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ANALYSIS OF NEUTRON RESONANCES IN FISSILE ELEMENTS:

PROGRAMS CØDILLI, CURVEPLØT, AND SIGMA

D. B. Adler and F. T. Adler

RELEASED FOR ANNOUNCEMENT

IN NUCLEAR SCIENCE ABSTRACTS

Department of Physics
University of Illinois
Urbana, Illinois

September, 1966

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ANALYSIS OF NEUTRON RESONANCES IN FISSILE ELEMENTS:

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D. B. Adler and F. T. Adler

ABSTRACT

An interrelated group of programs has been developed for the analysis of low energy neutron cross sections of fissile elements. The method of analysis is based on the multilevel expansion of the cross sections. The basic program, CØDILLI, consists of a combination of interdependent Subroutines. This facilitates not only the adaptation to other computers but it also allows freedom to incorporate specific experimental information such as resolution functions or statistical errors. The numerical determination of the resonance parameters is performed by the standard least squares techniques which make use of the Gauss linearization method for nonlinear trial functions.

Program SIGMA provides for the calculation of capture and scattering cross sections from fitted total and fission cross section data, as well as for various methods of comparing different cross section models. Program CURVEPLØT provides for multilevel analysis without least-squares fitting and it also provides for a graphical representation of the cross sections by means of a CALCOMP plotter.

A description of the programs and of their modus operandi are given in the appendices together with the listings in the FØRTRAN II version used at the University of Illinois.

I. INTRODUCTION

The programs CØDILLI, CURVEPLØT, and SIGMA described below belong to a family of FØRTRAN II programs written for the purpose of analyzing the low energy neutron cross sections of fissile elements⁽¹⁾ with the multilevel formalism as described in previous reports.⁽²⁾

The program CØDILLI has been written for analysis of experimental data by least squares fitting. It can handle simultaneously 32 levels as well as take into account the effects of 20 extra levels for which the resonance parameters are known. Some or all of these extra levels may be located in the energy region chosen for the fitting of the unknown levels. Thus, it is easily possible to take care of the effects of known impurities in the targets, or to utilize already existing information on the level structure.

To analyze a given set of data with the program CØDILLI, some detailed information is needed on the condition of the measurement such as the resolution function and the effective temperature, and on the statistical errors connected with the experiment.

Also, the process of data analysis cannot be automatized entirely; it is necessary to postulate level locations and estimates for the level widths in order to begin the evaluation. These preliminary values for level locations and total widths have to be obtained either by inspection of the experimental curves, or from existing compilations of resonance parameters.

The least squares analysis is based on the conventional solution of the normal equations.⁽³⁾ Nonlinear parameters are also analyzed by the application of the Gauss method of linearization.⁽⁴⁾

The program CØDILLI provides as output on cards the parameters for the multilevel expansion obtained from the fitting and lists of the values of the experimental cross section data together with the apparent cross section curve, i.e., the trial function resulting from the least squares fitting process, as well as relative deviations and evaluated standard deviations.

The results of the fitting frequently require additional calculations in order to be understood or evaluated. A satellite program, CURVEPLØT, has been written for this purpose. Similar to CØDILLI, CURVEPLØT analyzes (without fitting) a set of cross-section data by comparing it for the same energy interval to the contribution of a given set of known multilevel parameters, which may be only a part of those derived from the fitting. For example, the contributions of negative energy levels can be studied in this manner.

The original version of CURVEPLØT, written for the IBM-7094 (1964), was later (1965) transcribed for the ILLIAC II in order to utilize a CALCOMP plotter for the graphic representation of the results. Recently (June, 1966) the CALCOMP plotter has become available for use also with the IBM-7094 at Illinois and a third version of CURVEPLØT is now being used on the 7094/CALCOMP.

Although CURVEPLØT shares with CØDILLI seven subroutines and therefore contains a large fraction of the same programming, such distribution of operations between CØDILLI and CURVEPLØT allows for an efficient use of the IBM-7094 computer at Illinois.

Users at different installations may find it, however, preferable to insert a CALCOMP plotting subroutine directly into the program CØDILLI.

It should be noted, however, that the program CURVEPLOT can provide a variety of additional pieces of information beyond that given by the least squares analysis as performed in CØDILLI.

Finally, the program SIGMA has been written to calculate the temperature broadened fission, capture, scattering, and total cross sections either from single-level data or from multilevel parameters. The program SIGMA has been designed as a complement of the fitting program. For example, when total and fission cross sections have been fitted, SIGMA can be used to establish the compatibility between the results of the two sets of parameters by calculating capture and scattering cross sections. It can also be used to investigate the effect of Doppler broadening, and more generally, the effects of changes in resonance parameters on the cross sections. For example, SIGMA has been used to compare cross sections obtained from single level and multilevel fits.

To facilitate the adaptation of these programs to a variety of experimental data and eventually to other computers, the different steps of the analytical procedure have been assigned as far as possible to separate subroutines. The program CØDILLI encompasses thirteen Subroutines, ten of which are in FØRTRAN II, while the Subroutines DINV (for double precision matrix inversion) DSQRT (double precision square root calculation), and the function ROUND (to round double precision numbers to single precision numbers) are in SCATRE.

Thus, in adapting CØDILLI to another computer only these three standard Subroutines would have to be replaced.

A modified version of CODILLI has also been written for the ILLIAC II computer of the University of Illinois. This version differs in memory requirements and in several subsidiary subroutines which are written in the ILLIAC II language NICAP, instead of in SCATRE. Because of the increased word length of ILLIAC II, it is possible to avoid the double precision arithmetic in the matrix inversion, and thus this version is faster than the IBM-7094 version of the program. The programs SIGMA and CURVEPLOT are entirely in FORTRAN II. These programs have been used extensively in analyzing experimental data with the IBM-7094 and with ILLIAC II.

The method of analysis is described in Section II, and the possible choices are derived for the trial function. The equations for the least squares analysis are derived in Section III. Section IV, V, VI contain the description of programs CODILLI and CURVE PLOT with the Subroutines pertaining to them.

Section VII gives a brief description of Routine SIGMA. Section VIII contains the final comments and conclusions. Input and Output for each program are described in Appendices A to D.

The listings of the FORTRAN programs are given in Appendices E to G.

II. METHOD OF ANALYSIS

A. The Multilevel Expansion

Least squares analysis requires the definition of a trial function, which here is obtained from the multilevel expansion, limited to a finite number of terms.⁽⁵⁾ The neglected levels are taken into account by inclusion of corresponding expansions for the immediately close resonances, whenever parameters for such resonances are available, and in all cases by inclusion of background terms. The general expansion for the total or the reaction cross section as presented in previous reports⁽⁵⁾ is given by:

$$\begin{aligned} \sqrt{E} \sigma_o^{(x)}(E) = & \frac{C}{\sqrt{E}} 2 (1 - \cos \omega) \\ & + C \sum_{k=1}^{\text{NRT} + \text{NOUT}} \frac{v_k (G_k^{(x)} \cos \omega + H_k^{(x)} \sin \omega) + (\mu_k - E) (H_k^{(x)} \cos \omega - G_k^{(x)} \sin \omega)}{(\mu_k - E)^2 + v_k^2} \\ & + C (A_1^{(x)} + A_2^{(x)} E + \dots + B_1^{(x)} E + B_2^{(x)} E^2 + \dots), \end{aligned} \quad (1)$$

where $C = 6.52 \times 10^5$ barns $\times$ eV.

Here $\mu_k - iv_k$ represents the k th pole of the collision matrix, so that μ_k represents the resonance energy and v_k the corresponding half-width of the k th level. The variable $\omega = 2WN\sqrt{E}$ represents the phase shift of the potential scattering, where WN expresses in appropriate units the nuclear "radius" when E is in eV. The phase ω is set equal to zero for any cross section, other than the total cross section. The index NOUT refers to the set of known, neighboring resonances, added to the NRT resonances, of which the parameters will be obtained by the least squares analysis. The set of NRT resonances refers to the totality of the fitted

resonances, and it contains NR resonances within the energy interval considered; it may also contain NEIGH resonances with unknown parameters in a region adjacent to the same interval. Such neighboring resonances have been used to analyze the "negative energy" levels of U-235, the contribution of which is essential in the lower energy region.

In the expansion (1) the meaning and the values of the background constants A_i , B_i depend on the particular energy interval in consideration, and on the contribution of the NOUT set; in particular, for $NOUT = 0$, A_1^T is expected to be larger than A_1^F , while if $NOUT \neq 0$ only the sum of A_1^T and of the NOUT contributions to σ_T has to be larger than the combined contributions of A_1^F and of the NOUT resonances to the fission cross section.

The parameters G, H of Eq. (1) are defined according to the specific cross section in consideration.⁽²⁾

A more convenient expression for the cross-section expansion given in (1) is obtained by introducing the following definitions for the unknowns:

$$X_k = \frac{G_k}{v_k}, \quad X_{NRT+k} = \frac{H_k}{v_k} \quad \text{for } k = 1, NR, \quad (2)$$

$$X_k = G_k v_k, \quad X_{NRT+k} = H_k v_k \quad \text{for } k = NR+1, \dots, NRT, \quad (2a)$$

$$X_k = A_i \quad \text{for } k = 2NRT + i \text{ and } i = 1, KNEG, \quad (2b)$$

$$X_k = B_i \quad \text{for } k = 2NRT + KN + i \text{ and } i = 1, KPOS, \text{ where} \quad (2c)$$

KNEG represents the number of background terms with negative powers of E, and KPOS refers similarly to terms with positive powers of E. Consistently, a new set of known vectors is defined:

$$\phi_k(E) = \frac{\cos \omega - y_k \sin \omega}{y_k^2 + 1} \quad \text{for } k = 1, \text{ NR} , \quad (3)$$

$$\phi_{\text{NRT} + k}(E) = \frac{y_k \cos \omega + \sin \omega}{y_k^2 + 1} \quad \text{for } k = 1, \dots \text{NR} , \quad (3a)$$

$$\left. \begin{aligned} \phi_k(E) &= \frac{\cos \omega - y_k \sin \omega}{v_k^2(1 + y_k^2)} \\ \phi_{\text{NRT} + k}(E) &= \frac{y_k \cos \omega + \sin \omega}{v_k^2(1 + y_k^2)} \end{aligned} \right\} \quad k = \text{NR} + 1 \dots \text{NRT} , \quad (3b)$$

$$\text{with } y_k = \frac{\mu_k - E}{v_k} ,$$

$$\phi_{2\text{NRT} + i}(E) = E^{1-i} \quad \text{for } i \neq 1, \text{ KNEG} , \quad (3c)$$

$$\phi_{2\text{NRT} + \text{KNEG} + i}(E) = E^i \quad \text{for } i = 1, \text{ KPOS} , \quad (3d)$$

and similar vectors, $\phi_J(E)$, for the NOUT terms. Using Eqs. (2) and (3), the expansion given in (1) now has the form,

$$\sqrt{E} \sigma_o^{(x)}(E) = \frac{2C}{\sqrt{E}} (1 - \cos \omega) + C \sum_{k=1}^{\text{NG}} X_k \phi_k(E) + C \sum_{J=1}^{2\text{NOUT}} X_J^0 \phi_J(E) , \quad (4) \quad \text{where}$$

$\text{NG} = 2 \text{NRT} + \text{KPOS} + \text{KNEG}$, and where X_J^0 are the known parameters of the NOUT resonances.

B) Doppler Broadening

In general, the Doppler broadened cross section is expressed by

$$\sqrt{E} \sigma_c^{(x)}(E) = \int K_D(E; E') \sqrt{E'} \sigma_o^{(x)}(E') dE', \quad (5)$$

where $K_D(E; E')$ is the Doppler broadening kernel, representing the effect of the medium temperature on the resonance lines. By applying this convolution to each term in (4) and with the notations:

$$\phi(E; T) = \int K_D(E; E') \phi(E') dE', \quad (6)$$

Equation (5) can now be written as an expansion, formally analogous to Eq. (4):

$$\sqrt{E} \sigma_c^{(x)}(E) = C \sum_{k=1}^{NG} X_k \phi_k(E; T) + C \sum_{J=1}^{2NOUT} X_J^0 \phi_J(E; T) + \frac{2C}{\sqrt{E}} (1 - \cos \omega), \quad (7)$$

where the broadening effects for the potential scattering term have been neglected.

It is useful to separate in Eq. (7) the unknown terms from the known contributions. Thus, the Doppler broadened cross section of Eq. (7) is written as

$$\sqrt{E} \sigma_c^{(x)}(E) = C \sum_{k=1}^{NG} X_k \phi_k(E; T) + \sqrt{E} \sigma_{Dis}^{(x)}(E), \quad (7a)$$

where

$$\sqrt{E} \sigma_{Dis}^{(x)}(E) \equiv \sqrt{E} \sigma_{pot} + C \sum_{J=1}^{2NOUT} X_J^0 \phi_J(E; T), \quad (8)$$

and

$$\sigma_{pot} \equiv \frac{2C}{E} (1 - \cos \omega). \quad (9)$$

In the programs CØDILLI and CURVEPLØT, this last term is automatically set equal to zero when (x) represents either fission or capture cross section.

C.) Doppler and Resolution Broadening: The Trial Function

In the program CØDILLI the trial function for the least squares fit is given in the general form

$$Y_{app}^{(x)}(E) = \sum_{k=1}^{NG} X_k^{(x)} P_k^{(x)}(E) + Y_o^{(x)}(E) , \quad (10)$$

where the connection with the theoretical cross section of Eqs. (7) and (7a) depends upon the nature of the measurement from which the data have been obtained. In Eq. (10) the functions $P_k(E)$ and $Y_o^{(x)}(E)$ are known functions of E , and contain temperature and resolution effects, while the quantities X_k are the unknown parameters.

For the case of fission or capture measurements, the resolution effects can be represented directly by defining an apparent cross section $\sigma_{app}^{(x)}(E)$ in terms of $\sigma_c^{(x)}(E)$ and of the resolution kernel $K_R(E;E')$, so that

$$\sqrt{E} \sigma_{app}^{(x)}(E) = \int K_R(E;E') \sigma_c^{(x)}(E') \sqrt{E'} dE' . \quad (11)$$

By combining now Eqs. (11) and (7a), one has

$$\sqrt{E} \sigma_{app}^{(x)}(E) = C \sum_{k=1}^{NG} X_k^{(x)} P_k(E) + C Y_o^{(x)}(E) , \quad (12)$$

where the known functions $P_k(E)$ and $Y_o^{(x)}$ are defined by:

$$P_k(E) = \int K_R(E; E') \phi_k(E'; T) dE' , \quad (13)$$

$$\begin{aligned} CY_o^{(x)}(E) &= \int K_R(E; E') \sigma_{Dis}^{(x)}(E') \sqrt{E'} dE' \\ &\equiv C \sum_{J=1}^{2NOUT} X_J^o P_J(E) . \end{aligned} \quad (14)$$

Equation (12) is thus, aside from the factor C, identical to Eq. (10), where

$$Y_{app}^{(x)}(E) = \frac{1}{C} \sqrt{E} \sigma_{app}^{(x)}(E) . \quad (15)$$

Simplifications in the evaluation of the vector components P_k and therefore also of $Y_o^{(x)}$, are possible in the following situations:

(a) Whenever the motion of the target nucleus is not affected strongly by the crystalline binding. Michaudon⁽⁶⁾ has indicated that when the crystalline binding is weak its effects can be accounted for by introducing appropriately an effective temperature associated with the Debye temperature of the sample.

In this case the Doppler kernel is described by a Gaussian; even if the conventional Gaussian should be replaced by the "exact Doppler broadening" kernel, it still would be possible to express the broadening effects in terms of ψ and X functions⁷ where, however, the integration variable would be $\sqrt{E}$ rather than E .

For the case of a Gaussian Doppler broadening kernel the vector components ϕ_k appearing in Eq. (7) and defined in Eq. (3a) can be written explicitly in terms of the line shape functions ψ and χ , as:

$$\phi_k(E;T) = \cos \omega \psi_k(E;T) - \sin \omega \chi_k(E;T), \quad (16)$$

$$\phi_{NRT+k}(E;T) = \cos \omega \chi_k(E;T) + \sin \omega \psi_k(E;T), \quad (17)$$

where T represents the appropriate effective temperature in the sense discussed above.⁶ Thus, the folding of Eqs. (16) and (17) with the resolution kernel reduces Eq. (13) to simple rather than double convolutions. While the same broadening prescription is applied also to the functions ϕ_T of the NOUT resonances, the functions ϕ_k given in Eq. (3b) are kept unbroadened. The reason for this lies in the fact that only the "tails" of such resonances, which usually are meant to represent negative energy levels, are taken into account, while some of the NOUT resonances may lie in the energy interval considered.

(b) Whenever, also, the resolution kernel can be approximated by a Gaussian, the convolutions of the type (13) can be shown to give

$$P_k(E) = \phi_k(E; T_R), \quad (18)$$

where the vectors $\phi_k(E; T_R)$ are formally defined by (16), (17), and T_R represents a fictitious E -dependent temperature, obtained by combining the width of the resolution function with the Doppler width.

The combined Gaussian width is given by:

$$\Delta'^2 = \Delta_D^2 + \Delta_R^2, \quad (19)$$

where the Doppler width is given by

$$\Delta_D^2 = 4 \frac{k T E}{A}, \quad (20)$$

and, for time-of-flight measurements, the resolution width is defined by^{6,8,9}

$$\Delta_R^2 = A E^3 + B E^2, \quad (21)$$

and where the values of the parameters A and B are defined by the experimental conditions. Thus the value of the fictitious temperature T_R is given by:

$$kT_R = \frac{\Delta_R^2 A}{4E} \quad (22)$$

For relatively small energy intervals, and for small values of Δ_R one may replace T_R by its average value and thus the evaluation of $P_k(E)$ is reduced to the relatively simple but approximate evaluation of line shape functions at fixed temperatures. These different cases which lead to different types of trial functions are encompassed in CØDILLI, and are distinguished by an index, JS, as follows:

JS = 1 corresponds to the last case (i.e., average T_R , constant over a given energy interval),

JS = 2 corresponds to the general case of a non-Gaussian resolution kernel with a Gaussian Doppler broadening [Eqs. (13) and (14)],

JS = 4 corresponds to the simplified case of a Gaussian resolution kernel combined with a Gaussian Doppler broadening [Eq. (19)].

For total cross sections,⁸ normally transmission data are to be fitted which are related to the experimental cross section $\sigma_{\text{exp}}^{(T)}(E)$ by the relation

$$Y_{\text{ex}}^{(T)}(E) = e^{-N\sigma_{\text{ex}}^{(T)}(E)}, \quad (23)$$

where N is the sample thickness in atoms/barn. The trial function is correspondingly defined by the convolution

$$Y_{\text{app}}^{(T)}(E) = \int K_R(E; E') e^{-N\sigma_c^{(T)}(E')} dE', \quad (24)$$

where K_R indicates the resolution kernel and $\sigma_c^{(T)}$ is the theoretical cross section as given in Eqs. (7) and (7a). This case is denoted in CØDILLI by the index JS = 3. In this case the unknown parameters, contained in $\sigma_c^{(T)}(E)$, appear in the trial function in a nonlinear manner. A linearization in the Gauss sense is therefore necessary, and it is possible if one has available an appropriate "initial" trial function containing preliminary values of the parameters. Indicating with X_k^0 such a set of initial parameters, the theoretical cross section of Eq. (7a) can be written as

$$\begin{aligned} \sigma_c^{(T)}(E) = \frac{C}{\sqrt{E}} & \left[\sum_{k=1}^{NG} X_k^0 \phi_k(E; T) + \sum_{J=1}^{2NOUT} X_J^0 \phi_J(E; T) \right] + \sigma_{\text{pot}} \\ & + \frac{C}{\sqrt{E}} \sum_{k=1}^{NG} \delta X_k \phi_k(E; T), \end{aligned} \quad (25)$$

where the parameters defined as unknown are here the increments

$$\delta X_k = X_k - X_k^0. \quad (26)$$

Numerically, the known part of Eq. (25) can be treated in analogy with the expression given by Eq. (8). Thus, generalizing the meaning of σ_{Dis} , one defines

$$\sigma_{\text{Dis}}^T(E) = \sigma_{\text{pot}} + \frac{C}{\sqrt{E}} \sum_{k=1}^{NG + 2NOUT} X_k^0 \phi_k(E; T), \quad (27)$$

so that

$$\sigma_c^T(E) = \frac{C}{\sqrt{E}} \sum_{k=1}^{NG} \delta X_k \phi_k(E; T) + \sigma_{\text{Dis}}^T(E). \quad (25a)$$

The desired linearization is obtained by assuming that

$$\frac{C}{\sqrt{E}} \sum_{k=1}^{NG} \delta X_k \phi_k(E; T) \ll \sigma_{\text{Dis}}^T(E),$$

Thus, one can write

$$e^{-N\sigma_c^T(E)} \approx e^{-N\sigma_{\text{Dis}}^T(E)} \left(1 - \frac{NC}{\sqrt{E}} \sum_{k=1}^{NG} \delta X_k \phi_k(E; T) \right). \quad (28)$$

Introducing into Eq. (24) the expression given by Eq. (28), one has finally

$$Y_{\text{app}}^T(E) = \int K_R(E; E') e^{-N\sigma_{\text{Dis}}^T(E')} dE' - \sum_{k=1}^{NG} NC \delta X_k \int K_R(E; E') e^{-N\sigma_{\text{Dis}}^T(E)} \phi_k(E'; T) dE' / \sqrt{E'}, \quad (29)$$

so that, defining

$$Y_O^T(E) = \int K_R(E; E') e^{-N\sigma_{\text{Dis}}^T(E')} dE' \quad (30)$$

$$P_k(E) = -NC \int K_R(E;E') e^{-N\sigma_{Dis}^T(E')} \phi_k(E';T) dE' / \sqrt{E'} , \quad (31)$$

Eq. (29) is reduced to the form

$$Y_{app}^T(E) = Y_o^T(E) + \sum_{k=1}^{NG} \delta X_k P_k(E) , \quad (32)$$

which is structurally similar to Eq. (10).

For cases in which $N\sigma \ll 1$ (thin sample) Eq. (24) can be simplified to give

$$Y_{app}^T(E) \sim \int K_R(E;E') [1 - N\sigma_c^T(E')] dE' , \quad (33)$$

and correspondingly the experimental transmission becomes:

$$Y_{ex}^T(E) \sim 1 - N\sigma_{ex}^T(E) . \quad (34)$$

In this case the trial function (33) has the same form as the resolution broadened function of the Eq. (15), ($JS = 4$ or $JS = 2$).

This last case has been used to derive initial parameters X^0 ; using the complete expansion with too small initial values of X^0 can lead to unstable solutions; (e.g., the parameters for the fission cross sections of levels where the capture is large are not suitable as initial values).

The trial functions discussed so far, which appear as options in CØDILLI, are listed in Table I. The expansions and symbols used in this Table reflect the actual structure of those Subroutines of CØDILLI (and of CURVEPLOT), which occur directly in the calculation of the trial function (Subroutines PHIFRM, DSIG, PLOT, SCRAMB; see Section V.)

For this reason, the functions listed in Table I are written in a general form, which does not contain the detailed definition of the functions P_k , ϕ_k , or σ_{Dis} . The particular choice of these functions is effectuated by a combination of input indices (defining the total number of unknowns NG, the known resonance parameters, NOUT, etc), and their actual definition is based on the initial set of level parameters, μ , ν , characterizing the resonances to be analyzed.

The function ϕ_k , as given by the set of Eqs. (3) to (3d) represent, for a given NG, the known functions appearing in the trial function, corresponding to the NG coefficients X_k , as listed in Eqs. (2) to (2d). Thus, the expansions of the form (4), or (7), give an analytical representation of the theoretical cross section which is a linear expansion in terms of the unknowns X_k . The values of μ , ν , are in practical cases either obtained by inspecting the experimental data, or suggested by previous results. There is, however, no certainty, at the start, that such "guesses" reproduce the data satisfactorily until the results are obtained. Corrections and improvements (possibly also the addition of levels) can be made by modifying the original "guesses," and repeating the fitting. This process, which is necessary whenever the number of levels (i.e., NG) has to be changed, can be described as a parametric study of the level parameters μ , ν (and of the level number) which is based on the same type of linear expansion as discussed above. When the level number (i.e., NG) needs no modification, parametrization can be effectuated within CØDILLI by selecting the value of an index, IEND, and providing as input the new set of "guesses." Such types of fitting are referred to as "linear fits," in contrast with the case in which, leaving unchanged the number of the levels,

Table I. Optional Form of the Trial Functions in CØDILLI

JB	$Y_{\text{exp}}(E_1)$	$Y_{\text{app}}(E_1) = \sum_k X_k P_k(E_1) + Y_0(E_1)$	$P_k(E_1)$	$Y_0(E_1)$	Comments
1	$\frac{\sqrt{E_1}}{C} \sigma_{\text{ex}}(E_1)$	$\frac{\sqrt{E_1}}{C} \sigma_c(E_1; T_R)^{**}$	$\phi_k(E_1; T_R)^{**}$	$\frac{\sqrt{E_1}}{C} \sigma_{\text{Dis}}(E_1)$	Gaussian Doppler kernel, with approximate treatment of Gaussian Resolution. See Eq. (22).
2	$\frac{\sqrt{E_1}}{C} \sigma_{\text{ex}}(E_1)$	$\int_0^\infty \frac{\sqrt{E}}{C} \sigma_c(E) K_R(E_1; E) dE$	$\int_0^\infty K_R(E_1; E) \phi_k(E; T) dE$	$\int_0^\infty K_R(E_1; E) \frac{\sqrt{E}}{C} \sigma_{\text{Dis}}(E) dE$	Gaussian Doppler kernel, arbitrary Resolution kernel: see Eqs. (12), (13) and (14).
3	$e^{-N\sigma_{\text{ex}}(E_1)}$	$\int_0^\infty e^{-N\sigma_c(E)} K_R(E_1; E) dE$	$\int_0^\infty K_R(E_1; E) e^{-N\sigma_{\text{Dis}}(E)} \phi_k(E; T) \frac{dE}{\sqrt{E}}$	$\int_0^\infty K_R(E_1; E) e^{-N\sigma_{\text{Dis}}(E)} dE$	Transmission: see Eqs. (30), (31), and (32)
4	$\frac{\sqrt{E_1}}{C} \sigma_{\text{ex}}(E_1)$	$\frac{\sqrt{E_1}}{C} \sigma_c(E_1; \Delta')^*$	$\phi_k(E_1; \Delta')^*$	$\frac{\sqrt{E_1}}{C} \sigma_{\text{Dis}}(E_1; \Delta')$	Gaussian Resolution and Doppler kernels; see Eqs. (19), (20), and (21).

