag{14}$$

where $P\int$ indicates Canchy's principal value, whereas ΔE and $\bar{E}$ are length and mid-point of the energy interval excluded from the sum. The first integral is the so-called distant-level parameter, usually denoted by R^∞_c, that describes the influence of the energy variation of s_c (including the vanishing of s_c below the ground state energy). Furthermore one can neglect the energy variation of s_c and R^∞_c in the interval if ΔE is small compared to the spacing of optical-model size resonances ($\sim$ 2 MeV). Then

$$K^o_{cc}(E) \approx k_c a_c R^\infty_c(\bar{E}) + 2k_c a_c s_c(\bar{E}) \text{ ar tanh } \frac{E-\bar{E}}{\Delta E/2} \quad . \tag{15}$$

The contribution of distant levels can thus be estimated from the level-statistical parameters R_c^∞ and s_c or, equivalently, from the effective nuclear radius

$$R_c' = a_c(1-R_c^\infty) \tag{16}$$

and the s-wave strength function

$$S_{co} = 2k_c a_c s_c \sqrt{\frac{1\ eV}{E-E_c}}\ . \tag{17}$$

After thus reducing the number of levels to a manageable size one can reduce the dimensionality of the matrix K. Following Reich and Moore (Refs. 7,8) one applies the Teichmann-Wigner channel elimination prescription (Ref. 6) to the photon channels and then introduces the approximation

$$\sum_{c\in\gamma} \Gamma_{\lambda c}^{1/2}\Gamma_{\mu c}^{1/2} \approx \delta_{\lambda\mu}\sum_{c\in\gamma}\Gamma_{\lambda c} = \delta_{\lambda\mu}\Gamma_{\lambda\gamma}, \tag{18}$$

where the summation is over photon channels and $\Gamma_{\lambda\gamma}$ is the total radiation width. This is justified by the usually large number of radiative transitions that can de-excite the compound state and by the fact that the $\Gamma_{\lambda c}^{1/2}$ are symmetrically distributed around zero so that the cross terms in the sum tend to cancel, in contrast to the terms with $\lambda=\mu$. The result is the Reich-Moore prescription

$$\begin{aligned} U_{cc'}^J &= \Omega_c\left[(1-iK)^{-1}(1+iK)\right]_{cc'}\Omega_{c'} \\ &= \Omega_c\left[2(1-iK)^{-1}-1\right]_{cc'}\Omega_{c'} \end{aligned} \tag{19}$$

$$K_{cc'} = \frac{1}{2} \sum_{\lambda} \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \quad , \tag{20}$$

valid inside the interval of explicitly given resonances ($\bar{E}-\Delta E/2<E_\lambda<\bar{E}+\Delta E/2$) and for particle channels ($c,c' \notin \gamma$). All cross sections except those for neutron capture can now be obtained from Eqs. (5), (6), while the capture cross sections must be calculated as

$$\sigma_{\gamma o} = \sigma_{To} - \sum_{x \notin \gamma} \sigma_{xo} = \pi \lambda\!\!\!^{-2}_n \sum_J g_J \left(1 - \sum_{x \notin \gamma} |U^J_{nx}|^2\right). \tag{21}$$

The last equation follows from the unitarity of the collision matrix. The Reich-Moore formalism as a genuine R matrix formalism guarantees this unitarity: The restriction (18) for the partial radiation widths affects neither the symmetry nor the reality of the K-matrix. The same is true for the approximation (11), (15) to the distant levels.

In the FANAC program s-wave cross sections are calculated according to the Eqs. (5), (6), (11), (15), (19), (20), (21). The number of particle channels is restricted to 2 (elastic channel plus at most one inelastic channel), so that 1-iK is at most a 2x2 matrix which is easily inverted.

2.2 Cross sections for $l \geq 1$

The cross sections for partial waves with $l \geq 1$ are described in FANAC by

$$\sigma_{T1} = \sum_{\lambda} (\sigma_o \psi)_\lambda + 4\pi \lambda\!\!\!^{-2}_n \cdot 3 \sin^2(k_n R'_1 - \arctan k_n R'_1), \tag{22}$$

$$\sigma_{x1} = \sum_{\lambda} \left(\frac{\Gamma_x}{\Gamma}\sigma_o\psi\right)_{\lambda} \qquad (x=n,n',\gamma) , \qquad (23)$$

where

$$\sigma_o = 4\pi\lambda\!\!\!^{-2}_n \, g_J \frac{\Gamma_n}{\Gamma} , \qquad (24)$$

$$\psi = \int_{-\infty}^{\infty} dE' \, \frac{\exp[-(E-E')^2/\Delta^2]}{\Delta\sqrt{\pi}} \, \frac{\Gamma^2/4}{(E'-E_o)^2+\Gamma^2/4} , \qquad (25)$$

$$\Delta = \sqrt{\frac{4kTE_o}{A}} . \qquad (26)$$

Thus levels associated with $l \geq 1$ are treated as Doppler-broadened, non-interfering resonances. The total cross section σ_{T1} contains also the potential-scattering term for p-wave scattering. Potential scattering for $l \geq 2$ and potential-resonance interference for $l \geq 1$ is neglected. The quantity kT in Eq. (26) is the Lamb-corrected (Ref. 9) sample temperature in energy units, E_o the resonance energy and A the nuclear mass devided by the neutron mass.

The cross sections are then

$$\sigma_T = \sigma_{To} + \sigma_{T1} , \qquad (27)$$

$$\sigma_x = \sigma_{xo} + \sigma_{x1} \qquad (x=n,n') , \qquad (28)$$

$$\sigma_\gamma = \sigma_T - \sigma_n - \sigma_{n'} . \qquad (29)$$

The cross section parameters are (for each isotope, spin and parity)

- the potential-scattering parameters
  R'_J and S_{oJ} for the s-wave channel(s) (cf. Eqs. (16), (17)),
  R'_1 for the p-wave (Eq. (22)),

- the resonance parameters
  E_λ, $\Gamma_{\lambda n}$, $\Gamma_{\lambda n'}$, $\Gamma_{\lambda\gamma}$ and, if $\Gamma_{n'} \neq 0$, the relative signs
  $\mathrm{sgn}(\Gamma_{\lambda n}^{1/2}\Gamma_{\lambda n'}^{1/2}) = \mathrm{sgn}(\gamma_{\lambda n}\gamma_{\lambda n'})$.

For non-monotopic samples the isotopic cross sections must, of course, be multiplied by the appropriate abundances (and, in the case of σ_γ, by the detection efficiencies) and summed over all isotopes present in the sample, as explained in the next section.

2.4 Capture yields

The capture yield can be written as a collision series,

$$Y = Y_o + Y_1 + Y_2 + \ldots\ldots \qquad (30)$$

where the subscripts 0, 1, 2,... refer to the number of scattering collisions after which capture occurs. In order to be more specific we need

- the probability $\exp(-n\sigma_T)$ for a neutron to traverse without interaction a layer of material of thickness n (atoms/b);

- the probability $dn(d\sigma_n/d\Omega)d\Omega$ that scattering into a solid-angle element $d\Omega$ occurs within an infinitesimal sample layer dn;

- the corresponding probability $dn\sigma_\gamma$ for capture in a layer dn.

We can then write, for a sample of uniform thickness n, and cross sections σ_T, $d\sigma_n/d\Omega$, σ_γ for the incident energy,

$$y_o = \int_o^n e^{-n'\sigma_T} dn' \sigma_\gamma$$

$$y_1 = \int_o^n e^{-n'\sigma_T} dn' \int_{4\pi} d\Omega \frac{d\sigma_n}{d\Omega} \int_o^{n_1} e^{-n'_1\sigma_{T1}} dn'_1 \sigma_{\gamma 1}$$

$$y_2 = \int_o^n e^{-n'\sigma_T} dn' \int_{4\pi} d\Omega \frac{d\sigma_n}{d\Omega} \int_o^{n_1} e^{-n'_1\sigma_{T1}} dn'_1 \int_{4\pi} d\Omega_1 \frac{d\sigma_{n1}}{d\Omega_1} \int_o^{n_2} e^{-n'_2\sigma_{T2}} dn'_2 \sigma_{\gamma 2}$$

etc. (31)

where the subscripts 1,2,... refer to the number of preceding scattering collisions. The cross sections σ_{Tk}, $\sigma_{\gamma k}$, $d\sigma_{nk}/d\Omega_k$ depend on the neutron energy after k scattering collisions, which in turn depends on the angles and nuclear masses involved in all preceding collisions. Similarly the maximum material thickness n_k that a neutron can traverse without interaction after the k-th scattering collision depends on the spatial and angular coordinates of all k preceding collisions.

Performing the last integration in each term y_k one finds

$$y_o = (1-e^{-n\sigma_T}) \frac{\sigma_\gamma}{\sigma_T}$$

$$y_1 = (1-e^{-n\sigma_T}) \frac{\sigma_n}{\sigma_T} \left\langle (1-e^{-n_1\sigma_{T1}}) \frac{\sigma_{\gamma 1}}{\sigma_{T1}} \right\rangle_1$$

$$y_2 = (1-e^{-n\sigma_T}) \frac{\sigma_n}{\sigma_T} \left\langle (1-e^{-n_1\sigma_{T1}}) \frac{\sigma_{n1}}{\sigma_{T1}} \left\langle (1-e^{-n_2\sigma_{T2}}) \frac{\sigma_{\gamma 2}}{\sigma_{T2}} \right\rangle_2 \right\rangle_1$$

etc. (32)

where the brackets

$$\left\langle \ldots \right\rangle_k \equiv \int_0^{n_k\sigma_{Tk}} dn'_k\sigma_{Tk} \frac{e^{-n'_k\sigma_{Tk}}}{1-e^{-n_k\sigma_{Tk}}} \int_{4\pi} \frac{d\Omega_k}{\sigma_{nk}} \frac{d\sigma_{nk}}{d\Omega_k} \ldots \qquad (33)$$

denote averages over all possible scattering angles Θ_k and azimuths ϕ_k ($d\Omega_k = d(\cos\Theta_k)d\phi_k$) and all possible places for the k-th collision, the frequency distributions on the right-hand side of Eq. (33) being properly normalized to unity. The upper limit $n_k\sigma_{Tk}$ for the spatial distribution of interaction points along the neutron trajectory is just the maximum number of mean free paths that a neutron can traverse before the k-th collision, i.e. the distance between the (k-1)-th collision point (or, for k=1, the entrance point) and the sample surface. The quantities occuring in Eq. (32) can be interpreted as "thin sample" scattering and capture yields $n_k\sigma_{nk}$ and $n_k\sigma_{\gamma k}$, corrected for beam attenuation (self-shielding) by the factors $(1-\exp(-n_k\sigma_{Tk}))/(n_k\sigma_{Tk})$.

Since each average $\left\langle \ldots \right\rangle_k$ implies three integrations as shown by Eq. (33) the dimensionality of the integrals to be calculated for y_k increases rapidly with k, and only the first-collision yield is a simple function of cross sections and sample thickness.

Already the second-collision yield looks rather awkward even in the simple case of infinite-slab geometry:

$$y_1 = (1-e^{-n\sigma_T})\frac{\sigma_n}{\sigma_T} \int_{-1}^{1} d\mu\ p(\mu)\ \left(1-\frac{1-e^{t-t'}}{t-t'}\ \frac{t}{1-e^{t}}\right) \qquad (34)$$

with

$$t \equiv \operatorname{sgn}\mu \cdot n\sigma_T, \qquad t' \equiv \operatorname{sgn}\mu \cdot \frac{n\sigma_{T1}}{\mu} \qquad (35)$$

where μ is the cosine of the scattering angle and $p(\mu)d\mu$ the probability for μ in $d\mu$.

Higher-order terms in the collision expansion are increasingly more complicated functionals of the cross sections σ_T, σ_n, σ_γ.

2.4 Monte Carlo calulation of multiple-collision yields

The Monte Carlo method is best suited to calculate multi-dimensional integrals like those in Eqs. 32. In our case one has to simulate a sufficient number of multiple-collision events by sampling the neutron beam profile for the entry point and then, for successive collisions, the path length before the collision from

$$p(s')ds' = \frac{e^{-s'}}{1-e^{-s}}\,ds' \qquad (0<s'<s), \qquad (36)$$

the c.m.s. scattering angle θ_c from

$$p(\mu_c)d\mu_c = \frac{d\mu_c}{2} \qquad (-1\leq\mu_c\equiv\cos\theta_c\leq 1), \qquad (37)$$

the azimuth ϕ_c from

$$p(\phi_c)d\phi_c = \frac{1}{2\pi}\,d\phi_c \qquad (0\leq\phi_c<2\pi)\,. \qquad (38)$$

In writing down Eq. 37 we assumed isotropic c.m.s. scattering. In this case the simplest sampling technique is applicable to all three distributions: One samples a distribution $p(x)dx$ by generating a random number ρ between 0 and 1 and solving the equation

$$\rho = \int_0^x p(x')dx' \qquad (39)$$

for x. From the sampled c.m.s. quantities μ_c and ϕ_c one gets the corresponding quantities in the lab system,

$$\mu = \frac{A\mu_c + 1}{\sqrt{A^2+2A\mu_c+1}} = \cos\theta, \tag{40}$$

$$\phi = \phi_c \tag{41}$$

and the new energy

$$E' = E\,\frac{A^2+2A\mu_c+1}{(A+1)^2} \tag{42}$$

Although Eqs. 40-42 are valid only for target nuclei at rest and purely elastic scattering they are used in FANAC for target nuclei in thermal motion and also for inelastic collisions. Now Monte Carlo tests with the TACASI code (Ref. 4) showed that in the absence of inelastic processes the stationary-target approximation does not lead to significant errors in multiple-collision capture yield calculations even for very thick samples, except perhaps for very light sample nuclei (see Ref. 4). Application of Eqs. 40-42 to inelastic collisions, however, has no justification other than convenience and the fact that for light and medium-weight nuclei inelastic scattering in the keV region is usually much less probable than elastic scattering. The FANAC code must therefore be used with caution if both inelastic scattering and multiple collisions are important, i.e. if $\sigma_{n'} \gtrsim \sigma_n >> \sigma_\gamma$ and $n\sigma_T \gtrsim 1$.

Once the point of collision and the angles are established for the k-th collision one can calculate E' and find the corresponding cross sections $\sigma_{Tk}=\sigma_T(E')$, $\sigma_{nk}=\sigma_n(E')$ and $\sigma_{\gamma k}=\sigma_\gamma(E')$. The sample thickness n_k to the surface is obtained as follows:

The polar angle Θ was introduced above as the lab scattering angle. This implies use of a reference frame which has its polar axis parallel to the pre-collision velocity of the neutron. For the calculation of n_k, however, a lab reference frame is needed in which the sample surface has a simple description. We therefore take as the lab system a reference frame which has its z-axis coincident with the axis of the cylindrical disc sample. The transformation between both reference frames can be established as follows.

Let the neutron directions before and after the collision be given by the unit vectors $\vec{\Omega}$ and $\vec{\Omega}'$. In order to calculate the co-ordinates of $\vec{\Omega}'$ from those of $\vec{\Omega}$ and from the scattering angles θ and ϕ we introduce an intermediate reference frame which has its z-axis parallel to $\vec{\Omega}$, so that

$$\vec{\Omega} = (0,0,1), \tag{43}$$

$$\vec{\Omega}' = (\sin\theta \cos\phi,\ \sin\theta \sin\phi,\ \cos\theta). \tag{44}$$

In the lab system we introduce polar co-ordinates by writing (see Fig. 1)

$$\vec{\Omega} = (\Omega_x,\ \Omega_y,\ \Omega_z) = (\sin\zeta \cos\eta,\ \sin\zeta \sin\eta,\ \cos\zeta) \tag{45}$$

Now a unit vector can be brought from the position (0,0,1) into the position $(\sin\zeta \cos\eta, \sin\zeta \sin\eta, \cos\zeta)$ by two successive rotations (Fig. 2):

(1) rotation about the y"-axis, through an angle ζ,

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\zeta & 0 & \sin\zeta \\ 0 & 1 & 0 \\ -\sin\zeta & 0 & \cos\zeta \end{pmatrix} \cdot \begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} , \quad (46)$$

(2) rotation about the z"-axis, through an angle η,

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\eta & -\sin\eta & 0 \\ \sin\eta & \cos\eta & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} . \quad (47)$$

Combining the two transformations and expressing the polar coordinates of $\vec{\Omega}$ by its Cartesian coordinates,

$$\begin{aligned} \cos\zeta &= \Omega_z \quad , \quad \cos\eta = \frac{\Omega_x}{\sqrt{1-\Omega_z^2}} \quad , \\ \sin\zeta &= \sqrt{1-\Omega_z^2} \quad , \quad \sin\eta = \frac{\Omega_y}{\sqrt{1-\Omega_z^2}} \quad , \end{aligned} \quad (48)$$

we find eventually the lab coordinates of $\vec{\Omega}'$

$$\begin{pmatrix} \Omega'_x \\ \Omega'_y \\ \Omega'_z \end{pmatrix} = \begin{pmatrix} \Omega_x\Omega_z(1-\Omega_z^2)^{-1/2} & -\Omega_y(1-\Omega_z^2)^{-1/2} & \Omega_x \\ \Omega_y\Omega_z(1-\Omega_z^2)^{-1/2} & \Omega_x(1-\Omega_z^2)^{-1/2} & \Omega_y \\ -(1-\Omega_z^2)^{+1/2} & 0 & \Omega_z \end{pmatrix} \cdot \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \quad (49)$$

If $\Omega_z^2 = 1$ this expression fails and is to be replaced by

$$\begin{pmatrix} \Omega'_x \\ \Omega'_y \\ \Omega'_z \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \Omega_z . \quad (50)$$

Now we can calculate $n_k \sigma_{Tk}$, the number of mean free paths in the direction $\vec{\Omega}$ between the last collision point, (x_o, y_o, z_o), and the sample surface. The equations of the neutron trajectory are

$$\frac{x-x_o}{\Omega_x} = \frac{y-y_o}{\Omega_y} = \frac{z-z_o}{\Omega_z} \quad , \tag{51,52}$$

Let the surfaces of the cylindrical-disc sample be given by

$$z = 0 \qquad \text{(front face)}, \tag{53}$$

$$z = n \qquad \text{(back face)}, \tag{54}$$

$$x^2+y^2 = r^2 \qquad \text{(cylinder surface)}, \tag{55}$$

where all distances are expressed in units of atoms/b.
The point where the neutron trajectory intersects the cylinder is defined by the solution of Eqs. 51, 52 and 55,

$$\begin{aligned} x &= x_o + \Omega'_x \, d_o \\ y &= y_o + \Omega'_y \, d_o \\ z &= z_o + \Omega'_z \, d_o \end{aligned} \tag{56}$$

with $$d_o = \frac{\sqrt{b^2+ac}-b}{a} \quad , \tag{57}$$

and $$a = \Omega_x^2+\Omega_y^2 \quad , \tag{58}$$

$$b = x_o \, \Omega_x + y_o \Omega_y \, , \tag{59}$$

$$c = r^2-x_o^2-y_o^2 \quad . \tag{60}$$

The quantity d_o is just the distance to the cylinder surface. This must be compared to the distance to the front face,

$$d_1 = -\frac{z_o}{\Omega_z} \quad , \tag{61}$$

if $\Omega_z<0$, and to the distance to the back face,

$$d_2 = \frac{n-z_o}{\Omega_z} \quad , \tag{62}$$

if $\Omega_z>0$, the smaller quantity being the distance n_k (in atoms/b) that the neutron must traverse before it can escape from the sample:

$$n_k = \begin{cases} \min(d,d_1) & \text{if } \Omega_z < 0 \quad , \\ d_o & \text{if } \Omega_z = 0 \quad , \\ \min(d,d_2) & \text{if } \Omega_z > 0 \quad . \end{cases} \tag{63}$$

One can now compute the quantities

$$[1-\exp(-n_k\sigma_{Tk})]\cdot\sigma_{nk}/\sigma_{Tk} \quad \text{and} \quad [1-\exp(-n_k\sigma_{Tk})]\cdot\sigma_{\gamma k}/\sigma_{Tk}$$

and eventually the products

$$\prod_{j=0}^{k-1}(1-e^{-n_j\sigma_{Tj}})\,\frac{\sigma_{nj}}{\sigma_{Tj}}\,(1-e^{-n_k\sigma_{Tk}})\,\frac{\sigma_{\gamma k}}{\sigma_{Tk}} \tag{64}$$

whose average over many such simulated multiple-collisions events constitutes the Monte Carlo estimate of y_k.

2.5 Detector efficiencies

For non-monotopic samples the cross sections from which the capture yields must be calculated are actually abundance-weighted sums over all isotopes present in the sample, $\sigma_T = \Sigma a_i \sigma_{Ti}$, $\sigma_x = \Sigma a_i \sigma_{xi}$, with the exception of the capture cross section for which the weighting must also account for the usual isotope dependence of the capture detector efficiency (see e.g. Ref. 10). The required quantity is not the yield itself but rather the "observable yield", $y\varepsilon \equiv \Sigma y_i \varepsilon_i$. It is obtained if the cross section for detected capture, $\sigma_\gamma \varepsilon \equiv \Sigma a_i \sigma_{\gamma i} \varepsilon_i$, is used instead of $\sigma_\gamma = \Sigma a_i \sigma_{\gamma i}$. For nuclei with low level density (in the light-to-medium mass range or near closed shells) capture γ-ray spectra fluctuate significantly from resonance to resonance. The efficiencies ε_i depend therefore on energy if the capture detector is sensitive to these fluctuations. To the extent that level-level interference may be neglected for the capture cross section one can assume a different γ-ray spectrum and hence a different efficiency associated with each resonance. The efficiency to be used at a given energy is then

$$\varepsilon_i = \frac{\sum_\lambda \varepsilon_{i\lambda}\ \sigma_{\gamma\lambda}}{\sum_\lambda \sigma_{\gamma\lambda}} \quad , \tag{65}$$

where each $\sigma_{\gamma\lambda}$ is a single-level Breit-Wigner resonance term for the i-th isotope.

2.6 Resolution function

The resolution function can usually be taken as Gaussian,

$$r(E,E')dE' = \frac{1}{W\sqrt{\pi}} e^{-(E-E')^2/W^2} dE, \qquad (66)$$

with

$$W^2 = E^2 \left[c_1 (\frac{\Delta L}{L})^2 + c_2 (\frac{\Delta t}{L})^2 E\right] \qquad (67)$$

where δL is the thickness of the capture sample and Δt the observed half width (FWHM) of the γ peak in the time-of-flight spectrum resulting from photons produced in the accelerator target together with each neutron pulse. This form of the resolution function accounts for

(1) finite burst width of the accelerator-pulsed neutron source (Δt)
(2) finite channel width of the flight time analyzer (Δt),
(3) flight path differences due to finite sample thickness (ΔL),
(4) effects of detector size such as path differences of capture gamma rays and scintillation photons (Δt),
(5) electronic time jitter (Δt).

The constants $c_1 = 2/3$ and $c_2 = (60.259\ \mathrm{MeV}^{1/2}\ \mathrm{ns}\ \mathrm{m}^{-1})^{-2}$ guarantee the correct variance.

3. The Code

The modular structure of the FANAC code is shown in Fig. 3. The main program is essentially a series of CALL statements for the various subroutines, with a loop on iterations. The iterative least-squares procedure stops when either the maximum number of iterations specified in the input is completed or chi-squared remains essentially unchanged in successive iterations, as explained in Sect. 1, Eqs. 3,4. Then input for another similar job can be read in.

3.1 Subroutines

Although comments are generously used throughout the code (see Appendix) a brief description of the various subroutines may help to understand their functions.

CARDIN

CARDIN is called by the main program to read card input and to print sample and time-of-flight run specifications. Spin factors and compound spins are calculated. Then subroutine PAROUT (see below) is called to print the cross section parameter input. In the present version of the FANAC code CARDIN also calls a special subroutine, ETEC, that corrects truncation errors in channel energies caused by the data acquisition system. If the input energies are free of such errors one can eliminate subroutine ETEC and the associated CALL ~~and WRITE~~ statements in CARDIN (cards 2240 to 2390).

INDEX

This subroutine provides, for each isotope and compound spin, subscripts structuring the one-dimensional arrays containing the cross section parameters and their uncertainties:

MP(I,J) is the subscript of the first of two potential-scattering parameters (the two are distant-level strength function and effective nuclear radius),

MR(I,J) is the subscript of the first resonance parameter (there are four for each resonance, E_o, Γ_n, Γ_n, and Γ_γ)

for the I-th isotope and the J-th compound spin.
Cross section parameters are counted;

MX is their total number,

MA is the number of those which must be adjusted.

