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STAX 2 : A Computer Program for Calculating Neutron Elastic and Inelastic Scattering Cross Sections by Means of the Optical Model and Moldauer's Theory

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STAX 2
A Computer Program for Calculating Neutron Elastic and Inelastic Scattering Cross Sections by Means of the Optical Model and Moldauer's Theory

Summary

This program computes the cross sections for neutron elastic and inelastic scattering using the optical model and Moldauer's theory, and searches for potential parameters which reproduce experimental cross sections.

Improvement is made in the treatment of the effect of resonance interference. The quantity "Q" characterizing this effect has been regarded as an arbitrary parameter in the calculations hitherto published. In the present program this quantity can be calculated considering its dependence on the strength function.

Calculation using the Hauser-Feshbach theory is also possible.

November 1969

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STAX 2
光学模型と Moldauer の理論による中性子弾性非弾性散乱断面積計算コード

要　旨

このコードは，光学模型と Moldauer の理論によって，中性子の弾性非弾性散乱の断面積を計算し，実験値を再現するポテンシャルパラメーターを求める．

これまでの計算では任意なパラメーターとしてあつかわれてきた，共鳴準位の干渉の効果を示す量“Q”を，強度関数への依存性を考慮することによって計算できるよう改良した．

Hauser-Feshbach の理論による計算も可能になっている．

1969年11月

日本原子力研究所東海研究所
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1. Introduction

STAX2 is a computer program for calculating neutron elastic and inelastic scattering cross sections using the optical model and Moldauer's theory, and can search for potential parameters which can reproduce experimental cross sections. Search is made on all potential parameters with respect to any combination of the following cross sections:

1) total cross section,
2) elastic scattering cross section (integral or differential),
3) inelastic scattering cross section for the first excited level (integral or differential).

Although there exist many optical model programs[1),2)], none of them seems to use Moldauer's theory for the calculation of compound nuclear process. The program NEARREX[3)], often used to compute reaction cross sections using Moldauer's theory, can not compute angular distributions and does not include an optical model routine. These are the reasons why the present program has been written.

In this program improvement is made in the treatment of the resonance interference by considering the dependence of the quantity $Q^{J\Pi}$, characterizing this effect, on the strength function.

2. Theory

We consider the scattering of neutrons by a target nucleus of mass M. The cross section σ_{el} for elastic scattering is composed of the shape elastic cross section σ_{se} and the compound elastic cross section σ_{c0}:

$$\sigma_{el}=\sigma_{se}+\alpha\sigma_{c0}. \qquad (1)$$

The quantity α is a correction factor equal to or less than unity and is used to approximately correct for the effect of other open channels than neutron channels, because this program can treat only neutrons. This guantity is also used when higher energy levels are not well known. For the inelastic channels we neglect the direct process and the cross sections are given by

$$\sigma_n=\alpha\sigma_{cn}, \qquad (2)$$

where n indicates the n-th excited state.

Cross sections computed in the present program are those in the center-of-mass system.

2.1 Shape Elastic Scattering——Optical Model

The shape elastic scttering is treated by the optical model. The optical potential employed in the present program is of the form

$$-Vf(r)-iWg(r)-V_{so}(\boldsymbol{l}\cdot\boldsymbol{\sigma})h(r), \qquad (3)$$

where

$$f(r)=\frac{1}{1+\exp[(r-r_0A^{1/3})/a]}, \qquad (4)$$

$$g(r)=\frac{4\exp[(r-r_sA^{1/3})/b]}{\{1+\exp[(r-r_sA^{1/3})/b]\}^2}, \qquad (5)$$

$$h(r)=-\lambda\!\!\!^{-}_{\pi}{}^2\frac{1}{r}\frac{d}{dr}g(r), \qquad (6)$$

$$\lambda\!\!\!^{-}_{\pi}=2.04264\,\mathrm{fm}. \qquad (7)$$

Each of the seven parameters V, W, V_{so}, r_s, a and b may have an energy dependence

$$V=\sum_{n=0}^{5} V^{(n)}E^n \quad \text{etc.,} \tag{8}$$

where E is the kinetic energy in the center-of-mass system.

The radial Schroedinger equation describing the scattering is

$$\left[-\frac{\hbar^2}{2\mu}\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right\}-Vf(r)-iWg(r)-C_l^{(\pm)}V_{so}h(r)-E\right]\varphi_l^{(\pm)}=0, \tag{9}$$

where $(\pm)$ corresponds to the value of coupled angular momentum $j=l\pm1/2$ of $\boldsymbol{l}$ and $\boldsymbol{\sigma}$, and

$$C_l^{(+)}=-l,\ C_l^{(-)}=l+1, \tag{10}$$

$$\mu=\frac{mM}{m+M}. \tag{11}$$

Here m is the neutron mass, which is 1. 008665 amu-^{12}C.

The scattering amplitude $\eta_l^{(\pm)}$ is obtained from the asymptotic behavior of the wave function:

$$\varphi_l^{(\pm)}(r)\underset{r\to\infty}{\sim} r(h_l^{(2)}(kr)+\eta_l^{(\pm)}h_l^{(1)}(kr)), \tag{12}$$

where $h_l^{(1)}$ and $h_l^{(2)}$ are the spherical Hankel functions and

$$k=\frac{1}{\lambda\!\!\!^{-}}=\sqrt{\frac{2\mu E}{\hbar^2}}. \tag{13}$$

The shape elastic cross section and the cross section for the formation of compound nucleus are given by

$$\sigma_{se}=\pi\lambda\!\!\!^{-2}\sum_l\{(l+1)|1-\eta_l^{(+)}|^2+l|1-\eta_l^{(-)}|^2\}, \tag{14}$$

$$\frac{d\sigma_{se}}{d\Omega}=\frac{\lambda\!\!\!^{-2}}{4}\left[|\sum_l\{(l+1)(1-\eta_l^{(+)})+l(1-\eta_l^{(-)})\}P_l(\cos\theta)|^2\right.$$
$$\left.+|\sum_l(\eta_l^{(+)}-\eta_l^{(-)})P_l^1(\cos\theta)|^2\right], \tag{15}$$

$$\sigma_c=\pi\lambda\!\!\!^{-2}\sum_l\{(l+1)T_l^{(+)}+lT_l^{(-)}\}, \tag{16}$$

where transmission coefficients $T_l^{(\pm)}$ are given by

$$T_l^{(\pm)}=1-|\eta_l^{(\pm)}|^2. \tag{17}$$

2. 2 Compound Nuclear Process——Moldauer's Theory

By using Moldauer's theory(4) differential cross section for the n-th excited state can be written in the following form:

$$\frac{d\sigma_{cn}}{d\Omega}=\frac{\lambda\!\!\!^{-2}}{2(2I_0+1)}\sum_{\mathrm{L}}B_{\mathrm{L}}P_{\mathrm{L}}(\cos\theta), \tag{18}$$

$$B_{\mathrm{L}}=B_{\mathrm{L}}^{(1)}+B_{\mathrm{L}}^{(2)}+B_{\mathrm{L}}^{(3)}, \tag{19}$$

$$B_{\mathrm{L}}^{(1)}=\frac{(-)^{I_n-I_0}}{4}\sum_{J\Pi ljl'j'}(2J+1)^2\delta(\pi_0(-)^l,\Pi)\delta(\pi_n(-)^{l'},\Pi)$$
$$\times\bar{Z}(ljlj;\tfrac{1}{2}L)W(jJjJ;\ I_0L)\bar{Z}(l'j'l'j';\tfrac{1}{2}L)W(j'Jj'J;\ I_nL)$$
$$\times\left\langle\frac{\Theta_{\mu,0lj}\Theta_{\mu,nl'j'}}{\Theta_\mu}\right\rangle_\mu^{J\Pi}, \tag{20}$$

$$B_{\mathrm{L}}^{(2)}=\frac{\delta(n,0)}{4}\sum_{J\Pi(lj)\neq(l'j')}(2J+1)^2\left\{\bar{Z}(ljl'j';\tfrac{1}{2}L)W(jJj'J;I_0L)\right\}^2$$
$$\times\delta(\pi_0(-)^l,\Pi)\delta(\pi_0(-)^{l'},\Pi)R_{lj;l'j'}B\left\langle\frac{\Theta_{\mu,0lj}\Theta_{\mu,0l'j'}}{\Theta_\mu}\right\rangle_\mu^{J\Pi}, \tag{21}$$

$$B_L^{(3)} = \frac{-\delta(n,0)}{4} \sum_{J\Pi ljl'j'} (2J+1)^2 \left\{ \bar{Z}(ljl'j'\,;\,\frac{1}{2}L) W(jJj'J\,;\,I_0 L) \right\}^2$$
$$\times \delta(\pi_0(-)^l, \Pi)\delta(\pi_0(-)^{l'}, \Pi) R_{lj;l'j'} Q_\mu{}^{J\Pi} \langle \Theta_{\mu,0lj} \rangle_\mu{}^{J\Pi} \langle \Theta_{\mu,0l'j'} \rangle_\mu{}^{J\Pi}, \tag{22}$$