* Δ' = combined Gaussian width, accounting for Doppler broadening and Resolution effects.

** T_R = effective fictitious temperature representing a combined averaged, Resolution and Doppler broadening.

the level parameters μ , ν are considered as unknown and are to be determined by the least squares fitting procedure. This part of CODILLI is referred to as "non-linear fit."

d) Trial Functions for Non-Linear Cases

The definition of the known functions ϕ_k is modified for "non-linear" fits.

As for the case of transmission functions, the usual Gauss linearization method is applied, in order to bring the normal equations from a non-linear into a linear form. ⁽⁴⁾ The method amounts to express the unbroadened cross section equation given in Eq. (4) as a Taylor expansion around a certain initial set of known parameters (μ_k^0 , ν_k^0 , X_{NRT+k}^0 , for the k th level), truncated at the first term. Indicating now with ϕ_k^0 the vector ϕ_k of Eqs. (3) to (3d), evaluated at μ_k^0 , ν_k^0 , Eq. (4) can be written to the first order as

$$\begin{aligned} \sqrt{E} \sigma_o^{(x)}(E) &= \sqrt{E} \sigma_{Dis}(E) \\ &+ C \sum_{k=1}^{NG} \left[X_k^0 \left(\phi_k^0(E) + \frac{\partial \phi_k^0(E)}{\partial \mu_k} \delta \mu_k + \frac{\partial \phi_k^0(E)}{\partial \nu_k} \delta \nu_k \right) \right. \\ &\left. + \delta X_k \phi_k^0(E) \right], \end{aligned} \quad (35)$$

where

$$\sqrt{E} \sigma_{Dis}^{(x)}(E) = \frac{2C}{\sqrt{E}} (1 - \cos \omega) + C \sum_{J=1}^{2NOUT} X_J^0 \phi_J(E) \quad (36)$$

Equation (35) contains the increments $\delta \mu$, $\delta \nu$, in a linear manner, suitable for the linear fitting. Here it becomes necessary to enlarge the dimensions and to redefine the vectors ϕ and X as follows:

$$X_k = X_k^0 + \delta X_k \quad \text{for } k = 1, \dots, 2NRT; \text{ and } k = 2NRT + 2NR + 1, \dots, NG \quad (37)$$

$$X_{2NRT + k} = X_k^0 \delta \mu_k \quad \text{for } k = 1, \dots, NR, \quad (37a)$$

$$X_{2NRT + NR + k} = X_k^0 \delta v_k \quad \text{for } k = 1, \dots, NR, \quad (37b)$$

so that consistently

$$\phi_k = \phi_k^0 \quad \text{for } k=1, \dots, 2NRT \text{ and } k=2NRT + 2NR + 1, \dots, NG \quad (38)$$

$$\phi_{2NRT + k} = \frac{\partial \phi_k^0}{\partial \mu_k} + \frac{X_{NRT + k}^0}{X_k^0} \frac{\partial \phi_{NRT + k}^0}{\partial \mu_k} \quad \text{for } k = 1, NR, \quad (38a)$$

$$\phi_{2NRT + NR + k} = \frac{\partial \phi_k^0}{\partial v_k} + \frac{X_{NRT + k}^0}{X_k^0} \frac{\partial \phi_{NRT + k}^0}{\partial v_k}, \quad \text{for } k = 1, NR, \quad (38b)$$

The Taylor expansion for the Doppler broadened cross section of Eq. (7), is formally identical to the expression (35) under the assumption of a Gaussian Doppler kernel. Here the vectors ϕ_k^0 pertaining to the NR resonances and defined in Eqs. (38) to (38b) are now replaced by the explicit expansions of the form (16) and (17), and, respectively, by their derivatives with respect to μ_k and v_k .

The NEIGH resonances, which are defined as external to the energy interval which is being analyzed, are handled by CØDILLI in a manner which is formally different. These levels contribute in fact only with "tails," for which the broadening effects are negligible. In the process of the non-linear "fitting" the NEIGH levels are included only linearly, that is the pertaining values of μ and v are not changed during the fitting.

In Table II are listed the expressions of X and ϕ for the case in which the expressions (16) and (17) are valid. These equations are derived and evaluated in the subroutine PHIFRM, which is shared by CØDILLI and CURVEPLOT (see Section V).

Consistently with the results and equations obtained previously for the resolution convolutions, in Eqs. (11) to (15) one can again derive for the trial function related to non-linear fitting an expansion of the form (10). The vector components P_k are defined similarly to (13) by

$$P_k(E) = \int K_R(E, E') \phi_k(E', T) dE' ,$$

where, however, $\phi_k(E', T)$, as the vector X , has $2NR$ extra components.

Table II. Vector ϕ and Vector X

NRT = NR + NEIGH		For Linear Fit	NG = NRT + KNEG + KPOS	NCO = NG - (KPOS + KNEG)
		For Non-Linear Fit	NG = NRT + NR + KNEG + KPOS	
Vector ϕ (E;T) For Linear and Non-Linear Fit			Vector X for Linear and Non-Linear Fit	
(NR)	$\left. \begin{aligned} \phi_k &= \psi_k \cos \omega - \chi_k \sin \omega \\ \phi_{\text{NRT} + k} &= \psi_k \sin \omega + \chi_k \cos \omega \end{aligned} \right\} k = 1, \text{NR}$		$\left. \begin{aligned} X_k &= GR_k = G_k/v_k \\ X_{\text{NRT} + k} &= GI_k = H_k/v_k \end{aligned} \right\} k=1 \dots \text{NR}$	
(NEIGH)	$\left. \begin{aligned} \phi_{\text{NR} + k} &= \frac{\cos \omega - x_k \sin \omega}{v_k^2 (1 + x_k^2)} \\ \phi_{\text{NRT} + \text{NR} + k} &= \frac{\sin \omega + x_k \cos \omega}{v_k^2 (1 + x_k^2)} \end{aligned} \right\} k = 1, \text{NEIGH}$		$\left. \begin{aligned} X_{\text{NR} + k} &= GR_k = G_k v_k \\ X_{\text{NRT} + \text{NR} + k} &= GI_k = H_k v_k \end{aligned} \right\} k=1, \text{NEIGH}$	
For Non-Linear Fit Only			For Non-Linear Fit Only	
(NR)	$\left. \begin{aligned} \phi_{2\text{NRT} + k} &= \frac{\partial \psi_k}{\partial \mu_k} \left(\cos \omega + \frac{GI_k^0}{GR_k^0} \sin \omega \right) + \frac{\partial \chi_k}{\partial \mu_k} \left(-\sin \omega + \frac{GI_k^0}{GR_k^0} \cos \omega \right) \\ \phi_{2\text{NRT} + \text{NR} + k} &= \frac{\partial \psi_k}{\partial v_k} \left(\cos \omega + \frac{GI_k^0}{GR_k^0} \sin \omega \right) + \frac{\partial \chi_k}{\partial v_k} \left(-\sin \omega + \frac{GI_k^0}{GR_k^0} \cos \omega \right) \end{aligned} \right\}$		$\left. \begin{aligned} X_{2\text{NRT} + k} &= GR_k^0 \delta \mu_k \\ X_{2\text{NRT} + \text{NR} + k} &= GR_k^0 \delta v_k \end{aligned} \right\} k = 1, \text{NR}$	
For Either Case			For Either Case	
(BACKGROUND CONSTANTS)	$\phi_{\text{NCO} + i} = E^{1-i}$	$i = 1, \text{KNEG}$	$X_{\text{NCO} + i} = A_i$	$i = 1, \text{KNEG}$
	$\phi_{\text{NCO} + \text{KNEG} + i} = E^i$	$i = 1, \text{KPOS}$	$X_{\text{NCO} + \text{KNEG} + i} = B_i$	$i = 1, \text{KPOS}$

III. LEAST SQUARES EQUATIONS

The set of experimental data analyzed by least squares in CØDILLI is initially scaled according to the choice of the trial function:

for JS = 1, 2, 4,

$$Y_{\text{ex}}(E_i) = \frac{\sqrt{E}}{C} \sigma_{\text{ex}}(E_i), \quad (39)$$

while for JS = 3,

$$Y_{\text{ex}}^T(E_i) = e^{-N \sigma_{\text{ex}}^T(E_i)}, \quad (40)$$

the value of N being provided by the subroutine WIDTH, in those cases in which it is variable, or otherwise given as an input datum. The data are consequently to be compared with the values of the appropriately chosen trial function, $Y_{\text{app}}(E_i)$, in terms of the basic least squares equations. These equations require that the values of the unknown parameters appearing in Y_{app} minimize the appropriately weighted sum of the squares of the deviations between Y_{app} and Y_{ex} , i.e., require that

$$S = \sum_{i=1}^{NP} [Y_{\text{ex}}(E_i) - Y_{\text{app}}(E_i)]^2 w_i, \quad (41)$$

be minimum. Here NP represents the number of data points chosen in a given energy interval. The quantities w_i represent here weights which

can be taken as proportional to the inverse of the squares of the

statistical errors. Such weights should normally be a part of the experimental data, and thus be made available with the data themselves, or by means of related information, such as statistical errors, or statistical variances.

For cases in which information of this type is not available, it may be possible to calculate analytical values for the weights corresponding to appropriate assumptions..

By expressing the condition of minimum for S , as

$$\frac{\partial S}{\partial X_k} = 0, \quad (42)$$

for $k = 1, NP$

the normal equations for the least squares fitting are derived. From the condition (42) one has:

$$\sum_{i=1}^{NP} [Y_{ex}(E_i) - Y_{app}(E_i)] w_i \frac{\partial Y_{app}(E_i)}{\partial X_k} = 0. \quad (42a)$$

Replacing now Y_{app} with the expansion of the form given by Eq. (10):

$$Y_{app}(E) = Y_0(E) + \sum_{k=1}^{NP} X_k P_k(E),$$

the normal equations are obtained:

$$\sum_j Q_{kj} X_j = R_k, \quad (43)$$

where

$$Q_{kj} = \sum_{i=1}^{NP} P_k(E_i) P_j(E_i) w_i, \quad (44)$$

and

$$R_k = \sum_{i=1}^{NP} P_k(E_i) [Y_{ex}(E_i) - Y_0(E_i)] w_i. \quad (45)$$

The solution of the system of equations (43) is the vector X , the components of which (see Table II) are interpreted in terms of the desired multilevel parameters. The reciprocal of Q , Q^{-1} , is the error matrix,

the elements of which are needed to evaluate the variances δX_k of the unknowns X_k and the standard deviations $\delta Y_{app}(E_1)$ of the trial function $Y_{app}(E_1)$ at each point E_1 . One has

$$\delta X_k = s \sqrt{Q_{kk}^{-1}}, \quad (46)$$

$$\delta Y_{app}(E_1) = s \sqrt{\sum_{kj} \frac{\partial Y_{app}(E_1)}{\partial X_k} \frac{\partial Y_{app}(E_1)}{\partial X_j} Q_{kj}^{-1}}, \quad (47)$$

where the value of s is a measure of the quality of the overall fitting procedure and is given by

$$s^2 = \frac{1}{N_D} \sum_{i=1}^{NP} [Y_{ex}(E_1) - Y_{app}(E_1)]^2 w_i. \quad (48)$$

In Eq. (48) $Y_{app}(E_1)$ is evaluated with the parameters X_k resulting from the fitting, and N_D represents the number of degrees of freedom

$$N_D = NP - NG - 1. \quad (49)$$

IV. CØDILLI: MAIN PROGRAM AND SUBROUTINES WEIGHT AND SIGWE CONNECTED DIRECTLY WITH THE LEAST SQUARES ANALYSIS

Through the MAIN program, the input data are read and stored. The experimental data are read and scaled according to Eq. (39) or (40) of Section III. The detailed sequence of the input data is described in Appendix A.

The sequence of calculations performed by CØDILLI is controlled from the MAIN program via two indices: the index NT, representing the number of nonlinear iterations requested, and the index IEND, which at the end branches to a selection of "READ" orders, designed to make available, in variety of combinations (see Appendix A) new values of the level parameters, keeping unchanged the data and the type of trial function.

The following Subroutines are called from the MAIN program: WEIGHT, SIGWE, SKIP, and WIDTH, and FUNCTION INVERT. Subroutines SKIP and WIDTH are described in Section V.

(4-1) Subroutine WEIGHT

Purpose: to provide, at each E value the statistical error attributed to the measured data points, as to evaluate the corresponding weight.

Usage: CALL WEIGHT (JWE)

Description of the Calculation:

The index JWE (an input index) provides for the selection among six currently available types of weights.

For JWE = 1: equal weights

JWE = 2: weights derived from statistical errors

which are provided by input and defined as
proportional to the values of the cross section.

JWE = 3: weights calculated as inversely pro-
portional to the square of the cross section value.

JWE = 4: Weights derived from statistical errors
which are provided as input.

JWE = 5: weights calculated as inversely pro-
portional to the cross section value.

JWE = 6: represents a special case in which the
energy interval of interest is parted in two energy
intervals of different, constant weights.

This subroutine, by its nature, is closely related to
the experimental data, and it should be regarded as
pliable; it is readily open to modifications, changes,
or additions. Numerically, the scaling of the weights
bears some consequence on the derivation of the solution
of the normal equations. In the present version of
WEIGHT the weights are scaled to give

$$\sum_{i=1}^{NP} w_i = NP.$$

(4-2) Subroutine SIGWE

Purpose: preparation and solution of the least squares equations
(normal equations), as given in Section III.

Usage: CALL SIGWE (JW)

Description of Calculation:

The subroutine is controlled by the index JW. There are two branches, entered from the MAIN program: (1) (JW = 2) for each energy point, E_i , the functions $P_k(E_i)$, $Y_o(E_i)$ as listed in Table I, are calculated (see Subroutine SCRAMB) and stored on a tape (Tape 9). The matrix Q_{kj} and the known vector R_k are constructed, as given in the Eqs. (44) and (45) of Section III. The system of normal equations is solved via the FUNCTION INVERT, which returns the error matrix stored in the locations previously occupied by Q, while the formerly unknown vector $\vec{X}$ is returned in the locations previously assigned to the vector $\vec{R}$. From these results, SIGWE evaluates and lists: RS = weighted sum of the square deviations, and the goodness of fit squared, s^2 , given in Eq. (48) of Section III. From the components of the vector $\vec{X}$, the subroutine evaluates and lists the resonance parameters GR and GI, as given in Table II. From the variances which are calculated as in Eq. (46) of section III, the errors of GR and GI are evaluated and listed. This branch of SIGWE is repeatedly entered, from the MAIN program, when "non-linear" iterations are wanted. In these cases new values of μ and ν , given $\mu_o + \delta\mu$, $\nu_o + \delta\nu$ (see Table II) are

also calculated and their variances are evaluated and listed. The requested number of non-linear fits is prescribed by the input index NT. This index is set as zero if only a linear fit is wanted.

(2) At the end of the last of the requested iterations, the MAIN code chooses the second branch of SIGWE. (JW = 3). Here the calculation deals with the re-evaluation of the function $\sigma_{app}(E_i)$, as obtained from $Y_{app}(E_i)$, of the theoretical, Doppler broadened cross section, $\sigma_c(E_i)$, as given in Eq. (7) of Section II; the deviation

$$\sigma_{ex} = \sigma_{app} ,$$

the corresponding percent deviation, and the standard deviation as defined in Eq. (47) of Section III, are listed for each E value.

The detailed description of the output is given in Appendix B. Parameter cards, containing level parameters and the corresponding parameters GR, GI are punched, as described in Appendix B.

(4-3) FUNCTION INVERT

This function prepares the storage location needed for the double precision inversion of Q. The inversion is obtained by calling the subroutine

DINV (written in SCATRE). The values of the error matrix (Q^{-1}) are rounded, from double to single precision, with the function ROUND, and returned to SIGWE in the original storage locations of Q. Similarly $\vec{X}$ is returned after rounding in $\vec{R}$ and the variances are calculated in double precision arithmetic (DSQRT, being used for the square root operation) and returned to SIGWE in the array VARX:

V. SUBROUTINES SHARED BY CØDILLI AND CURVEPLØT:

SHAPE: PHIFRM, DSIG, PLØT, SCRAMB, WIDTH: SKIP

The subroutines SHAPE and PHIFRM together with the functions DSIG and PLØT are related directly to the cross-section formulae used in CØDILLI and described in Section II. Subroutine SCRAMB uses the previous subroutines and functions, in order to evaluate the quantities relevant to the construction of the trial functions (see Table I). Subroutine WIDTH contains all the information relevant to evaluate the resolution effects: as such, WIDTH contains in principle different information for each set of data. Finally, the subroutine SKIP has only editorial tasks, such as print a title and date on the top of the output pages. Thus, the description of SKIP will be skipped.

(5-1) Subroutine SHAPE

Purpose: evaluation of the line shape functions ψ and χ .

Usage: CALL SHAPE (J, X, T, PSI, CHI, IIN)

Description: The index J controls the two branches:

- (a) J = 1 initialization of the calculation and
- (b) J = 2 evaluation of the line shape functions $\psi(x,t)$ $\chi(x,t)$, having specified the values of x and t immediately before the calling sequence:

$$x = \frac{\mu_k - E}{v_k},$$

where E is the variable energy and μ_k , v_k are the parameters of the kth resonance,

$$t = \frac{kT}{A v_k^2}$$

is the ratio of the square Doppler width to the square half-width of the resonance, kT being the medium temperature in eV, E the variable energy, and A the atomic mass number of the element in question. The method of calculation is based on the application of Cauchy's integral to the approximate expansion of the convolution kernel in rational functions.¹⁰⁾ The index IIN is, for this version of SHAPE, a dummy index.

(5-2) Function DSIG(EN)

Purpose: to calculate the contribution of the "distant" known resonances, in the form

$$\frac{\sqrt{E}}{CC} \sigma_{\text{Dis}}(E) ,$$

for a given set of known^{*)} resonance parameters NOUT. This contribution includes the potential scattering, and it is given in Eq. (8) of Section II. Doppler and resolution effects are included, according to the choice of the trial function. The results are transmitted by DSIG(EN), EN being the variable energy.

*) These resonances are also referred to as "external" resonances, although among them may be included known resonances lying within the energy range considered.

(5-3) Function PLOT (EN)

Purpose: to calculate, for a given value of the energy EN, the theoretical cross section

$$\frac{\sqrt{E}}{C} \sigma_c(E)$$

as given in Eq. (7a) of Section II. The term arising from potential scattering and NOUT levels is obtained by DSIG(EN). The results are transmitted by PLOT(EN), EN being the variable energy.

(5-4) Subroutine PHIFRM

Purpose: to evaluate, for a given value of E, the complete set of vector components $\phi_k(E;T)$ as defined in Table II.

Usage: CALL PHIFRM(EN): all other variables are in common.

Description of the Calculation:

The calculation of the vector ϕ , as given in Table II, is performed in PHIFRM, through a set of internal branches. These are controlled by indices which distinguish linear from non-linear fits (Index IND), total from reaction cross section (Index INDE), and single level from multi-level parameters (Index LS). Except for the components related to the NEIGH resonances and to the background constants (KNEG; KPOS) all ϕ components are calculated via subroutine SHAPE:

(5-5) Subroutine SCRAMB

Purpose: to provide, at each value of E , the complete set of the vector components $P_k(E)$, and the function $Y_o(E)$, for any one of the choices of the trial function (index JS).

Usage: CALL SCRAMB(EN; YZER). All other variables are in common.

Description of the Calculation

The resolution kernel, $K_R(E_i, E)$, is introduced in SCRAMB as a built-in function, GAUSSF (Z).

In the enclosed listing of this subroutine,

$K_R(E_i, E)$ is coded as a Gaussian function. For cases in which the experimental conditions indicate the use of a different type of resolution kernel, the function GAUSSF (Z) should be replaced by the appropriate resolution function.*

The functions calculated in SCRAMB are listed in Table I. For the cases corresponding to $JS = 2$ and $JS = 3$, $K_R(E_i, E)$ is used with 64-steps Simpson integration scheme, to derive $P_k(E_i)$ and $Y_o(E_i)$. In either case, the functions utilized in the folding operation are provided, respectively, by PHIFRM [$\phi_k(E)$] and DSIG [$\sigma_{Dis}(E)$].

The limits of integration are defined, at each E_i , by the interval of width $8HR$, HR being the energy dependent resolution width, transmitted to SCRAMB by SUBROUTINE WIDTH. It might be worthwhile to recall here

* Case encountered in practice: the resolution function suggested by L. Bolliger for the analysis of his Pu-239 data.

some numerical experiments made during the course of the code checking. By defining appropriately the values of HR, SCRAMB (JS = 2) was used to reproduce, with a Gaussian convolution, the values of the ψ function as obtained independently by SHAPE. The 64 steps of the Simpson integration and the choice of the integration limits $E_i - 4HR$, $E_i + 4HR$, i.e.

$$\int_{-\infty}^{\infty} \rightarrow \int_{E_i - 4HR}^{E_i + 4HR}$$

reproduced the values given by SHAPE to the sixth significant figure, thus guaranteeing accuracy.

For the cases JS = 1, 4 Subroutine SCRAMB provides directly $P_k(E_i)$ and $Y_o(E_i)$ according to the respective prescriptions for the broadening, by directly calling PHIFRM and DSIG. The results thus obtained, in either PROGRAM, CØDILLI and CURVEPLØT, are stored on a tape (tape 9). In CØDILLI such values provide the necessary parts to evaluate first the elements of the inverse error matrix (Subroutine SIGWE), and to reconstruct, after the fitting, the function Y_{app} . In CURVEPLØT only this last calculation is needed, in order to list and plot the function Y_{app} .

(5-6) Subroutine WIDTH

Purpose: to provide at each value E the value HR of the resolution width, defined as the half-width at $1/e$ of the maximum of a Gaussian function, and measured in eV.

Usage: CALL WIDTH(EN,,HR)

Description of the Calculation:

The resolution width, HR, is defined as a function of E and depends on several parameters related to the measurement. For time-of-flight measurements such parameters are defined by the channel width, the burst width, the moderation time, the flight path, etc., and HR can be evaluated as

$\sqrt{aE^2 + bE^3}$ a, and b being assigned by the conditions of the experiment. For this reason, this subroutine has been, so far, written anew for each particular set of data analyzed, depending on the available information. Users at other installations may however devise a "universal" WIDTH subroutine reflecting the requirements of broad classes of experiments.

This subroutine is also expected to provide, for transmission data, the values of N (atoms/barn), referred to, in the code, as DENS, whenever these values are changing within the energy interval analyzed.

VI. CURVEPLOT AND SUBROUTINES SIGPLT AND GRAPH

DIRECTLY RELATED TO THE PLOTTING DEVICE (CALCOMP)

The MAIN program of curve plot does not differ logically from the last part of the MAIN of CØDILLI. CURVEPLOT does not execute any fitting, but simply reevaluates the cross section using as input parameters the parameter cards obtained from CØDILLI. (See Appendix A and Appendix C). The Subroutine SIGWE of CØDILLI is here replaced by SIGPLT, which duplicates the second branch of SIGWE.

The Subroutine GRAPH establishes the necessary link between the calculated variables and their graphic representation with the CALCOMP PLOTTER. One input option of CURVEPLOT, for JS = 3, differs from CØDILLI. The details are described in Appendix C.

VII. ROUTINE SIGMA

Purpose: To evaluate energy dependent Doppler broadened cross sections, either from multilevel or from single level parameters, in order to compare cross sections obtained from different sources, to study temperature effects, as well as to analyze numerically the role of the multilevel parameters. A choice is available (Index ISIG) in order to evaluate either the contribution of the symmetrical functions ψ , or the contributions of the asymmetrical functions χ . In these cases, the calculation ends in evaluating also the complete multilevel expansion.

The routine also satisfies the need, often arising in single level calculations, of estimating the values of the $1/v$ background constants.

Description of the calculation:

The resonance parameters are read from the subroutine BWSIG, which can evaluate cross sections of mixtures of resonance absorbers in the form given in Section 2, equation (1), with Doppler broadening. A distinction is made between single and multilevel parameters, in a first branch of BWSIG. In the first case, BWSIG evaluates, from the well known single level parameters of the BNL tables, symmetrical parameters GR. In the second case, the parameters GR, GI, obtained from total and fission cross section fitting are read from input cards. From the total cross section parameters are calculated the parameters for the resonance scattering, thus by difference the capture parameters are derived.⁽²⁾

The second branch of BWSIG evaluates Doppler broadened cross sections, from the established set of GR, GI parameters (without "remembering" whether derived from single or from multilevel input). For a given energy interval, also the resonance integrals

$$\int \sigma \frac{dE}{E} \text{ are calculated.}$$

In the single level case, an option can be made whether the background constants, A_1^F , A_1^T are to be evaluated from the thermal values provided as input. The Doppler broadening line shape functions are evaluated via SHAPE.

In Appendix D the input and output of Sigma are described.

VIII. CONCLUSIONS AND COMMENTS ON FURTHER WORK

The programs and subroutines described in this report should not be considered the product of experts in computer science, but rather, represent an effort to construct a tool useful for the analysis of neutron resonances, hopefully of practical interest. Therefore, it will appear to the expert that several parts should be simplified, rewritten and made more efficient.

At present, while these programs are being used, changes and improvements are being investigated, not with the pretense of perfecting the computer aspects, but with the aim of making these tools more flexible and complete.

The following changes are being envisaged:

- a) Introduction of a convergence criterion for the nonlinear cases and replacement of the Gauss method by more modern computer-oriented techniques. This will involve use of Tape or Disc memory on the IBM-7094 in order to record values of the parameters obtained by previous iterations.
- b) Provisions for the simultaneous analysis of pairs of cross sections (e.g. total and fission, or fission and capture cross sections). This planned program also requires the use of additional memory, such as tape or disc on the 7094.
- c) A generalized subroutine WIDTH, useful for a wide range of experimental data.
- d) Generalization of the fitting of the total cross section by including the potential scattering term among the unknowns, and also by removing the restriction of the hard-sphere model (implied in the present equations).