CONIJ

This subroutine calculates certain constants for each isotope (I):

D(I) is a constant which multiplied by $\sqrt{E}$ gives the Doppler width Δ (see Eq. 26),

CT(I,J) and CG(I,J) give $2\pi\lambda\!\!\!^{-2} a g_J$ and $\pi\lambda\!\!\!^{-2} a g_J$ after division by the neutron energy (a: abundance, g_j: spin factor)

MEV

MEV converts energies and resonance widths from keV to MeV and calculates the adjusted quantities $\Gamma_n^{1/2}$ and $\Gamma_{n'}^{1/2}$ from the input quantities Γ_n and $\Gamma_{n'}$, taking over the signs so that $\operatorname{sgn} \Gamma_n^{1/2} = \operatorname{sgn} \Gamma_n$, $\operatorname{sgn} \Gamma_{n'}^{1/2} = \operatorname{sgn} \Gamma_{n'}$.

CONE

This subroutine, called by the main program, calculates for each iteration the coefficients

$$A_{\mu\nu} = \sum_i \frac{y_{i,\mu}}{\delta\eta_i} \frac{y_{i,\nu}}{\delta\eta_i} , \tag{69}$$

$$c_\mu = \sum_i \frac{y_{i,\mu}}{\delta\eta_i} \frac{\eta_i - y_i}{\delta\eta_i} \tag{70}$$

of the normal equations

$$\sum_\nu A_{\mu\nu} (x_\nu - x_{o\nu}) = c_\mu \tag{71}$$

for the linearized least-squares problem, where

$x_{o\nu}$ is the initial approximation to the ν-th adjusted parameter,

x_ν the improved value to be calculated,

y_i the i-th calculated capture yield

$y_{i,\mu}$ its derivative with respect to the μ-th adjusted parameter,

η_i the i-th observed capture yield and

$\delta\eta_i$ its uncertainty.

The y_i and $y_{i,\mu}$ are calculated by numeric broadening of yields and yield derivatives obtained from the subroutines PRY, SEY and MUY. Strictly speaking the derivatives $y_{i,\mu}$ are taken as those of the primary yields because of the difficulty to get derivatives from Monte Carlo calculations. This is tantamount to neglect of errors and uncertainties in calculated multiple collision yields, so that $(\eta_i - y_i)/\delta\eta_i = (\eta_{oi} - y_{oi})/\delta\eta_i$. In other words, measured yields are reduced in each step to primary yields by subtraction of calculated multiple-collision contributions. The resulting primary yields are then fitted by parameter adjustment.

The required resolution function values come from the subroutines TGAUSS or CHISQ4. Numeric integration according to Simpson's rule is performed by subroutine SIMP. Furthermore CONE prints a table of measured and calculated yields (for details see Sect. 3.3 below).

PRY

PRY produces unbroadened primary capture yields (y_o in Eq. 32) and derivatives for the calling subroutine CONE. First an equidistant energy grid is established on the basis of the smallest resolution and Doppler width encountered. The grid is chosen so that for each incident energy E at least five integrand points are available between E-Δ and E+Δ for the resolution broadening, Δ being the Doppler width. If the resolution width and/or the energy interval to be analysed is very much larger than Δ it may happen that the number of grid points exceeds the available storage (201 points within six resolution widths, a total of 2048 grid points). In this case the Doppler width is artificially increased until the narrow resonances are sufficiently broad to allow an adequate description with the available number of grid points. This leaves s-wave results unaffected but p-wave results only to the extent that sample-thickness effects are small. It should be realized that such an artificial raise in temperature tends to increase the primary yield because the self-shielding factor $(1-\exp(-n\sigma_T))/(n\sigma_T)$ across a narrow

resonance increases. On the other hand multiple-collision yields are reduced because the sample becomes more transparent in the peak region. Thus a partial compensation could be expected even in cases where the sample is not "thin" ($n\sigma_T \ll 1$) at resonance. For narrow levels, whose width is much smaller than the average neutron energy loss per collision ($\Delta^2+(\Gamma/2)^2 \ll (2E/A)^2$), the self-shielding effect predominates, however, and the peak area parameters $g\Gamma_n\Gamma_\gamma/\Gamma$ calculated with artificially raised temperature are somewhat too small. If the limitation to 2048 internal grid points causes the difficulties one can avoid temperature readjustment by reducing the analysis interval, treating only one resonance at a time in the extreme case.

The internal grid extends beyond the boundaries of the analysis region in order to allow proper resolution broadening and multiple-collision treatment at these boundaries.

Ater having established the internal grid PRY calculates observable primary yields including efficiencies and their derivatives for all grid points. The required cross sections and cross section derivatives come from subroutine XSECT, efficiency weighting factors (Eq.65) from subroutine EFFI (see below).

SEY

SEY, called from CONE, calculates secondary yields according to Eq. 34 for all internal grid points. Since Eq. 34 is approximate and neglects effects of lateral sample extension and higher-order collisions the results are only used as weights for importance sampling in the Monte Carlo subroutine MUY.

MUY

MUY simulates multiple-collision events and calculates multiple-collision yields for all internal grid energies.

The principle of importance sampling is applied. This means that small capture yield contributions are computed with lower statistical accuracy (less neutron histories) than large contributions, in order to keep costs low. One tries to maximize the accuracy of $\Sigma_k y_k$ with the constraint $\Sigma_k N_k = N$, where the subscript $k=0,1,2,\ldots$ gives the number of completed scattering collisions, N_k is the number of simulations for the k-th order capture yield y_k and N the total number of simulations. With the plausible assumption that the accuracy of y_k is proportional to $1/\sqrt{N_k}$ one gets, by solving the extremum problem,

$$N_{k+1} : N_k = y_{k+1} : y_k \tag{72}$$

Accordingly the initial number of histories for each grid point is taken as

$$N_1 = \frac{y_1}{\max y_1} N_o \tag{73}$$

where N_o, the maximum number of simulations per grid point, is specified in the input and pertains to the energy point where y_1 has its maximum (In order to get sufficient statistics N_1 is set equal to 10 if Eq. 73 gives less). For higher-order collisions (k>1) N_{k+1} can be estimated with the geometric series approximation

$$y_{k+1} : y_k = y_k : y_{k-1} \tag{74}$$

as

$$N_{k+1} = N_k \frac{y_k}{y_{k-1}} \quad , \quad \text{if } y_k \leq y_{k-1} \, . \tag{75}$$

For $y_k > y_{k-1}$ one encounters difficulties since not enough pre-collision angles, coordinates and energies are stored. In order to avoid "splitting" /Ref. 11/ we set

$$N_{k+1} = N_k \quad , \quad \text{if } y_k > y_{k-1} \; . \tag{75}$$

MUY starts the simulations of N_1 multiple-collision events by sampling for each one the profile of the incident beam: The neutron density in the beam is taken as constant up to a certain fraction (EDGE) of the sample radius, as zero beyond. (In the present version EDGE is set equal to 0.8). After having thus established the points of incidence MUY samples coordinates and angles for N_1 first collisions. Scattering is taken as isotropic in the center-of-mass system as mentioned before. The new energies (Eq. 42) and the corresponding cross sections are found next, the latter by linear interpolation between stored values. The new direction cosines (Eq. 40,41,49) and the number of mean free paths, $n_1\sigma_{T1}$, between the collisionpoints and the sample surface (Eq. 56-63) are then calculated. Finally the scattered and captured fractions of the incident neutrons can be computed. Averaging the latter over all N_1 first collisions one gets the desired Monte Carlo estimate of y_1.

After establishing, on the basis of y_1, the number N_1 of second collisions to be simulated /Eq.74/ the computation proceeds in exact analogy to second, then to third etc. collisions until, after k collisions, N_{k+1} drops below 0.5, or until the 20th collision is completed.

For the relatively short flight paths used in Van-de-Graaff measurements the times spent by neutrons inside the sample may constitute noticeable fractions of the total registered flight times. Therefore MUY keeps track of these time delays and deposits calculated yields in correspondingly shifted

energy bins, applying some additional spreading so that the statistical fluctuations of the Monte Carlo results are smoothed out to a certain degree.

A last point should be mentioned. For the multiple-collision simulation the atomic weight of all sample nuclei is taken as the same, namely as that of the first isotope in the input. The small errors introduced in lab scattering angles and energies (cf. Eqs. 41,43) are usually tolerable in view of the other approximations invoked. If hydrogen or other very light nuclei contribute significantly to multiple scattering, however, it may be necessary to take the predominant scatterer as the first isotope in the input.

For users of the TACASI code (Ref. 4) it may be pointed out that the method adopted in MUY corresponds to the "FS-mode" (finite sample, stationary target nuclei) in TACASI.

EFFI

Subroutine EFFI, called by PRY in case not all resonance efficiencies are equal, provides energy-dependent efficiencies according to Eq. 65.

XSECT

Subroutine XSECT, called by PRY, calculates the required cross sections, cross section derivatives and transmission values for a given energy. Cross sections for the pure first isotope are also calculated for purpose of impurity correction.The formalism utilized for partial waves with $l=0$ and $l\geq 1$ is described in Sects. 2.1 and 2.2 above. The inverse of the matrix $1-iK$ (cf. Eq. 19) and its derivatives are furnished by the subroutine KMAT.

KMAT

Subroutine KMAT, called by XSECT, calculates K-matrix elements (Eq. 20), their derivatives and the elements of $(1-iK)^{-1}$.

CHOBAN

The solution of the system of normal equations (71) for the improved parameter vector requires inversion of the matrix $(A_{\mu\nu})$. This is accomplished by the subroutine CHOBAN. The method employed is that of Choleski and Banachiewicz as described e.g. in Ref. 12. The result is the covariance matrix $(B_{\mu\nu})$.

ADJ

The improved parameter vector is calculated in subroutine ADJ by multiplication of the covariance matrix $(B_{\mu\nu})$ into the deviation vector c_μ (Eq. 70) and addition of the resulting adjustment vector to the unadjusted parameter vector. The uncertainties of the adjusted parameters are calculated as

$$\delta x_\mu = \sqrt{B_{\mu\mu} \frac{\chi^2}{N-M}} \qquad (76)$$

where χ^2 is the sum of squared deviations over all N utilized data points and M the number of adjusted parameters.

For strong multiple-collision capture the convergence could be improved if the adjustment vector was reduced by 20-30 % in each step. In the present FANAC version the reduction factor (FUDGE) is set equal to 0.75 (see DATA statement).

KEV

The subroutine KEV converts energies and resonance widths back to keV prior to printing and plotting.

YPLOT

Plots of the results are prepared by subroutine YPLOT which calls a standard plotting subroutine PLOTA in use at the Karlsruhe nuclear research center (Ref. 1). The meaning of the arguements of PLOTA is explained on comment cards (see appendix) in order to facilitate replacement of PLOTA by equivalent plotting subroutines elsewhere.

PAROUT

At the start and after each iteration the cross section parameters and associated information such as abundances, atomic weigths, spin quantum numbers etc. are printed by PAROUT as illustrated in Sect. 3.3 below.

SIMP

The subroutine SIMP performs integrations according to Simpson's rule. It is utilized in the resolution-broadening calculation in CONE.

VOIGT

The subroutine VOIGT is an adaptation of the subroutine PSIXI of the group-constant programm MIGROS (Ref. 13). It calculates the symmetric and asymmetric Doppler-broadened line shape functions (Voigt profiles)

$$\psi(x,\beta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dx'}{\beta} \exp\left[-\left(\frac{x-x'}{\beta}\right)^2\right] \frac{1}{1+x'^2} \quad , \qquad (77)$$

$$\phi(x,\beta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dx'}{\beta} \exp\left[-\left(\frac{x-x'}{\beta}\right)^2\right] \frac{x'}{1+x'^2} \qquad (77')$$

that are needed in subroutine XSECT for the description of narrow resonances as described in Sect. 2.2 above, and for calculation of the associated cross section derivatives. The calculation is based on the representation

$$\psi(x,\beta) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} dy\, e^{-y^2} \frac{1+x^2+\beta^2y^2}{(1-x^2+\beta^2y^2)^2+4x^2} \quad , \qquad (78)$$

$$\phi(x,\beta) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} dy\, e^{-y^2} \frac{1+x^2-\beta^2y^2}{(1-x^2+\beta^2y^2)^2+4x^2} \quad , \qquad (78')$$

where $y = (x'-x)/\beta$. The numerical integration is performed according to the trapezoidal rule with $\Delta y = 0.7$. Unless

$$\beta < \frac{\Delta y}{\pi} \quad \text{and} \quad \frac{x^2-1}{\beta^2} + \frac{2\pi}{\beta\Delta y} > 25 \ , \tag{79}$$

which means unless Doppler broadening is very small ($\Delta \lesssim 0.1\ \Gamma$) and the energy very far from the peak, the following correction terms are added:

$$\delta\psi = \frac{2\sqrt{\pi}}{\beta} \exp\left(-\frac{x^2-1}{\beta^2} - \eta\right) \frac{\cos\xi\,(e^{-\eta}-\cos\zeta)-\sin\xi\sin\zeta}{(e^{-\eta}-\cos\zeta)^2+\sin^2\zeta} \tag{80}$$

$$\delta\phi = -\frac{2\sqrt{\pi}}{\beta} \exp\left(-\frac{x^2-1}{\beta^2} - \eta\right) \frac{\sin\xi\,(e^{-\eta}-\cos\zeta)+\cos\xi\sin\zeta}{(e^{-\eta}-\cos\zeta)^2+\sin^2\zeta} \tag{80'}$$

$$\text{with} \quad \xi = \frac{2x}{\beta^2} \ , \quad \eta = \frac{2\pi}{\beta\Delta y} \ , \quad \zeta = \frac{2\pi x}{\beta\Delta y} \ . \tag{81}$$

TGAUSS

This subroutine yields values of a truncated Gaussian distribution, normalized to unity, for the resolution-broadening calculation. The truncation limits are at $\pm\ 2\cdot\sqrt{2}$ standard deviations from the center.

CHISQ4

This subroutine is included in the present description to show the use of a skew resolution function, in this case of a χ^2-distribution with four degrees of freedom. It was actually applied to certain Fe-56 data, as shown by the call statement in subroutine CONE (the atomic weight, 56, was used as the criterion). With the information given in the comments it is easy to change the subroutine so as

to produce χ^2-distributions with other degrees of freedom, i.e. different skewness.

RANDOM

This function calls a(pseudo-)random-number generator (RANDU for IBM installations, for instance) and yields random numbers between 0 and 1. If necessary, RANDU can be replaced by an equivalent random number generator.

3.2 Input description

All numeric input must be given as FORTRAN-readable floating-point numbers. The present version of the program uses card input. As a rule 10 card columns are reserved for each number (the exception being the last two items on "resonance cards", see below). Within this field the number can be placed arbitrarily in F format, for E format the usual rules apply. This structure permits complete ommission of resonances or of data points from the input. One can easily change the number of resonances or data points by simply adding or removing input cards. Isotopic or spin reassigment of a given resonance requires nothing but repositioning of one "resonance card" in the input deck.

All energies must be given in keV, all channel radii in fm, all flight-time increments in ns, all lengths (flight paths, sample dimensions) in m. If other units are preferred it is easy to change the corresponding input and output formats by means of FORTRAN scale factors (along with the units in the printed table headings).

Input formats are essentially the same as for the FANAL code (Ref. 2) so that the same "isotope", "potential-scattering" and "resonance cards" (see below) can be used

for both codes. This has proved very convenient for parallel shape analysis of both capture and transmission data.

Each potential-scattering or resonance parameter is followed by an initial "uncertainty". If this uncertainty is set equal to zero the associated parameter is treated as constant, otherwise the parameter is adjusted in each iterative step.

The fact that the same input structure is used both in FANAL und FANAC is the reason that certain parameters such as distant-level strength functions or effective radii can be declared as adjustable although this is not practical in capture data analysis since capture yields depend on these quantities only weakly through self-shielding factors and multiple-collision yields.

The card input is structured as follows.

1st Card (Title Card)

Columns 1 - 80 Arbitrary alphameric text. This text appears on the print-out and also on the plots.

2nd Card (Analysis and Iteration Characteristics)

Columns 1 - 10 Lower boundary E_{min} (keV),

" 11 - 20 upper boundary E_{max} (keV) of the range of explicitly treated resonances, i.e. of the range for which the extracted parameters (including the distant-level strength function and the effective nuclear radius, Eqs. 15-17) are valid. Note that ΔE and $\bar{E}$ in Eq. 15 are calculated as $\Delta E = E_{max} - E_{min}$, $\bar{E} = (E_{max} + E_{min})/2$.

" 21 - 30 Effective temperature T(K), cf.Eq. 26, taken as the same for all isotopes.

" 31 - 40 Largest relative variation $\delta\chi^2/\chi^2$ between sucessive iterations (cf.Eq. 3) which is considered as sufficient to terminate the iterative process and to declare convergence achieved (values of order 1 to 5 % were found to be reasonable).

" 41 - 50 Maximum number of iterations to be followed through.

3rd Card (Isotope Card)

The isotope which contributes most to multiple-collision capture should come first, as its atomic mass is used to determine all energy losses and lab angles.

Columns 1 - 10 Isotopic abundance a of the first sample nuclide (i.e. fraction of sample atoms belonging to this nuclide).

Columns	11 - 20	Atomic mass of first sample nuclide divided by neutron mass (it is usually sufficient to use simply the nucleon number A).
"	21 - 30	Nuclear spin quantum number I of the first nuclide.
"	31 - 40	Effective nuclear radius R'_1 (fm) for p-wave scattering of the first nuclide (see Eq. 22).

4th Card (Potential-Scattering Card)

Columns	1 - 10	Effective s-wave strength function $S_{I+1/2}$ of first nuclide. ($S_{I+1/2}$ and $R'_{I+1/2}$ determine the influence of distant levels on s-wave scattering, see Eqs. 15-17).
"	11 - 21	Initial uncertainty+) of $S_{I+1/2}$.
"	21 - 30	Effective radius $R'_{I+1/2}$(fm) of first nuclide (see Eq. 16).
"	31 - 40	Initial uncertainty+) of $R'_{I+1/2}$.
"	41 - 50	Threshold $E_{I+1/2}$ (keV) for first inelastic channel, first isotope, compound spin I+1/2 (see text below Eq. 1o).

5th Card (Resonance Card)

Columns	1 - 10	Resonance energy E_o (keV), lab system,
"	11 - 20	Initial uncertainty+) of E_o,
"	21 - 30	Neutron width Γ_n (keV),
"	31 - 40	Initial uncertainly+) of E_o,
"	41 - 50	Partial width for inelastic scattering $\Gamma_{n'}$ (keV) with the sign of $\gamma_n\gamma_{n'}$ (see text after Eq. 10),
"	51 - 60	Initial uncertainty+) of $\Gamma_{n'}$,
"	61 - 70	Radiation width Γ_γ (keV).
"	71 - 75	Initial uncertainty+) of $\Gamma\gamma$.

+) The preceding parameter is kept constant if the uncertainty is zero, otherwise it is adjusted.

Columns 76 - 80 Detection efficiency ε (see Eq. 65 where this quantity is denoted by $\varepsilon_{i\lambda}$), may include gamma ray absorption, gamma spectrum fraction above detector threshold, intrinsic detector efficiency etc.

As a rule the smallest partial width should be varied (if necessary), otherwise convergence may be bad.

A similar "resonance card" follows for each s-wave resonance with spin I+1/2 belonging to the first isotope. If this isotope has non-zero ground state spin, s-wave neutrons can excite also resonances with spin I-1/2. For this second possible compound spin a similar set of cards must be prepared, consisting of at least a "potential-scattering card" and optionally a number of "resonance cards". If, for a given isotope and compound spin, no "resonance cards" are encountered, only the potential-scattering cross section is calculated.

So-called p-,d-,... wave levels, i.e. resonances which can only be excited by neutrons with $l \geq 1$, $l \geq 2$,..., must be treated as levels of additional (pseudo-) isotopes, with vanishing s-wave scattering ($S_J = R'_J = 0$). For each occurring spin factor g_J there must be one pseudo-isotope, with I (ground state spin quantum number) set equal to zero and the abundance set equal to $g_J a$ (a: true abundance). In Sect. 4 below this is illustrated for p- and d-wave levels of ^{56}Fe+n (g_J=1,2 and 3). For most levels with $l \geq 1$, however, spins are unknown and only the combination $g_J \Gamma_n \Gamma_\gamma / \Gamma$ can be estimated from the capture data. One must then use average values for g_J and Γ_γ to calculate the corresponding Γ_n and use these figures as input (see the example in Sect. 4). This is quite adequate if self-shielding and (multiple) scattering are unimportant ($n\sigma_T << 1$) or dominated by s-wave scattering ($\sigma_{T1} << \sigma_{To}$, Eq. 27). In this case the capture yields depend

mainly on $g_J\Gamma_n\Gamma_\gamma/\Gamma$, i.e. on the "unshielded" resonance area. For thick samples and relatively small s-wave cross sections, however, it can make a difference whether a resonance with given peak area is treated as narrow and high (large g_J) or as broad and low (small g_J).

If the capture sample contains other isotopes (sample impurities, oxygen in oxides, hydrogen in adsorbed moisture etc.) completely analogous input cards must be prepared for each nuclide: an "isotope card" followed by a "potential-scattering card" plus "resonance cards" (optional) for I+1/2, then for I-1/2 if I>0. Up to ten isotopes and pseudo-isotopes can be handled.

The cards specifying the cross section parameters are followed by other cards carrying information for up to five time-of-flight runs. For each run one needs a "sample card", a "time-of-flight card", "capture yield data cards" and one blank card:

Sample Card

Columns	1 - 10	Sample thickness n (atoms/b), i.e. total number of sample atoms per barn.
	11 - 20	Sample radius r (atoms/b), see Eq. 55.

Time-of-flight Card

Columns	1 - 10	Flight path L (m), to mid-plane of sample.
"	11 - 20	Sample thickness ΔL (m), see Eq. 67.
"	21 - 30	Full width at half maximum of gamma peak, Δt (ns), see Eq. 67.
"	31 - 40	maximum number N_o of Monte Carlo multiple-collision event simulations per energy point, see Eq. 73.
"	41 - 50	Time shift (ns) to correct for small time-zero channel differences between time-of-flight runs (can usually be left blank).

Capture Yield Card

Columns	1 - 10	Energy E_i (keV)
	11 - 20	Capture yield divided by sample "thickness", η_i/n (b).
	21 - 30	Uncertainty $\delta\eta_i/n$ (b).
	31 - 40	Energy E_{i+1} (keV).
	41 - 50	Capture yield divided by sample "thickness", η_{i+1}/n (b).
	51 - 60	Uncertainty $\delta\eta_{i+1}/n$ (b).

Thus two data points including their uncertainties can be put on each "capture yield card". Up to 512 experimental points (total for all TOF runs) can be simultaneously fitted. It is to be noted that energies are given explicitly, i.e. regularity or equidistance on a time-of-flight scale is not required (in contrast to the FANAL code, Ref. 2). Pairs of data points not to be used for the fit can thus be taken out quite easily.

The last capture yield card from a given time-of-flight run (which may contain a single data point) must be followed by a blank card. Two blank cards signal the end of the whole input.

Input for other calculations may follow, i.e. problems can be stacked.

In addition to the card input there are a few quantities which are specified by DATA or other statements in the program:

- the adjustment reduction factor FUDGE in subroutine ADJ (DATA statement),
- the ratio of beam radius to sample radius, EDGE, in subroutine MUY (DATA statement),
- the minimum number of first collisions per grid energy in subroutine MUY (card no. 11830).
- The constants A,B,C in subroutine CHISQ4 refer to 4 degrees of freedom as explained on comment cards in CHISQ4.

3.3 Output description

The output consists of print-out and plots.

The print-out shows first the contents of "title", "isotope", "potential-scattering", "resonance" and "time-of-flight" cards and some additional derived information such as compound spins. This is followed by tables of measured and calculated capture cross section data (observed yields divided by sample "thickness" y/n and capture cross sections σ_γ). These quantities are calculated for the sample composition and include detector efficiencies.Subsequently the values of the squared-error sum χ^2 and of Gauss' error adjustment factor $\sqrt{\chi^2/(N-M)}$ are printed (N: number of data prints, M: number of adjusted parameters). For a good fit the error adjustment factor should be close to 1.

Ater that one gets a table with the adjusted and constant parameters and their uncertainties. The latter are the square roots of the corresponding diagonal elements of the covariance matrix, multiplied by the error adjustment factor. The covariance matrix elements result from the experimental uncertainties by normal error propagation (in linear approximation), the error adjustment factor characterizes the goodness of the fit.

If the maximum number of iterative steps exceeds 1 a similar printout (yield table plus improved parameters) is obtained for each completed step. If the number is set equal to 1 the cross section of the pure first isotope is also calculated. In this way the code can be used to generate and plot Doppler-broadened cross sections corrected for all experimental effects such as sample impurities, instrumental resolution, detector efficiency, self-shielding, and multiple scattering.