where I_n and π_n are the spin and parity of the n-th excited state (the ground state is denoted by $n=0$), J and Π are the total angular momentum and parity, and $\delta(n, m)$ is Kronecker's symbol. The coefficients $\bar{Z}$ and W are the Blatt-Biedenharn and the Racah coefficients, and

$$Q^{J\Pi} = \frac{2B}{N^2}\left[1 - \Phi_0\left(\frac{\langle \Theta_\mu \rangle_\mu{}^{J\Pi}}{2N^2}\right)\right], \tag{23}$$

$$B = |b_{nlj}|^2, \tag{24}$$

$$R_{lj;l'j'} = Re(b_{0lj} b_{0l'j'}{}^*)/B. \tag{25}$$

Here B is assumed to be independent of (nlj).
The function Φ_0 is defined by

$$\Phi_0(x) = 1 - \frac{1}{x}\left[1 - \frac{1}{x} e^{-x} \sinh x\right] - \frac{1}{x} \mathrm{Ei}(-x)\left[\cosh x - \frac{1}{x} \sinh x\right], \tag{26}$$

and

$$\Theta_\mu = \sum_{nlj} \Theta_{\mu,nlj}. \tag{27}$$

Other quantites $\Theta_{\mu,nlj}$, b_{nlj} and N are defined in ref.[4] and the average $\langle \ \ \rangle_\mu{}^{J\Pi}$ is taken over the compound levels μ which have a spin and parity of $J\Pi$. The quantity $\langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi}$ is proportional to the strength function $\langle \Gamma_{\mu,nlj}/D \rangle_\mu{}^{J\Pi}$, and is related to the transmission coefficient T_{nlj} by

$$T_{nlj} = \langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi} - \frac{Q^{J\Pi}}{4} \{ \langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi} \}^2. \tag{28}$$

Assuming a χ^2-distribution with ν degrees of freedom for $\Theta_{\mu,nlj}$ we obtain[5]

$$\left\langle \frac{\Theta_{\mu,nlj} \Theta_{\mu,n'l'j'}}{\Theta_\mu} \right\rangle_\mu^{J\Pi} = \frac{\langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi} \langle \Theta_{\mu,n'l'j'} \rangle_\mu{}^{J\Pi}}{\langle \Theta_\mu \rangle_\mu{}^{J\Pi}} S_{nlj;n'l'j'}{}^{J\Pi}, \tag{29}$$

$$S_{nlj}{}^{J\Pi}{}_{;n'l'j'} = \int_0^\infty dt \frac{1 + 2\delta_{nn'}\delta_{ll'}\delta_{jj'}}{f_{nlj} f_{n'l'j'} \prod_{n''l''j''}{}^{J\Pi} f_{n''l''j''}{}^{\nu/2}}, \tag{30}$$

where the product in the denominator is taken over all channels which have a total angular momentum and parity of $J\Pi$, and

$$f_{nlj} = 1 + \frac{\langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi}}{\langle \Theta_\mu \rangle_\mu{}^{J\Pi}} \frac{2t}{\nu}. \tag{31}$$

Various quantites given above have limited ranges of magnitude:

$$1 \geq B \geq 0, \tag{32}$$

$$N \geq 1, \tag{33}$$

$$1 \geq R_{lj;l'j'} \geq -1, \tag{34}$$

$$R_{lj;lj} = 1, \tag{35}$$

$$2 \geq Q^{J\Pi} \geq 0, \tag{36}$$

and in the limit of $\Gamma/D \rightarrow 0$ they become

$$B = 1, \tag{37}$$

$$N = 1, \tag{38}$$

$$R_{lj;l'j'} = 1, \tag{39}$$

$$Q^{J\Pi} = 2. \tag{40}$$

The quantity $R_{lj;l'j'}$ for $(lj) \neq (l'j')$ is assumed to be independent of $(lj\,;\,l'j')$ in the present program. This quantity does not affect the cross sections when the spin of the target nucleus is zero.

In the calculations hitherto published, $Q^{J\Pi}$ was treated as a constant neglectnig its dependence on $\langle \Theta_{\mu,nlj} \rangle_\mu{}^{J\Pi}$. However, this treatment sometimes results in negative values[6] for the compound elastic cross sections for some partial waves, when many channels are open and the constant is not taken sufficiently small. This difficulty is avoided if Eq. (28) is solved for $\langle\Theta_{\mu,nlj}\rangle_{\mu}{}^{J\Pi}$ by considering the functional dependence of $Q^{J\Pi}$ on $\langle\Theta_{\mu,nlj}\rangle_{\mu}{}^{J\Pi}$ given by Eq. (23). Both treatment of $Q^{J\Pi}$ are possible in the present program.

The largest possible $Q^{J\Pi}$ is given for $B=1$ and $N=1$.

By putting b_{nlj} to zero and $S_{nlj;n'l'j'}{}^{J\Pi}$ to unity, B and $Q^{J\Pi}$ become zero and the Hauser-Feshbach formula is obtained in Eqs. (18)-(22).

3. Fitting to Experimental Cross Sections

Fitting the calculation to experimental cross sections is made by minimizing the quantity χ^2 defined by

$$\chi^2=\left\{W_t\left(\frac{\sigma_t^{\mathrm{cal}}-\sigma_t^{\mathrm{exp}}}{\Delta\sigma_t}\right)^2+W_{\mathrm{el}}\left(\frac{\sigma_{\mathrm{el}}^{\mathrm{cal}}-\sigma_{\mathrm{el}}^{\mathrm{exp}}}{\Delta\sigma_{\mathrm{el}}}\right)^2+W_1\left(\frac{\sigma_1^{\mathrm{cal}}-\sigma_1^{\mathrm{exp}}}{\Delta\sigma_1}\right)^2\right.$$
$$+W_{\mathrm{ela}}\sum_\theta\left(\frac{\dfrac{d\sigma_{\mathrm{el}}^{\mathrm{cal}}(\theta)}{d\Omega}-\dfrac{d\sigma_{\mathrm{el}}^{\mathrm{exp}}(\theta)}{d\Omega}}{\Delta\dfrac{d\sigma_{\mathrm{el}}(\theta)}{d\Omega}}\right)^2+W_{1\mathrm{a}}\sum_\theta\left.\left(\frac{\dfrac{d\sigma_1^{\mathrm{cal}}(\theta)}{d\Omega}-\dfrac{d\sigma_1^{\mathrm{exp}}(\theta)}{d\Omega}}{\Delta\dfrac{d\sigma_1(\theta)}{d\Omega}}\right)^2\right\}$$
$$/(W_t+W_{\mathrm{el}}+W_1+\sum_\theta W_{\mathrm{ela}}+\sum_\theta W_{1\mathrm{a}}), \tag{41}$$

where σ_t is the total cross section, "cal" and "exp" indicate the calculated and the experimental cross sections, Δ indicates the experimental uncertainty, and W_t etc. are weighting factors which may be arbitrarily chosen. Search for the "best" parameters is made on any number of parameters $V^{(0)}$, $W^{(0)}$, $V_{\mathrm{so}}{}^{(0)}$, $r_0{}^{(0)}$, $r_s{}^{(0)}$, $a^{(0)}$ and $b^{(0)}$ by means of Gauss-Newton's method.

For brevity we denote the set of parameters to be searched for by $\{x_i\}$ and the cross sections to be fitted by $\{\sigma_\alpha\}$. Around $\{x_i{}^{(n)}\}$ the cross sections are approximated by

$$\sigma_\alpha{}^{\mathrm{cal}}(\{x_i{}^{(n)}+\delta x_i\})=\sigma_\alpha{}^{\mathrm{cal}}(\{x_i{}^{(n)}\})+\sum_i\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}(\{x_i{}^{(n)}\})}{\partial x_i}\delta x_i, \tag{42}$$

where $\{x_i{}^{(n)}\}$ indicates the parameters obtained after the n-th iteration. The parameters which minimize χ^2 can be obtained by

$$\sum_{\alpha j}\frac{W_\alpha}{(\Delta\sigma_\alpha)^2}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_i}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_j}\delta x_j=\sum_\alpha\frac{W_\alpha(\sigma_\alpha{}^{\mathrm{exp}}-\sigma_\alpha{}^{\mathrm{cal}})}{(\Delta\sigma_\alpha)^2}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_i}. \tag{43}$$