- e) The fitting procedure can also be generalized by introducing constraints through the usual Lagrange multiplier method. For example, constraints could be chosen in the following form:

$$\int_{E_i - \Delta}^{E_i + \Delta} \sigma_{\text{ex}}(E') (E')^j dE' = \int_{E_i - \Delta}^{E_i + \Delta} \sigma_{\text{app}}(E') (E')^j dE' .$$

Here, the case $j = 0$ corresponds to the "equal areas" requirements, i.e. that integrals over certain energy ranges for the experimental cross sections should match the corresponding integrals for the calculated cross sections. Similarly, for $j = -1$, the requirement is imposed that the resonance integral calculated from the theoretical cross section will match the resonance integral calculated from the experimental cross section points. Such requirements could be an aid in simplifying the handling of different normalizations for different experiments, and also perhaps induce stability in non-linear fitting. For the lower energy regions, and certain experiments, another possible constraint could be the requirement that the calculated cross section curve match the "recommended values" of the thermal cross sections.

Other changes of practical nature can be suggested and could easily be achieved, at other installations:

- a) Use of CALCOMP plotting directly with ~~CODILLI~~ and SIGMA*
- b) The possibility of reading the experimental data from a tape*
- c) Enlargement of the memory storage to include more levels either by use of tapes or disc or by adaption of the program to a more powerful computer (e.g. an IBM 360).

* These possibilities were at one time included in these programs, and later removed, in order to speed up the turn-around time of the computations at Illinois.

The memory limitations of these programs presented here in their current version are given in Table III for the use of the reader. It should be emphasized that the transition from the Illinois FORTRAN II used in these programs to the standard IBM FORTRAN II or the FORTRAN 63 (not available at Illinois) requires only minor changes. The transition to FORTRAN IV, which will become desirable once an IBM 360 becomes available at Illinois, may require more changes, but not basic changes in logic or structure of the programs.

TABLE III LIMITATIONS OF CURRENT VERSIONS OF THE PROGRAMS

USED AT THE UNIVERSITY OF ILLINOIS

CODILLI	7094	ILLIAC II
NP	≤ 1000	≤ 600
NR + NEIGH	≤ 32	≤ 20
(NR > 0)		
NOUT	≤ 20	≤ 10
NG	≤ 85	≤ 20
<u>CURVEPLOT</u>		
NP	≤ 1000	≤ 1000
NR + NEIGH	≤ 42	≤ 20
NOUT	≤ 40	≤ 40
<u>SIGMA</u>		
NUMBI	≤ 5	$= 1$
NO(I)	≤ 80	≤ 80

List of symbols used in the input of CØDILLI and CURVE PLØT.

A-1) CONSTANTS USED IN THE INPUT

- TEMP = kinetic energy of the target nucleus, in eV.
- ATM = atomic mass number of the nucleus.
- DENS = number of atoms per barn (characterizing the thickness of the sample in transmission measurements).
- WN = nuclear radius in units of $\text{eV}^{-1/2}$, such that, when E is in eV, $\text{WN} \sqrt{E} = ka$, where k is the wave number and a is the nuclear radius.
- C = 6.52×10^5 barns * eV.

A-2) INDICES CONTROLLING THE TRIAL FUNCTION AND THE CODE OPERATION.

- NP: number of data points.
- INDE: selects the cross section equation: for total cross section, INDE = 1, for reaction cross section, INDE = 0. This last case causes the code to set equal zero the potential scattering contribution, which is instead evaluated when INDE = 1.
- NT: represents the wanted number of nonlinear iterations. NT = 0 causes the code to limit the fitting to the linear fit only.
- LS: selects the multilevel analysis (LS = 2) or a "single level" analysis (LS = 1). In the latter case, only the symmetrical contributions are introduced in the trial function, thus only GR parameters are fitted. This case entails only linear fits.

IPR : provides test outputs for the normal equation:

normally $IPR = 0$. If $IPR = 1$ the matrix elements of the error matrix before and after the inversion are printed out. This option is useful, as a partial (BCD) dump, in dubious cases. (e.g., over- or under-flow during the inversion).

JS : selects one out of four types of trial functions (see section 2), as follows:

JS = 1 For reaction cross sections. Doppler and resolution kernels are assumed to have a Gaussian form and are combined into one Doppler-type Gaussian kernel, having an averaged effective temperature.

JS = 2 For reaction cross sections. The Doppler broadening kernel is assumed to have a Gaussian form, and it is folded with a resolution kernel of arbitrary form. The convolution is evaluated with a 64 steps Simpson integration.

JS = 3 For total cross sections. The calculated transmission function (evaluated with a Doppler-broadened cross section) is folded into a resolution kernel of arbitrary form. The convolution is performed with a 64 steps Simpson integration.

JS = 4 For reaction cross sections. Doppler and resolution broadening are assumed to have Gaussian form and are combined into one Gaussian kernel, having a combined width, in which the resolution width is evaluated at each energy point.

- NE: This index, if set equal to 64 in CØDILLI, satisfies a purely editorial task. It is, however, used differently in CURVE PLØT (See Appendix C.).
- NR: number of resonance levels to be fitted inside the energy interval of interest.
- NEIGH: number of resonance levels to be fitted, neighboring the energy interval of interest. With NEIGH the "tails" of external levels having unknown parameters can be evaluated and fitted. The use of NEIGH is necessary for fitting negative energy levels.
- NOUT: number of resonance levels, either outside the energy interval of interest, or inside, whose parameters are known. With NOUT the "tails" of external (known) levels can be evaluated, or impurities of known concentration, and of known elements can be accounted for, and finally well fitted internal levels can be subtracted to facilitate the fitting of other resonances, especially in nonlinear cases.
- KNEG ≤ 3 (also referred to as KN) represents the number of constants in the expansion $A_1 + A_2/E + A_3/E^2$ so that for KNEG = 1 only A_1 is evaluated; KNEG = 2 A_1 and A_2 are evaluated.
- KPOS ≤ 5 represents the number of terms in the expansion $B_1E + B_2E^2 + \dots + B_5E^5$ so that for KPOS = 1 only B_1 is evaluated; KPOS = 2 B_1 and B_2 are evaluated, etc.
- JWE causes the subroutine weight to select one among six types of weights to be inserted into the least squares equations. (See Section IV).

JWE = 1 equal weights

JWE = 2 weights derived from statistical errors which are provided by input and defined as proportional to the values of the cross section.

JWE = 3 weights calculated as inversely proportional to the square of the cross section value.

JWE = 4 weights derived from statistical errors which are provided by input.

JWE = 5 weights calculated as inversely proportional to the cross section value.

JWE = 6 Special case requiring an additional input card. In this case the data are separated in two regions having different, constant weights. The additional input card contains the two weights and the energy value separating the two regions.

IEND: This index, punched in the column 1 of the last card of the deck, causes the calculation to branch as follows:

IEND = 1 to read from start a completely new set of data for a new problem. (e.g. a fission cross section fit after a total cross section fit).

For IEND = 2,3,4,5,6,7,8,9

the original set of data is reanalyzed, keeping fixed all indices, but varying the values of the parameters. The new parameters, set after the IEND card, can be selected as follows:

- IEND = 2 a new set of NR guesses
- = 3 a new set of NEIGH guesses
- = 4 a new set of NOUT parameters
- = 5 new NR and NEIGH guesses
- = 6 new NR guesses and new NOUT parameters
- = 7 new NEIGH guesses and new NOUT parameters
- = 8 this branch is dummy (IEND = 8 at start)
- = 9 a new set of NR and NEIGH guesses and of NOUT parameters

Note: in each choice, the sets not named remain unchanged, as in the previous fit. All choices involving NEIGH and NOUT require that such indices are non-zero.

A-3) EXPERIMENTAL DATA

Experimental Data are read from cards, each card having the form:

E = energy value

Y = cross section in barns

DEL= statistical error, or a related quantity, expected in the cases JWE = 2,4.

A-4) RESONANCE PARAMETERS

Guesses for NR + NEIGH resonances have to be provided on cards for CØDILLI each card containing a value for the resonance energy μ and the resonance half-width ν . For the case JS = 3 (Transmission) these cards must provide the estimated values GR°, GI° of the parameters.

Known parameters for NOUT resonances must also be supplied if NOUT $\neq$ 0. Usually these parameters are available on cards from previous outputs of CØDILLI.

A-5) INPUT FORMAT FOR CØDILLI and CURVE PLØT

Card 1 comment card with ID number in Col. 73-80.

Card 2 comment card FØRMAT (3A6,A2)

Card 3 CONSTANTS: TEMP, ATM, DENS, WN, C FØRMAT (5E15.4)

Card 4 indices: NP, INDE, NT, LS, IPR, JS, NI FØRMAT (7I5)

Card 5 indices: NR, NEIGH, NOUT, KNEG, KPOS, JWE FØRMAT (6I5)

These cards are followed by

NP data cards FORMAT (3E 15.8)

NR + NEIGH* cards containing the "guesses" for μ , ν

FORMAT (2E15.4)

NOUT cards containing known parameters μ , ν , GR, GI

FORMAT (4E15.4)

IEND* FØRMAT (I4)

* not for CURVEPLØT, see Appendix D.

APPENDIX B

OUTPUT OF CØDILLI

The first page describes and reproduces the input. A quantity EPS is printed, which establishes an upper limit to the sum of the squares of the weighted deviation, RS, so that for $RS > EPS$ no output on cards is obtained.

The pages following the first contain the print-out of the following quantities derived from the fitting:

DET = determinant of the matrix Q

$RS = S^2$, as given in Section 3,

$CHISQ = \frac{S^2}{N_D}$, $GF = \sqrt{CHISQ}$, ND = number of free parameters.

This line is followed by NR lines each containing a set of values.

GR, VAR = δGR , MU, VAR = $\delta \mu$

and NR lines containing

GI, VAR = δGI , NU, VAR = $\delta \nu$.

For NEIGH resonances the fitting being always linear, the NEIGH lines contain again

GR, δGR , MU

GI, δGI , NU

but no variances for μ and ν are provided. Finally, the background constants A_i , B_i , are printed.

For each fit NR + NEIGH parameter cards are punched, in the FORMAT (4E15.4), containing

μ, ν, GR, GI , level number and input identification number.

These cards can be used as follows:

- 1) as NOUT, for other runs
- 2) as input for the SUBROUTINE BWSIG (See Section 8) which is used in the routine SIGMA and in other existing programs, which utilize resonance parameters.

After the last fitting iteration has been executed, CØDILLI lists

E , σ_{ex} (EXP. SIGMA)

σ_{app} (APP. SIGMA)

(see Section 2)

σ_{c} (CAL. SIGMA)

Deviations = $\sigma_{\text{ex}} - \sigma_{\text{app}}$

percent error

Standard deviation (see Section 3)

Finally, the value of $\sigma_{\text{app}}(E)$ and of $A_1/\sqrt{E}$ are calculated at $E = .025$ eV and printed.

Last, a list is given of the parameters $G = GR * v$, $H = GI * v$ and $\text{SUM} = \sum_k H_k$ is evaluated. The last line reproduces IEND.

APPENDIX C

COMMENTS ON CURVEPLOT

The Input to CURVEPLOT is identical to the input to CODILLI except

- a) NR + NEIGH cards: the "guesses" are here replaced by the corresponding parameter cards, containing the values of GR, GI parameters which have been punched by CODILLI.
- b) The NOUT parameter cards are followed by cards containing the background constant(s) A_i, B_i (FORMAT E 15.4) as obtained by CODILLI in the same run from which the NR + NEIGH parameters have been obtained.
- c) A title card for the graph, (read by the Subroutine GRAPH).
- d) The card IEND is eliminated. Subsequent runs, can be obtained, however, since CURVEPLOT ends on the first "READ" order.
- e) The Case JS = 3 is the only one differing from the pattern.

This case requires additional input, that is an additional set of NR + NEIGH parameters, to be set after the background constant(s) but before the title card.

Upon test on JS, CURVEPLOT searches for the second set of parameters. Here, two cases are considered, depending whether the curve plotted is expected to reproduce the actual trial function (linearized transmission) or the exact transmission.

For the first case, the initial set of parameters GR^0, GI^0 is the same used in CODILLI to initialize the fitting (See Appendix A and Section II) and the additional set is the one of the GR, GI fitted by CODILLI and punched on cards for the JS = 3 case. In this case, CURVEPLOT computes

the differences between GR and GR° , GI and GI° , and reconstructs the genuine linearized trial function.

For the second case, the first set of input parameters is the one of the GR, GI fitted by CODILLI and punched on cards, and the additional set is instead blank. This provides the appropriate mechanism (via the index NI) to evaluate the transmission curve corresponding to the fitted parameters where such parameters appear now in a nonlinear manner in the function Y_{app} .

The output of CURVEPLOT differs from the one of CODILLI, in the following parts:

- a) no quantities connected with the solution of the normal equations are provided (hence no RS, CHISQ, or standard deviations), but the input is again reproduced.
- b) A "CALCOMP" graph reproducing σ_{ex} and σ_{app} is delivered via the Subroutine GRAPH.

APPENDIX D

D-1) LIST OF SYMBOLS AND INPUT OF ROUTINE SIGMA

a) BWSIG symbols

NUMBI = number of resonance absorbers

CONST = $6.52 \cdot 10^5$ eV * barn

ATM(I) = atomic mass number

WN(I) = nuclear radius in $\text{eV}^{-1/2}$

GFACT(I) = $\bar{g}_J$, average g factor

LS(I) = 1 for single level parameters
2 for multilevel parameters

NO(I) = number of resonance level

} for the
Ith nuclear
species

LS = 1, single_level_case

DE(I,K) = energy level E_k

DW(I,K) = Γ_{nk}

GRA(I,K) = Γ_{kF}

GRG(I,K) = $\Gamma_{k\gamma}$

ALFA(I,K) = Γ_{kn}°

} for the
kth level
of the Ith species.

LS = 2, multilevel_case

DE(I,K) = μ_k	}	for the kth level of the fission cross section of the Ith species
DW(I,K) = $\dot{v}_k$		
GRA(I,K) = GR_k^F		
GIA(I,K) = GI_k^F		

and similar symbols for total cross section parameters;

CF1(I), CF2(I), CF3(I)	fission background constants	}	for the Ith species
BF1(I), BF5(I)			
CT1(I), CT2(I)	total background constants		
BT1(I),			

where CF1 = A_1 CF2 = A_2 CF3 = A_3 , etc.

BF1 = B_1 BF2 = B_2 BF3 = B_3 , etc.

for fission and similarly for total cross sections.

TEMP = kinetic energy of the mixture in eV

b) Symbols of Sigma:

EMAX = maximum value of E	}	in eV
EMIN = minimum value of E		
DELE = energy interval dE		

ISIG For ISIG = 1 the resonance integrals and average α are printed, at the end of the energy interval.

ISIG = 2 the calculated cross section contains only the symmetrical contributions.

ISIG = 3 the calculated cross section contains only the asymmetrical contributions.

IEND = 2 the calculation branches to the final output,
skipping the calculation of the background constants.

a) BWSIG cards

Followed by 2 NO cards containing

or

FORMAT (4E 15.4)

Fission, Total.

TEMP card - contains TEMP, FORMAT (E10.4)

b) SIGMA cards

E card contains EMAX, EMIN, DELE, NUMB I (FORMAT 3E15.8,I5)

Indices

1) ISIG FORMAT(I 5)

2) IEND (needed only if ISIG = 1) FORMAT (I 5)

Note: if ISIG $\neq$ 1, no IEND card is needed, but another ISIG.

Eventually ISIG = 1 should appear followed by IEND.

D-3 OUTPUT OF ROUTINE SIGMA

A first part of the output is a list of parameters, two lines per level, as follows

$$\mu, GR^F, GR^Y, GR^N, GR^T$$

$$\nu, GI^F, GI^Y, GI^N, GI^T$$

where GR^Y, GI^Y, GR^N, GI^N are calculated in BWSIG for LS = 2, from total and fission parameters, and for LS = 1, directly from single level parameters. The background constants and the value of TEMP are then printed out.

The second part is a listing of calculated values:

$$E, \sigma_t, \sigma_n, \alpha, \sigma_\gamma, \sigma_F$$

and finally the reaction rates, and $\bar{\alpha}$ are printed out.

FASTRAN

PROGRAM CODILLI--LEAST SQUARES FITTING OF NUCLEAR RESONANCE DATA. CODLI 1

CODLI 2

N.B. THE FOLLOWING SUBROUTINES ARE NEEDED BUT NOT LISTED--SEE WRITEUP. CODLI 3

SYSTEM, SYSERR, ERROR, FTRAP, (RTN), (FIL), (STH), .PRINT, (SCH), (CSH), CODLI 4

.LOOK, .READ, SQRT, EXP, SIN, COS, EXP(2, (SLO), (SLI)) CODLI 5

CODLI 6

N.B. THIS PROGRAM SHOULD BE COMPILED ON FORTRAN II ONLY----- CODLI 7

FOR NECESSARY CHANGES IF COMPILED ON OTHER VERSIONS OF FORTRAN, SEE CODLI 8

WRITEUP. CODLI 9

CODLI 10

MAIN PROGRAM--INITIALIZE, READ INPUT DATA. CODLI 11

DATA READ FROM CARDS ONLY DUE TO CHANGES OF MARCH, 1966. CODLI 12

CODLI 13

DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000) CODLI 14

1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI CODLI 15

2(32),POS(5),VARX(66),A(28),PHI(66) CODLI 16

COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC, CODLI 17

1NP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,CCODLI 18

23,POS,X,T,PST,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI CODLI 19

EQUIVALENCE (W,DEL) CODLI 20

DIMENSION SAVEFU(32),SAVEGU(32) CODLI 21

CALL FTRAP CODLI 22

1001 CALL SHAPE (1,X,X,X,X,2) CODLI 23

IEND=8 CODLI 24

1 CALL SKIP(1) CODLI 25

CALL SKIP(2) CODLI 26

READ 5000,TEMP,ATM,DENS,WN,CC CODLI 27

5000 FORMAT (5E15.8) CODLI 28

WOT6,5001,TEMP,ATM,DENS,WN,CC CODLI 29

5001. FORMAT (6H0TEMP=F8.4,5H ATM=F5.0,6H DENS=E15.8,4H WN=E15.8,4H CC= CODLI 30

1 E15.8) CODLI 31

READ 102,NP,INDE,NT,LS,IPR,JS,NI CODLI 32

READ 102,NR,NEIGH,NOUT,KNEG,KPOS,JWE CODLI 33

WOT6,102,NP,INDE,NT,LS,IPR,JS,NI CODLI 34

WOT6,102,NR,NEIGH,NOUT,KNEG,KPOS,JWE CODLI 35

MAU=KNEG CODLI 36

MUP=KPOS CODLI 37

GO TO (20,21), LS CODLI 38

20 TLEVEL=6HSINGLE CODLI 39

GO TO 23 CODLI 40

21 TLEVEL=6HMULTI- CODLI 41

23 FISTOT=6HTOTAL CODLI 42

INFG=0 CODLI 43

BACK=2HNO CODLI 44

IF(KNEG) 25,25,24 CODLI 45

24 INEG=KNEG-1 CODLI 46

BACK=2H A CODLI 47

202 FORMAT(18H0THIS RUN CONTAINS15,23H DATA POINTS, AND IS A A6,8HRUN CODLI 48

1WITH13,29H NON-LINEAR ITERATIONS USING A6,24H LEVEL PARAMETERS. I CODLI 49

2PR=12,1H./15H TRIAL FUNCTION12,1H,14,19H INTEGRATION STEPS.) CODLI 50

1202 FORMAT(18H THIS RUN CONTAINS13,19H INSIDE RESONANCES,13,21H NEIGHBCODLI 51

10R RESONANCES,13,20H OUTSIDE RESONANCES,A2,21H BACKGROUND CONSTANTCODLI 52

2,712,31H TERMS OF NEG. POWERS OF E, AND12,50H TERMS OF POS. POWERSCODLI 53

3 OF E, USING WEIGHTING OPTION12,1H.) CODLI 54

102 FORMAT(1115) CODLI 55

25 IF(INDE) 31,30,31 CODLI 56

30 WN=0. CODLI 57

FISTOT=6HFISS. CODLI 58

31 DO 34 I=1,NP CODLI 59

34 READ 104,E(I),Y(I),DEL(I) CODLI 60

	WOT6,202,NP,FISTOT,NT,TLEVEL,IPR,JS,NI	CODLI 61
	WOT6,1202,NR,NEIGH,NOUT,BACK,INEG,KPOS,JWE	CODLI 62
104	FORMAT(4F15.8)	CODLI 63
	SUME=0.	CODLI 64
303	DO 304 I=1,NP	CODLI 65
304	SUME=SUME + E(I)	CODLI 66
5	CALL WEIGHT	CODLI 67
	GO TO (40,40,42,40),JS	CODLI 68
40	DO 41 I=1,NP	CODLI 69
41	Y(I)=Y(I)/CC*SQRT(E(I))	CODLI 70
	GO TO 997	CODLI 71
42	DO 43 I=1,NP	CODLI 72
	CALL WIDTH(F(I),HR)	CODLI 73
43	Y(I)=EXP(-DENS*Y(I))	CODLI 74
997	WRITE OUTPUT TAPE 6,1103	CODLI 75
1103	FORMAT (30HCGUESSES FOR INSIDE RESONANCES)	CODLI 76
	DO 3 I=1,NR	CODLI 77
	READ 104,FU(I),GU(I),GR(I),GI(I)	CODLI 78
	WOT6,203,I,FU(I),GU(I),GR(I),GI(I)	CODLI 79
203	FORMAT (15,4H MU=F15.8,4H NU=F13.8,4H GR=E15.8,4H GI=E15.8)	CODLI 80
	SAVEFU(I)=FU(I)	CODLI 81
9004	SAVEGU(I)=GU(I)	CODLI 82
3	CONTINUE	CODLI 83
	GO TO(26,9002,9002,9002,6,9,9002,26,6),IEND	CODLI 84
26	IF (NEIGH) 6,8,6	CODLI 85
6	KMIN=NR+1	CODLI 86
	KMAX=NR+NEIGH	CODLI 87
	WRITE OUTPUT TAPE 6,1104	CODLI 88
1104	FORMAT (32HCGUESSES FOR NEIGHBOR RESONANCES)	CODLI 89
	DO 7 K=KMIN,KMAX	CODLI 90
	READ 104,FU(K),GU(K),GR(K),GI(K)	CODLI 91
7	WOT6,203,K,FU(K),GU(K),GR(K),GI(K)	CODLI 92
	GO TO(8,9002,9002,9002,9002,9002,9,8,9),IEND	CODLI 93
8	IF(NOUT) 9,9002,9	CODLI 94
9	WRITE OUTPUT TAPE 6,1105	CODLI 95
1105	FORMAT (34HOPARAMETERS FOR OUTSIDE RESONANCES)	CODLI 96
	DO 10 K=1,NOUT	CODLI 97
	READ 104,DL(K),DW(K),DGR(K),DGI(K)	CODLI 98
10	WRITE OUTPUT TAPE 6,210,K,DL(K),DW(K),DGR(K),DGI(K)	CODLI 99
210	FORMAT (15,4H DL=F15.8,4H DW=F13.8,5H DGR=E15.8,5H DGI=E15.8)	CODLI 100
9002	DO 9003 I=1,NR	CODLI 101
	FU(I)=SAVEFU(I)	CODLI 102
9003	GU(I)=SAVEGU(I)	CODLI 103
	READ 9999,IEND	CODLI 104
9999	FORMAT(11)	CODLI 105
9001	IND=1	CODLI 106
	NC=0	CODLI 107
	WRITE OUTPUT TAPE 6,1108,EPS	CODLI 108
1108	FORMAT (5H0EPS=E15.8)	CODLI 109
	CALL SKIP (2)	CODLI 110
	WOT6,11	CODLI 111
11	FORMAT (11H"LINEAR FIT")	CODLI 112
	NG=LS*(NR+NEIGH)+MAU+MUP	CODLI 113
	CALL SIGWE(2)	CODLI 114
	IF(NT) 19,18,19	CODLI 115
19	IND=2	CODLI 116
	NG=4*NR+MAU+2*NEIGH+MUP	CODLI 117
16	NC=NC+1	CODLI 118
	IF (NT-NC) 18,17,17	CODLI 119
17	CALL SKIP (2)	CODLI 120
	WOT6,1109,NC	CODLI 121

APPENDIX E - page 3

1109	FORMAT (22HONON-LINEAR FIT NUMBER13)	CODLI122
	CALL SIGWE(2)	CODLI123
	GO TO 16	CODLI124
18	CALL SIGWE(3)	CODLI125
	WOT6,9998,IEND	CODLI126
9998	FORMAT (6H0IEND=11)	CODLI127
	CALL SKIP (2)	CODLI128
	GO TO(1,997,6,9,997,997,6,1,997),IEND	CODLI129
	END	CODLI130