For each iterative step a plot is produced which contains all experimental points and their error bars together with the calculated values in curve form. The text of the title card appears under each plot. If only one iteration is requested a second plot is obtained showing the Doppler-broadened capture cross section of the pure first isotope.

For the last set of parameters neither capture yield nor χ^2 values are calculated, printed or plotted. If the convergence criterion, Eq. 3, with reasonably chosen ε is satisfied there should be no significant change with respect to the preceding step.

4. Example

Fig. 4 shows the input cards for a realistic fitting problem which illustrates most features of FANAC:

Data from two measurements, taken with the same Fe_2O_3 sample enriched to 99.7 % ^{56}Fe but with slightly different resolution, were to be analyzed between 21.6 and 41.1 keV (for experimental details see Ref. 3, 14). The range of explicitly treated ^{56}Fe-resonances with l=0 (including a subthreshold level at -3.9 keV) was taken as -6 to 100 keV, the effective temperature as 300 K and the convergence threshold (ε in Eq. 3) as 3 %.

The cards for s-wave levels are followed by those for narrow resonances with $l \geq 1$ which are represented as levels of three fictitious isotopes with target spin zero and abundance of 0.997 = 99.7 % (for g_J=1), 2·0.997 = 1.994 (for g_J=2) and 3·0.997 = 2.991 (for g_J=3), as explained in the input description (Sect. 3.2). Potential scattering for l=1 is represented by an effective nuclear radius of 5.4 fm of the first fictitious isotope.

The only important impurity was oxygen. Its smooth cross section is specified by a potential-scattering card without resonance cards following. Its relative abundance is 1.5 corresponding to the stoichiometric ratio in Fe_2O_3. This means that the sample thickness must be given in Fe-atoms per barn. Alternatively one could have given the total number of all (iron and oxygen)nuclei per barn in the sample along with relative abundances of $(2/5)\cdot 0.997\cdot g_J$ for ^{56}Fe and 3/5 for oxygen.

Sample, run and capture yield cards for the utilized two time-of-flight runs follow.

Fig. 5-7 show the cross section parameter input and the tables with measured and calculated yields and cross sections (inclusive of detector efficiencies) as they are printed by the computer.Fig.8 shows the corresponding plots. Convergence, i.e. less than 5 % variation of χ^2, was formally reached after four iterations. The final value $\sqrt{\chi^2/(M-N)} = 1.288$ is close enough to unity to indicate that input data, input errors and mathematical model (cross section formalism, multiple-collision treatment, resolution function) are reasonably consistent with each other. A slightly better χ^2 might be achieved with a more exact resolution function, but no significant change in resonance parameters is expected.

A few words on input preparation may be appropriate.
First estimates of the resonance energies were obtained directly from the capture data by inspection. The starting value for the radiation width of the broad s-wave resonance near 27.6 keV was taken from the "barn book" (Ref. 15). The peak area parameters $g_J\Gamma_n\Gamma_\gamma/\Gamma$ of the narrow levels were estimated from the data by equating the observed peak areas to the theoretical thin-sample expression,

$$\delta E \sum_i \frac{\eta_i}{n} = \frac{\bar{a}\varepsilon}{n} 2\pi\lambda\!\!\!^{-2} g_J \frac{\Gamma_n\Gamma_\gamma}{\Gamma} \qquad (82)$$

where the sum extends over the peak, δE is the spacing of the data points near the peak, χ^2 is calculated at resonance and the other symbols have the same meaning as before (a: abundance, ε: detection efficiency for the resonance). From a Bayesian analysis of available values of $g_J\Gamma_n$, $g_J\Gamma_\gamma$ and $g_J\Gamma_n\Gamma_\gamma/\Gamma$ for ^{56}Fe+n the radiation widths for p- and d- wave resonances were known to be close to 0.33 and 0.6 eV, respectively. The same type of analysis was used to select spins and parities by Monte Carlo sampling. The resulting g_J and Γ_γ were then used to calculate the input values of Γ_n from the estimated $g_J\Gamma_n\Gamma_\gamma/\Gamma$. For each observed resonance the smaller of the two partial widths was adjusted. The efficiency factors assigned to individual resonances were estimated from observed capture gamma ray spectra. They also include an estimated correction for quasi-prompt capture of resonance-scattered neutrons in the immediate vicinity of the sample (cf.Refs. 3,10).

The print-out shows that the temperature was raised artificially to 6368 K in order to avoid difficulties with the equidistant internal energy grid as explained in Sect. 3.1 (subroutine PRY). One can treat the narrow resonances separately to avoid or at least reduce this automatic temperature change. Taking for example only the data between 22.1 and 23.2 keV, i.e. analyzing only the peak near 22.75 keV, one gets a much smaller change to only 1171 K. Nevertheless, the resulting $g_J\Gamma_n\Gamma_\gamma/\Gamma$ is essentially unchanged.

A similar insensitivity exists with respect to the correct spin factor: if all spin factors are set equal to 1 (i.e. all narrow levels are assigned to the same fictitious isotope with a = 0.997) the results are essentially unchanged. The reason is the same as before: In our example s-wave scattering of ^{56}Fe and ^{16}O predominates even near the peaks of the narrow levels. Therefore changes in g_J or in the temperature, which otherwise would affect the peak area through the beam-attenuation

factor $(1-\exp(-n\sigma_T)) / (n\sigma_T)$, have no great influence. In other cases, however, where s-wave scattering does not predominate, spin and (unless $\Gamma << \Delta$) temperature effects may be important.

Multiple-collision contributions in this example are seen to be of the order of few percent near the peaks of the narrow resonances but quite substantial near the broad peak near 27.6 keV and in the valleys between resonances.

The CPU time for the whole job (3 iterations, 12 adjusted parameters, a maximum of 30 Monte Carlo multiple-collision event simulations per grid point) was 3 min 19 sec on an IBM/370-168 computer. The memory space required was 476 k bytes.

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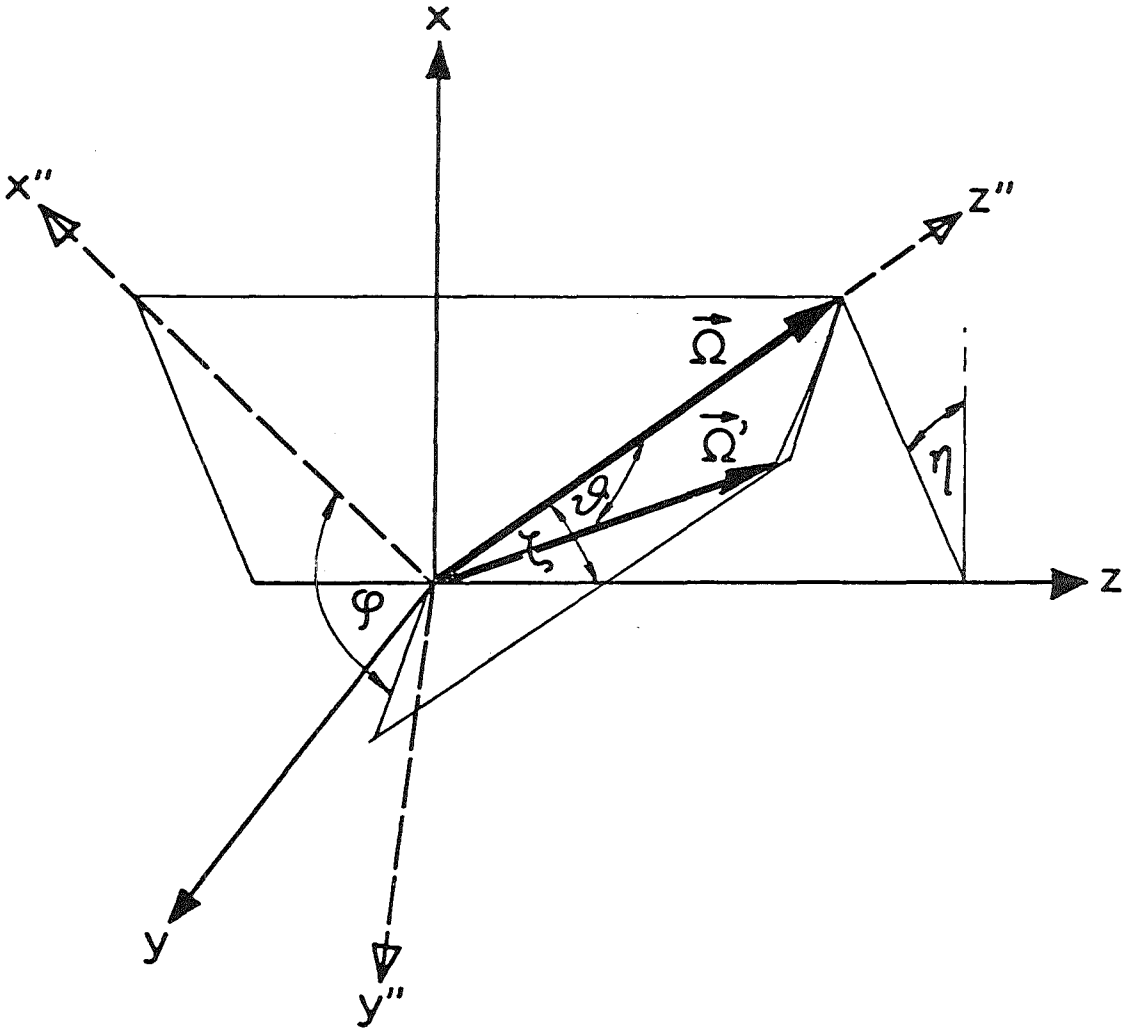


Figure 1. Neutron directions $\vec{\Omega}$, $\vec{\Omega}'$ (before and after collision, resp.) and angles ζ, η, ϑ, φ, and their positions relative to the laboratory system (x, y, z) and to the system S'' (x'', y'', z''), in which $\vec{\Omega}$ has the coordinates (0, 0, 1).

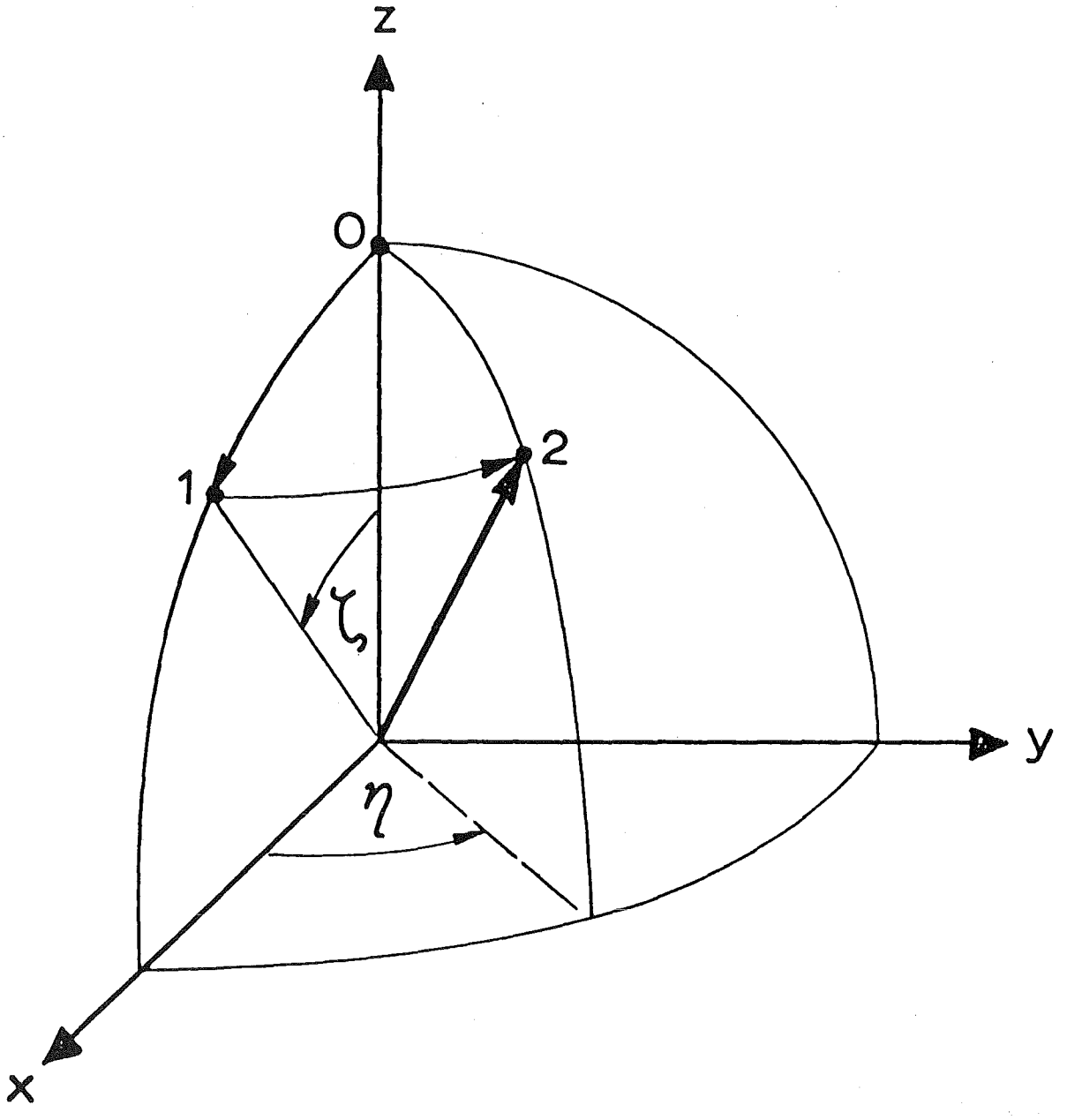


Figure 2. Two-step rotation of a vector from the position (0, 0, 1) into the position ($\sin\zeta \cos\eta$, $\sin\zeta \sin\eta$, $\cos\zeta$).

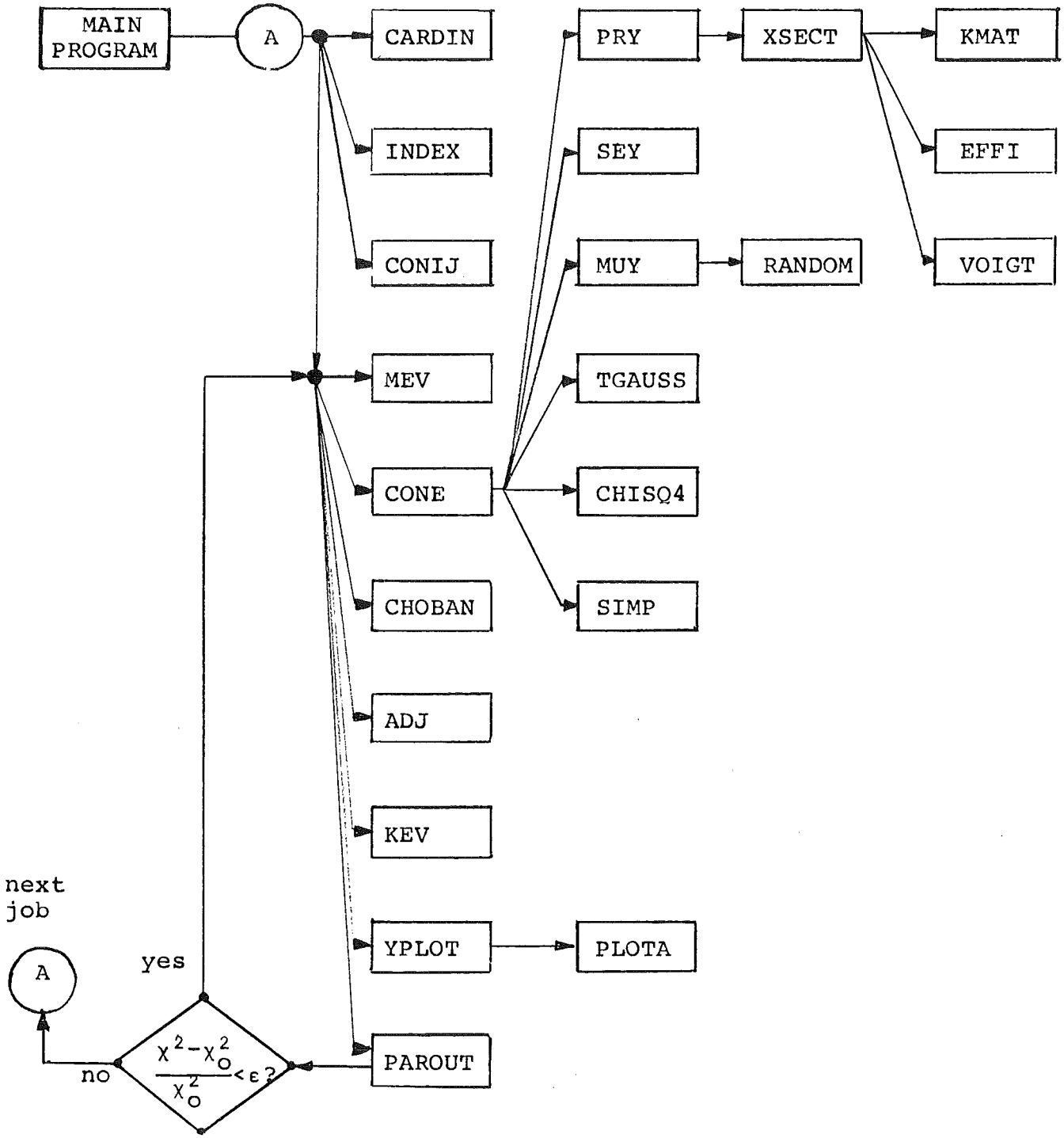
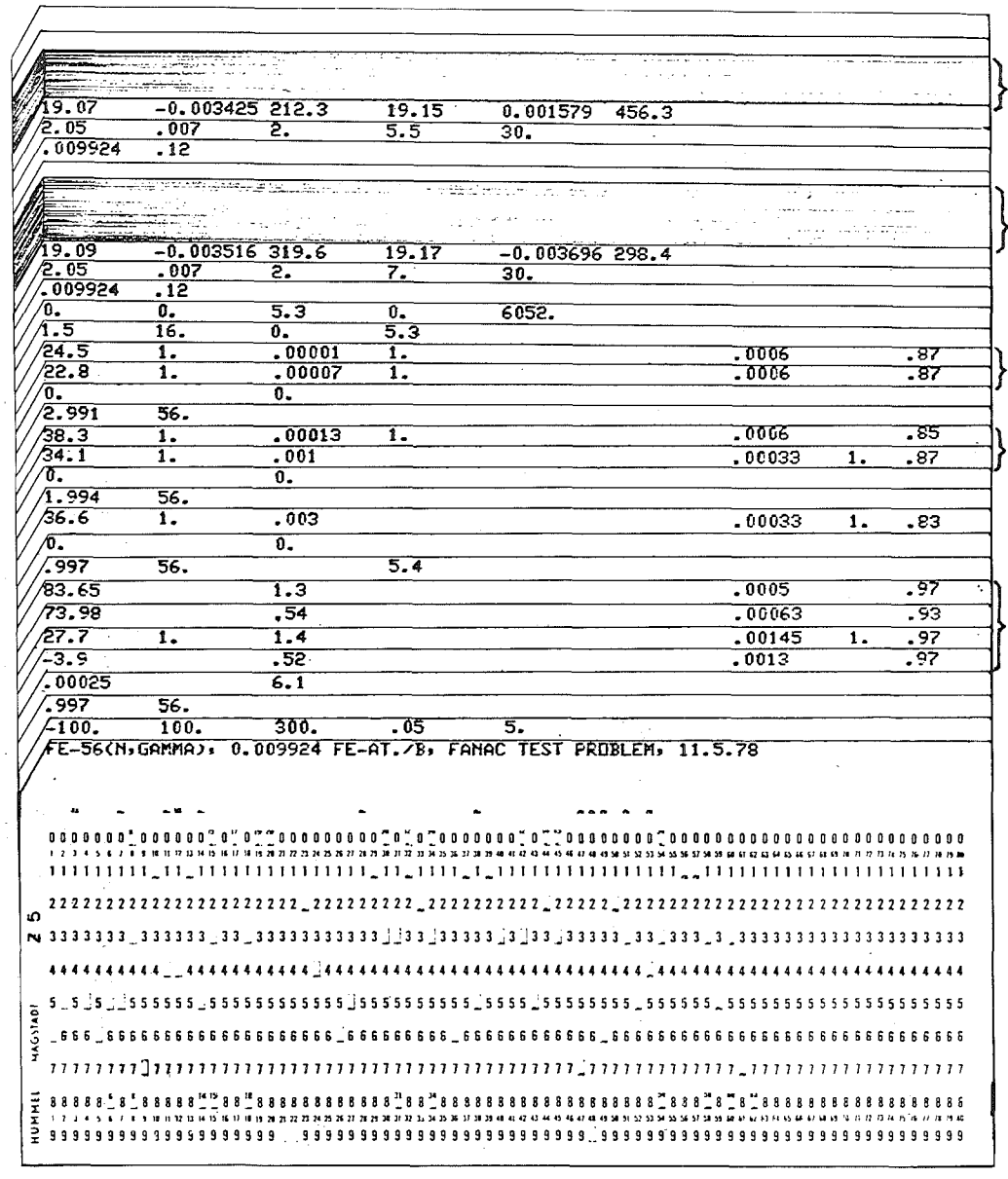


Fig. 3 FANAC program structure



blank card (end of job)
blank card
capture yield cards } 2nd time-of-flight run
time-of-flight card
sample card
blank card
capture yield cards } 1st time-of-flight run
time-of-flight card
sample card
potential-scattering card } ^{16}O
isotope card
resonance cards } $l \geq 1$, $g=3$
potential-scattering card
(pseudo-)isotope card
resonance cards } $l \geq 1$, $g=2$ } ^{56}Fe
potential-scattering card
(pseudo-)isotope card
resonance card } $l \geq 1$, $g=1$
potential-scattering card
(pseudo-)isotope card
resonance cards } $l=0$
potential-scattering card
isotope card
analysis and iteration characteristics
title card

Fig. 4 -- Card input for analysis of two sets of capture yield data taken with the same Fe_2O_3 sample enriched to 99.7 % ^{56}Fe but slightly differing resolution. See text (Sect. 4) for further details.

FE-56(N,GAMMA), 0.009924 FE-AT./B, FANAC TEST PROBLEM, 11.5.78

EXPLICIT-RESONANCE RANGE: -100.000 ... 100.000 KEV
EFFECTIVE TEMPERATURE: 300.0 KELVIN
MAXIMUM TOLERABLE CHI**2 CHANGE: 0.0500 (RELATIVE)
MAX. NUMBER OF ITERATIVE STEPS: 5.

SPECIFICATIONS OF UTILIZED MEASUREMENTS:

MMENT. NO.	SAMPLE THICKNESS (NUCLEI/B)	SAMPLE RADIUS (NUCLEI/B)	FLIGHT PATH (M)	SAMPLE THICKNESS (M)	CHANNEL WIDTH (NS)	FWHM GAMMA PEAK (NS)	MONTE CARLO HISTORIES	TIME SHIFT CORRECTION (NS)
1	9.924E-03	1.200E-01	2.0500	0.0070	2.000	7.000	30.	0.0
2	9.924E-03	1.200E-01	2.0500	0.0070	2.000	5.500	30.	0.0

CROSS SECTION PARAMETERS:

ABUN-DANCE	ATOMIC WEIGHT	TARGET SPIN	P-WAVE RADIUS (FM)	COMP. SPIN	S-WAVE STRENGTH FUNCTION /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.	DETECT. EFFIC.
0.9970	56.0	0.0	0.0	0.5	2.500E-04 0.0	6.100 0.0	0.0	-3.900 0.0	5.200E-01 0.0	0.0 0.0	1.300E-03 0.0	0.970
								27.700 1.000	1.400E+00 0.0	0.0 0.0	1.450E-03 0.100E+01	0.970
								73.980 0.0	5.400E-01 0.0	0.0 0.0	6.300E-04 0.0	0.930
								83.650 0.0	1.300E+00 0.0	0.0 0.0	5.000E-04 0.0	0.970
0.9970	56.0	0.0	5.400	0.5	0.0 0.0	0.0 0.0	0.0	36.600 1.000	3.000E-03 0.0	0.0 0.0	3.300E-04 0.100E+01	0.830
1.9940	56.0	0.0	0.0	0.5	0.0 0.0	0.0 0.0	0.0	34.100 1.000	1.000E-03 0.0	0.0 0.0	3.300E-04 0.100E+01	0.870
								36.300 1.000	1.300E-04 0.100E+01	0.0 0.0	6.000E-04 0.0	0.850
2.990	56.0	0.0	0.0	0.5	0.0 0.0	0.0 0.0	0.0	22.800 1.000	7.000E-05 0.100E+01	0.0 0.0	6.000E-04 0.0	0.870
								24.500 1.000	1.000E-05 0.100E+01	0.0 0.0	6.000E-04 0.0	0.870
1.5000	56.0	0.0	5.300	0.5	0.0 0.0	5.3 0.0	6052.000					

EFFECTIVE TEMPERATURE : 8249. DEG. KELVIN,
RESULTING DOPPLER WIDTH: 31.133 EV AT 19.092 KEV

Fig. 5 - Beginning of FANAC print-out: content of input cards excepting capture yields. The last two lines are a warning that the effective temperature was raised artificially in order to reduce the number of internal grid points (see text).