This equation can be solved easily. However, since we neglected higher order terms of $\{\delta x_i\}$ in Eq. (42), this equation is not very accurate when some of the eigenvalues of the matrix

$$\left(\sum_\alpha\frac{W_\alpha}{(\Delta\sigma_\alpha)^2}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_i}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_j}\right)$$

are small, and such circumstances may often happen because of the well known optical potential ambiguities. For this reason Eq. (43) is not solved as it is. We define a symmetric marix and column vectors in the parameter space:

$$(A_{ij})=\left(\sum_\alpha\frac{W_\alpha}{(\Delta\sigma_\alpha)^2}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_i}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_j}\delta x_i{}^{\max}\delta x_j{}^{\max}\right), \tag{44}$$

$$(b_i)=\left(\sum_\alpha\frac{W_\alpha(\sigma_\alpha{}^{\mathrm{cal}}-\sigma_\alpha{}^{\mathrm{exp}})}{(\Delta\sigma_\alpha)^2}\frac{\partial\sigma_\alpha{}^{\mathrm{cal}}}{\partial x_i}\delta x_i{}^{\max}\right), \tag{45}$$

$$(\delta\xi_i)=\left(\frac{\delta x_i}{\delta x_i{}^{\max}}\right), \tag{46}$$

where $\{\delta x_i{}^{\max}\}$ is introduced in order to make the magnitude of A_{ij} uniform and also to set a limit for $\{\delta x_i\}$, and is given as follows:

$$\left.\begin{aligned}&\delta V^{max}=\delta W^{max}=\delta V_{so}{}^{max}=3.0\,\text{MeV},\\&\delta r_0{}^{max}=0.05\,\text{fm},\\&\delta r_s{}^{max}=0.1\,\text{fm},\\&\delta a^{max}=0.07\,\text{fm},\\&\delta b^{max}=0.1\,\text{fm}.\end{aligned}\right\}\tag{47}$$

Then Eq. (43) can be written as

$$\boldsymbol{A}\delta\boldsymbol{\xi}=\boldsymbol{b}. \tag{48}$$

The matrix $\boldsymbol{A}$ is diagonalized by a orthogonal matrix $\boldsymbol{U}$:

$$\boldsymbol{U}\boldsymbol{A}\boldsymbol{U}^t=\boldsymbol{D}=\begin{pmatrix}\lambda_1 & & 0\\ & \lambda_2 & \\ 0 & & \ddots\end{pmatrix}. \tag{49}$$

Solution of Eq. (48) is given by

$$\delta\boldsymbol{\xi}=\boldsymbol{U}^t\delta\boldsymbol{\eta}, \tag{50}$$

$$\delta\boldsymbol{\eta}=\boldsymbol{D}^{-1}\boldsymbol{U}\boldsymbol{b}. \tag{51}$$

Because of the reason mentioned above, we neglect small eigenvalues and replace $\boldsymbol{D}^{-1}$ by $\tilde{\boldsymbol{D}}^{-1}$, the elements of which are given by

$$\tilde{D}_{ij}{}^{-1}=\begin{cases}\dfrac{\delta_{ij}}{\lambda_i}, & if\ \ |\lambda_i|\geq\varepsilon\\ 0, & if\ \ |\lambda_i|<\varepsilon,\end{cases} \tag{52}$$

where ε is a small number defined below in Eq. (57). Furthermore, since the approximation (42) is valid only in the neighbourhood of $\{x_i{}^{(n)}\}$, $\delta\eta$ is truncated as follows:

$$\delta\eta_i=\begin{cases}\widetilde{\delta\eta}_i, & if\ \ |\widetilde{\delta\eta}_i|\leq 1\\ \dfrac{\widetilde{\delta\eta}_i}{|\widetilde{\delta\eta}_i|}, & if\ \ |\widetilde{\delta\eta}_i|>1,\end{cases} \tag{53}$$

where

$$\widetilde{\delta\boldsymbol{\eta}}=\tilde{\boldsymbol{D}}^{-1}\boldsymbol{U}\boldsymbol{b}. \tag{54}$$

At $\{x_i{}^{(n)}+\delta x_i\}$, χ^2 is expected to decrease by

$$\Delta\chi^2=\sum_{i,\lambda_i\geq|\varepsilon|}\lambda_i(\delta\eta_i)^2 \tag{55}$$

in the same approximation as above. When $\chi^2(\{x_i{}^{(n)}\})-\chi^2(\{x_i{}^{(n)}+\delta x_i\})\geq\frac{\Delta\chi^2}{4}$, $\{x_i{}^{(n)}+\delta x_i\}$ is taken as $\{x_i{}^{(n+1)}\}$. When $\chi^2(\{x_i{}^{(n)}\})-\chi^2(\{x_i{}^{(n)}+\delta x_i\})\leq\frac{\Delta\chi^2}{4}$, we consider the approximation (42) to be not good and compute χ^2 at $\{x_i{}^{(n)}+\frac{1}{2}\delta x_i\}$. Then $\{x_i{}^{(n+1)}\}$ is obtained by approximating $\chi^2(x_i{}^{(n)}+\alpha\delta x_i\})$ by a quadratic polynomial of α.

This parameter search is stopped when one of the following conditions is encountered:

1) a specified number of iteration has been made,
2) specified calculation time has elapsed,
3) χ^2 has become smaller than a specified value $\chi^2{}_{min}$,
4) $\chi^2(\{x_i{}^{(n)}\})-\chi^2(\{x_i{}^{(n+1)}\})\leq 0.01\,\chi_{min}{}^2$.

The matrix $\boldsymbol{A}$ is diagonalized by means of Jacobi's method and the accuracy of diagonalization is taken as

$$\varepsilon'=\frac{10^{-K}}{N_p}\sum A_{ii}, \tag{56}$$

where N_p is the number of the parameter to be searched for and K is usually set equal to five unless otherwise specified. The ε in Eq. (52) is given by

$$\varepsilon=10\,N_p\varepsilon'. \tag{57}$$

Derivative $\frac{\partial \sigma_\alpha}{\partial x_i}$ is approximated by

$$\frac{\sigma_\alpha(x_i^{(n)}+\Delta x_i)-\sigma_\alpha(x_i^{(n)})}{\Delta x_i}, \tag{58}$$

where $\{\Delta x_i\}$ is given as follows:

$$\left.\begin{array}{l}\Delta V=\Delta W=\Delta V_{so}=0.1\,\text{MeV},\\ \Delta r_0=r_s=\Delta a=\Delta b=0.01\,\text{fm}.\end{array}\right\} \tag{59}$$

In computing $\sigma_\alpha(\{x_i^{(n)}+\Delta x_i\})$ two methods are employed:

(A) $\sigma_\alpha(\{x_i^{(n)}+\Delta x_i\})$ is calculated rigorously,

(B) only the shape elastic cross section and the cross section for the formation of compound nucleus are calculated, and the cross sections through compound process are approximated as follows:

$$\sigma_{cn}(x_i^{(n)}+\Delta x_i)=\frac{\sigma_c(x_i^{(n)}+\Delta x_i)}{\sigma_c(x_i^{(n)})}\sigma_{cn}(x_i^{(n)}), \tag{60}$$

$$\frac{d\sigma_{cn}(x_i^{(n)}+\Delta x_i)}{d\Omega}=\frac{\sigma_c(x_i^{(n)}+\Delta x_i)}{\sigma_c(x_i^{(n)})}\frac{d\sigma_{cn}(x_i^{(n)})}{d\Omega}. \tag{61}$$

Method (B) is inferior in accuracy to method (A), but requires much shorter calculation time especially when many channels are open. In most cases method (B) is preferred.

4. Methods of Numerical Calculation

4.1 Solution of the Schroedinger Equation

Equation (9) is solved by means of Noumerov's method[7] in the internal region. Rewriting Eq. (9) as

$$\frac{d^2}{dr^2}\varphi_l^{(\pm)}=D_l^{(\pm)}\varphi_l^{(\pm)}, \tag{62}$$

and defining the quantity

$$\Psi_l^{(\pm)}=\left(1-\frac{h^2}{12}D_l^{(\pm)}\right)\varphi_l^{(\pm)}, \tag{63}$$

we can replace Eq. (9) by the recurrence relation

$$\Psi_l^{(\pm)}(r_n)=\left[2+\frac{h^2D_l^{(\pm)}(r_{n-1})}{1-\frac{h^2}{12}D_l^{(\pm)}(r_{n-1})}\right]\Psi_l^{(\pm)}(r_{n-1})-\Psi_l^{(\pm)}(r_{n-2}), \tag{64}$$

where

$$r_n=r_1+(n-1)h \tag{65}$$

and $h=0.25$ fm unless otherwise specified. Two values $\Psi_l^{(\pm)}(r_1)$ and $\Psi_l^{(\pm)}(r_2)$ are necessary for solving Eq. (65). These values are obtained by expanding the functions in power series of r:

$$\varphi_l^{(\pm)}(r)=\sum_{n=0}^{\infty}b_{ln}^{(\pm)}r^{n+l+1}, \tag{66}$$

$$D_l^{(\pm)}(r)=\frac{l(l+1)}{r_2}-\frac{K_l^{(\pm)}}{r}-\sum_{n=0}^{\infty}a_{ln}^{(\pm)}r^n, \tag{67}$$

where

$$K_l^{(\pm)}=\frac{2\mu\lambda_\pi^2V_{so}C_l^{(\pm)}}{\hbar^2}\frac{}{a}\frac{\exp(-r_0A^{1/3}/a)}{\{1+\exp(-r_0A^{1/3}/a)\}^2}, \tag{68}$$

$$a_{ln}{}^{(\pm)}=\frac{2\mu}{\hbar^2}[E\delta_{n0}+f_n V+4ig_n W+(n+2)\lambda_\pi{}^2 V_{so}C_l{}^{(\pm)}f_{n+2}]. \tag{69}$$