\$	FASTRAN		
C	SUBROUTINE SIGWE--INITIALIZE, PERFORM LEAST SQUARES FIT, PLOT	SGWEC	1
C	CURVE	SGWEC	2
C		SGWEC	3
C	SUBROUTINE SIGWE(JW)	SGWEC	4
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	SGWEC	5
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GIS	SGWEC	6
	2(32),POS(5),VARX(66),A(28),PHI(66)	SGWEC	7
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	SGWEC	8
	INP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,CI,C2,CS	SGWEC	9
	23,POS,X,T,PSI,CHI,VARX ,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	SGWEC	10
	EQUIVALENCE (W,DEL)	SGWEC	11
	DIMENSION GRO(33),PAM(65)	SGWEC	12
	GO TO (1001,1002,1003),JW	SGWEC	13
1001	RETURN	SGWEC	14
1002	DO 1 K=1,NG	SGWEC	15
	R(K)=0.0	SGWEC	16
	PAM(K)=0.	SGWEC	17
	DO 1 J=1,NG	SGWEC	18
1	Q(K,J)=0.	SGWEC	19
C	PREPARE ARRAYS FOR FIT	SGWEC	20
	REWIND 9	SGWEC	21
	VARX(66)=0.	SGWEC	22
	NRT=NR +NEIGH	SGWEC	23
	KP=1	SGWEC	24
50	FN =E(KP)	SGWEC	25
	WE=W(KP)**2	SGWEC	26
	CALL SCRAMB(TEN,YO)	SGWEC	27
	WRITE TAPE 9,YO,(PHI(I),I=1,NG)	SGWEC	28
	YE=Y(KP)-YO	SGWEC	29
3	DO 7 J=1,NG	SGWEC	30
	R(J)=R(J)+YE*PHI(J)/WE	SGWEC	31
	DO 7 K=1,NG	SGWEC	32
7	Q(J,K)=Q(J,K)+PHI(J)*PHI(K)/WE	SGWEC	33
	KP=KP+1	SGWEC	34
	IF (KP=NP) 50,50,60	SGWEC	35
C	TEST OUTPUT	SGWEC	36
60	IF(IPR) 51,51,52	SGWEC	37
52	WOT6,92	SGWEC	38
	DO 53 I=1,NG	SGWEC	39
	WOT6,93,I,(Q(I,J),J=1,NG)	SGWEC	40
53	WOT6,94,R(I)	SGWEC	41
92	FORMAT(//1X,1HI60X,6HQ(I,J)56X,4HR(I))	SGWEC	42
93	FORMAT(1HO12,7E16.8/(3X,7E16.8))	SGWEC	43
94	FORMAT(118X,E15.8)	SGWEC	44
51	REWIND 9	SGWEC	45
	I=INVERT(NG)	SGWEC	46
	WOT6,95,DET(2),I	SGWEC	47
95	FORMAT(13HODETERMINANT=E14.8,5X,4HINV=I2)	SGWEC	48
	IF(IPR) 55,55,54	SGWEC	49
54	WOT6,96	SGWEC	50
96	FORMAT(1HO57X,7HINVERSF)	SGWEC	51
	DO 56 I=1,NG	SGWEC	52
6	WOT6,93,I,(Q(I,J),J=1,NG)	SGWEC	53
	CALL SKIP(2)	SGWEC	54
C	EVALUATE SOLUTIONS	SGWEC	55
55	DO 57 I=1,NG	SGWEC	56
57	PAM(I)=R(I)	SGWEC	57
C	VARX(I) IS NOW CALCULATED IN INVERSION SUBROUTINE.	SGWEC	58
C	EVALUATE FITNESS	SGWEC	59
	RS=0.	SGWEC	60

DO 14 KP=1,NP	SGWEC 61
WE=W(KP)*W(KP)	SGWEC 62
READ TAPE 9,YZER,(PHI(I),I=1,NG)	SGWEC 63
PART=0.	SGWEC 64
DO 140 I=1,NG	SGWEC 65
140 PART=PART+R(I)*PHI(I)	SGWEC 66
14 RS=RS+((Y(KP)-YZER-PART)**2)/WE	SGWEC 67
REWIND 9	SGWEC 68
ND=NP-NG-1	SGWEC 69
D=FLOATF(ND)	SGWEC 70
XYZ=RS/D	SGWEC 71
GF=SQRT(XYZ)	SGWEC 72
WOT6,115,RS,GF,XYZ,NR	SGWEC 73
115 FORMAT(///4H RS=E15.8,4H GF=E15.8,8H CHI SQ=E15.8,4H NR=15)	SGWEC 74
DO 6000 K=1,NG	SGWEC 75
6000 VARX(K)=VARX(K)*GF	SGWEC 76
C DEFINITION OF PARAMETERS	SGWEC 77
GO TO (469,469,470,469), JS	SGWEC 78
469 DO 18 J=1,NRT	SGWEC 79
IF (J-NR) 463,463,462	SGWEC 80
463 GRO(J)=GR(J)	SGWEC 81
462 GR(J)=PAM(J)	SGWEC 82
GO TO (1018, 1462) , LS	SGWEC 83
1462 J2 =NRT+J	SGWEC 84
GI(J)=PAM(J2)	SGWEC 85
GO TO 18	SGWEC 86
1018 GI(J)=0.0	SGWEC 87
18 CONTINUE	SGWEC 88
GO TO (919,20),IND	SGWEC 89
470 DO 471 J=1,NG	SGWEC 90
PAM(J)=-PAM(J)*100.0/CC	SGWEC 91
471 VARX(J)=VARX(J)*100.0/CC	SGWEC 92
DO 472 J=1,NRT	SGWEC 93
J2=NRT+J	SGWEC 94
GRO(J)=GR(J)	SGWEC 95
GR(J)=GR(J)+PAM(J)	SGWEC 96
472 GI(J)=GI(J)+PAM(J2)	SGWEC 97
GO TO (919,20),IND	SGWEC 98
20 DO 17 J=1,NR	SGWEC 99
J3=2*NRT+J	SGWEC100
J4=J3+NR	SGWEC101
VARX(J3)=VARX(J3)/GRO(J)	SGWEC102
VARX(J4)=VARX(J4)/GRO(J)	SGWEC103
FU(J)=FU(J)+PAM(J3)/GRO(J)	SGWEC104
17 GU(J)=GU(J)+PAM(J4)/GRO(J)	SGWEC105
919 IF(MUP) 19,10,13	SGWEC106
13 DO 12 J=1,MUP	SGWEC107
K=NG-MAU-MUP+J	SGWEC108
12 POS(J)=PAM(K)	SGWEC109
19 IF (MAU) 24,26,24	SGWEC110
24 GO TO (21,22,23),MAU	SGWEC111
21 C1=PAM(NG)	SGWEC112
C2=0.	SGWEC113
C3=0.	SGWEC114
GO TO 599	SGWEC115
22 C1=PAM(NG-1)	SGWEC116
C2=0.	SGWEC117
C3=PAM(NG)	SGWEC118
GO TO 599	SGWEC119
23 C1=PAM(NG-2)	SGWEC120
C2=PAM(NG-1)	SGWEC121

	C3=PAM(NG)	SGWEC122
	GO TO 599	SGWEC123
26	C1=0.	SGWEC124
	C2=0.	SGWEC125
	C3=0.	SGWEC126
C	OUTPUT OF PARAMETERS	SGWEC127
599	WRITE OUTPUT TAPE 6,9999	SGWEC128
9999	FORMAT(///12X,2HGR17X,3HVAR18X,2HMU17X,3HVAR)	SGWEC129
	DO 600 I=1,NR	SGWEC130
	II=2*NRT+I	SGWEC131
	GO TO (597,600),IND	SGWEC132
597	II=66	SGWEC133
600	WOT6,601,I,GR(I),VARX(I),FU(I),VARX(II)	SGWEC134
601	FORMAT(13,E17.8,3E20.8)	SGWEC135
	WRITE OUTPUT TAPE 6,607	SGWEC136
607	FORMAT(712X,2HGI,17X,3HVAR,18X,2HNU,17X,3HVAR)	SGWEC137
	DO 605 I=1,NR	SGWEC138
	II=NRT+I	SGWEC139
	III=2*NRT+NR+I	SGWEC140
	GO TO (596,605),IND	SGWEC141
596	III=66	SGWEC142
	GO TO (1605,605),LS	SGWEC143
1605	II=66	SGWEC144
605	WOT6,601,I,GI(I),VARX(II),GU(I),VARX(III)	SGWEC145
	IF (NEIGH) 602,602,603	SGWEC146
603	WRITE OUTPUT TAPE 6,604	SGWEC147
604	FORMAT(///23H NEIGHBORING RESONANCES/12X,2HGR,17X,3HVAR,18X,2HNU)	SGWEC148
	IMIN=NR+1	SGWEC149
	DO 608 I=IMIN,NRT	SGWEC150
608	WOT6,601,I,GR(I),VARX(I),FU(I)	SGWEC151
	WRITE OUTPUT TAPE 6,622	SGWEC152
622	FORMAT(12X,2HGI,17X,3HVAR,18X,2HNU)	SGWEC153
	DO 620 I=IMIN,NRT	SGWEC154
	II=NRT+I	SGWEC155
	GO TO*(1620,620),LS	SGWEC156
01620	II=66	SGWEC157
620	WOT6,601,I,GI(I),VARX(II),GU(I)	SGWEC158
C	ROUTINE NOW PRINTS HEADING FOR MUP CONSTANTS AND OUTPUTS VALUES	SGWEC159
602	IF(MAU+MUP) 25,25,611	SGWEC160
611	WOT6,612	SGWEC161
612	FORMAT(10H-CONSTANTS)	SGWEC162
	IF(MAU) 615,615,619	SGWEC163
619	WOT6,625	SGWEC164
225	FORMAT(12X,2HAI17X,3HVAR18X,2HA217X,3HVAR18X,2HA317X,3HVAR)	SGWEC165
	GO TO (311,312,313),MAU	SGWEC166
313	IMIN=NG-2	SGWEC167
	GO TO 314	SGWEC168
312	IMIN=NG-1	SGWEC169
	WOT6,615,(PAM(I),VARX(I),I=IMIN,NG)	SGWEC170
315	FORMAT(2E20.8,40X,2E20.8)	SGWEC171
	GO TO 615	SGWEC172
311	IMIN=NG	SGWEC173
	WOT6,616,(PAM(I),VARX(I),I=IMIN,NG)	SGWEC174
316	FORMAT(6E20.8)	SGWEC175
615	IF(MUP) 25,25,325	SGWEC176
325	IMIN=NG-MAU	SGWEC177
	WOT6,617	SGWEC178
317	FORMAT(1H011X,2HB117X,3HVAR18X,2HB217X,3HVAR18X,2HB317X,3HVAR)	SGWEC179
	MIN=IMIN-MUP+1	SGWEC180
	GO TO(318,318,318,319,319),MUP	SGWEC181
318	WOT6,616,(PAM(I),VARX(I),I=MIN,IMIN)	SGWEC182

GO TO 25	SGWEC183
319 WOT6,320,(PAM(I),VARX(I),I=MIN,IMIN)	SGWEC184
320 FORMAT(6E20.8/1H011X,2HB417X,3HVAR18X,2HB517X,3HVAR/4E20.8)	SGWEC185
25 CONTINUE	SGWEC186
IF(JS-3) 400,40,400	SGWEC187
400 IF(EPS-RS) 45,40,40	SGWEC188
40 PUNCH 10005,(FU(I),GU(I),GR(I),GI(I),NC,I,A(13),A(14),I=1,NRT)	SGWEC189
10005 FORMAT(4E15.7,I6,I5,1X,A6,A2)	SGWEC190
WOT6,41	SGWEC191
41 FORMAT(25HOPARAMETER CARDS PUNCHED.)	SGWEC192
45 RETURN	SGWEC193
C PLOT CURVE	SGWEC194
1003 CONTINUE	SGWEC195
LINES=0	SGWEC196
CALL SKIP(2)	SGWEC197
10001 WOT6,418	SGWEC198
418 FORMAT(1H014X,6HENERGY6X,10HEXP. SIGMA6X,10HAPP. SIGMA6X,10HCAL. S	SGWEC199
11GMA7X,9HDEVIATION3X,13HPERCENT ERROR2X,14HSTD. DEVIATION)	SGWEC200
DO 10040 IEN=1,NP	SGWEC201
EN=E(IEN)	SGWEC202
406 S=SQRT(EN)	SGWEC203
READ TAPE 9,YAPP,(PHI(I),I=1,NG)	SGWEC204
NJS=JS	SGWEC205
JS=1	SGWEC206
SIGMA=PLOT(EN)/S*CC	SGWEC207
JS=NJS	SGWEC208
DO 10065 I=1,NG	SGWEC209
10065 YAPP=YAPP+R(I)*PHI(I)	SGWEC210
IF(JS-3) 10060,10050,10060	SGWEC211
10050 CALL WIDTH(EN,HR)	SGWEC212
YE=-ELOG(Y(IEN))/DENS	SGWEC213
SFACT= 1.0/(DENS*YAPP)	SGWEC214
YAPP=-ELOG(YAPP)/DENS	SGWEC215
GO TO 10070	SGWEC216
10060 YAPP=YAPP/S*CC	SGWEC217
YE=Y(IEN)/S*CC	SGWEC218
SFACT=CC/S	SGWEC219
10070 SD=0.	SGWEC220
DO 10080 K=1,NG	SGWEC221
DO 10080 L=1,NG	SGWEC222
10080 SD=SD+Q(K,L)*PHI(K)*PHI(L)	SGWEC223
SD=SQRT(SD)*GF*SFACT	SGWEC224
RESID=YE-YAPP	SGWEC225
PCER=RESID*100.0/YE	SGWEC226
10000 LINES=LINES+1	SGWEC227
IF(LINES-50) 10040,10040,10042	SGWEC228
10042 CALL SKIP(2)	SGWEC229
WOT6,418	SGWEC230
LINES=1	SGWEC231
10040 WOT6,529,IEN,EN,YE,YAPP,SIGMA,RESID,PCER,SD	SGWEC232
529 FORMAT(I5,7(1X,F15.4))	SGWEC233
SIGMA=PLOT(.025)/7.15811388*CC	SGWEC234
CONS=C1/.15811388*CC	SGWEC235
CALL SKIP(2)	SGWEC236
WOT6,530,SIGMA,CONS	SGWEC237
530 FORMAT(17HOAT E=.025,SIGMA=E14.8,24H AND CONTRIBUTION OF A1=E14.8)	SGWEC238
430 SUM=0.	SGWEC239
WRITE OUTPUT TAPE 6,3133	SGWEC240
3133 FORMAT (18HOINSIDE RESONANCES)	SGWEC241
DO 431 K=1,NRT	SGWEC242
IF (K-NR) 1431,1431,1430	SGWEC243

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30 WRITE OUTPUT TAPE 6,3134	SGWEC244
3134 FORMAT(20H0NEIGHBOR RESONANCES)	SGWEC245
G=GR(K)/GU(K)	SGWEC246
H=GI(K)/GU(K)	SGWEC247
GO TO 1432	SGWEC248
1431 G=GR(K)*GU(K)	SGWEC249
H=GI(K)*GU(K)	SGWEC250
1432 SUM=SUM+H	SGWEC251
431 WRITE OUTPUT TAPE 6,531,K,G,H	SGWEC252
531 FORMAT (110,3H G=E15.8,3H H=E15.8)	SGWEC253
WRITE OUTPUT TAPE 6,532,SUM	SGWEC254
532 FORMAT (5H0SUM=E15.8)	SGWEC255
10004 RETURN	SGWEC256
END	SGWEC257

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S	FASTRAN		
C	FUNCTION DSIG--CALCULATE CONTRIBUTION OF SUBTRACTED RESONANCES	DSIGC	1
C	AND POTENTIAL SCATTERING.	DSIGC	2
C		DSIGC	3
C	FUNCTION DSIG(EN)	DSIGC	4
C	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	DSIGC	5
C	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GID	DSIGC	6
C	2(32),POS(5),VARX(66),A(28),PHI(66)	DSIGC	7
C	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	DSIGC	8
C	1NP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,CD	DSIGC	9
C	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	DSIGC	10
C	EQUIVALENCE (W,DEL)	DSIGC	11
C	SQ = SORT(EN)	DSIGC	12
C	ARG = 2.*WN*SQ	DSIGC	13
C	SI=SIN(ARG)	DSIGC	14
C	CO=COS(ARG)	DSIGC	15
C	DSIG=0.	DSIGC	16
C	IF (NOUT) 1,2,1	DSIGC	17
1	DO 14 K = 1,NOUT	DSIGC	18
C	X=(DL(K)-EN)/DW(K)	DSIGC	19
C	IF(JS-4)20,10,20	DSIGC	20
10	CALL WIDTH(EN,HR)	DSIGC	21
C	T=EN *TEMP/((DW(K)*DW(K))*(ATM+1.0))+(HR*HR)/(DW(K)*DW(K))*0.25	DSIGC	22
C	GO TO 30	DSIGC	23
20	T=(EN*TEMP)/((ATM+1.0)*(DW(K)**2))	DSIGC	24
30	CALL SHAPE(2,X,T,PSI,CHI,2)	DSIGC	25
14	DSIG=DSIG+(DGR(K)*CO+DGI(K)*SI)*PSI+(DGI(K)*CO-DGR(K)*SI)*CHI	DSIGC	26
2	DSIG = 2./SQ*(1.-CO)+DSIG	DSIGC	27
C	RETURN	DSIGC	28
C	END	DSIGC	29

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\$	FASTRAN	
C	FUNCTION PLOT--GIVEN VALUES OF RESONANCE PARAMETERS AND ENERGY,	PLOT 1
C	COMPUTE CROSS SECTION * SQUARE ROOT OF ENERGY.	PLOT 2
C		PLOT 3
	FUNCTION PLOT (EN)	PLOT 4
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	PLOT 5
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI	PLOT 6
	2(32),POS(5),VARX(66),A(28),PHI(66)	PLOT 7
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	PLOT 8
	INP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,C	PLOT 9
	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	PLOT 10
	EQUIVALENCE (W,DEL)	PLOT 11
	S=SQRT(EN)	PLOT 12
423	ARG=2.*WN*S	PLOT 13
	SI=SIN(ARG)	PLOT 14
	CO=COS(ARG)	PLOT 15
428	CONS=C1+C2/EN+C3/EN**2	PLOT 16
	IF(MUP) 29,29,301	PLOT 17
301	DO 31 J=1,MUP	PLOT 18
31	CONS=CONS+POS(J)*EN**J	PLOT 19
29	PLOT = CONS+DSIG(FN)	PLOT 20
	NRT=NR+NEIGH	PLOT 21
	DO 429 K=1,NRT	PLOT 22
	X=(FU(K)-EN)/GU(K)	PLOT 23
	IF (K-NR) 1428,1428,1429	PLOT 24
1429	PH1=(CO-X*SI)/((1.+X**2)*GU(K)**2)	PLOT 25
	PH2=(SI+X*CO)/((1.+X**2)*GU(K)**2)	PLOT 26
	GO TO 429	PLOT 27
1428	T=TEMP*EN/((ATM+1.)*GU(K)**2)	PLOT 28
	CALL SHAPE (2,X,T,PSI,CHI,2)	PLOT 29
	PH1=PSI*CO-CHI*SI	PLOT 30
	PH2=PSI*SI+CHI*CO	PLOT 31
429	PLOT=PLOT+GR(K)*PH1+GI(K)*PH2	PLOT 32
	RETURN	PLOT 33
	END	PLOT 34

\$	FASTRAN	
(	SUBROUTINE PHIFRM--CALCULATE VECTOR PHI AS IN TRIAL FUNCTION 1.	PHFMC 1
(		PHFMC 2
	SUBROUTINE PHIFRM(EN)	PHFMC 3
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	PHFMC 4
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI	PHFMC 5
	2(32),POS(5),VARX(66),A(28),PHI(66)	PHFMC 6
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	PHFMC 7
	1NP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,CPH	PHFMC 8
	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NT	PHFMC 9
	EQUIVALENCE (W,DEL)	PHFMC 10
	NRT=NR+NEIGH	PHFMC 11
	ARG=2.*WN*SQRT(EN)	PHFMC 12
	SI=SIN(ARG)	PHFMC 13
	CO=COS(ARG)	PHFMC 14
	DO 5 KR=1,NRT	PHFMC 15
	X=(FU(KR)-EN)/GU(KR)	PHFMC 16
	IF (KR-NR) 466,466,1061	PHFMC 17
1061	KR2=NRT+KR	PHFMC 18
	PHI(KR)=(CO-X*SI)/((1.+X**2)*GU(KR)**2)	PHFMC 19
	GO TO (5, 1062) , LS	PHFMC 20
1062	PHI(KR2)=(CO*X*SI)/((1.+X**2)*GU(KR)**2)	PHFMC 21
	GO TO 5	PHFMC 22
466	IF (JS-4) 20,10,20	PHFMC 23
10	CALL WIDTH (EN,HR)	PHFMC 24
	T = EN *TEMP/((GU(KR)*GU(KR))*(ATM+1.0))+(HR*HR)/	PHFMC 25
	1(GU(KR)*GU(KR))*0.25	PHFMC 26
	GO TO 30	PHFMC 27
20	T = EN*TEMP/((ATM+1.0)*(GU(KR)*GU(KR)))	PHFMC 28
30	CALL SHAPE (2,X,T,PSI,CHI,2)	PHFMC 29
468	GO TO (61,59),IND	PHFMC 30
C	GAUSS METHOD ONLY	PHFMC 31
59	KR3=2*NRT+KR	PHFMC 32
	KR4=KR3+NR	PHFMC 33
	IF (TEMP) 469,469,470	PHFMC 34
470	DEPSI=(CHI-X*PSI)/(2.*T)	PHFMC 35
	DECHI=(1.-PSI-X*CHI)/(2.*T)	PHFMC 36
	GO TO 471	PHFMC 37
469	DEPSI=-2.*PSI*CHI	PHFMC 38
	DECHI=DEPSI*X+PSI	PHFMC 39
471	TEPSI=DECHI-PSI	PHFMC 40
	TECHI=-DEPSI-CHI	PHFMC 41
	PHI(KR3)= ((DEPSI*CO-DECHI*SI)+GI(KR)/GR(KR)*(DEPSI*SI+DECHI*CO))/	PHFMC 42
1	GU(KR)	PHFMC 43
	PHI(KR4)= -((TEPSI*CO-TECHI*SI)+GI(KR)/GR(KR)*(TEPSI*SI+TECHI*CO))/	PHFMC 44
1	GU(KR)	PHFMC 45
	COMMON TO BOTH FITS	PHFMC 46
61	PHI(KR)=PSI*CO-CHI*SI	PHFMC 47
	GO TO (5, 1063) , LS	PHFMC 48
1063	KR2=NRT+KR	PHFMC 49
	PHI(KR2)=PSI*SI+CHI*CO	PHFMC 50
5	CONTINUE	PHFMC 51
	IF(MUP)11,11,91	PHFMC 52
91	DO 101J=1,MUP	PHFMC 53
	K=NG-MAU-MUP+J	PHFMC 54
101	PHI(K)=FN**J	PHFMC 55
11	IF (MAU) 8,3,8	PHFMC 56
8	GO TO (2,4,6),MAU	PHFMC 57
2	PHI(NG)=1.	PHFMC 58
	GO TO 3	PHFMC 59
4	PHI(NG-1)=1.	PHFMC 60

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PHI(NG)=1./EN**2

PHFMC 61

GO TO 3

PHFMC 62

6 PHI(NG-2)=1.

PHFMC 63

PHI(NG-1)=1./EN

PHFMC 64

PHI(NG)=1./EN**2

PHFMC 65

3 RETURN

PHFMC 66

END

PHFMC 67

\$	FASTRAN	SHPEC	1
	FORTRAN II SUBROUTINE SHAPE FOR THE EVALUATION OF THE	SHPEC	2
	DOPPLER LINE SHAPE FUNCTIONS PSI(X,T) AND CHI(X,T).	SHPEC	3
C	F.T.ADLER, Y.D.NALIBOFF, J.L.DAVIDOV	SHPEC	4
	SUBROUTINE SHAPE (J,X,T,PSI,CHI,IIN)	SHPEC	5
	FREQUENCY 1(0,50),3(0,1,50),6(1,0,50),7(1,0,50),11(50,0),16(4,1,0)	SHPEC	6
	FREQUENCY 210(1,0,1),23(1,0,1),250(1,0,1),260(1,0,1),26(1,0,1),	SHPEC	7
1	27(1,0,1),28(1,0,1),29(1,0,1),30(1,0,1),320(1,0,1),330(1,0,1),	SHPEC	8
2	33(1,0,1),34(1,0,1),35(1,0,1),36(1,0,1),440(1,0,1),45(0,1,1)	SHPEC	9
	DIMENSION A(6),CR(5),CI(5),PR(5),PI(5),PS(5),CH(5),RPS(5),RCH(5)	SHPEC	10
	DIMENSION C1(2),C2(2),C3(2),C4(2),C5(2),C6(2)	SHPEC	11
1	GO TO (2,3),J	SHPEC	12
2	A(1)=2.5052367	SHPEC	13
	A(2)=1.2831204	SHPEC	14
	A(3)=0.2264718	SHPEC	15
	A(4)=0.1306469	SHPEC	16
	A(5)=-0.0202490	SHPEC	17
	A(6)=0.0039132	SHPEC	18
	CR(1)=0.	SHPEC	19
	CR(2)=1.09147804	SHPEC	20
	CR(3)=-2.30555691	SHPEC	21
	CR(4)=-CR(2)	SHPEC	22
	CR(5)=-CR(3)	SHPEC	23
	CI(1)=1.32271498	SHPEC	24
	CI(2)=1.29081178	SHPEC	25
	CI(3)=1.17416680	SHPEC	26
	CI(4)=CI(2)	SHPEC	27
	CI(5)=CI(3)	SHPEC	28
	PR(1)=0.	SHPEC	29
	PR(2)=-10.9663038	SHPEC	30
	PR(3)=24.240703	SHPEC	31
	PR(4)=-PR(2)	SHPEC	32
	PR(5)=-PR(3)	SHPEC	33
	PI(1)=6.1043246	SHPEC	34
	PI(2)=1.1317230	SHPEC	35
	PI(3)=-78.663636	SHPEC	36
	PI(4)=PI(2)	SHPEC	37
	PI(5)=PI(3)	SHPEC	38
	RPS(1)=0.21117643	SHPEC	39
	RPS(2)=0.081635073	SHPEC	40
	RPS(3)=-0.0050439914	SHPEC	41
	RPS(4)=RPS(2)	SHPEC	42
	RPS(5)=RPS(3)	SHPEC	43
	RCH(1)=0.	SHPEC	44
	RCH(2)=0.16088151	SHPEC	45
	RCH(3)=-0.0098666871	SHPEC	46
	RCH(4)=-RCH(2)	SHPEC	47
	RCH(5)=-RCH(3)	SHPEC	48
	C1(1)=1.	SHPEC	49
	C2(1)=3.	SHPEC	50
	C3(1)=15.	SHPEC	51
	C4(1)=105.	SHPEC	52
	C5(1)=945.	SHPEC	53
	C6(1)=10395.	SHPEC	54
	C1(2)=.33333333	SHPEC	55
	C2(2)=.1	SHPEC	56
	C3(2)=.23802524E-01	SHPEC	57
	C4(2)=.46295795E-02	SHPEC	58
	C5(2)=.75757575E-03	SHPEC	59
	C6(2)=.10683761E-03	SHPEC	60
	TWOPI=6.283185307		