ITERATION STEP 1, TIME-OF-FLIGHT RUN NO. 1

SAMPLE THICKNESS: 9.924E-03 NUCLEI/B
FLIGHT PATH : 2.050E+00 M

NEUTRON ENERGY (KEV)	MEASURED YIELD-OVER-THICKNESS (MILLI-BARN)		CALCULATED VALUES (MILLI-BARN)	FROM MULT. COLLISIONS (PERCENT)	CALCULATED CROSS SECTION (MILLI-BARN)	
19.092	-3.516 ±	11.237	0.820	10.717	0.797 ±	0.0
19.165	-3.696 ±	11.024	0.837	10.374	0.758 ±	0.0
19.238	11.694 ±	10.936	0.838	10.283	0.721 ±	0.0
19.312	15.888 ±	10.899	0.857	9.834	0.858 ±	0.0
19.386	13.596 ±	10.782	0.890	9.186	0.840 ±	0.0
19.461	0.583 ±	10.536	0.902	8.890	0.871 ±	0.0
19.536	-0.288 ±	10.429	0.906	9.105	0.912 ±	0.0
19.611	-10.203 ±	10.346	0.922	9.500	0.900 ±	0.0
19.687	-9.814 ±	10.265	0.946	9.825	0.865 ±	0.0
19.764	-0.696 ±	10.135	0.961	10.061	0.830 ±	0.0
19.841	-5.967 ±	9.965	0.984	10.139	1.013 ±	0.0
19.918	14.104 ±	9.972	1.016	10.087	0.962 ±	0.0
19.996	10.227 ±	9.777	1.033	9.818	0.983 ±	0.0
20.074	19.817 ±	9.869	1.033	9.499	0.966 ±	0.0
20.153	5.213 ±	9.602	1.051		0.941 ±	0.0
20.232	6.458 ±	9.532	1.07		.986 ±	0.0
.311	-1.806 ±	9.389			0 ±	0.0
	-2.365 ±	9.218			±	0.0
	7.094 ±	9.009				0.0
	±	8.				0.0
						0
35.				69.858		
35.886				57.996	0.	
36.074				46.813	0.64	
36.264	15.905 ±		.699	33.926	0.575 ±	
36.455	31.526 ±	4.004	15.628	19.698	0.548 ±	
36.648	46.688 ±	5.136	25.949	9.554	1.306 ±	
36.842	41.927 ±	4.738	40.961	4.050	132.666 ±	0.
37.039	17.675 ±	3.058	47.858	4.560	0.757 ±	0.0
37.235	10.338 ±	2.667	6.516	38.939	0.451 ±	0.0
37.434	6.997 ±	2.527	3.719	74.388	0.453 ±	0.0
37.635	12.981 ±	2.722	4.228	42.027	0.355 ±	0.0
37.837	16.515 ±	2.890	5.394	43.648	0.382 ±	0.0
38.041	19.946 ±	3.072	7.892	24.078	0.408 ±	0.0
38.246	32.576 ±	3.909	13.416	13.880	0.403 ±	0.0
38.453	50.792 ±	5.384	22.841	10.035	50.482 ±	0.0
38.662	29.836 ±	3.700	32.941	8.255	0.457 ±	0.0
38.873	4.133 ±	2.423	24.773	11.779	0.301 ±	0.0
39.085	3.667 ±	2.362	3.091	90.396	0.321 ±	0.0
39.299	6.985 ±	2.438	2.617	89.108	0.345 ±	0.0
39.515	4.174 ±	2.362	2.029	86.297	0.326 ±	0.0
39.732	2.301 ±	2.310	1.664	84.372	0.254 ±	0.0
39.952	2.682 ±	2.293	1.274	81.375	0.247 ±	0.0
40.173	4.059 ±	2.289	1.152	80.664	0.226 ±	0.0
40.396	3.631 ±	2.258	1.093	79.577	0.236 ±	0.0
40.621	0.015 ±	1.500	0.959	76.704	0.231 ±	0.0
40.848	-1.193 ±	2.202	0.739	70.430	0.233 ±	0.0
41.076	-2.439 ±	2.175	0.545	61.223	0.221 ±	0.0
41.307	2.433 ±	2.165	0.437	54.023	0.246 ±	0.0
41.539	1.252 ±	2.131	0.313	41.205	0.156 ±	0.0
41.774	7.016 ±	2.23	0.203	19.086	0.183 ±	0.0
42.010	-0.751 ±	2.093	0.194	17.463	0.182 ±	0.0
42.249	4.109 ±	2.141	0.193	17.360	0.155 ±	0.0
42.489	1.765 ±	2.093	0.190	17.017	0.163 ±	0.0
42.732	0.327 ±	2.065	0.186	16.246	0.162 ±	0.0
42.977	2.096 ±	2.054	0.183	15.465	0.153 ±	0.0
			0.179	14.859	0.171 ±	0.0

ITERATION STEP 1, TIME-OF-FLIGHT RUN NO. 2

SAMPLE THICKNESS: 9.924E-03 NUCLEI/B
FLIGHT PATH : 2.050E+00 M

NEUTRON ENERGY (KEV)	MEASURED YIELD-OVER-THICKNESS (MILLI-BARN)		CALCULATED VALUES (MILLI-BARN)	FROM MULT. COLLISIONS (PERCENT)	CALCULATED CROSS SECTION (MILLI-BARN)	
19.069	-3.425 ±	7.271	0.822	10.240	0.743 ±	0.0
19.142	1.579 ±	7.205	0.825	10.070	0.775 ±	0.0
19.215	3.532 ±	7.173	0.842	9.962	0.750 ±	0.0
19.289	11.569 ±	7.207	0.858	10.102	0.899 ±	0.0
19.363	-0.340 ±	7.036	0.922	9.936	0.899 ±	0.0
19.437	0.39. ±	6.998	0.949	10.162	0.862 ±	0.0
19.512	-4.090 ±	6.920	0.944	10.362	0.866 ±	0.0
19.588	6.316 ±	6.878	0.942	10.167	0.879 ±	0.0
19.664	8.615 ±	6.849	0.930	9.886	0.87 ±	0.0
19.740	-4.166 ±	6.753	0.925	9.729	0.876 ±	0.0
19.817	-3.056 ±	6.699	0.952	9.553	0.903 ±	0.0
19.894	5.738 ±	6.645	0.997	9.063	1.011 ±	0.0
19.972	10.679 ±	6.662	1.008	8.294	1.022 ±	0.0
20.050	0.934 ±	6.474	1.005	7.847	0.975 ±	0.0
20.128	14.243 ±	6.580	1.006	8.124	0.981 ±	0.0
20.207	9.867 ±	6.433	1.020	8.718	1.034 ±	0.0
20.287	12.333 ±	6.490	1.071	9.063	1.055 ±	
20.367	0.604 ±	6.742	1.122	9.011	1.1	
20.447	6.992 ±	6.321	1.137	9.133		
98	6.611 ±	6.226				
	7.690 ±	6.114				
	±	6.067				
					.6623 ±	0.0
35.			.2		0.623 ±	0.0
36.023			7.104	44.602	0.671 ±	0.0
36.212	11.67 ±	..	11.447	18.943	0.532 ±	0.0
36.403	24.937 ±	2.992	22.901	7.064	0.953 ±	0.0
36.596	56.094 ±	5.409	44.717	3.745	342.833 ±	0.0
36.790	45.599 ±	4.651	58.695	3.533	0.929 ±	0.0
36.985	16.877 ±	2.380	3.999	63.298	0.469 ±	0.0
37.182	4.804 ±	1.758	3.033	86.008	0.457 ±	0.0
37.381	7.036 ±	1.601	3.979	77.645	0.481 ±	0.0
37.581	6.578 ±	1.769	4.655	67.726	0.363 ±	0.0
37.783	10.738 ±	1.916	6.337	36.912	0.389 ±	0.0
37.986	21.081 ±	2.593	11.314	16.351	0.380 ±	0.0
38.191	42.248 ±	4.309	22.693	8.599	1.209 ±	0.0
38.398	58.916 ±	5.774	38.949	5.632	3.024 ±	0.0
38.607	29.767 ±	3.195	24.113	10.886	0.304 ±	0.0
38.817	10.291 ±	1.894	3.474	91.491	0.329 ±	0.0
39.029	4.059 ±	1.660	3.490	91.775	0.303 ±	0.0
39.242	7.362 ±	1.651	2.755	89.984	0.295 ±	0.0
39.458	2.628 ±	1.648	1.993	86.676	0.308 ±	0.0
39.675	4.884 ±	1.665	1.536	84.498	0.244 ±	0.0
39.894	2.802 ±	1.589	1.292	82.762	0.246 ±	0.0
40.114	5.309 ±	1.640	0.976	77.053	0.247 ±	0.0
40.337	5.105 ±	1.618	0.952	76.774	0.230 ±	0.0
40.562	4.648 ±	1.598	0.864	73.986	0.245 ±	0.0
40.788	2.443 ±	1.524	0.635	65.978	0.227 ±	0.0
41.016	1.846 ±	1.493	0.563	63.771	0.222 ±	0.0
41.246	1.535 ±	1.481	0.403	53.577	0.170 ±	0.0
41.478	0.842 ±	1.476	0.203	19.151	0.167 ±	0.0
41.713	1.958 ±	1.500	0.199	17.127	0.158 ±	0.0
41.949	4.846 ±	1.571	0.201	16.497	0.165 ±	0.0
42.187	1.990 ±	1.519	0.198	16.429	0.162 ±	0.0
42.427	0.307 ±	1.495	0.195	16.208	0.171 ±	0.0
42.669	1.064 ±	1.457	0.193	15.839	0.193 ±	0.0
42.913	3.207 ±	1.409	0.187	16.021	0.160 ±	0.0

CHI SQARED: 1.103E+01
ERROR ADJUSTMENT FACTOR: 1.801E+00
ITERATION STEP: 1

Fig. 6 - Print-out of measured and calculated apparent capture cross sections (capture yields divided by sample thickness) and true capture cross section for the first iterative step, i. e. prior to parameter adjustment. The last lines show χ^2 and the error adjustment factor $\sqrt{\chi^2/(I-M)}$, Eq. 76.

CROSS SECTION PARAMETERS:

ABUN-DANCE	ATOMIC WEIGHT	TARGET SPIN	P-WAVE RADIUS (FM)	COMP. SPIN	S-WAVE STRENGTH FUNCTION /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.	DETECT. EFFIC.
0.9970	56.0	0.0	0.0	0.5	2.500E-04 0.0	6.100 0.0	0.0	-3.900 0.0	5.200E-01 0.0	0.0 0.0	1.300E-03 0.0	0.970
								27.478 0.038	1.400E+00 0.0	0.0 0.0	1.224E-03 0.414E-04	0.970
								73.980 0.0	5.400E-01 0.0	0.0 0.0	6.300E-04 0.0	0.930
								83.650 0.0	1.300E+00 0.0	0.0 0.0	5.000E-04 0.0	0.970
0.9970	56.0	0.0	5.400	0.5	0.0 0.0	0.0 0.0	0.0	36.641 0.008	3.000E-03 0.0	0.0 0.0	3.366E-04 0.222E-04	0.830
1.9940	56.0	0.0	0.0	0.5	0.0 0.0	0.0 0.0	0.0	34.118 0.006	1.000E-03 0.0	0.0 0.0	3.795E-04 0.238E-04	0.870
								38.278 0.007	2.349E-04 0.185E-04	0.0 0.0	6.000E-04 0.0	0.850
2.9910	56.0	0.0	0.0	0.5	0.0 0.0	0.0 0.0	0.0	22.754 0.005	6.705E-05 0.461E-05	0.0 0.0	6.000E-04 0.0	0.870
								24.488 0.037	7.365E-06 0.207E-05	0.0 0.0	6.000E-04 0.0	0.870
1.5000	16.0	0.0	5.300	0.5	0.0 0.0	5.3 0.0	6051.988					

CONVERGENCE AFTER 3 ITERATION(S).

Fig. 7 - Print-out of final parameters after convergence has been declared. It should be noticed that for the narrow resonances (with $\ell \geq 1$, members of level sequences with zero s-wave radius) only the product $g\Gamma_n\Gamma_\gamma/\Gamma$ (with g absorbed in the abundance as far as input is concerned) is meaningful, not Γ_n or Γ_γ separately.

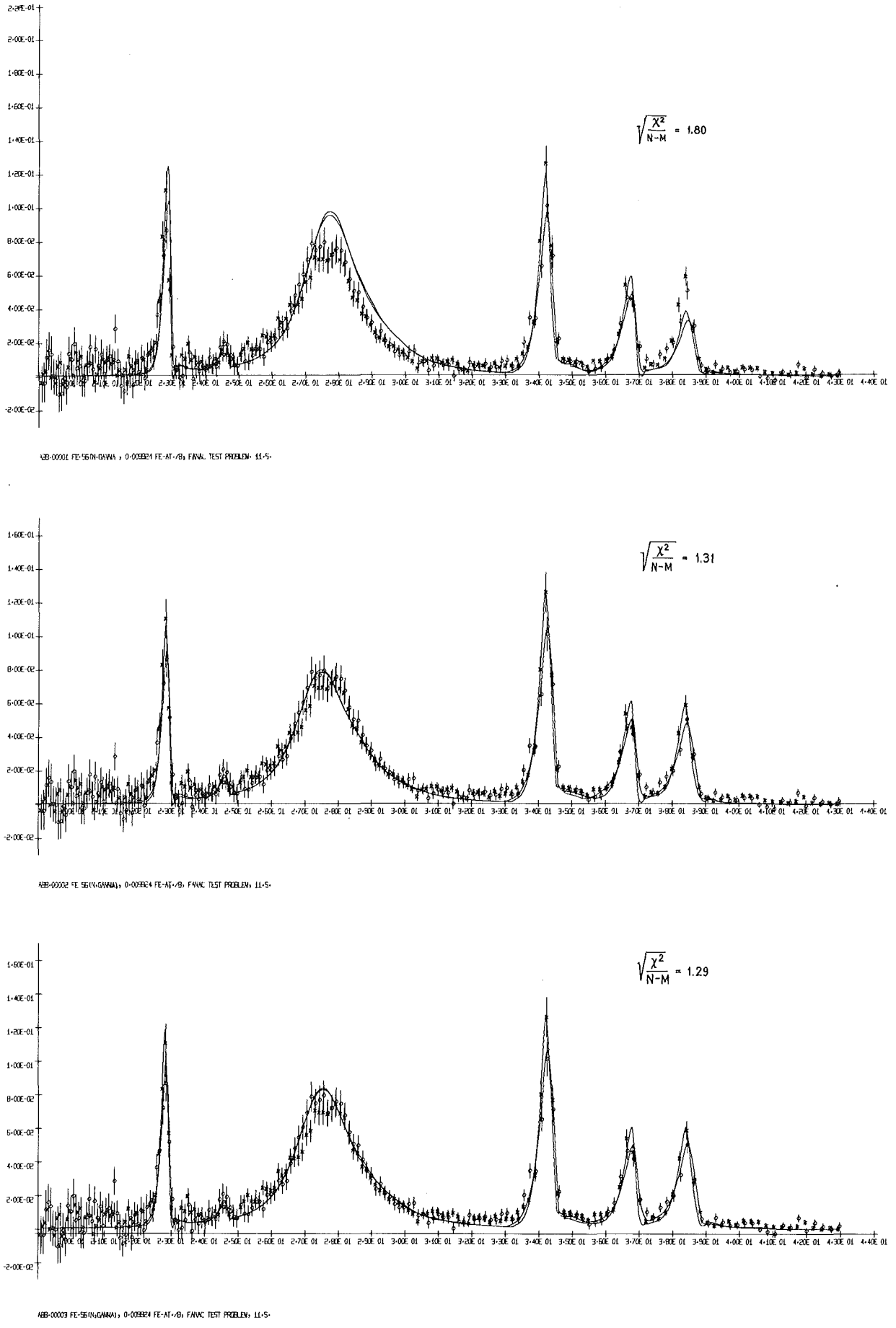


Fig. 8 - Plots produced along with the print-out shown in Figs. 5-7 illustrating progress of fit. Top corresponds to input parameters. The two solid lines correspond to the two experimental runs with slightly different resolution.