The coefficients f_n and g_n are the derivatives of potentials and are given by the following equations:

$$f_n=F_n(r_0, a) \tag{70}$$

$$g_n=-b(n+1)F_n(r_s, b), \tag{71}$$

$$F_0(r, c)=[1+\exp(rA^{1/3}/c)]^{-1}, \tag{72}$$

$$F_{n+1}(r, c)=\frac{1}{c(n+1)}\left[-F_n(r, c)+\sum_{k=0}^{n}F_k(r, c)F_{n-k}(r, c)\right]. \tag{73}$$

The expansion coefficients of $\varphi_l{}^{(\pm)}$ are given by

$$b_{l0}{}^{(\pm)}=1, \tag{74}$$

$$b_{l1}{}^{(\pm)}=-\frac{K_l{}^{(\pm)}}{2(l+1)}, \tag{75}$$

$$b_{ln}{}^{(\pm)}=\frac{-1}{n(2l+n+1)}\left[K_l{}^{(\pm)}b_{l n-1}{}^{(\pm)}+\sum_{k=0}^{n-2}b_{lk}{}^{(\pm)}a_{l n-k-2}{}^{(\pm)}\right]. \tag{76}$$

Only the first eight terms are taken in the expansion of $\varphi_l{}^{(\pm)}$.

Because of the singularity of $l(l+1)/r^2$, Eq. (64) is not accurate in the neighbourhood of $r=0$. Therefore r_1 and r_2 should be taken as large as possible. Error of $\varphi_l{}^{(\pm)}$ due to the truncation of the power series (66) is of the order of

$$\frac{(Kr)^8}{9!}\varphi_l{}^{(\pm)}(r), \tag{77}$$

where

$$K=\sqrt{\frac{2\mu}{\hbar^2}(E+V)}. \tag{78}$$

We require $\varphi_l{}^{(\pm)}(r_2)$ to be accurate to 10^{-5} and take r_2 as

$$r_2=\frac{1.2}{K}. \tag{79}$$

4.2 Determination of Scattering Amplitude

Scattering amplitude $\eta_l{}^{(\pm)}$ is obtained by matching the internal wave function with the external wave function (12):

$$\frac{\varphi_l{}^{(\pm)}(r_M)}{\varphi_l{}^{(\pm)}(r_{M-1})}=\frac{r_M}{r_{M-1}}\cdot\frac{h_l{}^{(2)}(kr_M)+\eta_l{}^{(\pm)}h_l{}^{(1)}(kr_M)}{h_l{}^{(2)}(kr_{M-1})+\eta_l{}^{(\pm)}h_l{}^{(1)}(kr_{M-1})}. \tag{80}$$

Matching radius r_M is determined by the requirement that at $r>r_M$ influence of the optical potential is negligible. By rewriting Eq. (9) as

$$\frac{d^2}{dr^2}\varphi_l{}^{(\pm)}+\left\{k^2-\frac{l(l+1)}{r^2}-v(r)\right\}\varphi_l{}^{(\pm)}=0, \tag{81}$$

relative error of $\varphi_l{}^{(\pm)}(r_M)$ introduced by neglecting $v(r)$ at $r>r_M$ can be shown to be of the order of

$$\frac{1}{k}\int_{r_M}^{\infty}drr^2v(r)h_l{}^{(1)}(kr)h_l{}^{(2)}(kr)\lesssim\frac{1}{k}\int_{r_M}^{\infty}dr|v(r)|. \tag{82}$$

The right hand side of the inequality becomes

$$\frac{|C|}{\alpha k}e^{-\alpha r_M} \tag{83}$$

for $v(r)=Ce^{-\alpha r}$. Therefore we require r_M to satisfy the following conditions

$$\left.\begin{aligned} &\frac{akV}{E}e^{\frac{r_0A^{1/3}-r_M}{a}}<10^{-6}, \\ &\frac{4bkW}{E}e^{\frac{r_sA^{1/3}-r_M}{a}}<10^{-6}, \\ &\frac{10k\lambda_\pi^2V_{so}}{aA^{1/3}E}e^{\frac{r_0A^{1/3}-r_M}{a}}<10^{-6}. \end{aligned}\right\} \tag{84}$$

4.3 Calculation of $Q^{J\Pi}$ and $\langle\Theta_{\mu,nlj}\rangle_\mu{}^{J\Pi}$

Equation (28) can be rewritten as

$$\Theta_c=\frac{2}{Q}\{1-\sqrt{QT_c}\} \tag{85}$$

and Θ_c may be regarded as a function of Q, where we denote $\langle\Theta_{\mu,nlj}\rangle_\mu{}^{J\Pi}$, T_{nlj} and $Q^{J\Pi}$ by Θ_c, T_c and Q for brevity. Then Eq. (23) becomes an equation with only one variable Q. This equation is solved by Newton's iteration method. Starting values are taken as

$$\Theta_c{}^{(0)}=T_c, \tag{86}$$

$$Q^{(0)}=\frac{2B}{N^2}\left(1-\Phi_0\left(\frac{\sum\limits_c\Theta_c{}^{(0)}}{2N^2}\right)\right), \tag{87}$$

and the next value is given by

$$Q^{(n+1)}=Q^{(n)}+\frac{\frac{2B}{N^2}\left\{1-\Phi_0\left(\frac{\sum\limits_c\Theta_c{}^{(n)}}{2N^2}\right)\right\}-Q^{(n)}}{1+\frac{B}{4N^2}\sum\limits_c\frac{\{\Theta_c{}^{(n)}\}^2}{\sqrt{1-Q_c{}^{(n)}T_c}}\Phi_0'\left(\frac{\sum\limits_c\Theta_c{}^{(n)}}{2N^2}\right)}, \tag{88}$$

where $\Phi_0'(x)$ is replaced by

$$100\{\Phi_0(x+0.01)-\Phi_0(x)\}. \tag{89}$$

Iteration is continued until

$$|\Theta_c{}^{(n+1)}-\Theta_c{}^{(n)}|<10^{-6} \tag{90}$$

is reached for all c.

4.4 Calculation of Width Fluctuation Factor

For brevity we denote the integral in Eq. (30) by

$$I=\int_0^\infty\frac{dt}{\prod\limits_k(1+\alpha_kt)^{\nu/2}}. \tag{91}$$

By the transformation

$$y=(1+\bar{\alpha}t)^{1-n} \tag{92}$$

the integral becomes

$$I=\frac{1}{(n-1)\bar{\alpha}}\int_0^1\frac{dy}{\prod\limits_k Y_k}, \tag{93}$$

where

$$n=\frac{1}{2}\sum_k\nu, \tag{94}$$

$$\bar{\alpha}=\frac{1}{n}\sum_k\alpha_k, \tag{95}$$

$$Y_k=\left(1-\frac{\alpha_k}{\bar{\alpha}}\right)y^{\frac{1}{n-1}}+\frac{\alpha_k}{\bar{\alpha}}. \tag{96}$$

The integrand is a monotonously decreasing function of y, and when values of α_k are scattered widely around their average $\bar{\alpha}$ it has a large derivative in the neighbourhood of $y=0$. In order to avoid this rapid variation further transformation

$$y=z^5 \tag{97}$$

is made and the integral becomes

$$I=\frac{5}{(n-1)\bar{\alpha}}\int_0^1 \frac{z^4}{\prod_k Y_k}dz, \tag{98}$$

which is evaluated by means of the 16-point Legendre-Gauss formula.

5. Subroutines

The following subroutines are used in the present program.

1. SUBROUTINE SEARCH searches for the "best" potential parameters.
2. SUBROUTINE EIGEN diagonalizes the matrix A in Eq. (49).
3. SUBROUTINE XSECT computes various cross sections.
4. SUBROUTINE DIFEQ solves the Schroedinger equation.
5. SUBROUTINE BESSEL AND BESSE2 compute the spherical Bessel and Neumann functions.
6. SUBROUTINE SHAPE computes the shape elastic cross section.
7. SUBROUTINE LEGND1 and LEGND2 compute the Legendre functions.
8. SUBROUTINE TRANS computes $Q^{J\Pi}$ and $\langle\Theta_{\mu,nlj}\rangle_\mu{}^{J\Pi}$.
9. SUBROUTINE PHAI computes the function Φ_0.
10. SUBROUTINE EI computes the exponential integral.
11. SUBROUTINE BLL computes B_L in Eq. (18).
12. FUNCTION S computes the width fluctuation factor.
13. SUBROUTINE FACTRL, FUNCTION DELT and EXDELT are used for computing the Clebsch-Gordan coefficient and the Racah coefficient.
14. FUNCTION CG0 computes the Clebsch-Gordan coefficient.
15. FUNCTION WRAC computes the Racah coefficient.