RETURN	SHPEC 61
3 IF (T) 5,4,5	SHPEC 62
4 PSI=1./(1.+X**2)	SHPEC 63
CHI=X*PSI	SHPEC 64
RETURN	SHPEC 65
5 X2=X*X	SHPEC 66
B1=1.+X2	SHPEC 67
B3=2.*T	SHPEC 68
B4=4.*T	SHPEC 69
RT=SQRT(B3)	SHPEC 70
C16=X/RT	SHPEC 71
C26=1./RT	SHPEC 72
210 IF (ABSF(X)-1.) 21,21,22	SHPEC 73
21 R=ABSF(C26)	SHPEC 74
W=X2	SHPEC 75
U=1.	SHPEC 76
V=1.	SHPEC 77
GO TO 23	SHPEC 78
22 R=ABSF(C16)	SHPEC 79
W=1./X2	SHPEC 80
U=-1.	SHPEC 81
V=X2	SHPEC 82
23 IF (R-12.53) 30,24,24	SHPEC 83
24 N=1	SHPEC 84
B6=B3/B1**2*V	SHPEC 85
250 IF (R-14.52) 37,25,25	SHPEC 86
25 F1=0.	SHPEC 87
F2=0.	SHPEC 88
260 IF (R-18.24) 38,26,26	SHPEC 89
26 IF (R-26.32) 39,27,27	SHPEC 90
27 IF (R-54.40) 40,28,28	SHPEC 91
28 IF (R-200.) 41,29,29	SHPEC 92
29 IF (R-16384.) 42,43,43	SHPEC 93
30 IF (R-.589) 31,31,48	SHPEC 94
31 N=2	SHPEC 95
B6=V/B4	SHPEC 96
G=X/R3	SHPEC 97
H=SQRT(T*3.1415927)	SHPEC 98
E=EXP((1.-X2)/B4)/B3	SHPEC 99
SI=SIN(G)	SHPEC100
CO=COS(G)	SHPEC101
320 IF (R-.456) 32,32,37	SHPEC102
32 F1=0.	SHPEC103
F2=0.	SHPEC104
330 IF (R-.318) 33,33,38	SHPEC105
33 IF (R-.191) 34,34,39	SHPEC106
34 IF (R-.084) 35,35,40	SHPEC107
35 IF (R-.0172) 36,36,41	SHPEC108
36 IF (R-.00017) 43,43,42	SHPEC109
37 F1=((((((13.*W-286.)*W+1287.)*W-1716.)*W+715.)*W-78.)*W+1.)*C6(N)*	SHPEC110
1 B6	SHPEC111
F2=((((((W-78.)*W+715.)*W-1716.)*W+1287.)*W-286.)*W+13.)*C6(N)*B6	SHPEC112
38 F1=((((((11.*W-165.)*W+462.)*W-330.)*W+55.)*W-1.)*U*C5(N)+F1)*B6	SHPEC113
F2=((((((W-55.)*W+330.)*W-462.)*W+165.)*W-11.)*U*C5(N)+F2)*B6	SHPEC114
39 F1=((((((9.*W-84.)*W+126.)*W-36.)*W+1.)*C4(N)+F1)*B6	SHPEC115
F2=((((((W-36.)*W+126.)*W-84.)*W+9.)*C4(N)+F2)*B6	SHPEC116
40 F1=((((((7.*W-35.)*W+21.)*W-1.)*U*C3(N)+F1)*B6	SHPEC117
F2=((((((W-21.)*W+35.)*W-7.)*U*C3(N)+F2)*B6	SHPEC118
41 F1=((((((5.*W-10.)*W+1.)*C2(N)+F1)*B6	SHPEC119
F2=((((((W-10.)*W+5.)*C2(N)+F2)*B6	SHPEC120
42 F1=((((((3.*W-1.)*U*C1(N)+F1)*R6	SHPEC121

F2=((W-3.)*U*C1(N)+F2)*B6	SHPEC122
3 F1=(1.+F1)	SHPEC123
F2=(1.+F2)	SHPEC124
440 IF (U) 45,44,44	SHPEC125
44 FF=F2	SHPEC126
F2=F1	SHPEC127
F1=FF	SHPEC128
45 IF (N-1) 46,46,47	SHPEC129
46 PSI=F2/B1	SHPEC130
CHI=F1/B1*X	SHPEC131
RETURN	SHPEC132
47 PSI=E*(CO*(H-F2)+X*SI*F1)	SHPEC133
CHI=E*(-SI*(H-F2)+X*CO*F1)	SHPEC134
RETURN	SHPEC135
48 IZ=1	SHPEC136
B2=-2.*X*RT	SHPEC137
DO 10 I=1,5	SHPEC138
6 IF (ABSF(X-CR(I)/CI(I))-0.005) 7,7,9	SHPEC139
7 IF (ABSF(CI(I)*RT-1.)-0.005) 8,8,9	SHPEC140
8 IZ=2	SHPEC141
PS(I)=RPS(I)	SHPEC142
CH(I)=RCH(I)	SHPEC143
S1=0.	SHPEC144
S2=0.	SHPEC145
GO TO 10	SHPEC146
9 Q1=B1+B2*CR(I)+B3*(CR(I)**2-CI(I)**2)	SHPEC147
Q2=(B2+B4*CR(I))*CI(I)	SHPEC148
D1=PR(I)*Q1-PI(I)*Q2	SHPEC149
D2=PI(I)*Q1+PR(I)*Q2	SHPEC150
D=D1**2+D2**2	SHPEC151
PS(I)=D2/D	SHPEC152
CH(I)=(CR(I)*D2-CI(I)*D1)/D	SHPEC153
10 CONTINUE	SHPEC154
11 GO TO (12,19),IZ	SHPEC155
12 P16=A(1)	SHPEC156
P26=0.	SHPEC157
C262=C16*C26**2.	SHPEC158
C162=C16**2-C26**2	SHPEC159
C16N=C162	SHPEC160
C26N=C262	SHPEC161
I=2	SHPEC162
15 P16=P16+A(I)*C16N	SHPEC163
P26=P26+A(I)*C26N	SHPEC164
16 IF (I-6) 17,18,18	SHPEC165
17 C1N=C162*C16N-C262*C26N	SHPEC166
C2N=C262*C16N+C162*C26N	SHPEC167
C16N=C1N	SHPEC168
C26N=C2N	SHPEC169
I=I+1	SHPEC170
GO TO 15	SHPEC171
18 D3=P16**2+P26**2	SHPEC172
SI=PI67/(2.*RT*D3)	SHPEC173
S2=(P26+X*P16)/(B4*D3)	SHPEC174
19 DO 20 I=1,5	SHPEC175
S1=S1+PS(I)	SHPEC176
20 S2=S2+CH(I)	SHPEC177
PSI=TWOPI*S1	SHPEC178
CHI=X*PSI-RT*TWOPI*S2	SHPEC179
RETURN	SHPEC180
END	SHPEC181

\$	FASTRAN	SCMBC	1
	SUBROUTINE SCRAMB(EN,YZER)	SCMBC	2
	OR CODILLI REVISED MAY 1966	SCMBC	3
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	SCMBC	4
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GIS	SCMBC	5
	2(32),POS(5),VARX(66),A(28),PHI(66),SIM(66)	SCMBC	6
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	SCMBC	7
	INP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,C	SCMBC	8
	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	SCMBC	9
	GAUSSF(Z)=EXP(-((EN-7)**27/(HR*HR)))	SCMBC	10
	GO TO (100,200,300,100),JS	SCMBC	11
100	YZER=DSIG(EN)	SCMBC	12
	CALL PHIFRM(EN)	SCMBC	13
	RETURN	SCMBC	14
200	FACT=1.0	SCMBC	15
	JSC=1	SCMBC	16
201	NGP1=NG+1	SCMBC	17
	GO TO 500	SCMBC	18
300	FACT = DENS*100.0	SCMBC	19
	IF(NI) 301,302,302	SCMBC	20
301	JSC=3	SCMBC	21
	NGP1=1	SCMBC	22
	GO TO 500	SCMBC	23
302	JSC=2	SCMBC	24
	GO TO 201	SCMBC	25
500	CALL WIDTH(EN,HR)	SCMBC	26
	H=HR/4.0	SCMBC	27
	FASP=1.0	SCMBC	28
	C = EN- 4.0*HR	SCMBC	29
	DO 530 I =1,NGP1	SCMBC	30
530	SIM(I) =0.0	SCMBC	31
	NPU = 1	SCMBC	32
531	S = SQRT(C)	SCMBC	33
	GO TO (501,502,503),JSC	SCMBC	34
501	PHI(NGP1) = DSIG(C)	SCMBC	35
	PL = 1.0	SCMBC	36
	CALL PHIFRM(C)	SCMBC	37
	GO TO 506	SCMBC	38
502	PHI(NGP1)=S	SCMBC	39
	PL=EXP(-(DENS*CC/S*PLOT (C)))/S	SCMBC	40
	CALL PHIFRM(C)	SCMBC	41
	GO TO 506	SCMBC	42
503	PHI(NGP1)=S	SCMBC	43
	PL=EXP(-(DENS*CC/S*PLOT (C)))/S	SCMBC	44
	GO TO 506	SCMBC	45
506	G = GAUSSF(C)	SCMBC	46
	DO 505 I =1,NGP1	SCMBC	47
505	SIM(I) = SIM(I) + FASP*G*PL*PHI(I)	SCMBC	48
	NPU = NPU+1	SCMBC	49
	IF(NPU-3) 507,508,509	SCMBC	50
507	C = EN+4.0*HR	SCMBC	51
	GO TO 531	SCMBC	52
508	C=C-H	SCMBC	53
	FASP=2.0	SCMBC	54
	GO TO 531	SCMBC	55
509	IF(NPU-34) 508,510,512	SCMBC	56
510	C = C-H/2.0	SCMBC	57
	FASP=4.0	SCMBC	58
	GO TO 531	SCMBC	59
512	IF(NPU-65) 511,511,529	SCMBC	60
511	C=C+H	SCMBC	60

FASP=4.0	SCMBC 61
GO TO 531	SCMBC 62
539 DO 526 I=1,NG	SCMBC 63
526 PHI(I)=.2350790104E-1*SIM(I)*FACT	SCMBC 64
540 YZER=.2350790104E-1*SIM(NGP1)	SCMBC 65
RETURN	SCMBC 66
END	SCMBC 67

\$	FASTRAN		
C	FUNCTION INVERT--PREPARE LEAST SQUARES MATRIX FOR DOUBLE PRECISION	INVT	1
C	INVERSION AND PARTIALLY COMPUTE VARIANCE OF PARAMETERS OBTAINED.	INVT	2
C		INVT	3
C	FUNCTION INVERT(DUMMY)	INVT	4
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	INVT	5
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI	INVT	6
	2(32),POS(5),VARX(66),AT(28),PHI(66)	INVT	7
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	INVT	8
	INP,NR,NT,MAI,NOUT,INDE,NEIGH,JWE,MUP,IPR,TEND,NG,IND,GR,GI,C1,C2,C	INVT	9
	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	INVT	10
	EQUIVALENCE (W,DEL)	INVT	11
	DIMENSION IPIVOT(65),INDEX(65,2)	INVT	12
	N=NG	INVT	13
	1 DO 2 I=1,NG	INVT	14
	Q(2*N,I)=Q(N,I)	INVT	15
	2 Q(2*N-1,I)=0.0	INVT	16
	R(2*N)=R(N)	INVT	17
	R(2*N-1)=0.0	INVT	18
	N=N-1	INVT	19
	IF(N) 3,3,1	INVT	20
	3 INVERT=DNVI(NG,130,I,Q,R,DET(2),PIVOT,IPIVOT,INDEX,65)	INVT	21
	DO 5 I=1,NG	INVT	22
	VARX(I)=ROUNDF(DSQRT(Q(2*I,I),PIVOT(2)))	INVT	23
	DO 4 N=1,NG	INVT	24
	4 Q(I,N)=ROUNDF(Q(2*I,N),Q(2*I-1,N))	INVT	25
	5 R(I)=ROUNDF(R(2*I),R(2*I-1))	INVT	26
	RETURN	INVT	27
	END	INVT	28
		INVT	29
DSQTC	115		

\$	SCATRE			DSQTC	
*	FUNCTION ROUND--ROUND DOUBLE PRECISION NUMBER TO SINGLE PRECISION			DSQTC	1
	ENTRY ROUND			DSQTC	2
ROUND	FRN			DSQTC	3
	TRA 1,4			DSQTC	4
	END			DSQTC	5
* UOI	DOUBLE PRECISION SQRT			DSQTC	6
	ENTRY DSQRT			DSQTC	7
	EVEN			DSQTC	8
U	BSS 2	TEMP STORAGE		DSQTC	9
DSQRT	CLA* 1,4			DSQTC	10
	TMI ERR	ERROR RETURN, X NEGATIVE		DSQTC	11
	SXA AA,1			DSQTC	12
	ACL =01770000000000	(P+128+127)*2**-8		DSQTC	13
	XCL			DSQTC	14
	LGL 8			DSQTC	15
	ALS 27	((P/2)-1)+128 = NEW CHARACTERISTIC		DSQTC	16
	STO COMMON+1			DSQTC	17
	TQP *+2	MQ IS + IF P IS ODD, USE Y/2 FOR Y		DSQTC	18
	LLS 1	MQ IS - IF P IS EVEN, USE Y		DSQTC	19
	LLS 5	6 BITS OF Y USED FOR TABLE LOOKUP		DSQTC	20
	PAX 0,1	OF INITIAL APPROXIMATION		DSQTC	21
	TXL A,1,15	TRA IF ARG NOT NORMAL		DSQTC	22
	LLS 25	AC=Y/16 OR -Y/16		DSQTC	23
	SLW COMMON			DSQTC	24
	VDH TABLE+16,1,19	DIVIDE BY INITIAL APPROX. (X0/4)		DSQTC	25
	LLS 16	MQ=Y/4X0 OR -Y/4X0		DSQTC	26
	XCL	AC=Y/4X0, MAYBE P BIT IS 1		DSQTC	27
	ADD TABLE+16,1	AC=((Y/2X0)+(X0/2))/2=X1/2		DSQTC	28
	STO COMMON+2			DSQTC	29
	CLA COMMON	AC=Y/16		DSQTC	30
	DVH COMMON+2			DSQTC	31
	XCA	AC=Y/8X1		DSQTC	32
	ALS 2			DSQTC	33
	ADD COMMON+2	AC=(Y/2X1)+(X1/2)=X2, FIXED POINT		DSQTC	34
	LRS 8			DSQTC	35
	RQL 28			DSQTC	36
	ADD COMMON+1	X2/2, FLOATING POINT		DSQTC	37
*				DSQTC	38
	DST U			DSQTC	39
	DLD* 1,4	ACMQ=A		DSQTC	40
	DFDH U	ACMQ=2A/X2		DSQTC	41
	SUB =00020000000000	ACMQ=A/2X2		DSQTC	42
	DFAD U	ACMQ=X3=SQRT(A)		DSQTC	43
	DST* 2,4	STORE RESULT		DSQTC	44
*				DSQTC	45
.AA	AXT **,1	RESTORE XR1		DSQTC	46
	TOV 3,4	RETURN		DSQTC	47
	TRA 3,4	RETURN		DSQTC	48
*				DSQTC	49
A	DLD* 1,4			DSQTC	50
	TZE AA-1	ZERO RETURN		DSQTC	51
	SXA SB,4			DSQTC	52
	CALL SYSWOT	PRINT ERROR MESSAGE		DSQTC	53
	TIX M,,4			DSQTC	54
SB	AXT **,4			DSQTC	55
	TRA AA			DSQTC	56
M	BCI 4,0DSQRT ARG NOT NORMAL			DSQTC	57
ERR	SXA SA,4			DSQTC	58
	CALL SYSWOT			DSQTC	59
	TIX MA,,4			DSQTC	60

	AXT	**4		DSQTC 61
	TRA	3,4		DSQTC 62
MA	BCI	4,0	DSORT ARG NEGATIVE	DSQTC 63
	DEC	.9960861B2	.25#SQRT(127/128)	DSQTC 64
	DEC	.9882118B2		DSQTC 65
	DEC	.9802742B2		DSQTC 66
	DEC	.9722718B2		DSQTC 67
	DEC	.9642030B2		DSQTC 68
	DEC	.9560662B2		DSQTC 69
	DEC	.9478594B2		DSQTC 70
	DEC	.9395810B2		DSQTC 71
	DEC	.9312290B2		DSQTC 72
	DEC	.9228014B2		DSQTC 73
	DEC	.9142962B2		DSQTC 74
	DEC	.9057110B2		DSQTC 75
	DEC	.8970438B2		DSQTC 76
	DEC	.8882919B2		DSQTC 77
	DEC	.8794530B2		DSQTC 78
	DEC	.8705243B2		DSQTC 79
	DEC	.8615030B2		DSQTC 80
	DEC	.8523864B2		DSQTC 81
	DEC	.8431711B2		DSQTC 82
	DEC	.8338540B2		DSQTC 83
	DEC	.8244316B2		DSQTC 84
	DEC	.8149003B2		DSQTC 85
	DEC	.8052562B2		DSQTC 86
	DEC	.7954951B2		DSQTC 87
	DEC	.7856128B2		DSQTC 88
	DEC	.7756046B2		DSQTC 89
	DEC	.7654655B2		DSQTC 90
	DEC	.7551904B2		DSQTC 91
	DEC	.7447735B2		DSQTC 92
	DEC	.7342088B2		DSQTC 93
	DEC	.7234898B2		DSQTC 94
	DEC	.7126076B2		DSQTC 95
	DEC	.7015608B2		DSQTC 96
	DEC	.6903351B2		DSQTC 97
	DEC	.6789238B2		DSQTC 98
	DEC	.6673174B2		DSQTC 99
	DEC	.6555055B2		DSQTC100
	DEC	.6434769B2		DSQTC101
	DEC	.6312191B2		DSQTC102
	DEC	.6187184B2		DSQTC103
	DEC	.6059600B2		DSQTC104
	DEC	.5929271B2		DSQTC105
	DEC	.5796712B2		DSQTC106
	DEC	.5659616B2		DSQTC107
	DEC	.5519851B2		DSQTC108
	DEC	.5376453B2	ETC	DSQTC109
	DEC	.5229125B2	.25#SQRT(35/128)	DSQTC110
TABLE	DEC	.5077524B2	.25#SQRT(33/128)	DSQTC111
MON	BSS	3	TEMP STORAGE	DSQTC112
	END			DSQTC113

\$	FASTRAN		
C	SUBROUTINE SKIP--READ AND PRINT PAGE HEADINGS.	SKIPC	1
C		SKIPC	2
C	N.B.--DAT1 IS A SUBROUTINE WICH OBTAINS THE DATE FROM THE MONITOR	SKIPC	3
C	AND STORES IT IN THE LOCATION OF THE ARGUMENT AND THE TWO FOLLOWING	SKIPC	4
C	LOCATIONS--I.E. FORWARD IN CORE.	SKIPC	5
C		SKIPC	6
	SUBROUTINE SKIP(INIT)	SKIPC	7
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	SKIPC	8
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI	SKIPC	9
	2(32),POS(5),VARX(66),A(28),PHI(66)	SKIPC	10
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,	SKIPC	11
	1NP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,C1,C2,C	SKIPC	12
	23,POS,X,T,PSI,CHI,VARX ,LS,NC,EPS,A,SUME,DENS,JS,PHI,NT	SKIPC	13
	EQUIVALENCE (W,DEL)	SKIPC	14
	DIMENSION DATE(3)	SKIPC	15
	GO TO (10,30),INIT	SKIPC	16
10	READ 20,(A(I), I=1,28)	SKIPC	17
20	FORMAT (13A6,A2)	SKIPC	18
	CALL DAT1(DATE(3))	SKIPC	19
	IPAGE=0	SKIPC	20
	RETURN	SKIPC	21
30	IPAGE=IPAGE + 1	SKIPC	22
	WOT6,40,(A(I),I=1,14),DATE(3),DATE(2),DATE(1),IPAGE,(A(I),I=15,28)	SKIPC	23
40	FORMAT (1H113A6,A2,10X,3A6,7X,4HPAGEI3/1H 13A6,A2,8X,27HPROGRAM COS	SKIPC	24
	1DILLI 7 AUG 1965)	SKIPC	25
	RETURN	SKIPC	26
	END	SKIPC	27

\$	FASTRAN	
C	SUBROUTINE WEIGHT--COMPUTE WEIGHTS FOR INPUT DATA.	WGHTC 1
C	WEIGHTS SCALED TO GIVE SUMW = NP	WGHTC 2
C		WGHTC 3
C	SUBROUTINE WEIGHT	WGHTC 4
	DIMENSION Q(130,65),R(130),DET(2),PIVOT(130),FU(32),GU(32),E(1000)	WGHTC 5
	1,Y(1000),DEL(1000),W(1000),DL(20),DW(20),DGR(20),DGI(20),GR(32),GI	WGHTC 6
	2(32),POS(5),VARX(66),A(28),PHI(66)	WGHTC 7
	COMMON Q,R,DET,PIVOT,FU,GU,E,Y, W,DL,DW,DGR,DGI,TEMP,ATM,WN,CC,WGHTC	WGHTC 8
	1NP,NR,NT,MAU,NOUT,INDE,NEIGH,JWE,MUP,IPR,IEND,NG,IND,GR,GI,CI,C2,CW	WGHTC 9
	23,POS,X,T,PSI,CHI,VARX,LS,NC,EPS,A,SUME,DENS,JS,PHI,NI	WGHTC 10
	EQUIVALENCE (W,DEL)	WGHTC 11
	GO TO (201, 202, 203, 204, 205, 206), JWE	WGHTC 12
C	EQUAL WEIGHTS	WGHTC 13
201	DO 4 K=1,NP	WGHTC 14
4	W(K)=1.0	WGHTC 15
	GO TO 15	WGHTC 16
C	PROPORTIONAL WEIGHTS	WGHTC 17
202	DO 5 K =1,NP	WGHTC 18
5	DEL(K) = Y(K)*DEL(K)	WGHTC 19
	GO TO 204	WGHTC 20
204	IF(JS=3) 2204,1204,2204	WGHTC 21
C	ERROR FOR SD(E)*SIGMA	WGHTC 22
2204	DO 7 K =1,NP	WGHTC 23
7	W(K) =SQRT(E(K))*DEL(K)*100.0/CC	WGHTC 24
	GO TO 15	WGHTC 25
C	ERROR FOR TRANSMISSION	WGHTC 26
1204	DO 77 K =1,NP	WGHTC 27
	EN=E(K)	WGHTC 28
	CALL WIDTH(EN,HR)	WGHTC 29
	FACT=DENS*DEL(K)*100.0	WGHTC 30
	Z=EXP(-DENS*Y(K))	WGHTC 31
77	W(K)=Z*FACT	WGHTC 32
	GO TO 15	WGHTC 33
C	1/Y**2 WEIGHTS	WGHTC 34
2203	IF(JS=3) 2203,1203,2203	WGHTC 35
2203	DO 6 K=1,NP	WGHTC 36
6	W(K)=Y(K)*SQRT(E(K))*100.0/CC	WGHTC 37
	GO TO 15	WGHTC 38
1203	DO 66 K=1,NP	WGHTC 39
	EN=E(K)	WGHTC 40
	CALL WIDTH(EN,HR)	WGHTC 41
66	W(K) =(EXP(-DENS*Y(K)))*100.0	WGHTC 42
	GO TO 15	WGHTC 43
C	1/Y WEIGHTS	WGHTC 44
2205	IF(JS=3) 2205,1205,2205	WGHTC 45
2205	DO 8 K=1,NP	WGHTC 46
8	W(K)=SQRT(ABS(F(Y(K)*SQRT(E(K)))/CC))*100.0	WGHTC 47
	GO TO 15	WGHTC 48
1205	DO 88 K=1,NP	WGHTC 49
	FN=F(K)	WGHTC 50
	CALL WIDTH(EN,HR)	WGHTC 51
	FACT = EXP(-DENS*Y(K))	WGHTC 52
	W(K) = SQRT(FACT)*100.0	WGHTC 53
	GO TO 15	WGHTC 54
206	READ ZIC,EZERO,WE1,WE2	WGHTC 55
210	FORMAT(3E15.8)	WGHTC 56
	DO 10 K=1,NP	WGHTC 57
	IF(E(K)-EZERO) 11,11,12	WGHTC 58
11	W(K)=1.0/SQRT(WE1)	WGHTC 59
	GO TO 10	WGHTC 60

12	W(K)=1.0/SQRT(WE2)	WGHTC 61
	CONTINUE	WGHTC 62
15	SUMW=0.0	WGHTC 63
	DO 1500 K=1, NP	WGHTC 64
1500	SUMW = SUMW + 1.0/(W(K)*W(K))	WGHTC 65
	XWE = FLOATF(NP)/SUMW	WGHTC 66
	FAWE = SQRT(XWE)	WGHTC 67
	DO 1501 K=1, NP	WGHTC 68
1501	W(K)=W(K)/FAWE	WGHTC 69
	EPS = 900.0*FLOATF(NP)	WGHTC 70
	RETURN	WGHTC 71
	END	WGHTC 72