APPENDIX

Listing of FANAC code

```
C     FANAC, MAIN PROGRAM                                                    000010
C                                                                            000020
C        NOTE TO NON-KFK USERS:                                              000030
C                                                                            000040
C        PLOTA(X,Y,N,NT,NP,NH,I,NS,NR,XMAX,XMIN,SX,YMAX,YMIN,SY,TEXT,ID)     000050
C        IS A STANDARD PLOTTER SUBROUTINE IN USE AT KFK (KARLSRUHE)          000060
C        WHICH MUST BE REPLACED BY AN EQUIVALENT  PLOTTER PACKAGE            000070
C        ELSEWHERE  THE ARGUMENTS ARE EXPLAINED IN SUBROUTINE YPLOT.         000080
C                                                                            000090
C        RANDU(IX,IY,RANDOM) EMPLOYED IN SUBROUTINE MUY                      000100
C        IS A RANDOM-NUMBER GENERATOR (IBM SUBROUTINE) YIELDING              000110
C        VARIATE VALUES UNIFORMLY DISTRIBUTED IN THE INTERVAL 0 ... 1        000120
C        AND MUST BE REPLACED BY AN EQUIVALENT IF UNAVAILABLE.               000130
C                                                                            000140
C                                                                            000150
C        FANAC SUMMARY:                                                      000160
C                                                                            000170
C        VERSION              : NOVEMBER 1977                                000180
C        PROGRAMMING LANGUAGE: FORTRAN IV                                    000190
C        PURPOSE              : SHAPE ANALYSIS OF NEUTRON CAPTURE DATA.      000200
C                               EXTRACTION OF RESONANCE PARAMETERS.          000210
C                               CALCULATION OF TRUE CROSS SECTION.           000220
C        METHOD               : SIMULTANEOUS LEAST-SQUARES FIT TO            000230
C                               SEVERAL  SETS OF TIME-OF-FLIGHT DATA         000240
C                               (TAKEN E.G. WITH DIFFERENT SAMPLES OR        000250
C                               FLIGHT PATHS).                               000260
C        FORMALISM            : MULTI-LEVEL R-MATRIX FORMULA WITH            000270
C                               1 ELASTIC AND 1 INELASTIC NEUTRON            000280
C                               CHANNEL PER COMPOUND SPIN AND PARITY.        000290
C                               CAPTURE CHANNELS ARE ELIMINATED WITH         000300
C                               TEICHMANN-WIGNER REDUCTION METHOD            000310
C                               FOLLOWING REICH AND MOORE.                   000320
C        CORRECTIONS          : DOPPLER BROADENING IS APPLIED ONLY TO        000330
C                               LEVEL SEQUENCES WITH ZERO S-WAVE RADIUS      000340
C                               (P-,D-...WAVE LEVELS) AS FANAC WAS           000350
C                               DEVELOPPED FOR STRUCTURAL MATERIALS          000360
C                               FOR WHICH DOPPLER BROADENING OF S-WAVE       000370
C                               LEVELS IS NEGLIGIBLE.                        000380
C                               YIELDS INCLUDE SELF-SHIELDING AND            000390
C                               MULTIPLE-SCATTERING CORRECTIONS.             000400
C                               RESOLUTION BROADENING WITH GAUSSIAN          000410
C                               OR CHI-SQUARE DISTRIBUTION IS FOLDED IN.     000420
C                               AN EFFICIENCY FACTOR CAN BE APPLIED TO       000430
C                               EACH RESONANCE TO TAKE ACCOUNT OF GAMMA      000440
C                               SPECTRUM FLUCTUATIONS.                       000450
C        DOCUMENTATION        : F. H. FROEHNER, REPORT KFK 2145 (1975)       000460
C                                                                            000470
C        SUBSCRIPT CONVENTIONS IN FANAC:                                     000480
C        I (MAX.   10) LABELS ISOTOPES,                                      000490
C        J (MAX.    2)   "    COMPOUND SPINS,                               000500
C        K (MAX. 2048)   "    MEASURED DATA POINTS,                         000510
C        L (MAX.   48)   "    RESONANCES,                                   000520
C        M (MAX.  200)   "    CROSS SECTION PARAMETERS                      000530
C                             (BOTH FIXED AND ADJUSTED),                    000540
C        N (MAX.    5)   "    TIME-OF-FLIGHT MEASUREMENTS.                  000550
C                                                                            000560
C        NOTE: FOR EACH SAMPLE NUCLIDE ONE MUST PREPARE INPUT FOR            000570
C        1 ISOTOPE WITH NONZERO S-WAVE RADIUS FOR ALL S-WAVE LEVELS,         000580
```

```
C         AND, IF P-,D-...WAVE LEVELS ARE PRESENT,                          000590
C         1 ISOTOPE WITH    ZERO S-WAVE RADIUS FOR NON-S-WAVE LEVELS.       000600
C         THE LATTER ARE TREATED WITHOUT MULTI-LEVEL OR POTENTIAL/          000610
C         RESONANCE INTERFERENCE.                                           000620
C         THIS APPROXIMATION MAY FAIL ABOVE 300-400 KEV.                    000630
C                                                                           000640
0001           COMMON                                                       000650
              1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQ0,                           000660
              2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),  000670
              3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RF(11),   000680
              4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),     000690
              5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(5,2),Y(512),DLY(5,2),     000700
              6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,M0,     000710
              7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),  000720
              8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  000730
              9F(201),RF(201)                                               000740
0002           COMMON /ABC/ A(20,20),B(20,20),C(20)                         000750
0003           DOUBLE PRECISION A,B                                         000760
0004           COMMON/I1/ SG1(2048),DLSGT1(2048)                            000770
0005           COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                     000780
C                                                                           000790
0006         1 CHISQ=0.                                                     000800
0007           CALL CARDIN                                                  000810
0008           CALL INDEX                                                   000820
0009           CALL CONTJ                                                   000830
0010           IZX=ZIT                                                      000840
0011           DO 2 IZ=1,IZX                                                000850
0012           CHISQ0=CHISQ                                                 000860
0013           CHISQ=0.                                                     000870
0014           CALL MEV                                                     000880
0015           CALL CONE                                                    000890
0016           CALL CHOBAN(MA,A,B)                                          000900
0017           CALL ADJ(IZ,MX,MA,KX(NX),CHISQ,X,DLX,B,C)                    000910
0018           CALL KEV                                                     000920
0019           CALL YPLOT                                                   000930
0020           CALL PAROUT                                                  000940
0021           VCHISQ=((CHISQ-CHISQ0)/CHISQ)**2                             000950
0022           DLCHSQ=SQRT(VCHISQ)                                          000960
0023           IF(DLCHSQ.LT.EPS)GO TO 3                                     000970
0024           WRITE(6,100)IZ                                               000980
0025       100 FORMAT(//' AFTER',I3,' ITERATION(S) NO CONVERGENCE YET.'//)  000990
0026         2 CONTINUE                                                     001000
0027           GO TO 1                                                      001010
0028         3 WRITE(6,101)IZ                                               001020
0029       101 FORMAT(//' CONVERGENCE AFTER',I3,' ITERATION(S).'//)         001030
0030           GO TO 1                                                      001040
0031           END                                                          001050
```

```
                C                                                                       C01060
0001                 SUBROUTINE CARDIN                                                  C01070
                C                                                                       C01080
                C                                                                       C01090
                C         CARDIN READS THE INPUT FROM CARDS                             C01100
                C                                                                       C01110
0002                 COMMON                                                             C01120
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 C01130
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), C01140
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         C01150
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          C01160
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           C01170
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,           C01180
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   C01190
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  C01200
                    9F(201),RF(201)                                                     C01210
0003                 DIMENSION TS(5)                                                    C01220
0004                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           C01230
                C                                                                       C01240
0005                 I=0                                                                C01250
0006                 N=0                                                                C01260
0007                 MX=0                                                               C01270
0008                 HI=(0.,.5)                                                         C01280
0009                 GI=(0.,1.)                                                         C01290
0010                1 READ(5,100,END=999)TITLE                                          C01300
0011              100 FORMAT(20A4)                                                      C01310
0012                 WRITE(6,101)TITLE                                                  C01320
0013              101 FORMAT(1H1//30X,20A4///)                                          C01330
0014                 READ(5,102)E1,E2,TEFF,EPS,ZIT                                      C01340
0015              102 FORMAT(5E10.5)                                                    C01350
0016                 WRITE(6,103)E1,E2,TEFF,EPS,ZIT                                     C01360
0017              103 FORMAT(//                                                         C01370
                   1' EXPLICIT-RESONANCE RANGE: ',F8.3,' ...',F8.3,' KEV'/           C01380
                   2' EFFECTIVE TEMPERATURE:          ',F8.1,' KELVIN'/              C01390
                   3' MAXIMUM TOLERABLE CHI**2 CHANGE: ',F8.4,'  (RELATIVE)'/        C01400
                   4' MAX. NUMBER OF ITERATIVE STEPS:  ',F8.0)                       C01410
0018                2 I=I+1                                                         C01420
                C         READ ISOTOPE CARD (I-TH ISOTOPE)                          C01430
                C            H(I)   : ABUNDANCE,                                    C01440
                C            AG(I)  : ATOMIC WEIGHT,                                C01450
                C            SPIN(I): TARGET SPIN,                                  C01460
                C            RP(I)  : EFFECTIVE RADIUS FOR P-WAVE SCATTERING (FM).  C01470
0019                 READ(5,104)H(I),AG(I),SPIN(I),RP(I)                            C01480
0020              104 FORMAT(4E10.5)                                                C01490
0021                3 G(I,1)=.5*(1.+2./(2.*SPIN(I)+1.))                             C01500
0022                 G(I,2)=1.-G(I,1)                                               C01510
0023                 IF(SPIN(I).EQ.0.)JX(I)=1                                       C01520
0024                 IF(SPIN(I).GT.0.)JX(I)=2                                       C01530
0025                 CS(I,1)=SPIN(I)+.5                                             C01540
0026                 CS(I,2)=SPIN(I)-.5                                             C01550
0027                 L=0                                                            C01560
0028                 J=1                                                            C01570
0029                 MN=MX+1                                                        C01580
0030                 MX=MN+1                                                        C01590
                C         READ POTENTIAL-SCATTERING CARD (I-TH ISOTOPE, J-TH SPIN)  C01600
                C            X(MN)  : S-WAVE STRENGTH FUNCTION,                     C01610
                C            DLX(MN): INITIAL UNCERTAINTY OF X(MN),                 C01620
                C            X(MX)  : EFFECTIVE RADIUS FOR S-WAVE SCATTERING (FM),  C01630
```

```
                C          DLX(MX): INITIAL UNCERTAINTY OF X(MX),                          001630
                C          ES(I,J): 1ST INELASTIC THRESHOLD (KEV).                         001640
                C       NOTE: PUT INITIAL UNCERTAINTY =0. FOR FIXED,                       001650
                C                              >0. FOR ADJUSTED PARAMETERS.                001660
0031                    READ(5,105)(X(M),DLX(M),M=MN,MX),ES(I,J)                           001670
0032              105 FORMAT(5E10.5)                                                       001680
0033                4 L=L+1                                                              001690
0034                  MN=MX+1                                                            001700
0035                  MX=MN+3                                                            001710
                C       READ RESONANCE CARD                                              001720
                C          X(MN)  : RESONANCE ENERGY (KEV),                              001730
                C          X(MN+1): NEUTRON WIDTH (KEV),                                 001740
                C          X(MN+2): PARTIAL WIDTH FOR INELASTIC SCATTER (KEV)            001750
                C          X(MX)  : RADIATION WIDTH (KEV)                                001760
                C          DLX(M) : INITIAL UNCERTAINTY OF X(M)                          001770
                C          EFF(I,J,L): CAPTURE DETECTION EFFICIENCY                      001780
0036                    READ(5,106)(X(M),DLX(M),M=MN,MX),EFF(I,J,L)                        001790
0037              106 FORMAT(7E10.5,2E5.3)                                                 001800
                C       CHECK CARD TYPE                                                  001810
0038                    IF(X(MX).NE.0.)   GO TO 4                                        001820
0039                    IF(J.LT.JX(I))    GO TO 5                                        001830
0040                    IF(DLX(MN).GE.1.) GO TO 6                                        001840
0041                                      GO TO 7                                        001850
                C       LAST CARD WAS POTENTIAL-SCATTERING CARD                          001860
0042                5 LX(I,J)=L-1                                                        001870
0043                  MX=MX-2                                                            001880
0044                  J=2                                                                001890
0045                  ES(I,J)=X(MN+2)                                                    001900
0046                  L=0                                                                001910
0047                  GO TO 4                                                            001920
                C       LAST CARD WAS ISOTOPE CARD                                       001930
0048                6 LX(I,J)=L-1                                                        001940
0049                  MX=MX-4                                                            001950
0050                  I=I+2                                                              001960
0051                  H(I)   =X(MN)                                                      001970
0052                  AG(I)  =DLX(MN)                                                    001980
0053                  SPIN(I)=X(MN+1)                                                    001990
0054                  RP(I)  =DLX(MN+1)                                                  002000
0055                  GO TO 3                                                            002010
                C       LAST CARD WAS SAMPLE CARD                                        002020
                C          XN(N): SAMPLE THICKNESS (NUCLEI/B)                            002030
                C          XR(N): SAMPLE RADIUS    (NUCLEI/B)                            002040
0056                7 LX(I,J)=L-1                                                        002050
0057                  MX=MX-4                                                            002060
0058                  IX=I                                                               002070
0059                  N=N+1                                                              002080
0060                  XN(N)=X(MN)                                                        002090
0061                  XR(N)=DLX(MN)                                                      002100
0062                  KH=0                                                               002110
                C       READ SPECIFICATIONS OF N-TH MEASUREMENT                          002120
                C          FP(N)  : FLIGHT PATH (M)                                      002130
                C          DLFP(N): SAMPLE THICKNESS (M)                                 002140
                C          TC(N)  : CHANNEL WIDTH (NS)                                   002150
                C          TB(N)  : FWHM OF GAMMA PEAK (NS)                              002160
                C          ZH(N)  : NUMBER OF MONTE CARLO HISTORIES PER ENERGY           002170
                C          TS(N)  : TIME SHIFT (NS) TO COMPENSATE ZERO-TIME ERRORS       002180
0063               12 READ(5,107)FP(N),DLFP(N),TC(N),TB(N),ZH(N),TS(N)                   002190
0064              107 FORMAT(6E10.5)                                                     002200
```

```
0065                8 KN=KH+1                                                          C02210
0066                  KH=KN+1                                                          C02220
                C       READ DATA CARD                                                 C02230
                C          EE(K) : EXPERIMENTAL ENERGY (KEV)                           C02240
                C          Y(K)  : EXPERIMENTAL YIELD                                  C02250
                C          DLY(K): EXPERIMENTAL YIELD UNCERTAINTY (%)                  C02260
0067            READ(5,108)(EE(K), Y(K),DLY(K),K=KN,KH)                                C02270
0068          108 FORMAT(6E10.5)                                                       C02280
                C       WAS THIS LAST DATA CARD?                                       C02290
                C       NOTE: LAST DATA CARD IS FOLLOWED BY A BLANK CARD (1 FOR EACH   C02300
                C             MEASUREMENT). A 2ND BLANK CARD SIGNALS END OF PROBLEM.   C02310
                C             INPUT FOR ANOTHER PROBLEM MAY FOLLOW.                    C02320
0069            IF(DLY(KH).NE.0.)GO TO 8                                               C02330
0070            DO 9 K=KN,KH                                                           C02340
0071            IF(DLY(K ).NE.0.)GO TO 9                                               C02350
0072            KX(N)=K-1                                                              C02360
0073            GO TO 10                                                               C02370
0074             9 CONTINUE                                                            C02380
0075            10 IF(KX(N).EQ.KH-2)GO TO 11                                           C02390
0076            READ(5,109)DUMMY                                                       C02400
0077          109 FORMAT(E10.5)                                                        C02410
0078            11 N=N+1                                                               C02420
0079            READ(5,110)XN(N),XR(N)                                                 C02430
0080          110 FORMAT(2E10.5)                                                       C02440
0081            KH=KX(N-1)                                                             C02450
                C       END OF INPUT?                                                  C02460
0082            IF(XN(N).GT.0.)GO TO 12                                                C02470
0083            NX=N-1                                                                 C02480
                C       CALCULATE ABSOLUTE ERROR                                       C02490
0084            KH=KX(NX)                                                              C02500
0085            DO 13 K=1,KH                                                           C02510
0086            DLY(K)=DLY(K)*ABS(Y(K))*.01                                            C02520
0087            13 CONTINUE                                                            C02530
                C       CHECK WHETHER ALL CAPTURE EFFICIENCIES ARE EQUAL               C02540
0088            LL=0                                                                   C02550
0089            EFC=1.                                                                 C02560
0090            DO 14 I=1,IX                                                           C02570
0091            JH=JX(I)                                                               C02580
0092            DO 15 J=1,JH                                                           C02590
0093            IF(LX(I,J).EQ.0)GO TO 15                                               C02600
0094            LH=LX(I,J)                                                             C02610
0095            DO 16 L=1,LH                                                           C02620
0096            LL=LL+1                                                                C02630
0097            IF(LL.EQ.1)EFC=EFF(I,J,L)                                              C02640
0098            IF(LL.GT.1.AND.EFF(I,J,L).NE.EFC)EFC=0.                                C02650
0099            16 CONTINUE                                                            C02660
0100            15 CONTINUE                                                            C02670
0101            14 CONTINUE                                                            C02680
                C       CORRECT TRUNCATION ERRORS OF ENERGIES AND PRINT MEASURED DATA  C02690
                C                                                                      C02700
                C                                                                      C02720
                C       WRITE RUN INFORMATION                                          C02730
0102            WRITE(6,113)                                                           C02740
0103          113 FORMAT(1HO///42H SPECIFICATIONS OF UTILIZED MEASUREMENTS: /           C02750
                  .            42H ========================================= /// 126H  C02760
                  1 MMENT.   SAMPLE      SAMPLE      FLIGHT      SAMPLE      CHANNEL   C02770
                  2    FWHM        MONTE       TIME SHIFT                     /126H  C02780
                  3 NO.      THICKNESS   RADIUS      PATH        THICKNESS   WIDTH     C02790
```

```
                     4    GAMMA PEAK  CARLO       CORRECTION                          /126H  002800
                     5           (NUCLEI/B)  (NUCLEI/B)  (M)          (M)          (NS)      002810
                     6    (NS)        HISTORIES   (NS)                                  /)  002820
0104                      DO 51 N=1,NX                                                       002830
0105                      WRITE(6,114)N,XN(N),XR(N),FP(N),DLFP(N),TC(N),TB(N),ZH(N),TS(N)    002840
0106                   51 CONTINUE                                                           002850
0107                  114 FORMAT(I3,1PE16.2,1PE12.3,0PF10.4,F12.4,F10.3,F12.3,F12.0,F12.3)  002860
                    C         WRITE CROSS SECTION PARAMETERS                               002870
                    C                                                                      002880
0108                      CALL PAROUT                                                      002890
                    C                                                                      002900
0109                      IF(IX.GT.10.OR.NX.GT.5.OR.KX(NX).GT.512)WRITE(6,115)IX,NX,KX(NX)  0029 0
0110                  115 FORMAT(1H //' TOO MUCH INPUT:', I6, ' ISOTOPES,'/                002920
                         1            '                ', I6, ' MEASUREMENTS,'/            002930
                         2            '                ', I6, ' DATA POINTS.')             002940
0111                      IF(IX    .GT. 10)IX    = 10                                      002950
0112                      IF(NX    .GT.  5)NX    =  5                                      002960
0113                      IF(KX(NX).GT.512)KX(NX)=512                                      002970
0114                      RETURN                                                           002980
0115                  999 STOP                                                             002990
0116                      END                                                              003000
```

```
                C                                                                   003010
                C                                                                   003020
0001                 SUBROUTINE ETEC(EE,Y,DLY,FP,TS,KX,NX)                          003030
                C                                                                   003040
                C        ETEC CORRECTS NONLINEARITIES OF THE TIME-OF-FLIGHT SCALE    003050
                C        CAUSED BY TOO FEW DIGITS USED FOR THE INPUT ENERGIES       003060
                C        BY A LINEAR LEAST-SQUARES FIT TO THE FLIGHT TIMES.         003070
                C           EE: ENERGIES (KEV), FIRST TRUNCATED, THEN CORRECTED     003080
                C           Y:  CAPTURE YIELD DATA (B)                              003090
                C           DLY:UNCERTAINTIES (B)                                   003100
                C           FP: FLIGHT PATH                                         003110
                C           TS: TIME SHIFT CORRECTION                               003120
                C           KX: ARRAY BOUNDARIES FOR Y AND DLY                      003130
                C           NX: NUMBER OF TIME-OF-FLIGHT RUNS                       003140
                C                                                                   003150
0002                 DIMENSION EE(512),Y(512),DLY(512),FP(5),TS(5),KX(5)            003160
0003                 WRITE(6,100)                                                   003170
0004               100 FORMAT(1H0//' INPUT DATA TO BE FITTED:'/                     003180
                   1          ' ========================'///                       003190
                   2' TRUNCATED   CORRECTED      CAPTURE YIELD'/                   003200
                   3'  ENERGY      ENERGY           DATA     '/                     003210
                   4'   (KEV)       (KEV)            (B)     ')                    003220
0005                 KH=0                                                           003230
0006                 DO 3 N=1,NX                                                    003240
0007                 KN=KH+1                                                        003250
0008                 KH=KX(N)                                                       003260
0009                 CC=TS(N)/(72.3*FP(N)*SQRT(1000.))                              003270
0010                 WRITE(6,101)                                                   003280
0011               101 FORMAT(1H /)                                                 003290
0012                 A11=0.                                                         003300
0013                 A12=0.                                                         003310
0014                 A22=0.                                                         003320
0015                 C1 =0.                                                         003330
0016                 C2 =0.                                                         003340
0017                    DO 1 K=KN,KH                                                003350
0018                    FK=K                                                        003360
0019                    ETA=1./SQRT(EE(K))                                          003370
0020                    A11=A11+1.                                                  003380
0021                    A12=A12+FK                                                  003390
0022                    A22=A22+FK**2                                               003400
0023                    C1 =C1+ETA                                                  003410
0024                    C2 =C2+ETA*FK                                               003420
0025                  1 CONTINUE                                                    003430
0026                 DET=A11*A22-A12*A12                                            003440
0027                 B11= A22/DET                                                   003450
0028                 B12=-A12/DET                                                   003460
0029                 B22= A11/DET                                                   003470
0030                 X1=B11*C1+B12*C2+CC                                            003480
0031                 X2=B12*C1+B22*C2                                               003490
0032                    DO 2 K=KN,KH                                                003500
0033                    FK=K                                                        003510
0034                    YK=X1+FK*X2                                                 003520
0035                    EO=EE(K)                                                    003530
0036                    EE(K)=1./YK**2                                              003540
0037                    WRITE(6,102)EO,EE(K),Y(K),DLY(K)                            003550
0038               102  FORMAT(F8.3,F12.3,F 2.6,2H+-,F8.6)                         003560
0039                  2 CONTINUE                                                    003570
0040                  3 CONTINUE                                                    003580
0041                 RETURN                                                         003590
0042                 END
```

```
                C                                                                       003600
                C                                                                       003610
0001                 SUBROUTINE PAROUT                                                  003620
                C                                                                       003630
                C         PAROUT PRINTS THE CROSS SECTION PARAMETERS                    003640
                C                                                                       003650
0002                 COMMON                                                             003660
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 003670
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 003680
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         003690
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),           003700
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           003710
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,           003720
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   003730
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  003740
                    9F(201),RF(201)                                                     003750
0003                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           003760
                C                                                                       003770
0004                 MH=MX                                                              003780
0005                 WRITE(6,99)                                                        003790
0006                99 FORMAT(1HI//' CROSS SECTION PARAMETERS:'/                        003800
                    1           ' ========================'/)                          003810
0007                 WRITE(6,100)                                                       003820
0008               100 FORMAT(     127H  ABUN-   ATOMIC  TARGET P-WAVE    COMP.  S-WAVE  003830
                    1   S-WAVE    INEL.     RESONANCE       PARTIAL WIDTHS FOR          003840
                    2   DETECT. /127H  DANCE   WEIGHT  SPIN   RADIUS    SPIN   STRENGTH 003850
                    3   RADIUS    THRESH.   ENERGY    EL.SCATT.   INEL.SCATT. CAPTURE   003860
                    4   EFFIC.  /127H                      (FM)                FUNCTION  003870
                    5   (FM)      (KEV)     (KEV)     (KEV)       (KEV)       (KEV)     003880
                    6           /127H                                           /UNCERT.  003890
                    7   /UNCERT.          /UNCERT.  /UNCERT.    /UNCERT.    /UNCERT.    003900
                    8           /)                                                      003910
0009                 MX=0                                                               003920
0010                 DO 1 I=1,IX                                                        003930
0011                 J=1                                                                003940
0012                 IF(LX(I,1).EQ.0)GO TO 2                                            003950