6. Input

The meaning and FORMAT of input cards are described below. Units of energy and length are MeV and fm, respectively.

CARD 1

(DATE(N), N=1, 3), (NAME(N), N=1, 3)

FORMAT (6 A 4)

Date and name.

CARD 2

(TITLE(N), N=1, 18)

FORMAT (18 A 4)

Title of the calculation.

CARD 3

FMASST, NOMASS, NLEV, NLOUT, ELAB, PHIPRE, DR, ITEST, IFDPR, NPRE.

FORMAT (F 12. 0, 3 I 6, F 6. 0, E 12. 3, F 6. 0, 3 I 6)

FMASST : Mass of the target nucleus in amu-C^{12}.

NOMASS: Mass number of the target nucleus.

NLEV : Number of levels. (≤ 25)

NLOUT : Cross sections are calculated only for the lowest NLOUT levels.

ELAB : Energy of the incident neutrons in the laboratory system.

PHIPRE : The factor 10^{-6} in (84) is replaced by PHIPRE, if PHIPRE$\neq$0.

DR : If ITEST$\neq$0, matrices $\boldsymbol{A}$, $\boldsymbol{b}$, $\boldsymbol{D}$ and $\boldsymbol{U}$ in Eqs. (44)-(49) are printed as output.

IFDPR : If IFDPR=1, $\{\Delta x_i\}$ in Eqs. (59) are replaced by the values on CARD 4. If IFDPR=2, $\{\delta x_i^{max}\}$ in Eqs. (47) are replaced by the values on CARD 5. If IFDPR=3, both quatities are replaced.

NPRE : If NPRE$\neq$0, the factor K in Eq. (56). is replaced by NPRE.

CARD 4 (Necessary only when IFDPR=1 or 3.)

(DPARA(N), N=1, 7)

FORMAT (7 F 6. 0)

: ΔV, ΔW, ΔV_{so}, Δr_0, Δr_s, Δa and Δb in Eqs. (59).

CARD 5 (Necessary only when IFDPR=2 or 3.)

(DRPMAX(N), N=1, 7)

FORMAT (7 F 6. 0)

: δV^{max}, δW^{max}, $\delta V_{so}{}^{max}$, $\delta r_0{}^{max}$, $\delta r_s{}^{max}$, δa^{max} and δb^{max} in Eqs. (47).

CARD 6

(EX(N), N=1, NLEV)

FORMAT (12 F 6. 0)

: Excitation energy of each levels in ascending order.

CARD 7

(SPIN(N), PARITY(N), N=1, NLEV)

FORMAT (12(F 5. 0, A 1))

: Spin and parity of each levels. Parities are punched as + or −.

CARD 8

NANGL, IFCM, IFCOS

FORMAT (3 I 6)

NANGL : Number of angles for which differential cross sections are calculated. (≤ 20)

IFCM : If IFCM=1, the values of angles are those of in the center-of-mass system, and if IFCM=0, they are in the laboratory system.

IFCOS : If IFCOS=1, angles are given by cosine, and if IFCOS=0, they are given in degrees.

CARD 9

(ANG(N) or COSIN(N), N=1, NANGL)

FORMAT (12 F 6. 0)

: Values of angles.

CARD 10

NSRCH0, NSRCH, CHIMIN, TIME, WGTOT, WGEL, WG 1, WGELA, WG 1 A.

FORMAT (2 I 6, 7 F 6. 0)

NSRCH0 and NSRCH: Number of iteration of the parameter search by method (B) and by method (A). Usually method (B) is tried first and then method (A), but if NSRCH<0, method (A) is tried first. Either may be zero.

CHIMIN : Search ends when χ^2 has become smaller than CHIMIN.

TIME : Search is interrupted when calculation time has exceeded TIME. TIME is given in minutes.

WGTOT, WGEL, WG 1, WGELA and WG 1 A:

Weighting factors W_t, W_{el}, W_1, W_{ela} and W_{1a} in Eq. (41).

CARD 11

IFV, VO, (VE(N), N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

IFV : When search is made for the depth V of real potential, * is punched for IFV.

VO : $V^{(0)}$ in Eq. (8).

VE(N) : $V^{(N)}$ in Eq. (8).

CARD 12

IFW, WO (WE(N) N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as CARD 11 for the depth W of imaginary potential.

CARD 13

IFVSO, VSOO, (VSOE(N) N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as CARD 11 for the depth V_{so} of spin-orbit potential.

CARD 14

IFRR, RRO, (RRE(N), N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as CARD 11 for the radius parameter r_0 of real potential

CARD 15

IFRS, RSO, (RSE(N), N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as CARD 11 for the radius parameter r_s of imaginary potential.

CARD 16

IFA, AO, (AE(N), N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as CARD 11 for the diffuseness a of real potential.

CARD 17

IFB, BO, (BE(N), N=1, 5)

FORMAT (A 1, F 11. 0, 5 F 12. 0)

: Same as Card 11 for the diffuseness b of imaginary potential.

CARD 18 (Necessary only when at least one of WGTOT, WGEL and WG 1 is not zero.)

STOTEX, ERTOT, SELEX, EREL, S1STEX, ERIST

FORMAT (6 F 6. 0)

STOTEX and ERTOT : Experimental total cross section and its uncertainty.

SELEX and EREL : Same as above for the elastic scattering cross section.

S1STEX and ER1ST : Same as above for the first level cross section.

(CARD 19–21 are for the experimental values of differential elastic scattering cross sections, and are necessary only when WGELA$\neq$0.)

CARD 19

ERRAT

FORMAT (F 6. 0)

: Uncertainly in cross section in percent. When ratios of uncertainty to cross section are different for various angles, ERRAT is set equal to zero and uncertainties are given on CARD 21.

CARD 20

(SELAEX(N), N=1, NANGL)

FORMAT (12 F 6. 0)

: Values of the differential cross section in mb/sr. For angles where experimental values are lacking, SELAEX (N) are set equal to zero. They are not included in the χ^2 calculation.

CARD 21 (Necessary only when ERRAT=0.)

(ERELA(N), N=1, NANGL)

FORMAT (12 F 6. 0)

: Uncertainty in the above values in mb/sr.

(CARD 22-24 are for the experimental values of differential inelastic scattering cross sections leading to the first excited state, and are necessary only when WG 1 A$\neq$0. The meaning of these cards are same as CARD 19-21.)

CARD 22

ERRAT

FORMAT (F 6. 0)

CARD 23

(S 1 AEX(N), N=1, NANGL)

FORMAT (12 F 6. 0)

CARD 24 (Necessary only when ERRAT=0.)

(ER 1 A(N), N=1, NANGL)

FORMAT (12 F 6. 0)

CARD 25

FCHI, IQCONS, QCONST, BC, REBB, FNR, COMP

FORMAT (F 6. 0, I 6, 5 F 6. 0)

FCHI : Degrees of freedom of the χ^2-distribution for $\Theta_{\mu,nlj}$. IF FCHI=0, cross sections are calculated by means of the Hauser-Feshbach theory.

IQCONS and QCONST: If IQCONS=0, $Q^{J\Pi}$ is calculated as described in Sec. 2. 2. If IQCONS=1, $Q^{J\Pi}$ is set equal to QCONST.

BC : B in Eq. (24).

REBB : $R_{lj;\,l'j'}$ for $(l'j)\neq(l'j')$ in Eq. (25).

FNR : N in Eq. (23).

COMP : α in Eqs. (1) and (2).

7. Requirement for Machine

This program is coded in FORTAN for a FACOM-230/60 computer which has a library subroutine CLOCK which gives the elapsed time in units of Second. Memory size required for this program is about 40K words.

The auther is indebted to S. Igarashi for making available the code ELIESE-2 and for advices. Comparison with the calculation by ELIESE-2 greatly facilitated the error checking of STAX 2. He also wishes to express his thanks to K. Tsukada, K. Okamoto and M. Maruyama for careful reading of the manuscript.

References

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Appendix A Sample Calculation

For illustration, the input and output of a calculation is shown below. In this culculation fitting is tried to the data of Zn at E_n=2.24 MeV by using the largest possible values of Q.