5	FASTRAN	
	CURVE PLOT--ORIGINALLY FOR ILLIAC, NOW ADAPTED TO 7094--GRAPH	CVPLT 1
	ROUTINE FOR CALCAMP USES 10-INCH PAPER	JANUARY, 1966 CVPLT 2
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000), DL(40),DW(40),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	CVPLT 3
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CC	CVPLT 4
	1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NCV	CVPLT 5
	2I	CVPLT 6
1001	CALL SHAPE (1,X,X,X,X,2)	CVPLT 7
1	CALL SKIP(1)	CVPLT 8
	CALL SKIP(2)	CVPLT 9
	READ 5000,TEMP,ATM,DENS,WN,CC	CVPLT 10
5000	FORMAT (5E15.8)	CVPLT 11
	WOT6,5001,TEMP,ATM,DENS,WN,CC	CVPLT 12
5001	FORMAT (6HOTEMP=F8.4,5H ATM=F5.0,6H DENS=E15.8,4H WN=E15.8,4H CC=	CVPLT 13
	1 E15.8)	CVPLT 14
	READ 102,NP,INDE,NT,LS,IPR,JS,NI	CVPLT 15
	READ 102,NR,NEIGH,NOUT,KNEG,KPOS,JWE	CVPLT 16
	WOT6,102,NP,INDE,NT,LS,IPR,JS,NI	CVPLT 17
	WOT6,102,NR,NEIGH,NOUT,KNEG,KPOS,JWE	CVPLT 18
	MAU=KNEG	CVPLT 19
	MUP=KPOS	CVPLT 20
	GO TO (20,21), LS	CVPLT 21
20	TLEVEL= 6HSINGLE	CVPLT 22
	GO TO 23	CVPLT 23
21	TLEVEL= 6HMULTI-	CVPLT 24
23	FISTOT= 6HTOTAL	CVPLT 25
	INEG=0	CVPLT 26
	BACK=0	CVPLT 27
	IF(KNEG) 25,25,24	CVPLT 28
24	INEG=KNEG-1	CVPLT 29
	BACK=0	CVPLT 30
202	FORMAT(18H0THIS RUN CONTAINS15,23H DATA POINTS, AND IS A A6,8HRUN	CVPLT 31
	1WITH13,29H NON-LINEAR ITERATIONS USING A6, 4H LEVEL PARAMETERS.	CVPLT 32
	2PR=12,1H./15H TRIAL FUNCTION12,1H,14,19H INTEGRATION STEPS.)	CVPLT 33
1202	FORMAT(18H THIS RUN CONTAINS13,19H INSIDE RESONANCES,13,21H NEIGHBCVPLT	CVPLT 34
	10R RESONANCES,13,20H OUTSIDE RESONANCES,A2,21H BACKGROUND CONSTANTCVPLT	CVPLT 35
	2,712,31H TERMS OF NEG. POWERS OF E, AND12,50H TERMS OF POS. POWERSCVPLT	CVPLT 36
	3 OF E, USING WEIGHTING OPTION12,1H.)	CVPLT 37
	102 FORMAT(1115)	CVPLT 38
	25 IF(INDE) 31,30,31	CVPLT 39
30	WN=0.	CVPLT 40
	FISTOT= 6HFISS.	CVPLT 41
	31 CONTINUE	CVPLT 42
	32 DO 34 I=1,NP	CVPLT 43
	34 READ 104,E(I),Y(I),DEL(I)	CVPLT 44
	33 CONTINUE	CVPLT 45
	WOT6,202,NP,FISTOT,NT,TLEVEL,IPR,JS,NI	CVPLT 46
	WOT6,1202,NR,NEIGH,NOUT,BACK,INEG,KPOS,JWE	CVPLT 47
104	FORMAT(4E15.8)	CVPLT 48
997	WRITE OUTPUT TAPE 6,1103	CVPLT 49
1103	FORMAT (30H GUESSES FOR INSIDE RESONANCES)	CVPLT 50
	DO 3 I=1,NR	CVPLT 51
	READ 104,FU(I),GU(I),GR(I),GI(I)	CVPLT 52
	WOT6,203,I,FU(I),GU(I),GR(I),GI(I)	CVPLT 53
203	FORMAT (15,4H MU=F15.8,4H NU=F13.8,4H GR=E15.8,4H GI=E15.8)	CVPLT 54
3	CONTINUE	CVPLT 55
26	IF (NEIGH) 6,8,6	CVPLT 56
6	KMIN=NR+1	CVPLT 57
	KMAX=NR+NEIGH	CVPLT 58
	WRITE OUTPUT TAPE 6,1104	CVPLT 59
		CVPLT 60

1104	FORMAT (32HOGUESSES FOR NEIGHBOR RESONANCES)	CVPLT 61
	DO 7 K=KMIN,KMAX	CVPLT 62
	READ 104,FU(K),GU(K),GR(K),GI(K)	CVPLT 63
7	WOT6,203,K,FU(K),GU(K),GR(K),GI(K)	CVPLT 64
8	IF(NOUT) 9,9002,9	CVPLT 65
9	WRITE OUTPUT TAPE 6,1105	CVPLT 66
1105	FORMAT (34HOPARAMETERS FOR OUTSIDE RESONANCES)	CVPLT 67
	DO 10 K=1,NOUT	CVPLT 68
	READ 104,DL(K),DW(K),DGR(K),DGI(K)	CVPLT 69
10	WRITE OUTPUT TAPE 6,210,K,DL(K),DW(K),DGR(K),DGI(K)	CVPLT 70
210	FORMAT (15,4H DL=F15.8,4H DW=F13.8,5H DGR=E15.8,5H DGI=E15.8)	CVPLT 71
9002	IF(MAU) 28,28,27	CVPLT 72
27	READ 104,C1,C2,C3	CVPLT 73
	WOT6,101,C1,C2,C3	CVPLT 74
101	FORMAT(4H0A1=E15.8,4H A2=E15.8,4H A3=E15.8)	CVPLT 75
28	IF(MUP) 35,35,29	CVPLT 76
29	READ 104,(POS(I),I=1,MUP)	CVPLT 77
	WOT6,103,(POS(I),I=1,MUP)	CVPLT 78
103	FORMAT(27HOPOSITIVE CONSTANTS B1...B5/E15.8)	CVPLT 79
35	NG=LS*(NR+NEIGH)+MAU+MUP	CVPLT 80
	NRT=NR+NEIGH	CVPLT 81
	IF(JS=3) 352,351,352	CVPLT 82
351	DO 52 I=1,NRT	CVPLT 83
	READ 50,GRX,GIX	CVPLT 84
50	FORMAT(30X,2E15.8)	CVPLT 85
	IF(GRX) 51,60,51	CVPLT 86
60	NI=-1	CVPLT 87
	GO TO 52	CVPLT 88
51	R(I)=(GR(I)-GRX)*CC/100.0	CVPLT 89
	GO TO(52,510),LS	CVPLT 90
510	II=NRT+I	CVPLT 91
	R(II)=(GI(I)-GIX)*CC/100.0	CVPLT 92
52	CONTINUE	CVPLT 93
	IF(NI)4005,4005,4004	CVPLT 94
4004	IF (MAU) 57,57,53	CVPLT 95
53	GO TO(54,55,56),MAU	CVPLT 96
54	R(NG)=-C1*CC/100.0	CVPLT 97
	GO TO 57	CVPLT 98
55	R(NG-1)=-C1*CC/100.0	CVPLT 99
	R(NG)=-C3*CC/100.0	CVPLT100
	GO TO 57	CVPLT101
56	R(NG-2)=-C1*CC/100.0	CVPLT102
	R(NG-1)=-C2*CC/100.0	CVPLT103
	R(NG)=-C3*CC/100.0	CVPLT104
57	IF(MUP) 49,49,58	CVPLT105
58	DO 59 I=1,MUP	CVPLT106
	II=NG-MAU-MUP+I	CVPLT107
59	R(II)=-POS(I)*CC/100.0	CVPLT108
	WOT6, 4000, JS	CVPLT109
	DO 4001 I=1, NRT	CVPLT110
	II= NRT+I	CVPLT111
4001	WOT6, 4002, I, FU(I), GU(I), R(I), R(II)	CVPLT112
1000	FORMAT (16H0TRIAL FUNCTION15, 5X, 23HLINEARIZED TRANSMISSION//37H0	CVPLT113
	IPARAMETERS OBTAINED FROM CODILLI FIT)	CVPLT114
4002	FORMAT (15, 4H MU=F15.8, 4H NU=F13.8, 4H RR=F15.8, 4H RI=E15.8)	CVPLT115
	GO TO 49	CVPLT116
4005	WOT6, 4003, JS	CVPLT117
4003	FORMAT (15H0TRIAL FUNCTION15,5X,21HCOMPLETE TRANSMISSION//)	CVPLT118
	GO TO 49	CVPLT119
352	DO 37 I=1,NRT	CVPLT120
	R(I)=GR(I)	CVPLT121

	GO TO(37,36),LS	CVPLT122
36	NRTI=NRT+I	CVPLT123
	R(NRTI)=GI(I)	CVPLT124
37	CONTINUE	CVPLT125
	IF(MAU) 39,39,38	CVPLT126
38	GO TO (44,45,46), MAU	CVPLT127
44	R(NG)=C1	CVPLT128
	GO TO 39	CVPLT129
45	R(NG-1)=C1	CVPLT130
	R(NG)=C3	CVPLT131
	GO TO 39	CVPLT132
46	R(NG-2)=C1	CVPLT133
	R(NG-1)=C2	CVPLT134
	R(NG)=C3	CVPLT135
39	IF(MUP) 49,49,47	CVPLT136
47	DO 48 I=1,MUP	CVPLT137
	II=NG-MAU-MUP+I	CVPLT138
48	R(II)=POS(I)	CVPLT139
49	CALL SIGPLT	CVPLT140
	GO TO 1	CVPLT141
	FND	CVPLT142

\$	FASTAN	
	FUNCTION PLOT--GIVEN VALUES OF RESONANCE PARAMETERS AND ENERGY,	PLOTP 1
	COMPUTE CROSS SECTION * SQUARE ROOT OF ENERGY.	PLOTP 2
C		PLOTP 3
	FUNCTION PLOTSG(EN)	PLOTP 4
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000),DL(40),DW(40),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	PLOTP 5
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CPL	PLOTP 6
	1C,NP,NR,MAI,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NPL	PLOTP 7
	2I	PLOTP 8
	S=SQRT(EN)	PLOTP 9
423	ARG=2.*WN*S	PLOTP 10
	SI=SIN(ARG)	PLOTP 11
	CO=COS(ARG)	PLOTP 12
428	CONS=C1+C2/EN+C3/EN**2	PLOTP 13
	IF(MUP) 29,29,301	PLOTP 14
301	DO 31 J=1,MUP	PLOTP 15
	31 CONS=CONS+POS(J)*EN**J	PLOTP 16
29	PLOT = CONS+DSIG(EN)	PLOTP 17
	NRT=NR+NEIGH	PLOTP 18
	DO 429 K=1,NRT	PLOTP 19
	X=(FU(K)-EN)/GU(K)	PLOTP 20
	IF (K-NR) 1428,1428,1429	PLOTP 21
1429	PH1=(CO-X*SI)/((1.+X**2)*GU(K)**2)	PLOTP 22
	PH2=(SI+X*CO)/((1.+X**2)*GU(K)**2)	PLOTP 23
	GO TO 429	PLOTP 24
1428	T=TEMP*EN/((ATM+1.)*GU(K)**2)	PLOTP 25
	CALL SHAPE (2,X,T,PSI,CHI,2)	PLOTP 26
	PH1=PSI*CO-CHI*SI	PLOTP 27
	PH2=PSI*SI+CHI*CO	PLOTP 28
429	PLOT=PLOT+GR(K)*PH1+GI(K)*PH2	PLOTP 29
	PLOTSG=PLOT	PLOTP 30
	RETURN	PLOTP 31
	END	PLOTP 32
		PLOTP 33

\$	FASTRAN	
	SUBROUTINE SIGPLT	SGPTP 1
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000),	DL(40),DW(4SGPTP 2
	10),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	SGPTP 3
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CS	SGPTP 4
	1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NS	SGPTP 5
	2I	SGPTP 6
	LINES=0	SGPTP 7
	CALL SKIP(2)	SGPTP 8
	NRT=NR+NEIGH	SGPTP 9
10001	WOT6,418	SGPTP 10
418	FORMAT(1H014X,6HENERGY6X,10HEXP. SIGMA6X,10HAPP. SIGMA6X,10HCAL. S	SGPTP 11
	1IGMA7X,9HDEVIATION3X,13HPERCENT ERROR2X,14HSTD. DEVIATION)	SGPTP 12
	DO 10040 IEN=1,NP	SGPTP 13
	EN=E(IEN)	SGPTP 14
406	S=SQRT(EN)	SGPTP 15
	YE=Y(IEN)	SGPTP 16
	CALL SCRAMB(EN,YAPP)	SGPTP 17
	NJS=JS	SGPTP 18
	JS=1	SGPTP 19
	SIGMA=PLOTSG(EN)/S*CC	SGPTP 20
	JS=NJS	SGPTP 21
	IF(NI) 10050,10061,10061	SGPTP 22
10061	DO 10065 I=1,NG	SGPTP 23
10065	YAPP = YAPP + R(I)*PHI(I)	SGPTP 24
	IF(JS-3)10060,10050,10060	SGPTP 25
10050	YAPP=-ELOG(YAPP)/DENS	SGPTP 26
	GO TO 10070	SGPTP 27
10060	YAPP=YAPP/S*CC	SGPTP 28
10070	RFSID=YE-YAPP	SGPTP 29
	PCER=RFSID*100.0/YE	SGPTP 30
	DEL(IEN)=YAPP	SGPTP 31
10000	LINES=LINES+1	SGPTP 32
	IF(LINES-50) 10040,10040,10042	SGPTP 33
10042	CALL SKIP(2)	SGPTP 34
	WOT6,418	SGPTP 35
	LINES=1	SGPTP 36
10040	WOT6,529,IEN,EN,YE,YAPP,SIGMA,RESID,PCER	SGPTP 37
529	FORMAT(15,7(1X,F15.4))	SGPTP 38
	SIGMA=PLOTSG(.025)/.15811388*CC	SGPTP 39
	CONS=C1/.15811388*CC	SGPTP 40
	CALL SKIP(2)	SGPTP 41
	WOT6,530,SIGMA,CONS	SGPTP 42
530	FORMAT(17HOAT E=.025,SIGMA=E14.8,24H AND CONTRIBUTION OF A1=E14.8)	SGPTP 43
430	SUM=0.	SGPTP 44
	WRITE OUTPUT TAPE 6,3133	SGPTP 45
3133	FORMAT (18HOINSIDE RESONANCES)	SGPTP 46
	DO 431 K=1,NRT	SGPTP 47
	IF (K-NR) 1431,1431,1430	SGPTP 48
1430	WRITE OUTPUT TAPE 6,3134	SGPTP 49
3134	FORMAT(20HONEIGHBOR RESONANCES)	SGPTP 50
	G=GR(K)/GU(K)	SGPTP 51
	H=GI(K)/GU(K)	SGPTP 52
	GO TO 1432	SGPTP 53
1431	G=GR(K)*GU(K)	SGPTP 54
	H=GI(K)*GU(K)	SGPTP 55
1432	SUM=SUM+H	SGPTP 56
431	WRITE OUTPUT TAPE 6,531,K,G,H	SGPTP 57
531	FORMAT (110,3H G=E15.8,3H H=E15.8)	SGPTP 58
	WRITE OUTPUT TAPE 6,532,SUM	SGPTP 59
532	FORMAT (5HOSUM=E15.8)	SGPTP 60

EMIN=E(1)
 EMAX=E(NP)
 CALL GRAPH

SGPTP 61
 SGPTP 62
 SGPTP 63
 SGPTP 64
 SGPTP 65

10004 RETURN
 END

FASTPAN

FUNCTION DSIG--CALCULATE CONTRIBUTION OF SUBTRACTED RESONANCES
AND POTENTIAL SCATTERING.

DSIGP 1

DSIGP 2

DSIGP 3

DSIGP 4

FUNCTION DSIG(EN)

DSIGP 5

DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000), DL(40),DW(40),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)

DSIGP 6

COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CDSIGP
1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,ND

DSIGP 7

DSIGP 8

2I

DSIGP 9

SQ = SQRT(EN)

DSIGP 10

ARG = 2.*WN*SQ

DSIGP 11

SI=SIN(ARG)

DSIGP 12

CO=COS(ARG)

DSIGP 13

DSIG=0.

DSIGP 14

IF (NOUT) 1,2,1

DSIGP 15

DO 14 K = 1,NOUT

DSIGP 16

X=(DL(K)-FN)/DW(K)

DSIGP 17

IF(JS-4)20,10,20

DSIGP 18

10 CALL WIDTH(EN,HR)

DSIGP 19

T=EN *TEMP/((DW(K)*DW(K))*(ATM+1.0))+(HR*HR)/(DW(K)*DW(K))*0.25

DSIGP 20

GO TO 30

DSIGP 21

20 T=(FN*TEMP)/((ATM+1.0)*(DW(K)**2))

DSIGP 22

30 CALL SHAPE(2,X,T,PSI,CHI,2)

DSIGP 23

14 DSIG=DSIG+(DGR(K)*CO+DGI(K)*SI)*PSI+(DGI(K)*CO-DGR(K)*SI)*CHI

DSIGP 24

2 DSIG = 2./SQ*(1.-CO)+DSIG

DSIGP 25

RETURN

DSIGP 26

END

DSIGP 27

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APPENDIX F - page 8

\$	FASTRAN		
C	SUBROUTINE PHIFRM--CALCULATE VECTOR PHI AS IN TRIAL FUNCTION 1.	PHFMP	1
C		PHFMP	2
	SUBROUTINE PHIFRM(EN)	PHFMP	3
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000), DL(40),DW(40)	PHFMP	4
	10),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	PHFMP	5
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CPHFMP	PHFMP	6
	1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NPHFMP	PHFMP	7
	2I	PHFMP	8
	NRT=NR+NEIGH	PHFMP	9
	ARG=2.*WN*SQRT(EN)	PHFMP	10
	SI=SIN(ARG)	PHFMP	11
	CO=COS(ARG)	PHFMP	12
	DO 5 KR=1,NRT	PHFMP	13
	X=(FU(KR)-EN)/GU(KR)	PHFMP	14
	IF (KR-NR) 466,466,1061	PHFMP	15
1061	KR2=NRT+KR	PHFMP	16
	PHI(KR)=(CO-X*SI)/((1.+X**2)*GU(KR)**2)	PHFMP	17
	GO TO (5, 1062) , LS	PHFMP	18
1062	PHI(KR2)=(CO*X*SI)/((1.+X**2)*GU(KR)**2)	PHFMP	19
	GO TO 5	PHFMP	20
466	IF (JS-4) 20,10,20	PHFMP	21
10	CALL WIDTH (EN,HR)	PHFMP	22
	T=EN *TEMP/((GU(KR)*GU(KR))*(ATM+1.0))+(HR*HR)/	PHFMP	23
	1(GU(KR)*GU(KR))*0.25	PHFMP	24
	GO TO 30	PHFMP	25
20	T = EN*TEMP/((ATM+1.0)*(GU(KR)*GU(KR)))	PHFMP	26
30	CALL SHAPE (2,X,T,PSI,CHI,2)	PHFMP	27
61	PHI(KR)=PSI*CO-CHI*SI	PHFMP	28
	GO TO (5, 1063) , LS	PHFMP	29
1063	KR2=NRT+KR	PHFMP	30
	PHI(KR2)=PSI*SI+CHI*CO	PHFMP	31
5	CONTINUE	PHFMP	32
	IF(MUP)11,11,91	PHFMP	33
91	DO 101J=1,MUP	PHFMP	34
	K=NG-MAU-MUP+J	PHFMP	35
101	PHI(K)=EN**J	PHFMP	36
11	IF (MAU) 8,3,8	PHFMP	37
8	GO TO (2,4,6),MAU	PHFMP	38
2	PHI(NG)=1.	PHFMP	39
	GO TO 3	PHFMP	40
4	PHI(NG-1)=1.	PHFMP	41
	PHI(NG)=1./EN**2	PHFMP	42
	GO TO 3	PHFMP	43
6	PHI(NG-2)=1.	PHFMP	44
	PHI(NG-1)=1./EN	PHFMP	45
	PHI(NG)=1./EN**2	PHFMP	46
3	RETURN	PHFMP	47
	END	PHFMP	48

\$	FASTRAN	
C	FORTRAN II SUBROUTINE SHAPE FOR THE EVALUATION OF THE	SHPEP 1
C	DOPPLER LINE SHAPE FUNCTIONS PSI(X,T) AND CHI(X,T).	SHPEP 2
C	F.T.ADLER, Y.D.NALIBOFF	SHPEP 3
	SUBROUTINE SHAPE (J,X,T,PSI,CHI,IIN)	SHPEP 4
	FREQUENCY 1(0,50),3(0,1,50),6(1,0,50),7(1,0,50),11(50,0),16(4,1,0)	SHPEP 5
	FREQUENCY 210(1,0,1),23(1,0,1),250(1,0,1),260(1,0,1),26(1,0,1),	SHPEP 6
1	27(1,0,1),28(1,0,1),29(1,0,1),30(1,0,1),320(1,0,1),330(1,0,1),	SHPEP 7
2	33(1,0,1),34(1,0,1),35(1,0,1),36(1,0,1),440(1,0,1),45(0,1,1)	SHPEP 8
	DIMENSION A(6),CR(5),CI(5),PR(5),PI(5),PS(5),CH(5),RPS(5),RCH(5)	SHPEP 9
	DIMENSION C1(2),C2(2),C3(2),C4(2),C5(2),C6(2)	SHPEP 10
1	GO TO (2,3),J	SHPEP 11
2	A(1)=2.5052367	SHPEP 12
	A(2)=1.2831204	SHPEP 13
	A(3)=0.2264718	SHPEP 14
	A(4)=0.1306469	SHPEP 15
	A(5)=-0.0202490	SHPEP 16
	A(6)=0.0039132	SHPEP 17
	CR(1)=0.	SHPEP 18
	CR(2)=1.09147894	SHPEP 19
	CR(3)=-2.30555691	SHPEP 20
	CR(4)=-CR(2)	SHPEP 21
	CR(5)=-CR(3)	SHPEP 22
	CI(1)=1.32271498	SHPEP 23
	CI(2)=1.29081178	SHPEP 24
	CI(3)=1.17416680	SHPEP 25
	CI(4)=CI(2)	SHPEP 26
	CI(5)=CI(3)	SHPEP 27
	PR(1)=0.	SHPEP 28
	PR(2)=-10.9663038	SHPEP 29
	PR(3)=24.240703	SHPEP 30
	PR(4)=-PR(2)	SHPEP 31
	PR(5)=-PR(3)	SHPEP 32
	PI(1)=6.1043246	SHPEP 33
	PI(2)=1.1317230	SHPEP 34
	PI(3)=-78.663636	SHPEP 35
	PI(4)=PI(2)	SHPEP 36
	PI(5)=PI(3)	SHPEP 37
	RPS(1)=0.21117643	SHPEP 38
	RPS(2)=0.081635073	SHPEP 39
	RPS(3)=-0.0050439914	SHPEP 40
	RPS(4)=RPS(2)	SHPEP 41
	RPS(5)=RPS(3)	SHPEP 42
	RCH(1)=0.	SHPEP 43
	RCH(2)=0.16088151	SHPEP 44
	RCH(3)=-0.0098666871	SHPEP 45
	RCH(4)=-RCH(2)	SHPEP 46
	RCH(5)=-RCH(3)	SHPEP 47
	C1(1)=1.	SHPEP 48
	C2(1)=3.	SHPEP 49
	C3(1)=15.	SHPEP 50
	C4(1)=105.	SHPEP 51
	C5(1)=945.	SHPEP 52
	C6(1)=10395.	SHPEP 53
	C1(2)=.33333333	SHPEP 54
	C2(2)=.1	SHPEP 55
	C3(2)=.23809524E-01	SHPEP 56
	C4(2)=.46296296E-02	SHPEP 57
	C5(2)=.75757575E-03	SHPEP 58
	C6(2)=.10683761E-03	SHPEP 59
	TWOPI=6.283185307	SHPEP 60

RETURN	SHPEP 61
IF (T) 5,4,5	SHPEP 62
PSI=1./(1.+X**2)	SHPEP 63
CHI=X*PSI	SHPEP 64
RETURN	SHPEP 65
5 X2=X*X	SHPEP 66
B1=1.+X2	SHPEP 67
B3=2.*T	SHPEP 68
B4=4.*T	SHPEP 69
RT=SQRT(B3)	SHPEP 70
C16=X/RT	SHPEP 71
C26=1./RT	SHPEP 72
210 IF (ARSF(X)-1.) 21,21,22	SHPEP 73
21 R=ABSF(C26)	SHPEP 74
W=X2	SHPEP 75
U=1.	SHPEP 76
V=1.	SHPEP 77
GO TO 23	SHPEP 78
22 R=ABSF(C16)	SHPEP 79
W=1./X2	SHPEP 80
U=-1.	SHPEP 81
V=X2	SHPEP 82
23 IF (R-12.53) 30,24,24	SHPEP 83
24 N=1	SHPEP 84
B6=B3/B1**2*V	SHPEP 85
250 IF (R-14.52) 37,25,25	SHPEP 86
25 F1=0.	SHPEP 87
F2=0.	SHPEP 88
260 IF (R-18.24) 38,26,26	SHPEP 89
26 IF (R-26.32) 39,27,27	SHPEP 90
27 IF (R-54.40) 40,28,28	SHPEP 91
28 IF (R-200.) 41,29,29	SHPEP 92
29 IF (R-16384.) 42,43,43	SHPEP 93
30 IF (R-.589) 31,31,48	SHPEP 94
31 N=2	SHPEP 95
B6=V/B4	SHPEP 96
G=X/B3	SHPEP 97
H=SQRT(1*3.1415927)	SHPEP 98
E=EXP((1.-X2)/B4)/B3	SHPEP 99
SI=SIN(G)	SHPEP100
CO=COS(G)	SHPEP101
320 IF (R-.456) 32,32,37	SHPEP102
32 F1=0.	SHPEP103
F2=0.	SHPEP104
330 IF (R-.318) 33,33,38	SHPEP105
33 IF (R-.191) 34,34,39	SHPEP106
34 IF (R-.084) 35,35,40	SHPEP107
35 IF (R-.0172) 36,36,41	SHPEP108
36 IF (R-.00017) 43,43,42	SHPEP109
37 F1=(((((13.*W-286.)*W+1287.)*W-1716.)*W+715.)*W-78.)*W+1.)*C6(N)*	SHPEP110
1 B6	SHPEP111
F2=(((((W-78.)*W+715.)*W-1716.)*W+1287.)*W-286.)*W+13.)*C6(N)*B6	SHPEP112
F1=(((((11.*W-165.)*W+462.)*W-330.)*W+55.)*W-1.)*U*C5(N)+F1)*B6	SHPEP113
F2=(((((W-55.)*W+330.)*W-462.)*W+165.)*W-11.)*U*C5(N)+F2)*B6	SHPEP114
39 F1=(((((9.*W-84.)*W+126.)*W-36.)*W+1.)*C4(N)+F1)*B6	SHPEP115
F2=(((((W-36.)*W+126.)*W-84.)*W+9.)*C4(N)+F2)*B6	SHPEP116
40 F1=(((((7.*W-35.)*W+21.)*W-1.)*U*C3(N)+F1)*B6	SHPEP117
F2=(((((W-21.)*W+35.)*W-7.)*U*C3(N)+F2)*B6	SHPEP118
41 F1=(((((5.*W-10.)*W+1.)*C2(N)+F1)*B6	SHPEP119
F2=(((((W-10.)*W+5.)*C2(N)+F2)*B6	SHPEP120
42 F1=((3.*W-1.)*U*C1(N)+F1)*B6	SHPEP121