0013                 MN=MX+1                                                            003960
0014                 MX=MN+5                                                            003970
0015                 WRITE(6,101)H(I),AG(I),SPIN(I),RP(I),CS(I,J),X(MN),X(MN+1),ES(I,J) 003980
                    1,X(MN+2),X(MN+3),X(MN+4),X(MX),EFF(I,J,1),(DLX(M),M=MN,MX)         003990
0016               101 FORMAT(F7.4,F8.1,F7.1,F9.3,F8.1,1PE12.3,0PF8.3,F9.3,F12.3,1P3E12.2 004000
                    1,0PF8.3/39X,E12.3,F8.3,9X,F12.3,3E12.3/)                           004010
0017                 GO TO 3                                                            004020
0018                 2 MN=MX+1                                                          004030
0019                 MX=MN+1                                                            004040
0020                 WRITE(6,102)H(I),AG(I),SPIN(I),RP(I),CS(I,1),X(MN),X(MX  ),ES(I,1) 004050
                    1,DLX(MN),DLX(MX)                                                   004060
0021                102 FORMAT(F7.4,F8.1,F7.1,F9.3,F8.1,1PE12.3,0PF8.3,F9.3/39X,E12.3,F8.3 004070
                    1/)                                                                 004080
0022                 GO TO 4                                                            004090
0023                 3 IF(LX(I,J).LE.1)GO TO 4                                          004100
0024                 LMX=LX(I,J)                                                        004110
0025                 DO 5 L=2,LMX                                                       004120
0026                 MN=MX+1                                                            004130
0027                 MX=MN+3                                                            004140
0028                 WRITE(6,103)(X(M),M=MN,MX),EFF(I,J,L),(DLX(M),M=MN,MX)             004150
0029               103 FORMAT(68X,F12.3,1P3E12.3,0PF8.3/68X,F12.3,3E12.3/)              004160
0030                 5 CONTINUE                                                         004170
```

```
0031                4 IF(J.EQ.JX(I))GO TO 1                                                004170
0032                  J=2                                                                  004180
0033                  IF(LX(I,2).EQ.0)GO TO 6                                              004190
0034                  MN=MX+1                                                              004200
0035                  MX=MN+5                                                              004210
0036                  WRITE(6,104)CS(I,2),X(MN),X(MN+1),ES(I,2),X(MN+2),X(MN+3),X(MN+4),   004220
                     1X(MX),EFF(I,J,1),(DLX(M),M=MN,MX)                                    004230
0037               104 FORMAT(31X,F8.1,1PE12.3,0PF8.3,F9.3,F12.3,1P3E12.3,0PF8.3/39X,E12.  004240
                     13,F8.3,9X,F12.3,3E12.3/)                                             004250
0038                  GO TO 3                                                              004260
0039                6 MN=MX+1                                                              004270
0040                  MX=MN+1                                                              004280
0041                  WRITE(6,105)CS(I,2),X(MN),X(MX),ES(I,2),DLX(MN),DLX(MX)              004290
0042               105 FORMAT(31X,F8.1,1PE12.3,0PF8.3,F9.3/39X,E12.3,F8.3/)                004300
0043                1 CONTINUE                                                             004310
0044                  MX=MH                                                                004320
0045                  IF(IZ.GT.0)RETURN                                                    004330
0046                  RETURN                                                               004340
0047                  END                                                                  004350
```

```
                C                                                                       004360
                C                                                                       004370
0001                 SUBROUTINE INDEX                                                   004380
                C                                                                       004390
                C        INDEX PROVIDES, FOR EACH ISOTOPE AND COMPOUND SPIN, SUBSCRIPTS 004400
                C        STRUCTURING THE CROSS SECTION PARAMETER ARRAYS X AND DLX.      004410
                C           MP(I,J): BEGIN OF POTENTIAL-SCATTERING PARAMETERS,          004420
                C           MR(I,J): BEGIN OF RESONANCE PARAMETERS                      004430
                C                    FOR THE I-TH ISOTOPE AND THE J-TH COMPOUND SPIN,   004440
                C           MX: TOTAL NUMBER OF PARAMETERS,                             004450
                C           MA: NUMBER OF ADJUSTED PARAMETERS.                          004460
                C                                                                       004470
0002                 COMMON                                                             004480
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 004490
                    21,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 004500
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         004510
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          004520
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),          004530
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,          004540
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   004550
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  004560
                    9F(201),RF(201)                                                     004570
0003                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           004580
                C                                                                       004590
0004                 MSUM=1                                                             004600
0005                 DO 1 I=1,IX                                                        004610
0006                 JH=JX(I)                                                           004620
0007                 DO 1 J=1,JH                                                        004630
0008                 MP(I,J)=MSUM                                                       004640
0009                 MR(I,J)=MSUM+2                                                     004650
0010               1 MSUM=MR(I,J)+4*LX(I,J)                                             004660
0011                 MX=MSUM-1                                                          004670
0012                 MA=0                                                               004680
0013                 DO 2 M=1,MX                                                        004690
0014                 IF(DLX(M).GT.0.)MA=MA+1                                            004700
0015               2 CONTINUE                                                           004710
0016                 IF(MX.GT.200.OR.MA.GT.20)WRITE(6,100)MX,MA                         004720
0017             100 FORMAT(1H//' TOO MANY PARAMETERS:',I6,' ALL TOGETHER,'/            004730
                    '                    ',I6,' ADJUSTED ONES.')
0018                 IF(MX.GT.200)MX=200                                                004740
0019                 IF(MA.GT. 20)MA= 20                                                004750
0020                 RETURN                                                             004760
0021                 END                                                                004770
```

```
                C                                                                       004780
                C                                                                       004790
0001                 SUBROUTINE MEV                                                     004800
                C                                                                       004810
                C         MEV CONVERTS ENERGIES FROM KEV TO MEV                         004820
                C                                                                       004830
0002                 COMMON                                                             004840
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQD,                                 004850
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 004860
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         004870
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),           004880
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           004890
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MD,           004900
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   004910
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  004920
                    9F(201),RF(201)                                                     004930
0003                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           004940
                C                                                                       004950
0004                 IF(IZ.GT.1)GO TO 1                                                 004960
0005                 E1=E1*.001                                                         004970
0006                 E2=E2*.001                                                         004980
0007                 DO 2 I=1,IX                                                        004990
0008                 JH=JX(I)                                                           005000
0009                 DO 2 J=1,JH                                                        005010
0010                 ES(I,J)=ES(I,J)*.001                                               005020
0011                 IF(LX(I,J).EQ.0)GO TO 2                                            005030
0012                 M1=MR(I,J)                                                         005040
0013                 M2=MR(I,J)+4*LX(I,J)-4                                             005050
0014                 DO 2 M=M1,M2,4                                                     005060
0015                 X(M)=X(M)*.001                                                     005070
0016                 X(M+1)=SIGN(SQRT(.001*ABS(X(M+1))),X(M+1))                         005080
0017                 X(M+2)=SIGN(SQRT(.001*ABS(X(M+2))),X(M+2))                         005090
0018                 X(M+3)=X(M+3)*.001                                                 005100
0019               2 CONTINUE                                                           005110
0020                 KH=KX(NX)                                                          005120
0021                 DO 3 K=1,KH                                                        005130
0022               3 EE(K)=.001*EE(K)                                                   005140
0023                 IF(IZ.EQ.1)RETURN                                                  005150
0024                 EMN=EMN*.001                                                       005160
0025                 DLE=DLE*.001                                                       005170
0026                 RETURN                                                             005180
0027                 END
```

```
                C                                                                       005190
                C                                                                       005200
0001                 SUBROUTINE CONIJ                                                   005210
                C                                                                       005220
                C        CONIJ YIELDS CONSTANTS FOR THE CROSS SECTION CALCULATION       005230
                C                                                                       005240
0002                 COMMON                                                             005250
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                005260
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),005270
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),        005280
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          005290
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),ZE(512),Y(512),DLY(512),          005300
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,          005310
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),  005320
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC, 005330
                    9F(201),RF(201)                                                    005340
0003                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           005350
                C                                                                       005360
0004                 DO 1 I=1,IX                                                        005370
0005                 AL(I)=1.+1./AG(I)                                                  005380
0006                 CO=H(I)*AL(I)**2                                                   005390
0007                 D(I)=SQRT(344.68*TEFF/AG(I))*.000001                               005400
0008                 JH=JX(I)                                                           005410
0009                 DO 2 J=1,JH                                                        005420
0010                 CT(I,J)=CO*G(I,J)                                                  005430
0011                 CG(I,J)=.5*CT(I,J)                                                 005440
0012               2 CONTINUE                                                           005450
0013               1 CONTINUE                                                           005460
0014                 RETURN                                                             005470
0015                 END
```

```
                C                                                                       005480
                C                                                                       005490
0001                 SUBROUTINE CONE                                                    005500
                C                                                                       005510
                C        CONE YIELDS THE COEFFICIENTS OF THE NORMAL EQUATIONS           005520
                C                                                                       005530
0002                 COMMON                                                             005540
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                005550
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),005560
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),        005570
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          005580
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),          005590
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,          005600
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),  005610
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC, 005620
                    9F(201),RF(201)                                                    005630
0003                 COMMON /ABC/ A(20,20),B(20,20),C(20)                               005640
0004                 DOUBLE PRECISION A,B                                               005650
0005                 COMMON/SEYCO/YS(2048)                                              005660
0006                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           005670
0007                 DIMENSION FS(201),DYC(201,20)                                      005680
                C                                                                       005690
                C        INITIALIZE                                                     005700
0008                 DO 1 M=1,MA                                                        005710
0009                 C(M)=0.                                                            005720
0010                 DO 1 MM=1,MA                                                       005730
0011                1 A(M,MM)=0.                                                        005740
0012                 KH=0                                                               005750
                C        BEGIN LOOP OF MEASUREMENTS                                     005760
0013                 DO 2 N=1,NX                                                        005770
                C        GET PRIMARY, SECONDARY AND MULTIPLE-COLLISION YIELDS           005780
                C                                                                       005790
0014                   CALL PRY                                                         005800
0015                   CALL SEY                                                         005810
0016                   CALL MUY                                                         005820
                C                                                                       005830
                C        CONSTANTS FOR RESOLUTION WIDTH                                 005840
0017                 V1=(DLFP(N)/FP(N))**2/5.                                           005850
0018                 V2=(TB(N)/(60.259*FP(N)))**2                                       005860
                C        WRITE TABLE HEADING                                            005870
0019                 WRITE(6,101)IZ,N,XN(N),FP(N)                                       005880
0020               101 FORMAT('1'//' ITERATION STEP',I3,', TIME-OF-FLIGHT RUN NO.',I3//  005890
                   118H SAMPLE THICKNESS:,1PE10.3,9H NUCLEI/B /                         005900
                   218H FLIGHT PATH     :,1PE10.3,2H M        /)                      005910
0021                 WRITE(6,102)                                                       005920
0022               102 FORMAT(                                                          005930
                   1' NEUTRON    MEASURED               CALCULATED   FROM MULT.   CALC 005940
                   2ULATED'/                                                          005950
                   3' ENERGY     YIELD-OVER-THICKNESS VALUES         COLLISIONS   CROS 005960
                   4S SECTION'/                                                       005970
                   5' (KEV)      (MILLI-BARN)           (MILLI-BARN) (PERCENT)    (MIL 005980
                   6LI-BARN)'/)                                                       005990
                C        BEGIN ENERGY LOOP                                          006000
0023                 KN=KH+1                                                        006010
0024                 KH=KX(N)                                                       006020
0025                 DO 3 KK=KN,KH                                                  006030
0026                 XL=(EE(KK)-EMN)/DLE+1.                                         006040
0027                 L=XL                                                           006050
```

```
0028                DD=XL-FLOAT(L)                                                  006050
0029                RW=EE(KK)*SQRT(V1+V2*EE(KK))                                    006060
0030                QD=DLE/RW                                                       006070
0031                KR=3./QD                                                        006080
0032                STL  =ST(L)  +DD*(ST(L+1)  -ST(L)  )                            006090
0033                SGL  =SG(L)  +DD*(SG(L+1)  -SG(L)  )                            006100
0034                DLSGL=DLSG(L)+DD*(DLSG(L+1)-DLSG(L))                            006110
0035                TL   =T(L)   +DD*(T(L+1)   -T(L)   )                            006120
                  C         SELF-SHIELDING EFFECT ON MEAN PATH LENGTH IN SAMPLE      006130
0036                DELXL=(2./(XN(N)*STL)-(1.+TL)/(1.-TL))*DLFP(N)/FP(N)*EE(KK)/DLE 006140
0037                XL=XL+DELXL                                                     006150
0038                L=XL                                                            006160
0039                DD=XL-FLOAT(L)                                                  006170
0040                IF(KR+L.GT.KKX)KR=KKX-L                                         006180
0041                IF(KR.GT.100)WRITE(6,100)IZ,KR                                  006190
0042              100 FORMAT(1H   I8,17H. ITERATION, KR =,I6,'READJUSTED TO 100'  ) 006200
0043                IF(KR.GT.100)KR=100                                             006210
                  C         PREPARE INTEGRANDS FOR RESOLUTION BROADENING           006220
0044                K1=101-KR                                                       006230
0045                K2=101+KR                                                       006240
                  C                                                                 006250
0046                  IF(AG(1).NE.56.)                                            006260
                    *   CALL TGAUSS(QD,RF,K2)                                     006270
0047                  IF(AG(1).EQ.56.)                                            006280
                    .   CALL CHISQ4(QD,RF,K2)                                     006290
                  C                                                                 006300
0048                DO 4 K=K1,K2                                                    006310
0049                LK=L+K-101                                                      006320
0050                F(K) =RF(K)*(YY(LK)+DD*(YY(LK+1)-YY(LK)))                       006330
0051                FS(K)=RF(K)*(YS(LK)+DD*(YS(LK+1)-YS(LK)))                       006340
0052                DO 4 M=1,MA                                                     006350
0053                DYC(K,M)=RF(K)*(DYY(LK,M)+DD*(DYY(LK+1,M)-DYY(LK,M)))           006360
0054              4 CONTINUE                                                        006370
                  C         RESOLUTION BROADENING:                                006380
                  C                                                                 006390
0055                  CALL SIMP(F ,K1,K2,Z(KK))                                   006400
0056                  CALL SIMP(FS,K1,K2,ZS)                                      006410
                  C                                                                 006420
0057                ZS=ZS/Z(KK)                                                     006430
0058                Z(KK)=Z(KK)/XN(N)                                               006440
0059                ZDEV=(Y(KK)-Z(KK))/DLY(KK)                                      006450
                  C         RESOLUTION BROADENING OF DERIVATIVES:                 006460
0060                DO 5 M=1,MA                                                     006470
                  C                                                                 006480
0061                  CALL SIMP(DYC(1,M),K1,K2,DZ(M))                             006490
                  C                                                                 006500
0062                DZ(M)=DZ(M)/DLY(KK)/XN(N)                                       006510
                  C         COEFFICIENTS OF THE NORMAL EQUATIONS                  006520
0063                C(M)=C(M)+DZ(M)*ZDEV                                            006530
0064                DO 5 MM=1,M                                                     006540
0065              5 A(M,MM)=A(M,MM)+DZ(M)*DZ(MM)                                    006550
0066                CHISQ=CHISQ+ZDEV**2                                             006560
                  C         PRINT TABLE ENTRY                                     006570
0067                WRITE(6,103)EE(KK),Y(KK),DLY(KK),Z(KK),ZS,SGL,DLSGL             006580
0068              103 FORMAT(' ',3PF7.3,F 7.4,' +',F8.3,F13.3,2PF13.3,3PF13.3,' +',F8.3) 006590
0069                WRITE(6,104)                                                    006600
0070              104 FORMAT('+',18X,' _',47X,' _')                                 006610
0071                3 CONTINUE                                                      006620
```

```
                C         END OF ENERGY LOOP                                    006630
0072              2 CONTINUE                                                    006640
                C         END OF LOOP OF MEASUREMENTS                           006650
0073                RETURN                                                      006660
0074                END                                                         006670
```

```
                C                                                                       006680
                C                                                                       006690
0001                 SUBROUTINE PRY                                                     006690
                C                                                                       006700
                C         PRY YIELDS THE PRIMARY YIELD, ITS DERIVATIVES AND THE         006710
                C         TRANSMISSION                                                  006720
                C         E: NEUTRON ENERGY                                             006730
                C         K: ENERGY-GRID LABEL                                          006740
                C                                                                       006750
0002                 COMMON                                                             006760
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 006770
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 006780
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AC(11),SPIN(11),RP(11),         006790
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          006800
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           006810
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,           006820
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   006830
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  006840
                    9F(201),RF(201)                                                     006850
0003                 COMMON /ABC/ A(20,20),B(20,20),C(20)                               006860
0004                 DOUBLE PRECISION A,B                                               006870
0005                 COMMON/I1/ SGI1(2048),DLSGI1(2048)                                 006880
0006                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           006890
                C                                                                       006900
0007                 KH=KX(N)                                                           006910
0008                 KN=1                                                               006920
0009                 IF(N.GT.1)KN=KX(N-1)+1                                             006930
                C         ENERGY GRID                                                   006940
0010                 EMIN=EE(KN)                                                        006950
0011                 EMAX=EE(KH)                                                        006960
0012                 V1=(DLFP(N)/FP(N))**2/1.5                                          006970
0013                 V2=(TB(N)/(60.259*FP(N)))**2                                       006980
0014                 RW1=EMIN*SQRT(V1+V2*EMIN)                                          006990
0015                 RW =EMAX*SQRT(V1+V2*EMAX)                                          007000
0016                 ET=2.*EMAX  *XR(N)*DLFP(N)/(XN(N)*FP(N))                           007010
0017                 EMN=EMIN-3.*RW1                                                    007020
0018                 EMX=EMAX+3.*RW +ET                                                 007030
                C         IS VALIDITY INTERVAL WIDE ENOUGH?                             007040
0019                 IWARN=0                                                            007050
0020                 HINT=.5*(EMX-EMN)                                                  007060
0021                 EBAR=.5*(EMX+EMN)                                                  007070
0022                 IF(E1.LE.EBAR-HINT)GO TO 22                                        007080
0023                 IWARN=1                                                            007090
0024                 E1=EBAR-HINT                                                       007100
0025              22 IF(E2.GE.EBAR+HINT)GO TO 23                                        007110
0026                 IWARN=1                                                            007120
0027                 E2=EBAR+HINT                                                       007130
0028              23 IF(IWARN.EQ.1)WRITE(6,101)E1,E2                                    007140
0029             101 FORMAT(///                                                         007150
                    1' WARNING: VALIDITY RANGE READJUSTED,'/                            007160
                    2' PARAMETERS ARE NOW VALID FROM',3PF8.3,' TO',3PF8.3,' KEV'/)      007170
                C         TAKE INTERNAL GRID INTERVAL (DLE) AS HALF THE SMALLEST DOPPLER 007180
                C         WIDTH. IF MORE THAN 2048 INTERNAL GRID POINTS RESULT, OR IF   007190
                C         MORE THAN 101 GRID POINTS FALL WITHIN THRICE THE LARGEST      007200
                C         RESOLUTION WIDTH,  THE DOPPLER WIDTH (I. E. THE TEMPERATURE)  007210
                C         MUST BE INCREASED.                                            007220
0030                 DLE=.5*D(1)*SQRT(EMIN)                                             007230
0031                 DLEJ=DLE                                                           007240
```

```
0032                  DLE1=3.*XN/1.E.                                                  007250
0033                  DLE2=(EMX-EMN)/2044.                                             
0034                  DLE=AMAX1(DLE0,DLE1,DLE2)                                        007270
0035                  IF(DLE.LE.DLE0)GO TO 2                                           007280
0036                  QQ=DLE/DLE0                                                      007290
0037                  TEFF=TEFF*QQ**2                                                  007300
0038                  DO 1 I=1,IX                                                      007310
0039                1 D(I)=D(I)*QQ                                                     007320
0040                  DW=D(1)*SQRT(EMIN )*1000000.                                     007330
0041                  EIN QQ=EMIN*1000.                                                007340
0042                  WRITE(6,100)TEFF,DW,EINQQ                                        007350
0043              100 FORMAT(25H0EFFECTIVE TEMPERATURE  :,F7.2,13H DEG. KELVIN,        007360
                     1/      25H RESULTING DOPPLER WIDTH:,F7.3, 6H EV AT,F9.3,4H KEV/) 007370
0044                2 KKX=(EMX-EMN)/DLE+1.                                           007380
                  C       BEGIN ENERGY LOOP                                        007390
0045                  E=EMN-DLE                                                        007400
0046                  DO 11 K=1,KKX                                                    007410
0047                  E=E+DLE                                                          007420
                  C       CALCULATE CROSS SECTIONS AND DERIVATIVES                 007430
                  C                                                                007440
0048                   CALL XSECT(E,K)                                                 007450
                  C                                                                007460
                  C       TRANSMISSION:                                            007470
0049                  T(K)=EXP(-XN(N)*ST(K))                                           007480
                  C       PRIMARY YIELD:                                           007490
0050                  YY(K)=(1.-T(K))*SG(K)/ST(K)                                      007500
                  C       DERIVATIVES:                                             007510
0051                  DO 3 M=1,MA                                                      007520
0052                  DYY(K,M)=YY(K)*(DSG(M)/SG(K)-DST(M)/ST(K))                       007530
                     1    +XN(N)*SG(K)*T(K)*DST(M)/ST(K)                             007540
0053                3 CONTINUE                                                       007550
                  C       CALCULATE CROSS SECTION ERRORS                           007560
0054                  VST=0.                                                           007570
0055                  VSG=0.                                                           007580
0056                  IF(IZ.EQ.1)GO TO 6                                               007590
0057                  DO 5 MM=1,MA                                                     007600
0058                  DO 4 ML=1,MA                                                     007610
0059                  VST=VST+DST(MM)*B(MM,ML)*DST(ML)                                 007620
0060                  VSG=VSG+DSG(MM)*B(MM,ML)*DSG(ML)                                 007630
0061                4 CONTINUE                                                       007640
0062                5 CONTINUE                                                       007650
0063                6 DLST(K)=SQRT(VST)                                              007660
0064                  DLSG(K)=SQRT(VSG)                                                007670
                  C       TREAT FIRST ISOTOPE SEPARATELY                           007680
0065                  VSGI1=0.                                                         007690
0066                  IF(IZ.EQ.1)GO TO 10                                              007700
0067                  IH=1                                                             007710
0068                  IF(H(2).EQ.H(1))IH=2                                             007720
0069                  JH=JX(IH)                                                        007730
0070                  MX1=MR(IH,JH)+4*LX(IH,JH)-1                                      007740
0071                  MA1=0                                                            007750
0072                  DO 7 M=1,MX1                                                     007760
0073                  IF(DLX(M).GT.0.)MA1=MA1+1                                        007770
0074                7 CONTINUE                                                       007780
0075                  DO 9 MM=1,MA1                                                    007790
0076                  DO 8 ML=1,MA1                                                    007800
0077                  VSGI1=VSGI1+DSG(MM)*B(MM,ML)*DSG(ML)                             007810
0078                8 CONTINUE                                                       007820
```