氏名	日付 / /	プログラム名	JOB NO.	カード色指定	PUNCH 73-80
所属	電話	研究テーマ番号	IBJOB DECKNAME	備考	YES □ NO □

```
1969-10-20  Y.TØMITA
      ZN-2.24MEV           Q-MAX
       65.289     65       4      4    2.24
   0.0   1.02  1.835  1.90
    0+      2+     2+     0+
    19
    0.     10.     20.     30.    40.     50.     60.     70.     80.     90.     100.    110.
  120.    130.    140.    150.    160.    170.    180.
   20             .25      5.             1.        1.
*         50.
*         10.
          10.
          1.2
          1.2
*         .65
*         .50
                              .690     .013
     0.
                        550.0   368.1   230.1   137.2   88.0    82.0    90.5   104.8   110.6
  112.0    95.3    92.0   102.2
                         16.0    13.0    10.0     7.8     5.4     5.1     5.4     6.0     6.0
   6.3     5.7     5.4     6.0
   1.0      0         1.        1.       1.       1.
```

ZN-2.24MEV Q-MAX 1969-10-20 Y.TOMITA

MASS OF TARGET NUCLEUS........ 65.2890
MASS NUMBER........................ 65
ENERGY IN LAB. SYSTEM......... 2.2400 MEV
ENERGY IN C.M. SYSTEM......... 2.2059 MEV

	GROUND	1ST	2ND	3RD
E	0.000	1.020	1.835	1.900
SPIN	0 +	2 +	2 +	0 +

INITIAL POTENTIAL PARAMETERS

POWERS OF E	0	1	2	3	4	5
* V	50.000	-0.000	-0.000	-0.000	-0.000	-0.000
* W	10.000	-0.000	-0.000	-0.000	-0.000	-0.000
VSO	10.000	-0.000	-0.000	-0.000	-0.000	-0.000
RR	1.200	-0.000	-0.000	-0.000	-0.000	-0.000
RS	1.200	-0.000	-0.000	-0.000	-0.000	-0.000
* A	0.650	-0.000	-0.000	-0.000	-0.000	-0.000
* B	0.500	-0.000	-0.000	-0.000	-0.000	-0.000

*'S INDICATE THE PARAMETERS TO BE SEARCHED FOR

EXPERIMENTAL CROSS SECTIONS (AND ERRORS)

1ST LEVEL CROSS SECTION... 0.690(0.013) BARN WEIGHT..... 1.000

ELASTIC ANGULAR DISTRIBUTION (MILLIBARN/STERAD.) WEIGHT..... 1.000

ANGLE	CROSS SECTION	ANGLE	CROSS SECTION	ANGLE	CROSS SECTION	ANGLE	CROSS SECTION
0.0	-0.0(-0.0)	10.0	-0.0(-0.0)	20.0	-0.0(-0.0)	30.0	550.0(16.0)
40.0	368.1(13.0)	50.0	230.1(10.0)	60.0	137.2(7.8)	70.0	88.0(5.4)
80.0	82.0(5.1)	90.0	90.5(5.4)	100.0	104.8(6.0)	110.0	110.6(6.0)
120.0	112.0(6.3)	130.0	95.3(5.7)	140.0	92.0(5.4)	150.0	102.2(6.0)
160.0	-0.0(-0.0)	170.0	-0.0(-0.0)	180.0	-0.0(-0.0)		

MQ UNDERFLOW AT 060067

ZN-2.24MEV Q-MAX 1969-10-20 Y.TOMITA

PARAMETER SEARCH

NO.	*V	*W	VSO	RR	RS	*A	*B	TOTAL CROSS SECTION	COMP.FORM. CROSS SECTION	ELASTIC CROSS SECTION TOTAL	SHAPE	COMPOUND	1ST LEVEL CROSS SECTION	CHI-SQUARE	TIME
0	50.000	10.000	10.000	1.200	1.200	0.650	0.500	3.324	1.863	2.243	1.460	0.783	0.683	7.305*	22.7
1*	53.231	10.413	10.000	1.200	1.200	0.615	0.611	3.467	1.953	2.346	1.514	0.832	0.724	2.689*	53.2
2*	54.885	9.091	10.000	1.200	1.200	0.586	0.604	3.309	1.848	2.260	1.461	0.799	0.681	0.624*	83.2

MQ UNDERFLOW AT 060067

NO.	*V	*W	VSO	RR	RS	*A	*B	TOTAL CROSS SECTION	COMP.FORM. CROSS SECTION	ELASTIC CROSS SECTION TOTAL	SHAPE	COMPOUND	1ST LEVEL CROSS SECTION	CHI-SQUARE	TIME
3*	54.801	9.338	10.000	1.200	1.200	0.597	0.594	3.312	1.865	2.252	1.447	0.805	0.688	0.610*	113.0

MQ UNDERFLOW AT 060067

NO.	*V	*W	VSO	RR	RS	*A	*B	TOTAL CROSS SECTION	COMP.FORM. CROSS SECTION	ELASTIC CROSS SECTION TOTAL	SHAPE	COMPOUND	1ST LEVEL CROSS SECTION	CHI-SQUARE	TIME
4*	54.801	9.299	10.000	1.200	1.200	0.596	0.595	3.312	1.863	2.254	1.449	0.805	0.687	0.609*	143.0

MQ UNDERFLOW AT 060067

FINAL POTENTIAL PARAMETERS

POWERS OF E	0	1	2	3	4	5
* V	54.801	-0.000	-0.000	-0.000	-0.000	-0.000
* W	9.299	-0.000	-0.000	-0.000	-0.000	-0.000
VSO	10.000	-0.000	-0.000	-0.000	-0.000	-0.000
RR	1.200	-0.000	-0.000	-0.000	-0.000	-0.000
RS	1.200	-0.000	-0.000	-0.000	-0.000	-0.000
* A	0.596	-0.000	-0.000	-0.000	-0.000	-0.000
* B	0.595	-0.000	-0.000	-0.000	-0.000	-0.000

*'S INDICATE THE PARAMETERS TO BE SEARCHED FOR

TOTAL CROSS SECTION.......... 3.312 BARN
ABSORPTION CROSS SECTION..... 1.863 BARN
SHAPE ELASTIC CROSS SECTION.. 1.449 BARN
CHI-SQUARE VALUE............. 0.609

TRANSMISSION COEFFICIENTS

LEVEL		GROUND	1ST	2ND	3RD
ECM (EXIT)		2.206	1.186	0.371	0.306
MESH		0.250	0.250	0.250	0.250
MATCH. RADIUS		14.979	15.236	15.991	16.241
L	L-S				
0	+	7.2579E-01	6.7528E-01	5.1629E-01	4.8683E-01
1	-	6.3922E-01	4.4889E-01	1.5751E-01	1.2659E-01
1	+	7.8605E-01	5.8511E-01	2.1475E-01	1.7277E-01
2	-	5.5007E-01	2.9226E-01	3.1704E-02	2.0422E-02
2	+	3.4701E-01	1.6961E-01	1.9508E-02	1.2748E-02
3	-	8.5040E-02	1.2634E-02	2.6281E-04	1.3600E-04
3	+	2.0112E-01	2.7640E-02	5.1735E-04	2.6552E-04
4	-	9.7385E-03	7.5084E-04	0.	0.
4	+	7.0109E-03	5.5110E-04	0.	0.
5	-	3.0413E-04	1.2353E-05	0.	0.
5	+	6.7813E-04	2.6867E-05	0.	0.
6	-	1.0997E-05	0.	0.	0.
6	+	1.5602E-05	0.	0.	0.

S-MATRIX ELEMENTS FOR THE ELASTIC CHANNELS

	L-S -		L-S +	
L	REAL PART	IMAGENARY PART	REAL PART	IMAGENARY PART
0			-2.18351E-01	4.75951E-01
1	3.19318E-01	-5.08737E-01	3.17079E-01	-3.36771E-01
2	5.84469E-01	-3.29129E-01	7.22493E-01	-3.62065E-01
3	9.56496E-01	8.69566E-03	8.93229E-01	3.20154E-02
4	9.95119E-01	1.76826E-04	9.96486E-01	2.08633E-03
5	9.99848E-01	1.01511E-04	9.99661E-01	1.73409E-04
6	9.99994E-01	4.33369E-06	9.99992E-01	1.34409E-05

VARIOUS STATISTICAL QUANTITIES

CALCULATION OF COMPOUND PROCESS WAS CARRIED OUT BY USING MOLDAUER'S THEORY

N = 1.000
BC= 1.000
REAL PART OF THE RELATIVE PHASE OF SQUARES OF REDUCED WIDTH AMPLITUDES BETWEEN DIFFERENT CHANNELS.... 1.000
DEGREE OF FREEDOM OF CHI-SQUARE DISTRIBUTION FOR SQUARES OF REDUCED WIDTH AMPLITUDE................. 1.000