	F2=((W-3.)*U*C1(N)+F2)*B6	SHPEP122
	F1=(1.+F1)	SHPEP123
	F2=(1.+F2)	SHPEP124
440	IF (U) 45,44,44	SHPEP125
44	FF=F2	SHPEP126
	F2=F1	SHPEP127
	F1=FF	SHPEP128
45	IF (N-1) 46,46,47	SHPEP129
46	PSI=F2/B1	SHPEP130
	CHI=F1/B1*X	SHPEP131
	RETURN	SHPEP132
47	PSI=F*(CO*(H-F2)+X*SI*F1)	SHPEP133
	CHI=F*(-SI*(H-F2)+X*CO*F1)	SHPEP134
	RETURN	SHPEP135
48	IZ=1	SHPEP136
	B2=-2.*X*RT	SHPEP137
	DO 10 I=1,5	SHPEP138
6	IF (ABSF(X-CR(I)/CI(I))-0.005) 7,7,9	SHPEP139
7	IF (ABSF(CI(I)*RT-1.)-0.005) 8,8,9	SHPEP140
8	IZ=2	SHPEP141
	PS(I)=RPS(I)	SHPEP142
	CH(I)=RCH(I)	SHPEP143
	S1=0.	SHPEP144
	S2=0.	SHPEP145
	GO TO 10	SHPEP146
9	Q1=B1+B2*CR(I)+B3*(CR(I)**2-CI(I)**2)	SHPEP147
	Q2=(B2+B4*CR(I))*CI(I)	SHPEP148
	D1=PR(I)*Q1-PI(I)*Q2	SHPEP149
	D2=PI(I)*Q1+PR(I)*Q2	SHPEP150
	D=D1**2+D2**2	SHPEP151
	PS(I)=D2/D	SHPEP152
	CH(I)=(CR(I)*D2-CI(I)*D1)/D	SHPEP153
10	CONTINUE	SHPEP154
11	GO TO (12,19),IZ	SHPEP155
12	P16=A(1)	SHPEP156
	P26=0.	SHPEP157
	C262=C16*C26**2.	SHPEP158
	C162=C16**2-C26**2	SHPEP159
	C16N=C162	SHPEP160
	C26N=C262	SHPEP161
	I=2	SHPEP162
15	P16=P16+A(I)*C16N	SHPEP163
	P26=P26+A(I)*C26N	SHPEP164
16	IF (I-6) 17,18,18	SHPEP165
17	C1N=C162*C16N-C262*C26N	SHPEP166
	C2N=C262*C16N+C162*C26N	SHPEP167
	C16N=C1N	SHPEP168
	C26N=C2N	SHPEP169
	I=I+1	SHPEP170
	GO TO 15	SHPEP171
18	D3=P16**2+P26**2	SHPEP172
	SI=P167/(2.*RT*D3)	SHPEP173
	S2=(P26+X*P16)/(B4*D3)	SHPEP174
19	DO 20 I=1,5	SHPEP175
	S1=S1+PS(I)	SHPEP176
20	S2=S2+CH(I)	SHPEP177
	PSI=TWOPI*S1	SHPEP178
	CHI=X*PSI-RT*TWOPI*S2	SHPEP179
	RETURN	SHPEP180
	END	SHPEP181

FASTLAN		
SUBROUTINE SCRAMB(EN,YZER)	SCMBP	1
DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000),	DL(40),DW(4	SCMBP 2
10),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	SCMBP	3
DIMENSION SIM(86)	SCMBP	4
COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,C	SCMBP	5
1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NS	SCMBP	6
2I	SCMBP	7
GAUSSF(Z)=EXP(-((EN-Z)**2/(HR*HR)))	SCMBP	8
GO TO (100,200,300,100),JS	SCMBP	9
100 YZER=DSIG(EN)	SCMBP	10
CALL PHIFRM(EN)	SCMBP	11
RETURN	SCMBP	12
200 FACT=1.0	SCMBP	13
JSC=1	SCMBP	14
201 NGP1=NG+1	SCMBP	15
GO TO 500	SCMBP	16
300 FACT = DENS*100.0	SCMBP	17
IF(N1) 301,302,302	SCMBP	18
301 JSC=3	SCMBP	19
NGP1=1	SCMBP	20
GO TO 500	SCMBP	21
302 JSC=2	SCMBP	22
GO TO 201	SCMBP	23
500 CALL WIDTH(EN,HR)	SCMBP	24
H=HR/4.0	SCMBP	25
FASP =1.0	SCMBP	26
W = EN- 4.0*HR	SCMBP	27
DO 530 I =1,NGP1	SCMBP	28
530 SIM(I) =0.0	SCMBP	29
NPU = 1	SCMBP	30
531 S = SQRT(W)	SCMBP	31
GO TO (501,502,503),JSC	SCMBP	32
501 PHI(NGP1) = DSIG(W)	SCMBP	33
PL = 1.0	SCMBP	34
CALL PHIFRM(W)	SCMBP	35
GO TO 506	SCMBP	36
502 PHI(NGP1)=S	SCMBP	37
PL=EXP(-(DENS*CC/S*PLOTSG(W)))/S	SCMBP	38
CALL PHIFRM(W)	SCMBP	39
GO TO 506	SCMBP	40
503 PHI(NGP1)=S	SCMBP	41
PL=EXP(-(DENS*CC/S*PLOTSG(W)))/S	SCMBP	42
GO TO 506	SCMBP	43
506 G = GAUSSF(W)	SCMBP	44
DO 505 I =1,NGP1	SCMBP	45
505 SIM(I) = SIM(I) + FASP*G*PL*PHI(I)	SCMBP	46
NPU = NPU+1	SCMBP	47
IF(NPU-3) 507,508,509	SCMBP	48
507 W = EN+4.0*HR	SCMBP	49
GO TO 531	SCMBP	50
508 W=W-H	SCMBP	51
FASP=2.0	SCMBP	52
GO TO 531	SCMBP	53
509 IF(NPU-34) 508,510,512	SCMBP	54
510 W =W-H/2.0	SCMBP	55
FASP=4.0	SCMBP	56
GO TO 531	SCMBP	57
512 IF(NPU-65) 511,511,539	SCMBP	58
511 W=W+H	SCMBP	59
FASP=4.0	SCMBP	60

GO TO 531	SCMBP 61
539 DO 526 I=1,NG	SCMBP 62
526 PHI(I)=.2350790104E-1*SIM(I)*FACT	SCMBP 63
540 YZER=.2350790104E-1*SIM(NGP1)	SCMBP 64
RETURN	SCMBP 65
END	SCMBP 66
	SCMBP 67

S	FASTRAN		
	SUBROUTINE SKIP--READ AND PRINT PAGE HEADINGS.	SKIPP	1
		SKIPP	2
C	N.B.--DAT1 IS A SUBROUTINE WICH OBTAINS THE DATE FROM THE MONITOR	SKIPP	3
C	AND STORES IT IN THE LOCATION OF THE ARGUMENT AND THE TWO FOLLOWING	SKIPP	4
C	LOCATIONS--I.E. FORWARD IN CORE.	SKIPP	5
C		SKIPP	6
	SUBROUTINE SKIP(INIT)	SKIPP	7
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000), DL(40),DW(4	SKIPP	8
	10),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	SKIPP	9
	DIMENSION DATE(3)	SKIPP	10
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,C	SKIPP	11
	1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NS	SKIPP	12
	21	SKIPP	13
	GO TO (10,30),INIT	SKIPP	14
	10 READ 20,(A(I),I=1,20)	SKIPP	15
	20 FORMAT(10A8)	SKIPP	16
	CALL DAT1(DATE(3))	SKIPP	17
	IPAGE=0	SKIPP	18
	RETURN	SKIPP	19
30	IPAGE=IPAGE + 1	SKIPP	20
	WOT6,40,(A(I),I=1,10),DATE(3),DATE(2),DATE(1),IPAGE,(A(I),I=11,20)	SKIPP	21
40	FORMAT(1H110A8,10X,3A6,7X,4HPAGE13/1H 10A8,8X,27HPROGRAM CURVE 4 2	SKIPP	22
	14 AUG 1965)	SKIPP	23
	RETURN	SKIPP	24
	END	SKIPP	25

\$	FASTRAN		
	SUBROUTINE GRAPH	GRPHP	1
	SUBROUTINE GRAPH FULL SCALE FOR 10-INCH PAPER (Y = 500 MAXIMUM)	GRPHP	2
	DIMENSION R(85),FU(42),GU(42),E(1000),Y(1000), DL(40),DW(40)	GRPHP	3
	10),DGR(40),DGI(40),GR(42),GI(42),POS(5),A(20),PHI(86),DEL(1000)	GRPHP	4
	COMMON R,FU,GU,E,Y,DEL,DL,DW,DGR,DGI,GR,GI,POS,A,PHI,TEMP,ATM,WN,CGR	GRPHP	5
	1C,NP,NR,MAU,NOUT,INDE,NEIGH,MUP,NG,C1,C2,C3,LS,DENS,EMAX,EMIN,JS,NGR	GRPHP	6
	2I	GRPHP	7
	DIMENSION TITLE (13)	GRPHP	8
	READ 9,TITLE	GRPHP	9
	9 FORMAT (13A6)	GRPHP	10
	FACTOR=(9.0/25.0)*(10.5/10.0625)	GRPHP	11
	PLT=.045/FACTOR	GRPHP	12
	CALL CCP1FR(FACTOR)	GRPHP	13
	JJJJ=1	GRPHP	14
	ZJ=100.	GRPHP	15
	AI = .5	GRPHP	16
	16 NOPTS = 0	GRPHP	17
	EMIN = E(1)	GRPHP	18
	EMAX = E(NP)	GRPHP	19
	DO 53 I = 1, NP	GRPHP	20
	IF (E(I) - EMIN) 51, 50, 50	GRPHP	21
	51 EMIN = E(I)	GRPHP	22
	50 IF (E(I) - EMAX) 53, 53, 52	GRPHP	23
	52 EMAX = E(I)	GRPHP	24
	53 CONTINUE	GRPHP	25
	GMIN = INTF (EMIN)	GRPHP	26
	XOFF = GMIN - AI	GRPHP	27
	XFACT=.25	GRPHP	28
	YOFF=-59.375	GRPHP	29
	YFACT=25.0	GRPHP	30
	CALL CCP1OS(XOFF,XFACT,YOFF,YFACT)	GRPHP	31
	MAX = XINTF (10.0 * (EMAX - GMIN))	GRPHP	32
	XMAX = (INTF (10.0 * EMAX))/ 10.0	GRPHP	33
	C DRAWS LOWER X MARKS	GRPHP	34
	DO 10 I = 1, MAX	GRPHP	35
	AI = I - 1	GRPHP	36
	CALL CCP1PL (XMAX - AI/10.0, 0.0, 13)	GRPHP	37
	10 CALL CCP1PL (XMAX - AI/10.0, 5.0, 12)	GRPHP	38
	C DRAWS RIGHT Y MARKS	GRPHP	39
	DO 11 I = 1, 51	GRPHP	40
	AI = I * 10 - 10	GRPHP	41
	CALL CCP1PL (EMAX + .1, AI, 13)	GRPHP	42
	11 CALL CCP1PL (EMAX + .125, AI, 12)	GRPHP	43
	C DRAWS UPPER X MARKS	GRPHP	44
	DO 12 I = 1, MAX	GRPHP	45
	AI = I-1	GRPHP	46
	CALL CCP1PL (XMAX - AI/10.0, 500.0, 13)	GRPHP	47
	12 CALL CCP1PL (XMAX - AI/10.0, 495.0, 12)	GRPHP	48
	C DRAWS LEFT Y MARKS	GRPHP	49
	DO 13 I = 1, 51	GRPHP	50
	AI = 510 - I*10	GRPHP	51
	CALL CCP1PL (GMIN, AI, 13)	GRPHP	52
	13 CALL CCP1PL (GMIN - .025, AI, 12)	GRPHP	53
	C DRAWS Y-LINES	GRPHP	54
	DO 1 I=1,5,2	GRPHP	55
	AI=100*I	GRPHP	56
	CALL CCP1PL(GMIN,AI-100.0,13)	GRPHP	57
	CALL CCP1PL(EMAX+.1,AI-100.0,12)	GRPHP	58
	CALL CCP1PL(EMAX+.1,AI,13)	GRPHP	59
		GRPHP	60

1 CALL CCP1PL(GMIN,AI,12)	GRPHP 61
C WRITES IDENTIFICATION ABOVE FIRST GRAPH	GRPHP 62
GO TO (1018,98), JJJJ	GRPHP 63
1018 CALL CCP1PP(XPOS,YPOS)	GRPHP 64
CALL CCP2SB (XPOS,YPOS+.125/FACTOR,.125,TITLE,0.0,78)	GRPHP 65
JJJJ=2	GRPHP 66
C DRAWS X-LINES AND VALUES	GRPHP 67
98 X = GMIN	GRPHP 68
18 IF (X - EMAX + .9) 19, 19, 48	GRPHP 69
19 S = (X - .0625 - XOFF)/XFACT	GRPHP 70
CALL CCP1PL (X, 500.0, 13)	GRPHP 71
CALL CCP1PL (X, 0.0, 12)	GRPHP 72
CALL CCP3NR (S,1.79, .308 , X, 0.0, 1)	GRPHP 73
X = X + 1.0	GRPHP 74
S = S + 4.0	GRPHP 75
CALL CCP3NR (S,1.79, .308 , X, 0.0, 1)	GRPHP 76
CALL CCP1PL (X, 0.0, 13)	GRPHP 77
CALL CCP1PL (X, 500.0, 12)	GRPHP 78
X = X + 1.0	GRPHP 79
GO TO 18	GRPHP 80
48 IF (X - EMAX - .1) 49, 49, 2	GRPHP 81
49 S = (X - .0625 - XOFF)/XFACT	GRPHP 82
CALL CCP1PL (X, 500.0, 13)	GRPHP 83
CALL CCP1PL (X, 0.0, 12)	GRPHP 84
CALL CCP3NR (S,1.79, .308 , X, 0.0, 1)	GRPHP 85
C DRAWS Y VALUES	GRPHP 86
2 ZJ=ZJ-100.	GRPHP 87
DO 15 I = 1, 6	GRPHP 88
AI=4*(I-1)	GRPHP 89
S = (GMIN - XOFF)/XFACT - 1.25	GRPHP 90
CALL CCP3NR (S, AI + 2.13,.308,ZJ, 0.0, -1)	GRPHP 91
15 ZJ=ZJ+100.	GRPHP 92
C DRAWS MU VALUES	GRPHP 93
IF (NR) 31, 31, 30	GRPHP 94
30 DO 4 I=1,NR	GRPHP 95
IF (FU(I) - EMIN) 4, 28, 28	GRPHP 96
28 IF (FU(I) - EMAX) 29, 29, 4	GRPHP 97
29 S = (FU(I) - XOFF)/XFACT	GRPHP 98
CALL CCP1PL (S, .87, 3)	GRPHP 99
CALL CCP2SY (S, 2.6, .1, 6, 0.0,-2)	GRPHP100
CALL CCP3NR(S-.25,(.60+.09*(-1.0)**I)*2.0-.13,.308,FU(I),0.0,3)	GRPHP101
4 CONTINUE	GRPHP102
31 CALL CCP1PL (E(I), Y(I), 13)	GRPHP103
DO 5 I = 1, NP	GRPHP104
3 U=(E(I)-XOFF)/XFACT	GRPHP105
V=(Y(I)-YOFF)/YFACT	GRPHP106
W=(DEL(I)-YOFF)/YFACT	GRPHP107
IF(U)5,6,6	GRPHP108
6 IF (W) 5, 20, 20	GRPHP109
20 IF (W - 21.9138) 23,23,21	GRPHP110
21 NOPTS = NOPTS + 1	GRPHP111
E(NOPTS) = E(I)	GRPHP112
DEL(NOPTS) = DEL(I) - 500.0	GRPHP113
Y(NOPTS) = 0.0	GRPHP114
IF (V - 21.9138) 25, 25, 22	GRPHP115
22 Y(NOPTS) = Y(I) - 500.0	GRPHP116
GO TO 5	GRPHP117
23 IF (V - 21.9138) 26, 26, 24	GRPHP118
24 NOPTS = NOPTS + 1	GRPHP119
E(NOPTS) = E(I)	GRPHP120
Y(NOPTS) = Y(I) - 500.0	GRPHP121

DEL(NOPTS) = 0.0	GRPHP122
GO TO 27	GRPHP123
25 CALL CCP2SY (U, V, PLT, 1, 0.0, -1)	GRPHP124
CALL CCP2SY (U, V, PLT, 1, 0.0, -2)	GRPHP125
GO TO 5	GRPHP126
26 CALL CCP2SY (U, V, PLT, 1, 0.0, -1)	GRPHP127
CALL CCP2SY (U, V, PLT, 1, 0.0, -2)	GRPHP128
27 CALL CCP2SY (U, W, PLT, 11, 0.0, -1)	GRPHP129
CALL CCP2SY (U, W, PLT, 11, 0.0, -2)	GRPHP130
5 CONTINUE	GRPHP131
IF (NOPTS) 7, 7, 8	GRPHP132
8 NP = NOPTS	GRPHP133
AI = EMAX - XOFF + 1.0	GRPHP134
CALL CCP1BA	GRPHP135
GO TO 16	GRPHP136
7 CALL CCP1PL (EMAX + 1.0, -59.375, -13)	GRPHP137
RETURN	GRPHP138
END	GRPHP139

\$	FASTRAN	
(	THIS ROUTINE CONTAINS 80 LEVELS FOR ONE ELEMENT, FOR USE ON 7094	SIGMA 1
(	AND OUTPUTS SIGT,SIGS,ALFA,SIGG,SIGF, AS FUNCTIONS OF ENERGY	SIGMA 2
C		SIGMA 3
C	WITH ISIG = 1 OUTPUTS REACTION RATES AND AVERAGE ALFA	SIGMA 4
C	INPUT WITH ISIG = 1 TO BE FOLLOWED BY A IEND CARD	SIGMA 5
C	WITH IEND = 1 THERMAL VALUES OF ABSORPTION AND FISSION ARE	SIGMA 6
C	EXPECTED, AND IN THIS CASE BACKROUND CONSTANTS ARE OUTPUT	SIGMA 7
C	WITH IEND = 2 NO BACKROUND CONSTANTS ARE EVALUATED	SIGMA 8
C		SIGMA 9
C	WITH ISIG = 2,3 NO IEND CARD EXPECTED, BUT NEXT NEW ISIG.	SIGMA 10
C		SIGMA 11
C	DIMENSION ALFA(80),BETA(80),GRA(80),GIA(80),SAVA(80),SAVT(80),GRN(	SIGMA 12
	180),GIN(80),SAVN(80)	SIGMA 13
	COMMON SIGT,SIGS,SIGA,SIGG,FISS,NR,ALFA,BETA,GRA,GIA,CT1,CF1,GRN,G	SIGMA 14
	1IN	SIGMA 15
	1 CALL BWSIG(1,X)	SIGMA 16
	CALL BWSIG(3,X)	SIGMA 17
	READ INPUT TAPE 7,10,EMAX,EMIN,DELE,NUMBI	SIGMA 18
	10 FORMAT(3E15.8,I5)	SIGMA 19
	50 READ INPUT TAPE 7,15,ISIG	SIGMA 20
	15 FORMAT(I5)	SIGMA 21
	GO TO(80,70,60),ISIG	SIGMA 22
C	CALCULATE ONLY ASYMMETRICAL CONTRIBUTIONS	SIGMA 23
	60 DO 61 K=1,NR	SIGMA 24
	SAVA(K)=GRA(K)	SIGMA 25
	SAVT(K)=ALFA(K)	SIGMA 26
	SAVN(K)=GRN(K)	SIGMA 27
	GRA(K)=0.0	SIGMA 28
	ALFA(K)=0.0	SIGMA 29
	61 GRN(K)=0.0	SIGMA 30
	WRITE OUTPUT TAPE 6,62,ISIG	SIGMA 31
	GO TO 81	SIGMA 32
C	CALCULATE ONLY SYMMETRICAL CONTRIBUTIONS	SIGMA 33
	70 DO 71 K=1,NR	SIGMA 34
	SAVA(K)=GIA(K)	SIGMA 35
	SAVT(K)=BETA(K)	SIGMA 36
	SAVN(K)=GIN(K)	SIGMA 37
	GIA(K)=0.0	SIGMA 38
	BETA(K)=0.0	SIGMA 39
	71 GIN(K)=0.0	SIGMA 40
	WRITE OUTPUT TAPE 6,72,ISIG	SIGMA 41
	GO TO 81	SIGMA 42
	62 FORMAT(7H0ISIG =15/32H CONTRIBUTION OF CHI TERMS ONLY//)	SIGMA 43
	72 FORMAT(7H0ISIG =15/32H CONTRIBUTION OF PSI TERMS ONLY//)	SIGMA 44
	82 FORMAT(7H0ISIG =15/62H CONTRIBUTION OF PSI AND CHI TERMS THAT IS	SIGMA 45
	1COMPLETE EXPANSION//)	SIGMA 46
	80 WRITE OUTPUT TAPE 6,82,ISIG	SIGMA 47
	81 WRITE OUTPUT TAPE 6,83,EMIN,EMAX	SIGMA 48
	83 FORMAT(7H0EMIN =F10.4,8H EMAX =F10.4/1H013X,6HENERGY15X,5HTOTAL10	SIGMA 49
	1X,10HSCATTERING15X,5HALPHA13X,7HCAPTURE13X,7HFISSION)	SIGMA 50
C	CALCULATION OF 1/E FLUX REACTION RATES (ISIG=1 AND IEND=2 ONLY)	SIGMA 51
	GO TO (211,222,222),ISIG	SIGMA 52
	11 FRATE=0.0	SIGMA 53
	GRATE=0.0	SIGMA 54
	210 RATES=0.0	SIGMA 55
	FACT1=.5*DFLE/EMIN	SIGMA 56
	FACT2=.5*DFLE/EMAX	SIGMA 57
	222 E=EMIN	SIGMA 58
	11 CALL BWSIG(2,E)	SIGMA 59
	GO TO (200,201,201),ISIG	SIGMA 60

00 IF(E-EMIN-DELE) 202,203,204	SIGMA 61
02 FACT=FACT1	SIGMA 62
GO TO 220	SIGMA 63
203 FACT=DELE/E	SIGMA 64
GO TO 220	SIGMA 65
204 IF(E-EMAX) 203,205,201	SIGMA 66
205 FACT=FACT2	SIGMA 67
220 FRATE=FRATE+FISS*FACT	SIGMA 68
GRATE=GRATE+SIGG*FACT	SIGMA 69
221 RATES=RATES+SIGS*FACT	SIGMA 70
201 IF(FISS -1.0E-03) 231,231,232	SIGMA 71
232 ALA=SIGG/FISS	SIGMA 72
GO TO 230	SIGMA 73
231 ALA=0.0	SIGMA 74
230 WRITE OUTPUT TAPE 6,12,E, SIGT ,SIGS , ALA ,SIGG ,FISS	SIGMA 75
12 FORMAT(6F20.4)	SIGMA 76
21 E=E+DELE	SIGMA 77
IF(E-EMAX)11,11,13	SIGMA 78
13 GO TO(111,112,113),ISIG	SIGMA 79
112 DO 122 K=1,NR	SIGMA 80
GIA(K)=SAVA(K)	SIGMA 81
BETA(K)=SAVT(K)	SIGMA 82
122 GIN(K)=SAVN(K)	SIGMA 83
GO TO 50	SIGMA 84
113 DO 123 K=1,NR	SIGMA 85
GRA(K)=SAVA(K)	SIGMA 86
ALFA(K)=SAVT(K)	SIGMA 87
123 GRN(K)=SAVN(K)	SIGMA 88
GO TO 50	SIGMA 89
111 READ INPUT TAPE 7,15,IEND	SIGMA 90
GO TO(114,115),IEND	SIGMA 91
114 READ INPUT TAPE 7,120,SIGATH ,SIGFTH	SIGMA 92
120 FORMAT(2E15.4)	SIGMA 93
116 WRITE OUTPUT TAPE 6,126, SIGATH ,SIGFTH	SIGMA 94
126 FORMAT(20H THERMAL ABSORPTION=E15.4,4X,20HTHERMAL FISSION =E15.4,4X,20H	SIGMA 95
147737H CALCULATED VALUES WITHOUT BACKGROUND771H013X,6HENERGY15X,5H	SIGMA 96
2TOTAL10X,10HSCATTERING15X,5HALPHA13X,7HCAPTURE13X,7HFISSION/)	SIGMA 97
E=.0253	SIGMA 98
CALL BWSIG(2,E)	SIGMA 99
ALA=SIGG/FISS	SIGMA100
WRITE OUTPUT TAPE 6,12,E,SIGT,SIGS,ALA,SIGG,FISS	SIGMA101
DIFA=SIGATH-SIGA	SIGMA102
127 DIFT=SIGFTH-FISS	SIGMA103
ESQ=SQRT(.0253)	SIGMA104
CT1=DIFA*ESQ	SIGMA105
CF1=DIFT*ESQ	SIGMA106
CCT1=CT1/(6.52E+05)	SIGMA107
CCF1=CF1/(6.52E+05)	SIGMA108
128 WRITE OUTPUT TAPE 6,129, CT1 ,CF1 ,CCT1,CCF1	SIGMA109
129 FORMAT(41H CALCULATED BACKGROUND CONSTANTS IN BARNS7712H ABSORPTIOS	SIGMA110
1N=E15.6,12HFISSION =E15.6//7H SCALED/13H ABSORPTION =E15.6,12HFS	SIGMA111
2ISSION =E15.6777)	SIGMA112
15 ALA=GRATE/FRATE	SIGMA113
252 WRITE OUTPUT TAPE 6,253 ,FRATE ,GRATE ,RATES ,ALA	SIGMA114
250 CONTINUE	SIGMA115
253 FORMAT(40H CALCULATED REACTION RATES FOR 1/E FLUX 7710H FISSION =E	SIGMA116
110.4,13H CAPTURE =E10.4,13H SCATTERING =E10.4,13H ALFA =E	SIGMA117
210.477)	SIGMA118
GO TO 1	SIGMA119
END	SIGMA120