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0079                9 CONTINUE                                                  007830
0080               10 DLSGI1(K)=SQRT(VSGI1)/H(1)                                007840
0081               11 CONTINUE                                                  007850
0082                  RETURN                                                    007860
0083                  END                                                       007870
```

```
                C                                                                       007880
                C                                                                       007890
0001                 SUBROUTINE XSECT(E,K)                                              007900
                C                                                                       007910
                C        XSECT CALCULATES CROSS SECTIONS AND DERIVATIVES.                007920
                C           E: NEUTRON ENERGY                                           007930
                C           K: ENERGY GRID SUBSCRIPT (INTERNAL OR "FINE" GRID)          007940
                C        S-WAVE CROSS SECTIONS ARE CALCULATED WITH THE REICH-MOORE       007950
                C        FORMALISM WITHOUT DOPPLER BROADENING.                          007960
                C        HIGHER-ORDER PARTIAL-WAVE CROSS SECTIONS ARE CALCULATED        007970
                C        WITH DOPPLER-BROADENED SINGLE-LEVEL EXPRESSIONS WITHOUT        007980
                C        RESONANCE/POTENTIAL INTERFERENCE.                              007990
                C                                                                       008000
0002                 COMMON                                                             008010
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQQ,                                 008020
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 008030
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         008040
                    4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),           008050
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           008060
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MQ,           008070
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   008080
                    8SC(2048),T(2048),YY(2048,20),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC, 008090
                    9F(201),RF(201)                                                     008100
0003                 COMMON/GQSR/DR11(20),DR21(20),DR22(20)                             008110
0004                 COMMON/II/ SGI1(2048),DLSGI1(2048)                                 008120
0005                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           008130
0006                 COMPLEX DR11,DR21,DR22,U11,DU11(20),U21,DU21(20),EX1,ZZZ           008140
                C        FUNCTION DEFINITION                                            008150
0007                 ABSQ(ZZZ)=REAL(ZZZ)**2+AIMAG(ZZZ)**2                               008160
                C                                                                       008170
0008                 M=0                                                                008180
0009                 ST(K)=0.                                                           008190
0010                 SG(K)=0.                                                           008200
0011                 SC(K)=0.                                                           008210
0012                 DO 50 II=1,MA                                                      008220
0013                 DST(II)=0.0                                                        008230
0014                 DSG(II)=0.0                                                        008240
0015              50 CONTINUE                                                           008250
0016                 PLQ2=1.3019/E                                                      008260
                C        POTENTIAL-SCATTERING PHASE FACTOR, PREPARATION:                 008270
0017                 AR1=(2.*E-E2-E1)/(E2-E1)                                           008280
0018                 AR1=AR1*0.95                                                       008290
0019                 ATGH=.5*ALOG((1.+AR1)/(1.-AR1))                                    008300
0020                 AR2=SQRT(1.E6*E)*ATGH                                              008310
0021                 DO 1 I=1,IX                                                        008320
                C        DOPPLER WIDTH                                                  008330
0022                 DW=D(I)*SQRT(E)                                                    008340
                C        CALCULATE POTENTIAL SCATTERING FOR P-WAVE                      008350
0023                 XK1=.21969*SQRT(E)/AL(I)                                           008360
0024                 XQ=XK1*RP(I)                                                       008370
0025                 X1=XQ-ATAN(XQ)                                                     008380
0026                 SP=H(I)*PLQ2*AL(I)**2*6.*SIN(X1)**2                                008390
0027                 ST(K)=ST(K)+SP                                                     008400
0028                 JH=JX(I)                                                           008410
0029                 DO 2 J=1,JH                                                        008420
0030                 M1=MP(I,J)+2                                                       008430
0031                 M2=MP(I,J)-2+4*LX(I,J)                                             008440
                C        S- OR P-WAVE LEVEL SEQUENCE?                                   008450
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0032                  IF(X(M1-1).EQ.0..AND.DLX(M1-1).EQ.0.)GO TO 7                      000845
                C         S-WAVE LEVELS:                                              000846
0033                  XT=CT(I,J)*PLQ2                                                   000847
0034                  XG=CG(I,J)*PLQ2                                                   000848
                C                                                                       000849
0035                    CALL KMAT(E)                                                    000850
0036                    CALL EFFI(E,K,EFK)                                              000851
                C                                                                       000852
                C         POTENTIAL-SCATTERING PHASE FACTOR:                          000853
0037                  AR3=X(M1-2)*AR2                                                   000854
0038                  XI1=-XK1*X(M1-1)+ATAN(AR3)                                        000855
0039                  EX1=CEXP(2.*GI*XI1)                                               000856
                C         COLLISION MATRIX ELEMENTS:                                  000857
0040                  U11=EX1*(2.*Z11-1.)                                               000858
0041                  U21=     2.*Z21                                                   000859
                C         TOTAL AND CAPTURE CROSS SECTION                             000860
0042                  ST(K)=ST(K)+XT*(1.-REAL(U11))                                     000861
0043                  SC0=XG*(1.-ABSQ(U11)-ABSQ(U21))                                   000862
0044                  SC(K)=SC(K)+SC0                                                   000863
0045                  SG(K)=SG(K)+SC0*EFK                                               000864
0046                  IF(SC(K).LT.1.E-7*ST(K))SC(K)=1.E-7*ST(K)                         000865
0047                  IF(SG(K).LT.1.E-7*ST(K))SG(K)=1.E-7*ST(K)                         000866
                C         DERIVATIVES WITH RESPECT TO POTENTIAL-SCATTERING PARAMETERS  000867
0048                  M0=M                                                              000868
0049                  IF(DLX(M1-2).EQ.0.)GO TO 8                                        000869
0050                  M=M+1                                                             000870
0051                  ABL= AR2/(1.+AR3**2)                                              000871
0052                  DU11(M)=2.*GI*ABL*U11                                             000872
0053                8 IF(DLX(M1-1).EQ.0.)GO TO 9                                        000873
0054                  M=M+1                                                             000874
0055                  ABL=-XK1                                                          000875
0056                  DU11(M)=2.*GI*ABL*U11                                             000876
0057                9 IF(LX(I,J).EQ.0.)GO TO 10                                       000877
                C         DERIVATIVES WITH RESPECT TO RESONANCE PARAMETERS             000878
0058                  DO 11 MM=M1,M2,4                                                  000879
0059                  DO 11 ML=1,4                                                      000880
0060                  MK=MM+ML-1                                                        000881
0061                  IF(DLX(MK).LE.0.)GO TO 11                                         000882
0062                  M=M+1                                                             000883
0063                  DU11(M)=GI*(Z11**2*DR11(M)+2.*Z11*Z21*DR21(M)+Z21**2*DR22(M))*EX1 000884
0064                  DU21(M)=Z21*Z11*DR11(M)+(Z21**2+Z11*Z22)*DR21(M)+Z21*Z22*DR22(M)  000885
0065                  DU21(M)=DU21(M)*GI                                                000886
0066               11 CONTINUE                                                          000887
0067               10 IF(M.EQ.M0)GO TO 2                                                000888
0068                  ML=M0+1                                                           000889
0069                  DO 12 MM=ML,M                                                     000890
0070                  DST(MM)=-XT*REAL(DU11(MM))                                        000891
0071                  DSG(MM)=-XT*REAL(DU11(MM)*CONJG(U11)+DU21(MM)*CONJG(U21))*EFK     000892
0072               12 CONTINUE                                                          000893
0073                  GO TO 2                                                           000894
                C         P-WAVE LEVELS:                                              000895
0074                7 IF(LX(I,J).EQ.0)GO TO 2                                         000896
0075                  CT1=CT(I,J)*PLQ2*2.                                               000897
0076                  L=0                                                               000898
                C         BEGIN RESONANCE LOOP                                        000899
0077                  DO 3 MM=M1,M2,4                                                   000900
0078                  L=L+1                                                             000901
0079                  GN=X(MM+1)**2                                                     000902
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0080                GX=X(MM+2)**2                                                   000930
0081                GT=GN+GX+X(MM+3)                                                000940
0082                QGT=EFF(I,J,L)*X(MM+3)/GT                                       000950
0083                MC=M                                                            000960
0084                IF(DLX(MM  ).NE.0.)M=M+1                                        000970
0085                IF(DLX(MM+1).NE.0.)M=M+1                                        000980
0086                IF(DLX(MM+2).NE.0.)M=M+1                                        000990
0087                IF(DLX(MM+3).NE.0.)M=M+1                                        001000
                C       APPROXIMATE 1/E-WIDTH OF DOPPLER BROADENED RESONANCE      001010
0088                HW=SQRT(DW**2+GT**2/2.77259)                                    001020
                C       IS LEVEL FAR AWAY AND HENCE NEGLIGIBLE?                   001030
0089                IF(ABS(E-X(MM)).GT.6.*HW)GO TO 3                                001040
0090                XV=2.*(E-X(MM))/GT                                              001050
0091                BV=2.*DW/GT                                                     001060
                C                                                                 001070
0092                  CALL VOIGT(XV,BV,PSI,PHI)                                   001080
                C                                                                 001090
0093                SO=CT1*GN/GT                                                    001100
0094                ST1=SO*PSI                                                      001110
0095                SG1=ST1*QGT                                                     001120
                C       CROSS SECTIONS                                            001130
0096                ST(K)=ST(K)+ST1                                                 001140
0097                SG(K)=SG(K)+SG1                                                 001150
0098                SC(K)=SC(K)+SG1/EFF(I,J,L)                                      001160
                C       ANY DERIVATIVES NEEDED?                                   001170
0099                IF(M.EQ.MO)GO TO 3                                              001180
0100                M=MC                                                            001190
0101                AO=-4./(GT*BV**2)                                               001200
0102                A1=AO*(   PHI-XV*PSI)                                           001210
0103                A2=AO*(1.-PSI-XV*PHI)                                           001220
                C       DERIVATIVES                                               001230
0104                IF(DLX(MM  ).EQ.0.)GO TO 6                                      001240
0105                M=M+1                                                           001250
0106                DST(M)=SO*A1                                                    001260
0107                DSG(M)=DST(M)*QGT                                               001270
0108              6 IF(DLX(MM+1).EQ.0.)GO TO 5                                      001280
0109                M=M+1                                                           001290
0110                DST(M)=SO*(2.*PSI/GN+A2)*X(MM+1)                                001300
0111                DSG(M)=DST(M)*QGT-2.*SG1*X(MM+1)/GT                             001310
0112              5 IF(DLX(MM+2).EQ.0.)GO TO 4                                      001320
0113                M=M+1                                                           001330
0114                DST(M)=SO*A2*X(MM+2)                                            001340
0115                DSG(M)=DST(M)*QGT-2.*SG1*X(MM+2)/GT                             001350
0116              4 IF(DLX(MM+3).EQ.0.)GO TO 3                                      001360
0117                M=M+1                                                           001370
0118                DST(M)=SO*A2*.5                                                 001380
0119                DSG(M)=DST(M)*QGT+(ST1*EFF(I,J,L)-SG1)/GT                       001390
0120              3 CONTINUE                                                        001400
                C       (END OF RESONANCE LOOP)                                   001410
0121              2 CONTINUE                                                        001420
                C       (END OF SPIN LOOP)                                        001430
0122                IF(ZIT.LE.1..AND.AG(I).EQ.AG(1))SIG1(K)=SC(K)/H(1)              001440
0123              1 CONTINUE                                                        001450
                C       (END OF ISOTOPE LOOP)                                     001460
0124                RETURN                                                          001470
0125                END                                                             001480
```

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                C                                                                       000590
                C                                                                       000600
0001                 SUBROUTINE KMAT(E)                                                 000610
                C                                                                       000620
                C         KMAT CALCULATES THE ELEMENTS OF THE MATRIX R=2*K               000630
                C         AND INVERTS THE MATRIX 1-I*K = 1-I*R/2.                       000640
                C                                                                       000650
0002                 COMMON                                                             000660
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 000670
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 000680
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         000690
                    4G(11,2),CS(11,2),X(2000),DLX(2000),ES(11,2),EFF(11,2,200),         000700
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           000710
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,           000720
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   000730
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  000740
                    9F(201),RF(201)                                                     000750
0003                 COMMON/GQSR/DR11(20),DR21(20),DR22(20)                             000760
0004                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           000770
                    1,FE,F1,F2,EX1,EX2,U11,U21,DU11(20),DU21(20),DET,R11,R21,R22        000780
0005                 COMPLEX DR11,DR21,DR22                                             000790
                C                                                                       000800
0006                 R11=(0.,0.)                                                        000810
0007                 R21=(0.,0.)                                                        000820
0008                 R22=(0.,0.)                                                        000830
0009                 IF(LX(I,J).EQ.0)GO TO 2                                            000840
                C         (GO TO 2 IF THERE ARE NO RESONANCES)                          000850
0010                 MO=M                                                               000860
0011                 IF(DLX(M1-2).NE.0.)M=M+1                                           000870
0012                 IF(DLX(M1-1).NE.0.)M=M+1                                           000880
0013                 DO 3 MM=M1,M2,4                                                    000890
0014                 SQ1=(E/ABS(X(MM)))**.25                                            000900
0015                 IF(E.LE.ES(I,J))SQ2=0.                                             000910
0016                 IF(E.GT.ES(I,J))SQ2=((E-ES(I,J))/ABS(X(MM)-ES(I,J)))**.25          000920
0017                 FE=1./(X(MM)-E-HI*X(MM+3))                                         000930
0018                 W1=SQ1*X(MM+1)                                                     000940
0019                 W2=SQ2*X(MM+2)                                                     000950
0020                 F1=W1*FE                                                           000960
0021                 F2=W2*FE                                                           000970
0022                 R11=R11+F1*W1                                                      000980
0023                 R21=R21+F2*W1                                                      000990
0024                 R22=R22+F2*W2                                                      001000
0025                 IF(DLX(MM).EQ.0.)GO TO 4                                           001010
0026                 M=M+1                                                              001020
0027                 DR11(M)=-F1*F1                                                     001030
0028                 DR21(M)=-F2*F1                                                     001040
0029                 DR22(M)=-F2*F2                                                     001050
0030               4 IF(DLX(MM+1).LE.0.)GO TO 5                                         001060
0031                 M=M+1                                                              001070
0032                 DR11(M)=F1*SQ1*2.                                                  001080
0033                 DR21(M)=F2*SQ1                                                     001090
0034                 DR22(M)=0.                                                         001100
0035               5 IF(DLX(MM+2).EQ.0.)GO TO 6                                         001110
0036                 M=M+1                                                              001120
0037                 DR11(M)=0.                                                         001130
0038                 DR21(M)=SQ2*F1                                                     001140
0039                 DR22(M)=SQ2*F2*2.                                                  001150
0040               6 IF(DLX(MM+3).LE.0.)GO TO 3                                         001160
```

```
0041                M=M+1                                                          010160
0042                DR11(M)=HI*F1*F1                                               010170
0043                DR21(M)=HI*F2*F1                                               010180
0044                DR22(M)=HI*F2*F2                                               010190
0045              3 CONTINUE                                                       010200
0046                M=MC                                                           010210
0047              2 DET=(1.-HI*R11)*(1.-HI*R22)-(HI*R21)**2                        010220
0048                Z11=(1.-HI*R22)/DET                                            010230
0049                Z21=(   HI*R21)/DET                                            010240
0050                Z22=(1.-HI*R11)/DET                                            010250
0051                RETURN                                                         010260
0052                END                                                            010270
```



```
                  C                                                              010280
                  C
0001                SUBROUTINE EFFI(E,K,EFK)                                     010290
                  C                                                              010300
                  C       EFFI YIELDS THE AVERAGE DETECTOR EFFICIENCY (EFK)      010310
                  C       FOR THE I-TH ISOTOPE AND THE J-TH COMPOUND SPIN        010320
                  C                                                              010330
0002                COMMON                                                       010340
                   1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                           010350
                   2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),  010360
                   3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),   010370
                   4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),     010380
                   5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),     010390
                   6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,     010400
                   7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),  010410
                   8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  010420
                   9F(201),RF(201)                                               010430
0003                COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                     010440
                  C                                                              010450
                  C       ANY RESONANCES?                                        010460
0004                IF(LX(I,J).EQ.0)RETURN                                       010470
0005                EFK=EFC                                                      010480
                  C       SAME EFFICIENCY FOR ALL RESONANCES?                    010490
0006                IF(EFC.NE.0.)RETURN                                          010500
0007                SUM=0.                                                       010510
0008                SOM=0.                                                       010520
0009                L=0                                                          010530
0010                M1=MP(I,J)+2                                                 010540
0011                M2=MP(I,J)-2+4*LX(I,J)                                       010550
0012                DO 1 MM=M1,M2,4                                              010560
0013                L=L+1                                                        010570
0014                GN=X(MM+1)**2*SQRT(E/ABS(X(MM)))                             010580
0015                GX=X(MM+2)**2                                                010590
0016                GT=GN+GX+X(MM+3)                                             010600
0017                TM=GN*X(MM+3)/(4.*(E-X(MM))**2+GT**2)                        010610
0018                SUM=SUM+TM*EFF(I,J,L)                                        010620
0019              1 SOM=SOM+TM                                                   010630
0020                EFK=SUM/SOM                                                  010640
0021                RETURN                                                       010650
0022                END                                                          010660
```

```
                C                                                               010670
                C                                                               010680
0001                  SUBROUTINE VOIGT(X,B,PSI,PHI)                             010690
                C                                                               010700
                C         CALCULATION OF SYMMETRIC VOIGT PROFILE                010710
                C         X    : DEVIATION FROM RESONANCE ENERGY IN UNITS OF HALF010720
                C                THE HALF WIDTH                                 010730
                C         B    : DOPPLER WIDTH IN THE SAME UNITS                010740
                C         PSI  : SYMMETRIC VOIGT PROFILE                        010750
                C        PHI : ASYMMETRIC   "      "                            010760
                C                                                               010770
                C         YY=Y*Y, GF=(2*DLY/SQRT(PI))*EXP(-YY) GIVEN FOR DLY=0.7010780
                C         C1=DLY/SQRT(PI),C2=DLY/PI FOR DLY=0.7, C3=2*SQRT(PI)  010790
                C                                                               010800
0002                  DIMENSION YY(8),GF(8)                                     010810
0003                  DATA YY/.49,1.96,4.41,7.84,12.25,17.64,24.01,31.36/       010820
0004                  DATA GF/.483893E0,.111259E0,.960100E-2,.310948E-3,        010830
                     1        .377965E-5,.172428E-7,.295226E-10,.189711E-13/    010840
0005                  DATA C1/.394933/,C2/.222817/,C3/3.544908/                 010850
                C                                                               010860
0006                  XX=X*X                                                    010870
0007                  BB=B*B                                                    010880
0008                  PSI=C1/(1.+XX)                                            010890
0009                  PHI=PSI                                                   010900
0010                  DO 1 N=1,8                                                010910
0011                  YYBB=YY(N)*BB                                             010920
0012                  AQ=(1.-XX+YYBB)**2+4.*XX                                  010930
0013                  A1=(1.+XX+YYBB)*GF(N)/AQ                                  010940
0014                  A2=(1.+XX-YYBB)*GF(N)/AQ                                  010950
0015                  PSI=PSI+A1                                                010960
0016                 1 PHI=PHI+A2                                               010970
0017                  PHI=PHI*X                                                 010980
0018                  IF(B.LE.C2)RETURN                                         010990
0019                  ETA=2./(C2*B)                                             011000
0020                  EXPO=(XX-1.)/BB+ETA                                       011010
0021                  IF(EXPO.GT.25.)RETURN                                     011020
0022                  XI=2.*X/BB                                                011030
0023                  ZETA=X*ETA                                                011040
0024                  ACOS=COS(XI)                                              011050
0025                  BSIN=SIN(XI)                                              011060
0026                  CCOS=EXP(-ETA)-COS(ZETA)                                  011070
0027                  DSIN=SIN(ZETA)                                            011080
0028                  F=C3*EXP(-EXPO)/((CCOS**2+DSIN**2)*B)                     011090
0029                  PSI=PSI+F*(ACOS*CCOS-BSIN*DSIN)                           011100
0030                  PHI=PHI-F*(BSIN*CCOS+ACOS*DSIN)                           011110
0031                  RETURN                                                    011120
0032                  END                                                       011130
```

```
                C                                                                       011130
                C
0001                 SUBROUTINE SEY                                                     011140
                C                                                                       011150
                C         SEY YIELDS THE SECONDARY CAPTURE YIELD FOR AN INFINITE SLAB    011160
                C         THE TARGET NUCLEI ARE TAKEN TO BE AT REST.                    011170
                C                                                                       011180
0002                 COMMON                                                             011190
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                011200
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),011210
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),        011220
                    4G(11,2),GS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),          011230
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),          011240
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,          011250
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),  011260
                    8SC(2046),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC, 011270
                    9F(201),RF(201)                                                    011280
0003                 COMMON/SEYCO/YS(2048)                                              011290
0004                 COMMON/SEYM/FS(2048),PG(2048),PN(2048),FX,AA                       011300
0005                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           011310
0006                 DIMENSION U(5),W(5)                                                011320
0007                 DATA U/.013046736,.067468317,.160295215,.28330230,.42556283/       011330
0008                 DATA W/.033335672,.074725675,.109543181,.13463336,.14776211/       011340
                C                                                                       011350
                C         SECONDARY CAPTURE YIELD (INFINITE SLAB APPROXIMATION)         011360
0009                 ISOT=1                                                             011370
0010                 FX=0.                                                              011380
0011                 AA=(1.+AG(1))**2                                                   011390
0012                 E=EMN-DLE                                                          011400
0013                 DO 1 K=1,KKX                                                       011410
0014                 E=E+DLE                                                            011420
0015                 S1=0.                                                              011430
0016                 S2=0.                                                              011440
0017                 GX=XN(N)*ST(K)                                                     011450
0018                 T2=EXP(-GX)                                                        011460
                C         INTEGRATION BY 10-POINT GAUSSIAN QUADRATURE                   011470
0019                 DO 2 J=1,2                                                         011480
0020                 DO 2 I=1,5                                                         011490
0021                 XX=(1.-U(I))*FLOAT(J-1)+U(I)*FLOAT(2-J)                            011500
0022                 ANU=XN(N)                                                          011510
0023               6 SQ=SQRT(AG(1)**2-1.+XX**2)                                         011520
0024                 EX=E*(XX+SQ)**2/AA                                                 011530
0025                 WX=(XX+SQ)**2/AG(1)/SQ                                             011540
0026                 XL=(EX-E)/DLE+1.                                                   011550
0027                 L=XL                                                               011560
0028                 IF(L.GT.1)GO TO 4                                                  011570
0029                 SST=ST(1)                                                          011580
0030                 SSG=SG(1)                                                          011590
0031                 GO TO 5                                                            011600
0032               4 DIFF=AMOD(XL,1.)                                                   011610
0033                 SST=ST(L)+DIFF*(ST(L+1)-ST(L))                                     011620
0034                 SSG=SG(L)+DIFF*(SG(L+1)-SG(L))                                     011630
0035               5 G1=WX*SSG/SST                                                      011640
0036                 TAO=SST/XX                                                         011650
0037                 IF(GX-XN(N)*TAO.EQ.0.)GO TO 10                                     011660
0038                 G2=(EXP(-ANU*TAO)-T2*EXP(-(ANU-XN(N))*TAO))/(GX-XN(N)*TAO)*G1      011670
0039                 GO TO 73                                                           011680
0040              10 G2=EXP(-ANU*TAO)                                                   011690
```

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0041              70 S1=S1+G1*W(I)                                                  011700
0042                 S2=S2+G2*W(I)                                                  011710
0043                 IF(ANU.EQ.0.)GO TO 2                                           011720
0044                 ANU=0.                                                         011730
0045                 XX=-XX                                                         011740
0046                 GO TO 6                                                        011750
0047               2 CONTINUE                                                       011760
                 C        SECONDARY CAPTURE YIELD                                 011770
0048                 SNI=ST(K)-SC(K)                                                011780
0049                 FS(K)=XN(N)*SNI  /2.*((1.-T2)/GX*S1-S2)                        011790
0050               1 IF(FS(K).GT.FX)FX=FS(K)                                        011800
0051                 I=ISOT                                                         011810
0052                 RETURN                                                         011820
0053                 END                                                            011830
```

```
                C                                                                       011840
                C                                                                       011850
0001                    SUBROUTINE MUY                                                  011860
                C                                                                       011870
                C           MUY YIELDS THE MULTIPLE-COLLISION CONTRIBUTION TO THE       011880
                C           CAPTURE YIELD. THERMAL MOTION OF THE TARGET NUCLEI IS       011890
                C           NEGLECTED. THE SAMPLE IS TAKEN AS A CYLINDRICAL DISK.       011900
                C           THE INCIDENT BEAM IS ASSUMED COAXIAL WITH THE SAMPLE,       011910
                C           OF CONSTANT FLUX DENSITY AND WITH THE RADIUS EQUAL TO       011920
                C           EDGE*XR(N) (XR(N) IS THE SAMPLE RADIUS).                    011930
                C                                                                       011940
0002                    COMMON                                                          011950
                       1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQ0,                              011960
                       2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2),  011970
                       3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),FP(11),      011980
                       4G(11,2),CS(11,2),X(200),DLX(200),ES(11,2),EFF(11,2,200),        011990
                       5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),        012000
                       6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,M0,        012010
                       7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20), 012020
                       8SC(2048),T(2048),YY(2048),DYY(2048,2),ZZ(512),Z(512),DZ(20),EFC, 012030
                       9F(201),RF(201)                                                  012040
0003                    COMMON/SEYCC/YS(2048)                                           012050
0004                    COMMON/SEYM/FS(2048),PG(2048),PN(2048),FX,AA                    012060
0005                    COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                        012070
0006                    DIMENSION NC(2048)                                              012080
0007                    DIMENSION EM(500),WG(500),WN(500),U(500),V(500),W(500),         012090
                       1XM(500),YM(500),ZM(500),SK(500)                                 012100
0008                    DATA EDGE/.5/                                                   012110
                C                                                                       012120
0009                    JSPIN=J                                                         012130
                C           CALCULATE NEEDED FUNCTIONS                                  012140
0010                    DO 11 K=1,KKX                                                   012150
0011                    YS(K)=0.                                                        012160
0012                    PG(K)=SG(K)/ST(K)                                               012170
0013                 11 PN(K)=1.-SC(K)/ST(K)                                            012180
                C           BEGIN ENERGY LOOP                                           012190
0014                    E=EMN-DLE                                                       012200
0015                    DO 50 KE=1,KKX                                                  012210
0016                    E=E+DLE                                                         012220
0017                    WN0=(1.-T(KE))*PN(KE)                                           012230
                C           INITIAL NUMBER OF HISTORIES (IMPORTANCE SAMPLING)           012240
0018                    NH=ZH(N)*FS(KE)/FX+.5                                           012250
0019                    NHX=ZH(N)                                                       012260
0020                    IF(NH.GT.NHX)NH=NHX                                             012270
0021                    IF(NH.LT. 10)NH=10                                              012280
0022                    CK=2.*DLFP(1)/FP(1)*E/DLE/XN(1)                                 012290
0023                    DO 13 J=1,NH                                                    012300
0024                    EM(J)=E                                                         012310
0025                    WN(J)=WN0                                                       012320
                C           INITIAL DIRECTION;                                          012330
0026                    W(J)=1.                                                         012340
                C           ADDITIONAL PATH LENGTH                                      012350
0027                    SK(J)=0.                                                        012360
                C           COORDINATES OF FIRST COLLISION                              012370
                C           (BEAM RADIUS SMALLER THAN SAMPLE RADIUS)                    012380
0028                    XM(J)=XR(N)*SQRT(RANDOM(D))*EDGE                                012390
0029                    YM(J)=0.                                                        012400
0030                 13 ZM(J)=-ALOG(1.-WN0/PN(KE)*RANDOM(D))/ST(KE)                     012410
```

```
0031                FKO=YY(KE)                                                      012410
0032                SQM=0.                                                          012420
                C       BEGIN COLLISION LOOP                                        012430
0033                DO 14 K=1,2                                                     012440
0034                YH=NH                                                           012450
                C       BEGIN HISTORY LOOP                                          012460
0035                DO 15 J=1,NH                                                    012470
                C       COSINE OF CMS SCATTERING ANGLE                              012480
0036                CTHC=2.*RANDOM(0)-1.                                            012490
0037                QQ=1.+AG(1)**2+2.*AG(1)*CTHC                                    012500
                C       LAB SCATTERING ANGLE                                        012510
0038                CTH=(1.+AG(1)*CTHC)/SQRT(QQ)                                    012520
0039                STH=SQRT(1.-CTH**2)                                             012530
                C       NEW LAB ENERGY                                              012540
0040                EM(J)=EM(J)*QQ/AA                                               012550
                C       NEW TOTAL CROSS SECTION, SCATTERING AND CAPTURE PROBABILITY 012560
0041                XL=(EM(J)-EMN)/DLE+1.                                           012570
0042                IF(XL.GT.1.E01)GO TO 16                                         012580
0043                SST=ST(1)                                                       012590
0044                PPN=PN(1)                                                       012600
0045                PPG=PG(1)                                                       012610
0046                GO TO 19                                                        012620
0047             16 L=XL                                                            012630
0048                DD=XL-FLOAT(L)                                                  012640
0049                SST=ST(L)+DD*(ST(L+1)-ST(L))                                    012650
0050                PPN=PN(L)+DD*(PN(L+1)-PN(L))                                    012660
0051                PPG=PG(L)+DD*(PG(L+1)-PG(L))                                    012670
                C       AZIMUTH                                                     012680
0052             19 PHI=6.28318*RANDOM(0)                                           012690
0053                CPH=COS(PHI)                                                    012700
0054                SPH=SIN(PHI)                                                    012710
                C       NEW DIRECTION COSINES                                       012720
0055                IF(W(J)**2.LT.0.999)GO TO 21                                    012730
0056                U(J)=STH*CPH*W(J)                                               012740
0057                V(J)=STH*SPH*W(J)                                               012750
0058                W(J)=CTH*W(J)                                                   012760
0059                GO TO 22                                                        012770
0060             21 RHO=SQRT(1.-W(J)**2)                                            012780
0061                UNEW=CTH*U(J)+STH*(W(J)*U(J)*CPH-V(J)*SPH)/RHO                  012790
0062                V(J)=CTH*V(J)+STH*(V(J)*W(J)*CPH+U(J)*SPH)/RHO                  012800
0063                W(J)=CTH*W(J)-STH*CPH*RHO                                       012810
0064                U(J)=UNEW                                                       012820
                C       DISTANCE TO SAMPLE SURFACE                                  012830
                C       DC: DISTANCE TO CYLINDER                                    012840
                C       DP: DISTANCE TO PLANE                                       012850
0065             22 DC=3.*XR(N)                                                     012860
0066                DP=DC                                                           012870
0067                IF(W(J).LT.-0.0001)DP=      -ZM(J) /W(J)                        012880
0068                IF(W(J).GT.+0.0001)DP=(XN(N)-ZM(J))/W(J)                        012890
0069                IF(W(J).LT.-0.9999.OR.W(J).GT.+0.9999)GO TO 23                  012900
0070                B1=U(J)**2+V(J)**2                                              012910
0071                B2=U(J)*XM(J)+V(J)*YM(J)                                        012920
0072                B3=XR(N)**2-XM(J)**2-YM(J)**2                                   012930
0073                IF(B2.GE.0.)DC=B3/(B2+SQRT(B2**2+B1*B3))                        012940
0074                IF(B2.LT.0.)DC=(SQRT(B2**2+B1*B3)-B2)/B1                        012950
0075             23 DIS=AMIN1(DC,DP)                                                012960
0076                DS=AMIN1(DIS*SST,60.)                                           012970
0077                IF(DS.LT.1.E-07) DS=1.E-07                                      012980
```