TOTAL SPIN PARITY	TOTAL STRENGTH FUNCTION	COMPOUND FORMATION CROSS SECTION	Q
1/2-	1.8829	0.192	1.002
1/2+	2.0458	0.217	0.963
3/2-	2.7752	0.471	0.822
3/2+	2.6063	0.330	0.851
5/2-	1.7579	0.076	1.033
5/2+	2.3614	0.312	0.897
7/2-	1.2413	0.241	1.189
7/2+	0.5782	0.012	1.483
9/2-	0.0419	0.000	1.926
9/2+	0.2124	0.011	1.740
11/2-	0.0293	0.001	1.945
11/2+	0.0013	0.000	1.996
13/2-	0.0000	0.000	2.000
13/2+	0.0006	0.000	1.998

GROUND 0.000 MEV. 0 +

LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	COMPOUND ELASTIC	SHAPE ELASTIC	TOTAL ELASTIC
0.00	1.000	0.00	1.000	135.10	852.59	987.69
10.00	0.985	10.15	0.984	128.40	800.28	928.68
20.00	0.940	20.30	0.938	111.45	660.24	771.69
30.00	0.866	30.44	0.862	91.37	475.11	566.48
40.00	0.766	40.57	0.760	74.36	294.34	368.70
50.00	0.643	50.68	0.634	62.56	155.05	217.61
60.00	0.500	60.77	0.488	54.77	72.00	126.77
70.00	0.342	70.83	0.328	49.18	39.08	88.25
80.00	0.174	80.87	0.159	45.38	38.12	83.50
90.00	0.000	90.89	-0.015	44.15	49.10	93.25
100.00	-0.174	100.87	-0.189	45.88	57.26	103.14
110.00	-0.342	110.83	-0.356	49.99	55.88	105.87
120.00	-0.500	120.77	-0.512	55.78	45.45	101.23
130.00	-0.643	130.68	-0.652	63.87	30.70	94.57
140.00	-0.766	140.57	-0.772	76.01	17.09	93.10
150.00	-0.866	150.44	-0.870	93.07	8.11	101.18
160.00	-0.940	160.30	-0.941	112.63	4.20	116.83
170.00	-0.985	170.15	-0.985	128.78	3.49	132.27
180.00	-1.000	180.00	-1.000	135.10	3.60	138.70
INTEGRATED CROSS SECTION..........				0.805	1.449	2.254

1ST 1.020 MEV. 2 +

LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION	LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION
0.00	1.000	0.00	1.000	54.17	100.00	-0.174	101.19	-0.194	54.13
10.00	0.985	10.21	0.984	54.33	110.00	-0.342	111.13	-0.361	54.46
20.00	0.940	20.41	0.937	54.73	120.00	-0.500	121.05	-0.516	54.87
30.00	0.866	30.60	0.861	55.12	130.00	-0.643	130.92	-0.655	55.19
40.00	0.766	40.78	0.757	55.28	140.00	-0.766	140.78	-0.775	55.27
50.00	0.643	50.92	0.630	55.14	150.00	-0.866	150.60	-0.871	55.08
60.00	0.500	61.05	0.484	54.78	160.00	-0.940	160.41	-0.942	54.69
70.00	0.342	71.13	0.323	54.37	170.00	-0.985	170.21	-0.985	54.32
80.00	0.174	81.19	0.153	54.07	180.00	-1.000	180.00	-1.000	54.17
90.00	0.000	91.21	-0.021	53.98					

INTEGRATED CROSS SECTION.......... 0.687

2ND 1.835 MEV. 2 +

LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION	LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION
0.00	1.000	0.00	1.000	23.01	100.00	-0.174	102.13	-0.210	22.26
10.00	0.985	10.37	0.984	22.99	110.00	-0.342	112.03	-0.375	22.36
20.00	0.940	20.74	0.935	22.94	120.00	-0.500	121.87	-0.528	22.50
30.00	0.866	31.08	0.856	22.86	130.00	-0.643	131.65	-0.665	22.64
40.00	0.766	41.39	0.750	22.74	140.00	-0.766	141.39	-0.781	22.77
50.00	0.643	51.65	0.620	22.59	150.00	-0.866	151.08	-0.875	22.88
60.00	0.500	61.87	0.471	22.44	160.00	-0.940	160.74	-0.944	22.95
70.00	0.342	72.03	0.309	22.32	170.00	-0.985	170.37	-0.986	22.99
80.00	0.174	82.13	0.137	22.24	180.00	-1.000	180.00	-1.000	23.01
90.00	0.000	92.16	-0.038	22.22					

INTEGRATED CROSS SECTION.......... 0.283

3RD 1.900 MEV. 0 +

LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION	LAB. ANGLE	LAB. COSINE	C.M. ANGLE	C.M. COSINE	CROSS SECTION
0.00	1.000	0.00	1.000	9.83	100.00	-0.174	102.34	-0.214	5.93
10.00	0.985	10.41	0.984	9.68	110.00	-0.342	112.23	-0.378	6.28
20.00	0.940	20.81	0.935	9.25	120.00	-0.500	122.06	-0.531	6.79
30.00	0.866	31.19	0.855	8.62	130.00	-0.643	131.82	-0.667	7.43
40.00	0.766	41.53	0.749	7.90	140.00	-0.766	141.53	-0.783	8.11
50.00	0.643	51.82	0.618	7.18	150.00	-0.866	151.19	-0.876	8.78
60.00	0.500	62.06	0.469	6.56	160.00	-0.940	160.81	-0.944	9.33
70.00	0.342	72.23	0.305	6.10	170.00	-0.985	170.41	-0.986	9.70
80.00	0.174	82.34	0.133	5.83	180.00	-1.000	180.00	-1.000	9.83
90.00	0.000	92.38	-0.041	5.78					

INTEGRATED CROSS SECTION.......... 0.089

TIME REQUIRED .... 176.5 SEC.

END-OF-DATA ENCOUNTERED ON SYSTEM INPUT FILE.