\$	FASTRAN	BWSIG 1
(	BWSIG DEC 5, 1964	BWSIG 2
(	CONTAINS 80 LEVELS FOR ONE ELEMENT ONLY FOR USE ON ILLIAC II	BWSIG 3
C	COMPATIBLE WITH ROUTINE SIGMA VALID FOR ILLIAC II	BWSIG 4
C		BWSIG 5
	SUBROUTINE BWSIG (JJJ,E)	BWSIG 6
	DIMENSION ATM(1),WN(1),GFACT(1),LS(1),NO(1),DE(1,80),DW(1,80),	BWSIG 7
	1 GRA(1,80),GRG(1,80),ALFA(1,80),FU(80),GU(80),BETA(1,80),VN(80),	BWSIG 8
	2 VI(80),AL(80),BE(80),GIN(1,80),GRN(1,80),GIG(1,80),	BWSIG 9
	3 CF1(1),CF2(1),CF3(1),CT1(1),CT2(1),CT3(1),	BWSIG 10
	4 SIGT(1),SIGS(1),SIGA(1),SIGG(1),FISS(1),	BWSIG 11
	5 EFFT(1,80),GRT(1,80),GIT(1,80),GIA(1,80),	BWSIG 12
	6 BF1(1),BF2(1),BF3(1),BF4(1),BF5(1),BT1(1),BT2(1),BT3(1),BT4(1),	BWSIG 13
	7 BT5(1)	BWSIG 14
	COMMON SIGT,SIGS,SIGA,SIGG,FISS,NR,ALFA,BETA,GRA,GIA,CT1,CF1,GRN,GB	BWSIG 15
	1IN	BWSIG 16
	GO TO (1001,1002,1003),JJJ	BWSIG 17
1001	CALL SHAPE (1,X,X,X,X,2)	BWSIG 18
	READ INPUT TAPE 7,311,NUMBI,CONST	BWSIG 19
311	FORMAT(I10,E10.4)	BWSIG 20
	I=1	BWSIG 21
	10 READ INPUT TAPE 7,300,ATM(I),WN(I),GFACT(I),LS(I),NO(I)	BWSIG 22
300	FORMAT(E10.2,2E10.4,2I5)	BWSIG 23
	NR=NO(I)	BWSIG 24
	IN=LS(I)	BWSIG 25
	GO TO (100,200),IN	BWSIG 26
C	SINGLE LEVEL	BWSIG 27
100	DO 101 K=1,NR	BWSIG 28
	READ INPUT TAPE 7,302,DE(I,K),DW(I,K),GRA(I,K),GRG(I,K)	BWSIG 29
	READ INPUT TAPE 7,302,ALFA(I,K)	BWSIG 30
101	WRITE OUTPUT TAPE 6,304,ATM(I),DE(I,K),DW(I,K),GRA(I,K),GRG(I,K)	BWSIG 31
304	FORMAT(37H SINGLE LEVEL INPUT PARAMETERS FOR U F4.0/5H ER=E10.4,7	BWSIG 32
	.1HGAMMAN=E10.4,7HGAMMAF=E10.4,7HGAMMAG=E10.4,12HGAMMAN-ZERO=E10.4//	BWSIG 33
	2/)	BWSIG 34
	TLEVEL=6HSINGLE	BWSIG 35
	DO 102 K=1,NR	BWSIG 36
	FU(K)=DE(I,K)	BWSIG 37
	FUFU=ABS(FU(K))	BWSIG 38
	IF(DW(I,K))103,103,104	BWSIG 39
103	YR=SQRT(FUFU)	BWSIG 40
	DW(I,K)=(YR*ALFA(I,K))/(2.0*GFACT(I))	BWSIG 41
	GO TO 106	BWSIG 42
104	IF(ALFA(I,K))105,105,106	BWSIG 43
105	YR=SQRT(FUFU)	BWSIG 44
	ALFA(I,K)=(DW(I,K)*2.0*GFACT(I))/YR	BWSIG 45
106	AL(K)=ALFA(I,K)	BWSIG 46
	GU(K)=(DW(I,K)+GRA(I,K)+GRG(I,K))/2.0	BWSIG 47
	BETA(I,K)=0.0	BWSIG 48
	BE(K)=0.0	BWSIG 49
	DW(I,K)=GU(K)	BWSIG 50
	VN(K)=GRA(I,K)	BWSIG 51
102	VI(K)=GRG(I,K)	BWSIG 52
	DO 110 K=1,NR	BWSIG 53
	FACT=AL(K)/(2.0*GU(K)*GU(K))	BWSIG 54
	GRN(I,K)=(FACT*AL(K))/(2.0*GFACT(I))	BWSIG 55
	GIN(I,K)=0.0	BWSIG 56
	ALFA(I,K)=AL(K)/(GU(K))	BWSIG 57
	GRA(I,K)=FACT*VN(K)	BWSIG 58
	GRG(I,K)=FACT*VI(K)	BWSIG 59
	GIA(I,K)=0.0	BWSIG 60
110	GIG(I,K)=0.0	

	READ INPUT TAPE 7,302,CF1(I),CF2(I),CF3(I),BF5(I)	BWSIG 61
	READ INPUT TAPE 7,302,BF1(I),BF2(I),BF3(I),BF4(I)	BWSIG 62
	READ INPUT TAPE 7,302,CT1(I),CT2(I),CT3(I),BT5(I)	BWSIG 63
	READ INPUT TAPE 7,302,BT1(I),BT2(I),BT3(I),BT4(I)	BWSIG 64
	GO TO 150	BWSIG 65
C	FROM LEAST SQUARES FITTING	BWSIG 66
200	DO 201 K=1,NR	BWSIG 67
	READ INPUT TAPE 7,302,DE(I,K),DW(I,K),GRA(I,K),GIA(I,K)	BWSIG 68
	READ INPUT TAPE 7,302,DE(I,K),DW(I,K),ALFA(I,K),BETA(I,K)	BWSIG 69
	FU(K)=DE(I,K)	BWSIG 70
	GU(K)=DW(I,K)	BWSIG 71
	AL(K)=ALFA(I,K)*GU(K)	BWSIG 72
201	BE(K)=BETA(I,K)*GU(K)	BWSIG 73
302	FORMAT(4E15.4)	BWSIG 74
	TLEVEL=6HMULTI-	BWSIG 75
	READ INPUT TAPE 7,302,CF1(I),CF2(I),CF3(I),BF5(I)	BWSIG 76
	READ INPUT TAPE 7,302,BF1(I),BF2(I),BF3(I),BF4(I)	BWSIG 77
	READ INPUT TAPE 7,302,CT1(I),CT2(I),CT3(I),BT5(I)	BWSIG 78
	READ INPUT TAPE 7,302,BT1(I),BT2(I),BT3(I),BT4(I)	BWSIG 79
C	PREPARE SCATTERING PARMAMETERS	BWSIG 80
	DO 203 K=1,NR	BWSIG 81
	VN(K)=0.0	BWSIG 82
203	VI(K)=0.0	BWSIG 83
	DO 204 K=1,NR	BWSIG 84
	DO 204 J=1,NR	BWSIG 85
	TAU=FU(J)-FU(K)	BWSIG 86
	OMEG=GU(J)+GU(K)	BWSIG 87
	FIO=AL(K)*AL(J)+BE(K)*BE(J)	BWSIG 88
	SIO=AL(K)*BE(J)-AL(J)*BE(K)	BWSIG 89
	FUNU=TAU*TAU+OMEG*OMEG	BWSIG 90
	VN(K)=VN(K)+(FIO*OMEG+SIO*TAU)/FUNU	BWSIG 91
204	VI(K)=VI(K)+(FIO*TAU-SIO*OMEG)/FUNU	BWSIG 92
	DO 205 K=1,NR	BWSIG 93
	GRNT(I,K)=VN(K)/(2.0*GFACT(I)*GU(K))	BWSIG 94
	YR=SQRT(ABSF(FU(K)))	BWSIG 95
205	GRG(I,K)=ALFA(I,K)-GRA(I,K)-GRN(I,K)*YR	BWSIG 96
	DO 208 K=1,NR	BWSIG 97
	TERM=ABSF(GIA(I,K)-BETA(I,K))	BWSIG 98
	IF(TERM-1.0E-06) 209,209,210	BWSIG 99
209	GIN(I,K)=0.0	BWSIG100
	GIG(I,K)=0.0	BWSIG101
	GO TO 208	BWSIG102
210	GIN(I,K)=VI(K)/(2.0*GFACT(I)*GU(K))	BWSIG103
	YR=SQRT(ABSF(FU(K)))	BWSIG104
	GIG(I,K)=BETA(I,K)-GIA(I,K)-GIN(I,K)*YR	BWSIG105
208	CONTINUE	BWSIG106
150	WRITE OUTPUT TAPE 6,310,TLEVEL,ATM(I),NO(I)	BWSIG107
310	FORMAT(1H1A6,23H LEVEL PARAMETERS FOR U F4.0,4H FOR 13,7H LEVELS)	BWSIG108
	DO 207 K=1,NR	BWSIG109
	WRITE OUTPUT TAPE 6,303,FU(K),GRA(I,K),GRG(I,K),GRN(I,K),ALFA(I,K)	BWSIG110
207	WOT6,1303,GU(K),GIA(I,K),GIG(I,K),GIN(I,K),BETA(I,K)	BWSIG111
303	FORMAT(4HOMU=E14.8,3X,4HGRF=E14.8,3X,4HGRG=E14.8,3X,4HGRN=E14.8,3XBWSIG112	
	1,5HALFA=E14.8)	BWSIG113
33	FORMAT(4H NU=E14.8,3X,4HGIIF=E14.8,3X,4HGIIG=E14.8,3X,4HGIN=E14.8,3XBWSIG114	
	1,5HBETA=E14.8)	BWSIG115
	WRITE OUTPUT TAPE 6,2303,CF1(I),CF2(I),CF3(I),BF1(I),BF2(I),BF3(I)	BWSIG116
	1,BF4(I),BF5(I)	BWSIG117
2303	FORMAT(35H BACKGROUND CONSTANTS SIGMA FISSION75H CF1=E10.4,5H CF2=BWSIG118	
	1E10.4,5H CF3=E10.4,5H BF1=E10.4,5H BF2=E10.4,5H BF3=E10.4,5H BF4=EBWSIG119	
	210.4,5H BF5=E10.477)	BWSIG120
	WRITE OUTPUT TAPE 6,2304,CT1(I),CT2(I),CT3(I),BT1(I),BT2(I),BT3(I)	BWSIG121

	1,BT4(I),BT5(I)	BWSIG122
04	FORMAT(35H BACKGROUND CONSTANTS SIGMA TOTAL /5H CT1=E10.4,5H CT2=BWSIG123	BWSIG123
	1E10.4,5H CT3=E10.4,5H BT1=E10.4,5H BT2=E10.4,5H BT3=E10.4,5H BT4=E10.4,5H BT5=E10.4/)	BWSIG124
	210.4,5H BT5=E10.4/)	BWSIG125
	I=I+1	BWSIG126
	IF(I-NUMBI)10,10,11	BWSIG127
11	WRITE OUTPUT TAPE 6,306,NUMBI	BWSIG128
306	FORMAT(1H0110,9H ELEMENTS)	BWSIG129
	RETURN	BWSIG130
C	ENERGY DEPENDENT CROSS SECTIONS	BWSIG131
1002	YR=SQRT(E)	BWSIG132
	DO 251 I=1,NUMBI	BWSIG133
	SIGT(I)=CT1(I)+CT2(I)/E+CT3(I)/(E*E)+BT1(I)*E+BT2(I)*(E**2)+BT3(I)*E+BT4(I)*(E**4)+BT5(I)*(E**5)	BWSIG134
	SIGA(I)=CF1(I)+CF2(I)/E+CF3(I)/(E*E)+BF1(I)*E+BF2(I)*(E**2)+BF3(I)*E+BF4(I)*(E**4)+BF5(I)*(E**5)	BWSIG135
	NR=NO(I)	BWSIG136
	SIGG(I)=0.0	BWSIG137
	ARG=2.0*WN(I)*YR	BWSIG138
	CCS=COS(ARG)	BWSIG139
	SCS=SIN(ARG)	BWSIG140
	SIGS(I)=2.0*(1.0-CCS)/YR	BWSIG141
	SIGT(I)=SIGT(I)+SIGS(I)	BWSIG142
	DO 252 K=1,NR	BWSIG143
	GRT(I,K)=ALFA(I,K)*CCS+BETA(I,K)*SCS	BWSIG144
	GIT(I,K)=BETA(I,K)*CCS-ALFA(I,K)*SCS	BWSIG145
	VN(K)=GRT(I,K)-ALFA(I,K)+GRN(I,K)*YR	BWSIG146
252	VI(K)=GIT(I,K)-BETA(I,K)+GIN(I,K)*YR	BWSIG147
	DO 253 K=1,NR	BWSIG148
	X=(DE(I,K)-E)/DW(I,K)	BWSIG149
	T=EFFT(I,K)*E	BWSIG150
	CALL SHAPE (2,X,T,PSI,CHI,2)	BWSIG151
	SIGT(I)=SIGT(I)+GRT(I,K)*PSI+GIT(I,K)*CHI	BWSIG152
	SIGS(I)=SIGS(I)+VN(K)*PSI+VI(K)*CHI	BWSIG153
253	SIGA(I)=SIGA(I)+GRA(I,K)*PSI+GIA(I,K)*CHI	BWSIG154
	SIGT(I)=CONST*SIGT(I)/YR	BWSIG155
	SIGS(I)=CONST*SIGS(I)/YR	BWSIG156
	FISS(I)=CONST*SIGA(I)/YR	BWSIG157
	SIGG(I)=SIGT(I)-SIGS(I)-FISS(I)	BWSIG158
251	SIGA(I)=FISS(I)+SIGG(I)	BWSIG159
	RETURN	BWSIG160
1003	READ INPUT TAPE 7,312,TEMP	BWSIG161
312	FORMAT(F10.4)	BWSIG162
	DO1350 I=1,NUMBI	BWSIG163
	NR=NO(I)	BWSIG164
	DO 350 K=1,NR	BWSIG165
350	EFFT(I,K)=TEMP/((ATM(I)+1.0)*DW(I,K)**2)	BWSIG166
1350	CONTINUE	BWSIG167
	WRITE OUTPUT TAPE6,1312,TEMP	BWSIG168
1312	FORMAT(20X,12HTEMPERATURE=F7.5,3HEV//)	BWSIG169
	RETURN	BWSIG170
	END	BWSIG171

\$	FASTRAN	
C	FORTRAN II SUBROUTINE SHAPE FOR THE EVALUATION OF THE	SHAPE 1
(	DOPPLER LINE SHAPE FUNCTIONS PSI(X,T) AND CHI(X,T).	SHAPE 2
C	F.T.ADLER, Y.D.NALIBOFF, J.L.DAVIDOV	SHAPE 3
	SUBROUTINE SHAPE (J,X,T,PSI,CHI,IIN)	SHAPE 4
	FREQUENCY 1(0,50),3(0,1,50),6(1,0,50),7(1,0,50),11(50,0),16(4,1,0)	SHAPE 5
	FREQUENCY 210(1,0,1),23(1,0,1),250(1,0,1),260(1,0,1),26(1,0,1),	SHAPE 6
1	27(1,0,1),28(1,0,1),29(1,0,1),30(1,0,1),320(1,0,1),330(1,0,1),	SHAPE 7
2	33(1,0,1),34(1,0,1),35(1,0,1),36(1,0,1),440(1,0,1),45(0,1,1)	SHAPE 8
	DIMENSION A(6),CR(5),CI(5),PR(5),PI(5),PS(5),CH(5),RPS(5),RCH(5)	SHAPE 9
	DIMENSION C1(2),C2(2),C3(2),C4(2),C5(2),C6(2)	SHAPE 10
1	GO TO (2,3),J	SHAPE 11
2	A(1)=2.5052367	SHAPE 12
	A(2)=1.2831204	SHAPE 13
	A(3)=0.2264718	SHAPE 14
	A(4)=0.1306469	SHAPE 15
	A(5)=-0.0202490	SHAPE 16
	A(6)=0.0039132	SHAPE 17
	CR(1)=0.	SHAPE 18
	CR(2)=1.09147894	SHAPE 19
	CR(3)=-2.30555691	SHAPE 20
	CR(4)=-CR(2)	SHAPE 21
	CR(5)=-CR(3)	SHAPE 22
	CI(1)=1.32271498	SHAPE 23
	CI(2)=1.29081178	SHAPE 24
	CI(3)=1.17416680	SHAPE 25
	CI(4)=CI(2)	SHAPE 26
	CI(5)=CI(3)	SHAPE 27
	PR(1)=0.	SHAPE 28
	PR(2)=-10.9663038	SHAPE 29
	PR(3)=24.240703	SHAPE 30
	PR(4)=-PR(2)	SHAPE 31
	PR(5)=-PR(3)	SHAPE 32
	PI(1)=6.1043246	SHAPE 33
	PI(2)=1.1317230	SHAPE 34
	PI(3)=-78.663636	SHAPE 35
	PI(4)=PI(2)	SHAPE 36
	PI(5)=PI(3)	SHAPE 37
	RPS(1)=0.21117643	SHAPE 38
	RPS(2)=0.081635073	SHAPE 39
	RPS(3)=-0.0050439914	SHAPE 40
	RPS(4)=RPS(2)	SHAPE 41
	RPS(5)=RPS(3)	SHAPE 42
	RCH(1)=0.	SHAPE 43
	RCH(2)=0.16088151	SHAPE 44
	RCH(3)=-0.0098666871	SHAPE 45
	RCH(4)=-RCH(2)	SHAPE 46
	RCH(5)=-RCH(3)	SHAPE 47
	C1(1)=1.	SHAPE 48
	C2(1)=3.	SHAPE 49
	C3(1)=15.	SHAPE 50
	C4(1)=105.	SHAPE 51
	C5(1)=945.	SHAPE 52
	C6(1)=10395.	SHAPE 53
	C1(2)=.33333333	SHAPE 54
	C2(2)=.1	SHAPE 55
	C3(2)=.23809524E-01	SHAPE 56
	C4(2)=.46296296E-02	SHAPE 57
	C5(2)=.75757575E-03	SHAPE 58
	C6(2)=.10683761E-03	SHAPE 59
	TWOPI=6.283185307	SHAPE 60

RETURN	SHAPE 61
3 IF (T) 5,4,5	SHAPE 62
4 PSI=1./(1.+X**2)	SHAPE 63
CHI=X*PSI	SHAPE 64
RETURN	SHAPE 65
5 X2=X*X	SHAPE 66
B1=1.+X2	SHAPE 67
B3=2.*T	SHAPE 68
B4=4.*T	SHAPE 69
RT=SQRT(B3)	SHAPE 70
C16=X/RT	SHAPE 71
C26=1./RT	SHAPE 72
210 IF (ABSF(X)-1.) 21,21,22	SHAPE 73
21 R=ABSF(C26)	SHAPE 74
W=X2	SHAPE 75
U=1.	SHAPE 76
V=1.	SHAPE 77
GO TO 23	SHAPE 78
22 R=ABSF(C16)	SHAPE 79
W=1./X2	SHAPE 80
U=-1.	SHAPE 81
V=X2	SHAPE 82
23 IF (R-12.53) 30,24,24	SHAPE 83
24 N=1	SHAPE 84
R6=B3/B1**2*V	SHAPE 85
250 IF (R-14.52) 37,25,25	SHAPE 86
25 F1=0.	SHAPE 87
F2=0.	SHAPE 88
260 IF (R-18.24) 38,26,26	SHAPE 89
26 IF (R-26.32) 39,27,27	SHAPE 90
27 IF (R-54.40) 40,28,28	SHAPE 91
28 IF (R-200.) 41,29,29	SHAPE 92
29 IF (R-16384.) 42,43,43	SHAPE 93
30 IF (R-.589) 31,31,48	SHAPE 94
31 N=2	SHAPE 95
B6=V/B4	SHAPE 96
G=X/B3	SHAPE 97
H=SQRT(T*3.1415927)	SHAPE 98
E=EXP((1.-X2)/B4)/B3	SHAPE 99
SI=SIN(G)	SHAPE100
CO=COS(G)	SHAPE101
320 IF (R-.456) 32,32,37	SHAPE102
32 F1=0.	SHAPE103
F2=0.	SHAPE104
330 IF (R-.318) 33,33,38	SHAPE105
33 IF (R-.191) 34,34,39	SHAPE106
34 IF (R-.084) 35,35,40	SHAPE107
35 IF (R-.0172) 36,36,41	SHAPE108
36 IF (R-.00017) 43,43,42	SHAPE109
37 F1=(((((13.*W-286.)*W+1287.)*W-1716.)*W+715.)*W-78.)*W+1.)*C6(N)*B6	SHAPE110
1 B6	SHAPE111
F2=(((((W-78.)*W+715.)*W-1716.)*W+1287.)*W-286.)*W+13.)*C6(N)*B6	SHAPE112
38 F1=(((((11.*W-165.)*W+462.)*W-330.)*W+55.)*W-1.)*U*C5(N)+F1)*B6	SHAPE113
F2=(((((W-55.)*W+330.)*W-462.)*W+165.)*W-11.)*U*C5(N)+F2)*B6	SHAPE114
39 F1=(((((9.*W-84.)*W+126.)*W-36.)*W+1.)*C4(N)+F1)*B6	SHAPE115
F2=(((((W-36.)*W+126.)*W-84.)*W+9.)*C4(N)+F2)*B6	SHAPE116
40 F1=(((((7.*W-35.)*W+21.)*W-1.)*U*C3(N)+F1)*B6	SHAPE117
F2=(((((W-21.)*W+35.)*W-7.)*U*C3(N)+F2)*B6	SHAPE118
41 F1=(((((5.*W-10.)*W+1.)*C2(N)+F1)*B6	SHAPE119
F2=(((((W-10.)*W+5.)*C2(N)+F2)*B6	SHAPE120
42 F1=(((((3.*W-1.)*U*C1(N)+F1)*B6	SHAPE121

	F2=((W-3.)*U*C1(N)+F2)*B6	SHAPE122
43	F1=(1.+F1)	SHAPE123
	F2=(1.+F2)	SHAPE124
440	IF (U) 45,44,44	SHAPE125
44	FF=F2	SHAPE126
	F2=F1	SHAPE127
	F1=FF	SHAPE128
45	IF (N-1) 46,46,47	SHAPE129
46	PSI=F2/B1	SHAPE130
	CHI=F1/B1*X	SHAPE131
	RETURN	SHAPE132
47	PSI=E*(CO*(H-F2)+X*S1*F1)	SHAPE133
	CHI=E*(-S1*(H-F2)+X*CO*F1)	SHAPE134
	RETURN	SHAPE135
48	IZ=1	SHAPE136
	B2=-2.*X*RT	SHAPE137
	DO 10 I=1,5	SHAPE138
6	IF (ABSF(X-CR(I))/CI(I))-0.005) 7,7,9	SHAPE139
7	IF (ABSF(CI(I)*RT-1.)-0.005) 8,8,9	SHAPE140
8	IZ=2	SHAPE141
	PS(I)=RPS(I)	SHAPE142
	CH(I)=RCH(I)	SHAPE143
	S1=0.	SHAPE144
	S2=0.	SHAPE145
	GO TO 10	SHAPE146
9	Q1=B1+B2*CR(I)+B3*(CR(I)**2-CI(I)**2)	SHAPE147
	Q2=(B2+B4*CR(I))*CI(I)	SHAPE148
	D1=PR(I)*Q1-PI(I)*Q2	SHAPE149
	D2=PI(I)*Q1+PR(I)*Q2	SHAPE150
	D=D1**2+D2**2	SHAPE151
	PS(I)=D2/D	SHAPE152
	CH(I)=(CR(I)*D2-CI(I)*D1)/D	SHAPE153
10	CONTINUE	SHAPE154
11	GO TO (I2,I9),IZ	SHAPE155
12	P16=A(1)	SHAPE156
	P26=0.	SHAPE157
	C262=C16*C26*2.	SHAPE158
	CI62=CI6**2-C26**2	SHAPE159
	C16N=C162	SHAPE160
	C26N=C262	SHAPE161
	I=2	SHAPE162
15	PI6=PI6+A(I)*C16N	SHAPE163
	P26=P26+A(I)*C26N	SHAPE164
16	IF (I-6) 17,18,18	SHAPE165
17	C1N=C162*C16N-C262*C26N	SHAPE166
	C2N=C262*C16N+CI62*C26N	SHAPE167
	*C16N=C1N	SHAPE168
	C26N=C2N	SHAPE169
	I=I+1	SHAPE170
	GO TO 15	SHAPE171
18	D3=P16**2+P26**2	SHAPE172
	SI=PI6/(2.*RT*D3)	SHAPE173
	S2=(P26+X*P16)/(B4*D3)	SHAPE174
19	DO 20 I=1,5	SHAPE175
	S1=S1+PS(I)	SHAPE176
20	S2=S2+CH(I)	SHAPE177
	PSI=TWOPI*S1	SHAPE178
	CHI=X*PSI-RT*TWOPI*S2	SHAPE179
	RETURN	SHAPE180
	END	SHAPE181

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