```
                C         INTERACTING FRACTION                                          013990
0078                WI=1.-EXP(-DS)                                                      014000
0079                WG(J)=WN(J)*WI*PPG                                                  014010
0080                WN(J)=WN(J)*WI*PPN                                                  014020
                C         KY: SUBSCRIPT OF GRID POINT WHERE YS IS TO BE ADDED TO YY     014030
0081                KY=KK-INT(CK*(SK(J)+(1.+DS-DS/WI)/SST)+.5)                          014040
                C         SMOOTHING OF MONTE CARLO CONTRIBUTION:                        014050
0082                DELS=1.                                                             014060
0083                IF(DS.LT.3.4E)DELS=DS*.2887                                         014070
0084                K1=CK*DELS/SST+0.5                                                  014080
0085                IF(K1.LT.3)K1=3                                                     014090
0086                WGY=WG(J)/(YH*FLOAT(2*K1+1))                                        014100
0087                K2=KY+K1                                                            014110
0088                K1=KY-K1                                                            014120
0089                IF(K2.LT.1.OR.K1.GT.KKX)GO TO 15                                    014130
0090                IF(K1.LT.1)K1=1                                                     014140
0091                IF(K2.GT.KKX)K2=KKX                                                 014150
0092                DO 12 KY=K1,K2                                                      014160
0093             12 YS(KY)=YS(KY)+WGY                                                   014170
                C         COORDINATES OF NEXT COLLISION                                 014180
0094                S=-ALOG(1.-WI*RANDOM(D))/SST                                        014190
0095                XM(J)=XM(J)+S*U(J)                                                  014200
0096                YM(J)=YM(J)+S*V(J)                                                  014210
0097                ZM(J)=ZM(J)+S*W(J)                                                  014220
0098                D=SQRT(XM(J)**2+YM(J)**2)                                           014230
0099                IF(D).LE.XR(N))GO TO 24                                             014240
                C         CORRECT POSSIBLE TRUNCATION ERRORS                            014250
0100                XM(J)=XM(J)/D*0.99999                                               014260
0101                YM(J)=YM(J)/D*0.99999                                               014270
0102                IF(ZM(J).GT.XN(N))ZM(J)=0.99999*XN(N)                               014280
0103             24 SK(J)=SK(J)+S                                                       014290
0104             15 CONTINUE                                                            014300
                C         END OF HISTORY LOOP                                           014310
0105                SUM=0.                                                              014320
0106                DO 29 J=1,NH                                                        014330
0107             29 SUM=SUM+WG(J)                                                       014340
                C         AVERAGE CAPTURE PROBABILITY                                   014350
0108                FK=SUM/YH                                                           014360
0109                SUM=SUM+FK                                                          014370
0110                NC(KE)=K+1                                                          014380
                C         NEW NUMBER OF HISTORIES                                       014390
0111                NNH=ZH(N)*FK**2/FKO/FX+.5                                           014400
0112                IF(NNH.LT.NH)NH=NNH                                                 014410
0113                IF(NH.LT.1)GO TO 52                                                 014420
0114                FKO=FK                                                              014430
0115             14 CONTINUE                                                            014440
                C         END OF COLLISION LOOP                                         014450
0116             52 CONTINUE                                                            014460
                C         END OF ENERGY LOOP                                            014470
0117                DO 3 K=1,KKX                                                        014480
0118              3 YY(K)=YY(K)+YS(K)                                                   014490
0119                J=JSPIN                                                             014500
0120                RETURN                                                              014510
0121                END                                                                 014520
```

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FORTRAN IV G1  RELEASE 2.0            MAIN            DATE = 78181        11/36/14            PAGE 0001

                      C                                                                        013530
                      C
0001                        FUNCTION RANDOM(KRRR)                                              013540
                      C                                                                        013550
                      C         (PSEUDO-)RANDOM NUMBER GENERATOR.                              013560
                      C                                                                        013570
0002                        DATA IY/32767/                                                     013580
0003                    1 IX=IY                                                                013590
0004                        CALL RANDU(IX,IY,RANDOM)                                           013600
0005                        IF(RANDOM.GT.0.)RETURN                                             013610
0006                        IY=32767                                                           013620
0007                        GO TO 1                                                            013630
0008                        END                                                                013640


FORTRAN IV G1  RELEASE 2.0            MAIN            DATE = 78181        11/36/14            PAGE 0001

                      C                                                                        013650
                      C
0001                        SUBROUTINE CHISQ4(X,Y,K)                                           013660
                      C                                                                        013670
                      C         CHISQN YIELDS VALUES OF A CHI-SQUARED DISTRIBUTION WITH N      013680
                      C         DEGREES OF FREEDOM                                             013690
                      C         X: INCREMENT OF INDEPENDENT VARIABLE DIVIDED BY                013700
                      C            SQRT(2*VARIANCE)                                            013710
                      C         Y: DEPENDENT VARIABLE MULTIPLIED BY INCREMENT                  013720
                      C         K: SUBSCRIPT AT UPPER LIMIT (SUBSCRIPT AT CENTER OF GRAVITY    013730
                      C            IS 101)                                                     013740
                      C         A: N/2                                                         013750
                      C         B: SQRT(N)*X                                                   013760
                      C         C: EXP(-N/2)/GAMMA(N/2)*B                                      013770
                      C                                                                        013780
0002                        DIMENSION Y(201)                                                   013790
0003                        A=2.                                                               013800
0004                        B=2.*X                                                             013810
0005                        C=.1353353*B                                                       013820
0006                        D=EXP(B)                                                           013830
0007                        E=1./D                                                             013840
                      C                                                                        013850
                      C         GO FROM CENTER OF GRAVITY TOWARDS SMALLER J                    013860
0008                        XI=A-B                                                             013870
0009                        F=C/E                                                              013880
0010                        DO 1 J=101,K                                                       013890
0011                        XI=XI+B                                                            013900
0012                        F=F*E                                                              013910
0013                    1 Y(J)=F*XI**(A-1.)                                                    013920
                      C         GO FROM CENTER OF GRAVITY TOWARDS LARGER J UNTIL DISTRIBUTION   013930
                      C         DROPS TO ZERO                                                  013940
0014                        I1=A/B                                                             013950
0015                        XI=A                                                               013960
0016                        F=C                                                                013970
0017                        DO 2 I=1,I1                                                        013980
0018                        J=101-I                                                            013990
0019                        XI=XI-B                                                            014000
0020                        F=F*D                                                              014010
0021                    2 Y(J)=F*XI**(A-1.)                                                    014020
                      C         COMPLETE BY FILLING WITH ZEROES                                014030
0022                        I1=I1+1                                                            014040
0023                        I2=K-101                                                           014050
0024                        DO 3 I=I1,I2                                                       014060
0025                        J=101-I                                                            014070
0026                    3 Y(J)=0.                                                              014080
0027                        RETURN                                                             014090
0028                        END                                                                014100
```

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FORTRAN IV G1  RELEASE 2.0            MAIN            DATE = 78181      11/36/14          PAGE 0001

                      C                                                                    014110
                      C
0001                        SUBROUTINE TGAUSS(X,Y,K)                                       014120
                      C                                                                    014130
                      C         TGAUSS YIELDS VALUES OF A TRUNCATED GAUSSIAN, NORMALIZED TO 1 014140
                      C         IF TRUNCATED AT TWICE THE 1/E-WIDTH (K*X=2)                014150
                      C            X: INCREMENT OF INDEPENDENT VARIABLE DIVIDED BY 1/E-WIDTH, 014160
                      C            Y: DEPENDENT VARIABLE TIMES INCREMENT,                  014170
                      C            K: SUBSCRIPT AT UPPER LIMIT (SUBSCRIPT AT MEDIAN IS 101) 014180
                      C                                                                    014190
0002                        DIMENSION Y(201)                                               014200
0003                        Y(101)=0.566342*X                                              014210
0004                        F1=EXP(-X*X)                                                   014220
0005                        F2=F1*F1                                                       014230
0006                           DO 1 I=102,K                                                014240
0007                           Y(I)=Y(I-1)*F1                                              014250
0008                           J=202-I                                                     014260
0009                           Y(J)=Y(I)                                                   014270
0010                      1    F1=F1*F2                                                    014280
0011                        RETURN                                                         014290
0012                        END                                                            014300
```

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FORTRAN IV G1  RELEASE 2.0            MAIN            DATE = 78181      11/36/14          PAGE 0001

                      C                                                                    014310
                      C
0001                        SUBROUTINE SIMP(Y,M,N,SUM)                                     014320
                      C                                                                    014330
                      C         SIMPSON'S RULE:                                            014340
                      C                                                                    014350
0002                        DIMENSION Y(201)                                               014360
0003                        SUM=0.                                                         014370
0004                        K1=M+1                                                         014380
0005                        K2=N-1                                                         014390
0006                        DO 1 K=K1,K2,2                                                 014400
0007                      1 SUM=SUM+Y(K-1)+4.*Y(K)+Y(K+1)                                  014410
0008                        SUM=SUM/3.                                                     014420
0009                        RETURN                                                         014430
0010                        END                                                            014440
```

```
                C                                                               014450
                C                                                               014460
0001                    SUBROUTINE CHOBAN(MX,A,B)                               014470
                C                                                               014480
                C       MATRIX INVERSION BY THE "SQUARE-ROOT" METHOD OF         014490
                C       CHOLESKI AND BANACHIEWICZ,                              014500
                C       MX: RANK                                                014510
                C       A:  ORIGINAL MATRIX                                     014520
                C       B:  INVERTED MATRIX                                     014530
                C                                                               014540
0002                    DOUBLE PRECISION A(20,20),B(20,20),U(20,20),SUM         014550
                C       CONSTRUCT "SQUARE-ROOT" MATRIX U                        014560
0003                    DO 2 N=1,MX                                             014570
0004                    DO 2 M=N,MX                                             014580
0005                    SUM=0.                                                  014590
0006                    DO 1 K=1,N                                              014600
0007                  1 IF(K.LT.N)SUM=SUM+U(M,K)*U(N,K)                         014610
0008                    IF(M.EQ.N)U(N,N)=DSQRT(A(N,N)-SUM)                      014620
0009                  2 IF(M.GT.N)U(M,N)=(A(M,N)-SUM)/U(N,N)                    014630
                C       CALCULATE INVERSE B                                     014640
0010                    DO 4 NN=1,MX                                            014650
0011                    N=MX-NN+1                                               014660
0012                    DO 4 MM=NN,MX                                           014670
0013                    M=MX-MM+1                                               014680
0014                    SUM=0.                                                  014690
0015                    DO 3 K=M,MX                                             014700
0016                  3 IF(K.GT.M)SUM=SUM-U(K,M)*B(K,N)                         014710
0017                    IF(M.EQ.N)SUM=SUM+1./U(M,M)                             014720
0018                    B(M,N)=SUM/U(M,M)                                       014730
0019                  4 IF(M.NE.N)B(N,M)=B(M,N)                                 014740
0020                    RETURN                                                  014750
0021                    END                                                     014760
```

```
                C                                                                       014770
                C                                                                       014780
0001                 SUBROUTINE ADJ(IZ,MX,MA,K,CHISQ,X,DLX,B,C)                         014790
                C                                                                       014800
                C         CALCULATION OF IMPROVED CROSS SECTION PARAMETERS BY            014810
                C         MUTIPLICATION OF COVARIANCE MATRIX B INTO DEVIATION VECTOR C.  014820
                C                                                                       014830
0002                 DIMENSION X(200),DLX(200),C(20)                                    014840
0003                 DOUBLE PRECISION B(20,20)                                          014850
0004                 DATA FUDGE/.75/                                                    014860
                C         CALCULATE GAUSS' ERROR ADJUSTMENT FACTOR                      014870
0005                 CF=SQRT(CHISQ/FLOAT(K-MA))                                         014880
0006                 WRITE(6,100)CHISQ,CF,IZ                                            014890
0007               100 FORMAT(1H //' CHI SQARED:              ',1PE10.3/               014900
                   1             ' ERROR ADJUSTMENT FACTOR:',1PE10.3/                 014910
                   2             ' ITERATION STEP:          ',I10//)                  014920
0008                 M=0                                                                014930
0009                 DO 2 MM=1,MX                                                       014940
0010                 IF(DLX(MM).LE.0.)GO TO 2                                           014950
0011                 M=M+1                                                              014960
0012                 XM=0.                                                              014970
0013                 DO 1 MN=1,MA                                                       014980
0014               1 XM=XM+B(M,MN)*C(MN)                                                014990
0015                 XM=XM*FUDGE                                                        015000
0016                 X(MM)=X(MM)+XM                                                     015010
0017                 DLX(MM)=DSQRT(B(M,M))                                              015020
0018                 DLX(MM)=DLX(MM)*CF                                                 015030
0019               2 CONTINUE                                                           015040
0020                 RETURN                                                             015050
0021                 END
```

```
                C                                                                       015060
                C                                                                       015070
0001                 SUBROUTINE KEV                                                     015080
                C                                                                       015090
                C        KEV CONVERTS ENERGIES FROM MEV TC KEV                          015100
                C                                                                       015110
0002                 COMMON                                                             015120
                    1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQO,                                 015130
                    2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 015140
                    3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),         015150
                    4G(11,2),CS(11,2),X(2000),DLX(2000),ES(11,2),EFF(11,2,200),         015160
                    5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),           015170
                    6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,MO,           015180
                    7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20),   015190
                    8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC,  015200
                    9F(201),RF(201)                                                     015210
0003                 COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                           015220
                C                                                                       015230
0004                 DO 1 I=1,IX                                                        015240
0005                 JH=JX(I)                                                           015250
0006                 DO 1 J=1,JH                                                        015260
0007                 ES(I,J)=ES(I,J)*1000.                                              015270
0008                 IF(LX(I,J).EQ.0)GO TO 1                                            015280
0009                 M1=MR(I,J)                                                         015290
0010                 M2=MR(I,J)+4*LX(I,J)-4                                             015300
0011                 DO 1 M=M1,M2,4                                                     015310
0012                 X(M)=X(M)*1000.                                                    015320
0013                 X(M+1)=X(M+1)*ABS(X(M+1))*1000.                                    015330
0014                 X(M+2)=X(M+2)*ABS(X(M+2))*1000.                                    015340
0015                 X(M+3)=X(M+3)*1000.                                                015350
0016                 IF(DLX(M  ).GT.0.)DLX(M  )=DLX(M  )*1000.                          015360
0017                 IF(DLX(M+1).GT.0.)DLX(M+1)=DLX(M+1)*SQRT(ABS(X(M+1))*.001)*2000.   015370
0018                 IF(DLX(M+2).GT.0.)DLX(M+2)=DLX(M+2)*SQRT(ABS(X(M+2))*.001)*2000.   015380
0019                 IF(DLX(M+3).GT.0.)DLX(M+3)=DLX(M+3)*1000.                          015390
0020               1 CONTINUE                                                           015400
0021                 KH=KX(NX)                                                          015410
0022                 DO 2 K=1,KH                                                        015420
0023               2 EE(K)=EE(K)*1000.                                                  015430
0024                 EMN=1000.*EMN                                                      015440
0025                 DLE=1000.*DLE                                                      015450
0026                 RETURN                                                             015460
0027                 END                                                                015470
```

```
                C                                                                       015470
                C                                                                       015480
0001                    SUBROUTINE YPLOT                                                015490
                C                                                                       015500
                C       YPLOT PREPARES PLOTS OF MEASURED AND CALCULATED CAPTURE YIELDS  015510
                C       AND, FOR IZ=0, A CROSS SECTION PLOT FOR THE PURE 1ST ISOTOPE.   015520
                C                                                                       015530
                C       PLOTA(X,Y,N,NT,NP,NH,I,NS,NR,XMAX,XMIN,SX,YMAX,YMIN,SY,TEXT,ID) 015540
                C       IS A KFK PLOT SUBROUTINE WITH THE FOLLOWING ARGUMENTS:          015550
                C                                                                       015560
                C        1. X     ARRAY OF ABSCISSAE                                    015570
                C        2. Y     ARRAY OF ORDINATES                                    015580
                C        3. N     NUMBER OF CO-ORDINATE PAIRS                           015590
                C        4. NT=1  PLOT POINT SYMBOLS                                    015600
                C             =2  DRAW LINE                                             015610
                C             =3  DRAW LINE WITH POINT SYMBOLS                          015620
                C        5. NP    CHOOSE NP-TH POINT SYMBOL (FROM A LIST) IF NT=1 OR 3  015630
                C        6. NH=1  HEIGHT OF POINT SYMBOL 0.12 IN.                       015640
                C             =2  HEIGHT OF POINT SYMBOL 0.16 IN.                       015650
                C             =3  HEIGHT OF POINT SYMBOL 0.24 IN.                       015660
                C        7. I=1   LINEAR INTERPOLATION  (FOR NT=2 OR 3)                 015670
                C            =2   QUADRATIC     ''        (FOR NT=2 OR 3)               015680
                C            =3   CUBIC         ''        (FOR NT=2 OR 3)               015690
                C        8. NS    SPACING: EVERY NS-TH POINT IS TO BE MARKED            015700
                C                 (FOR NT=3)                                            015710
                C        9. NR=0  DRAW ONTO EXISTING PLOT                               015720
                C             =1  BEGIN NEW PLOT, (XMAX-XMIN)/(YMAX-YMIN) = 1           015730
                C             =2                  -''-                    = 2           015740
                C             =3                  -''-                    = 3           015750
                C             =4                  -''-                    = 4           015760
                C            >=5                  -''-                    = 1.5         015770
                C                 (NH,XMAX,XMIN,SX,YMAX,YMIN,SY,TEXT NEED NOT BE        015780
                C                 SPECIFIED FOR NR=0)                                   015790
                C        10. XMAX MAXIMAL ABSCISSA                                      015800
                C        11. XMIN MINIMAL ABSCISSA                                      015810
                C        12. SX   X-INCREMENT CORRESPONDING TO 0.01 IN.                 015820
                C        13. YMAX MAXIMAL ORDINATE                                      015830
                C        14. YMIN MINIMAL ORDINATE                                      015840
                C        15. SY   Y-INCREMENT CORRESPONDING TO 0.01 IN.                 015850
                C        16. TEXT FIGURE CAPTION, 60 ALPHAMERIC CHARACTERS              015860
                C        17. ID   FIGURE NUMBER                                         015870
                C                                                                       015880
0002                     COMMON                                                         015890
                        1HI,GI,Z11,Z21,Z22,IZ,CHISQ,CHISQ0,                            015900
                        2I,IX,J,JX(11),KX(5),L,LX(11,2),M,MA,MX,N,NX,KKX,MP(11,2),MR(11,2), 015910
                        3TITLE(20),ZIT,EPS,E1,E2,TEFF,H(11),AG(11),SPIN(11),RP(11),    015920
                        4G(11,2),GS(11,2),X(2000),DLX(2000),ES(11,2),EFF(11,2,200),    015930
                        5FP(5),DLFP(5),TC(5),TB(5),ZH(5),EE(512),Y(512),DLY(512),      015940
                        6XN(6),XR(6),TMX,AL(10),D(10),CT(10,2),CG(10,2),M1,M2,M0,      015950
                        7DLE,EMN,ST(2048),DLST(2048),DST(20),SG(2048),DLSG(2048),DSG(20), 015960
                        8SC(2048),T(2048),YY(2048),DYY(2048,20),ZZ(512),Z(512),DZ(20),EFC, 015970
                        9F(201),RF(201)                                                015980
0003                     COMMON/I1/ SGI1(2048),DLSGI1(2048)                             015990
0004                     DIMENSION EF(2),YF(2),EK(2048)                                 016000
0005                     COMPLEX HI,GI,Z11,Z21,Z22,DZ11,DZ21,DZ22                       016010
                C                                                                       016020
                C           ENERGY RANGE OF PLOTS (SAME FOR 1ST AND 2ND PLOT):          016030
0006                     KH=KX(1)                                                       016040
```

```
0007                EMIN=EE(1)                                                  016040
0008                EMAX=EE(KH)                                                 016050
0009                IF(NX.EQ.1)GO TO 2                                          016060
0010                DO 1 N=2,NX                                                 016070
0011                KN=KX(N-1)+1                                                016080
0012                KH=KX(N)                                                    016090
0013                EMIN=AMIN1(EMIN,EE(KN))                                     016100
0014                EMAX=AMAX1(EMAX,EE(KH))                                     016110
0015              1 CONTINUE                                                    016120
0016              2 EBER=(EMAX-EMIN)*1.001                                      016130
0017                ILG=ALOG10(EBER)                                            016140
0018                IF(EBER.LT.1.)ILG=ILG-1                                     016150
0019                DEK=10.0**ILG                                               016160
0020                EBER=EBER/DEK                                               016170
0021                BER=10.                                                     016180
0022                IF(EBER.LE.5.  )BER=5.                                      016190
0023                IF(EBER.LE.2.5 )BER=2.5                                     016200
0024                IF(EBER.LE.1.25)BER=1.25                                    016210
0025                BER=BER*DEK                                                 016220
0026                EMIN=FLOAT(INT(25.*EMIN/BER))*BER/25.                       016230
0027                EMAX=EMIN+BER                                               016240
0028                SE=0.0025*BER                                               016250
                  C      CAPTURE YIELD RANGE OF 1ST PLOT:                     016260
0029                YMAX=0.                                                     016270
0030                KH=0                                                        016280
0031                DO 4 N=1,NX                                                 016290
0032                KN=KH+1                                                     016300
0033                KH=KX(N)                                                    016310
0034                DO 3 KK=KN,KH                                               016320
0035                IF(Y(KK)+DLY(KK).GT.YMAX)YMAX=Y(KK)+DLY(KK)                 016330
0036              3 CONTINUE                                                    016340
0037              4 CONTINUE                                                    016350
0038                YBER=YMAX*22./25.*1.2                                       016360
0039                ILG=ALOG10(YBER)                                            016370
0040                IF(YBER.LT.1.)ILG=ILG-1                                     016380
0041                DEK=10.0**ILG                                               016390
0042                YBER=YBER/DEK                                               016400
0043                BER=11.                                                     016410
0044                IF(YBER.LE.5.5)BER=5.5                                      016420
0045                IF(YBER.LE.4.4)BER=4.4                                      016430
0046                IF(YBER.LE.2.2)BER=2.2                                      016440
0047                IF(YBER.LE.1.1)BER=1.1                                      016450
0048                BER=BER*DEK                                                 016460
0049                YMIN=-BER*3./22.                                            016470
0050                YMAX= BER                                                   016480
0051                SY=0.001*BER*25./22.                                        016490
0052                KH=0                                                        016500
0053                DO 8 N=1,NX                                                 016510
0054                KN=KH+1                                                     016520
0055                KH=KX(N)                                                    016530
                  C     NP: NUMBER OF POINTS TO BE PLOTTED                    016540
0056                NP=KH-KN+1                                                  016550
                  C      PLOT CALCULATED YIELDS AS CURVE (1ST PLOT)           016560
0057                IF(N.EQ.1)CALL PLOTA(EE    ,Z     ,NP,2,0,1,3,0,2,EMAX,EMIN,SE,  016570
                   1YMAX,YMIN,SY,TITLE,IZ)                                      016580
0058                IF(N.GT.1)CALL PLOTA(EE(KN),Z(KN),NP,2,0,1,3,0,0,EMAX,EMIN,SE,  016590
                   1YMAX,YMIN,SY,TITLE,IZ)                                      016600
                  C      PLOT MEASURED POINTS (1ST PLOT)                      016610
```

```
0059                  IF(N.LE.3)NS=N-1                                                  016620
0060                  IF(N.EQ.2)NS=4                                                    016630
0061                  IF(N.GE.4)NS=N+3                                                  016640
0062                  CALL PLOTA(EE(KN),Y(KN),NP,1,NS,1,3,3,0,EMAX,EMIN,SE,ZMAX,ZMIN,SZ,  016650
                     1D,0)                                                              016660
                    C         PLOT ERROR BARS OF MEASURED POINTS (1ST PLOT)            016670
0063                  DO 5 KK=KN,KH                                                     016680
0064                  EF(1)=EE(KK)                                                      016690
0065                  EF(2)=EE(KK)                                                      016700
0066                  YF(1)=Y(KK)+DLY(KK)                                               016710
0067                  YF(2)=Y(KK)-DLY(KK)                                               016720
0068                  IF(YF(2).LT.YMIN)YF(2)=YMIN                                       016730
0069                  CALL PLOTA(EF,YF,2,2,0,1,1,0,0,EMAX,EMIN,SE,YMAX,YMIN,SY,0,0)     016740
0070                5 CONTINUE                                                          016750
0071                8 CONTINUE                                                          016760
0072                  IF(ZIT.GE.1.)RETURN                                               016770
                    C         PLOT CAPTURE CROSS SECTION OF PURE FIRST ISOTOPE (2ND PLOT)  016780
                    C         CROSS SECTION RANGE OF 2ND PLOT:                        016790
0073                  EK(1)=EMN                                                         016800
0074                  DO 6 K=2,KKX                                                      016810
0075                  EK(K)=EK(K-1)+DLE                                                 016820
0076                6 CONTINUE                                                          016830
0077                  K1=(EMIN-EK(1))/DLE+2.                                            016840
0078                  K2=(EK(KKX)-EMAX)/DLE                                             016850
0079                  K2=KKX-K2-1                                                       016860
0080                  IF(K1.LT.  1)K1=  1                                               016870
0081                  IF(K2.GT.KKX)K2=KKX                                               016880
0082                  NP=K2-K1+1                                                        016890
0083                  SMIN=0.                                                           016900
0084                  SMAX=0.                                                           016910
0085                  DO 7 K=K1,K2                                                      016920
0086                  IF(SGI1(K).GT.SMAX)SMAX=SGI1(K)                                   016930
0087                7 CONTINUE                                                          016940
0088                  SBER=SMAX*1.2                                                     016950
0089                  ILG=ALOG10(SBER)                                                  016960
0090                  IF(SBER.LT.1.)ILG=ILG-1                                           016970
0091                  DEK=10.0**ILG                                                     016980
0092                  SBER=SBER/DEK                                                     016990
0093                  BER=12.5                                                          017000
0094                  IF(SBER.LE.6.25)BER=6.25                                          017010
0095                  IF(SBER.LE.5.  )BER=5.                                            017020
0096                  IF(SBER.LE.2.5 )BER=2.5                                           017030
0097                  IF(SBER.LE.1.25)BER=1.25                                          017040
0098                  SMAX=BER*DEK                                                      017050
0099                  SS=0.001*SMAX                                                     017060
0100                  CALL PLOTA(EK(K1),SGI1(K1),NP,2,0,1,3,0,2,EMAX,EMIN,SE,           017070
                     1SMAX,SMIN,SS,TITLE,IZ)                                            017080
0101                  RETURN                                                            017090
0102                  END                                                               017100
```