Appendix B Symbolic listing of STAX 2

```
C       STAX2        MAIN PROGRAM
C           OPTICAL MODEL AND MOLDAUER'S THEORY
C
       DIMENSION
      1                  ANG(19),COSIN(19),ANGLAB(19,25),COSLAB(19,25),
      2                  ANGCM(19,25),
      5                  LNAME(25),HALF(2),ISPIN(25),SIGLS(2)
C
       COMMON   /CFAC/FACO,FAC(100),EFACO,FFAC(100) /CDFG/DFGO
      1         /CLEV/NLEV,EX(25),SPIN(25),NPAR(25),NLMAX(25),DJ,NLMAXA
      2         /CSTA/T(11,2,25),TH(11,2,25),THTOT(21,2),Q(21,2),IQCONS,
      3               QCONST,FNR2,BC,REBB,FCHI,COMP
      4         /CKIN/EN(25),FK(25),HM,PLAM,PLAMO,PLAM1,FNM13,COMPAI
      5         /CWAV/PHIPRE,DR,DRN(25),RMATN(25)
      6         /CPOT/PARA(7),VE(5),WE(5),VSOE(5),RRE(5),RSE(5),AE(5),
      7               BE(5)
      8         /CCRS/NANGL,STOT,SABS,SEL,SSEL,SG(25),SELA(19),SSELA(19),
      9               SGA(19,25),PLAMEL
       COMMON   /CTON/TITLE(18),DATE(3),NAME(3),IFPARA(7),TIME1
       COMMON   /CEXP/IFEXP,WEIGHT,WGTOT,WGEL,WG1,
      1               WGELA,WG1A,STOTEX,ERTOT,SELEX,EREL,S1STEX,ER1ST,
      2               SELAEX(19),ERELA(19),S1AEX(19),ER1A(19)
      4         /CINT/XI0(8),WI0(8),XI1(8),XI2(8),XL1(8),XL2(8),
      5               XD1(8),XD2(8)
       COMPLEX        YETA(11,2)
       COMMON   /CYET/YETA/COMJ/NJMIN,NJMAX,NLMAXO(3),COSCM(19,25),IFFL
      1         /CDPR/CHIMIN,NPARA,PARA1(7),DPARA(7),DRPMAX(7),RAT(7),
      2               IDPAR(7),NPRE
C
       EQUIVALENCE     (IFV,IFPARA(1)),(IFW,IFPARA(2)),(IFVSO,IFPARA(3)),
      1                (IFRR,IFPARA(4)),(IFRS,IFPARA(5)),(IFA,IFPARA(6)),
      2                (IFB,IFPARA(7)),
      3                (VO,PARA(1)),(WO,PARA(2)),(VSOO,PARA(3)),
      4                (RRO,PARA(4)),(RSO,PARA(5)),(AO,PARA(6)),
      5                (BO,PARA(7))
C
       INTEGER         PARITY(25),PLUS,TIME1,TEND,TIME2
       DATA       PLUS,MINUS/1H+,1H-/,ISTAR/1H*/,HALF/2H  ,2H/2/,
      1           SIGLS/1H-,1H+/,
      2           LNAME(1)/4HGRD./,LNAME(2)/4H 1ST/,LNAME(3)/4H 2ND/,
      3           LNAME(4)/4H 3RD/,LNAMEO/4H OTH/,
      4           FMN/1.008665/,AMUMEV/.02392386/,COMPAI/2.04264/,
      7           DFGO/5.0/
       DATA        XI0/          .09501251,.28160355,.45801678,.61787624,
      1                          .75540441,.86563120,.94457502,.98940093/,
      2            WI0/          .18945061,.18260342,.16915652,.14959599,
      3                          .12462897,.09515851,.06225352,.02715246/
C
       CALL   OVERFL(NOVFL)
       CALL   FACTRL
       DO  5 I=1,8
       XI1(I)=(1.+XI0(I))*.5
       XI2(I)=(1.-XI0(I))*.5
       XL1(I)=2.*ALOG(XI1(I))
       XL2(I)=2.*ALOG(XI2(I))
       XD1(I)=XI1(I)**(DEGO-1.)

     5 XD2(I)=XI2(I)**(DEGO-1.)
    10 CALL   CLOCK(TIME1)
       READ (5,1010) DATE,NAME
  1010 FORMAT(18A4)
       READ (5,1010) TITLE
       READ (5,1020) FMASST,NOMASS,NLEV,NLOUT,ELAB,PHIPRE,DR,ITEST,IFDPR
      1              ,NPRE
       IF (PHIPRE.EQ.0.) PHIPRF=1.E-6
       IF (DR.EQ.0.) DR=.25
       NPRE=MAXO(NPRE,5)
  1020 FORMAT (F12.0,3I6,F6.0,E12.3,F6.0,3I6)
       IF (IFDPR.EQ.1.OR.IFDPR.EQ.3) GO TO 1021
       DPARA(1)=.1
       DPARA(2)=.1
       DPARA(3)=.1
       DPARA(4)=.005
       DPARA(5)=.005
       DPARA(6)=.003
       DPARA(7)=.003
       GO TO 1022
  1021 READ (5,1030)DPARA
  1022 FNM13=(FLOAT(NOMASS))**(1./3.)
       IF (NLOUT.EQ.0) NLOUT=NLEV
       IF (IFDPR.EQ.2.OR.IFDPR.EQ.3) GO TO 1024
       DRPMAX(1)=3.0
       DRPMAX(2)=3.0
       DRPMAX(3)=3.0
       DRPMAX(4)=.05
       DRPMAX(5)=.1
       DRPMAX(6)=.07
       DRPMAX(7)=.1
       GO TO 1025
  1024 READ (5,1030) DRPMAX
  1025 READ (5,1030) (EX(N),N=1,NLEV)
  1030 FORMAT (12F6.0)
       DO  1035 I=1,7
  1035 RAT(I)=DRPMAX(I)/DPARA(I)
       READ (5,1040) (SPIN(N),PARITY(N),N=1,NLEV)
  1040 FORMAT (12(F5.0,A1))
       DO  1041 N=1,NLEV
       NPAR(N)=1
       IF (PARITY(N).EQ.MINUS) NPAR(N)=-1
       IF (NPAR(N).EQ.1) PARITY(N)=PLUS
  1041 CONTINUE
       DJ=SPIN(1)-AINT(SPIN(1)+.1)+.5
       ECM=ELAB*FMASST/(FMN+FMASST)
       FMREL=FMN*FMASST/(FMN+FMASST)
       HM=FMREL*2.*AMUMEV
       READ (5,1050) NANGL,IFCM,IFCOS
  1050 FORMAT (12I6)
       RAD=3.1415927/180.
       IF (IFCOS.NE.0) GO TO 1090
       READ (5,1030) (ANG(NA),NA=1,NANGL)
       DO  1080 NA=1,NANGL
  1080 COSIN(NA)=COS(RAD*ANG(NA))
       GO TO 1105

  1090 READ (5,1030) (COSIN(NA),NA=1,NANGL)
       DO  1100 NA=1,NANGL
  1100 ANG(NA)=ARCOS(COSIN(NA))/RAD
  1105 DO  1140 N=1,NLEV
       EN(N)=ECM-EX(N)
       IF (EN(N).LE.0.) GO TO 1150
       FK(N)=SQRT(EN(N)*HM)
       GAM=FMN/(FMASST*SQRT(EN(N)/ECM))
       IF  (IFCM.NE.0) GO TO 1120
       DO  1110 NA=1,NANGL
       ANGLAB(NA,N)=ANG(NA)
       COSLAB(NA,N)=COSIN(NA)
       SQR2=1.-GAM**2*(1.-COSIN(NA)**2)
       IF (SQR2.LT.0.)    GO TO 1108
       COSCM(NA,N)=COSIN(NA)*SQRT(SQR2)
      1              -GAM*(1.-COSIN(NA)**2)
       ANGCM(NA,N)=ARCOS(COSCM(NA,N))/RAD
       GO TO 1110
  1108 ANGLAB(NA,N)=0.
       COSLAB(NA,N)=1.
       ANGCM(NA,N)=0.
       COSCM(NA,N)=1.
  1110 CONTINUE
       GO TO 1140
  1120 DO  1130 NA=1,NANGL
       COSLAB(NA,N)=(GAM+COSIN(NA))/SQRT(1.+GAM*(GAM+2.*COSIN(NA)))
       ANGLAB(NA,N)=ARCOS(COSLAB(NA,N))/RAD
       ANGCM (NA,N)=ANG(NA)
  1130 COSCM (NA,N)=COSIN(NA)
  1140 CONTINUE
       GO TO 1300
  1150 NLEV=N-1
       IF (NLOUT.GT.NLEV) NLOUT=NLEV
  1300 DO  1310 N=1,3
  1310 NLMAXO(N)=0
       CALL   OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98765)
 98765 FORMAT (/////5X,15H*****MAIN    2 ////)
       IFFL=0
       IF (NLEV.LE.4) GO TO 2000
       DO  1410 N=5,NLEV
       M10=(N-1)/10
       M1=N-10*M10-1
       LNAME(N)=LNAMEO+M1*8**6
       IF (M10.NE.0) LNAME(N)=LNAME(N)+22*8**10+M10*8**9
  1410 CONTINUE
  2000 READ (5,2010) NSRCHO,NSRCH,CHIMIN,TIME,WGTOT,WGEL,WG1,WGELA,WG1A
  2010 FORMAT (2I6,7F6.0)
       TEND=TIME1+INT(TIME*60.)
       IFEXP=1
       IF (WGTOT.EQ.0..AND.WGEL.EQ.0..AND.WG1.EQ.0..AND.WGELA.EQ.0..AND.
      1    WG1A.EQ.0.) IFEXP=0
       READ (5,2020) IFV,VO,(VE(I),I=1,5)
       READ (5,2020) IFW,WO,(WE(I),I=1,5)
       READ (5,2020) IFVSO,VSOO,(VSOE(I),I=1,5)
       READ (5,2020) IFRR,RRO,(RRE(I),I=1,5)
       READ (5,2020) IFRS,RSO,(RSE(I),I=1,5)
       READ (5,2020) IFA,AO,(AE(I),I=1,5)
       READ (5,2020) IFB,BO,(BE(I),I=1,5)
  2020 FORMAT (A1,F11.0,5F12.0)
       IF (WGTOT.EQ.0..AND.WGEL.EQ.0..AND.WG1.EQ.0.) GO TO 2030
       READ (5,1030) STOTEX,ERTOT,SELEX,EREL,S1STEX,ER1ST
  2030 IF (WGELA.EQ.0.)     GO TO 2060
       READ (5,1030) ERRAT
       READ (5,1030) (SELAEX(NA),NA=1,NANGL)
       IF (ERRAT.EQ.0.) GO TO 2050
       DO  2040 NA=1,NANGL
  2040 ERELA(NA)=ERRAT*SELAEX(NA)*.01
       GO TO 2060
  2050 READ (5,1030) (ERELA(NA),NA=1,NANGL)
  2060 IF (WG1A.EQ.0.)GO TO 2100
       READ (5,1030) ERRAT
       READ (5,1030) (S1AEX(NA),NA=1,NANGL)
       IF (ERRAT.EQ.0.) GO TO 2080
       DO  2070 NA=1,NANGL
  2070 ER1A(NA)=ERRAT*S1AEX(NA)*.01
       GO TO 2100
  2080 READ (5,1030) (ER1A(NA),NA=1,NANGL)
C
  2100 NPARA=0
       DO  2110 I=1,7
       IF (IFPARA(I).NE.ISTAR) GO TO 2110
       NPARA=NPARA+1
       IDPAR(NPARA)=I
  2110 CONTINUE
       N1=0.
       N2=0.
       DO  2140 NA=1,NANGL
       IF (WGELA.EQ.0.) GO TO 2130
       IF (SELAEX(NA).GT.0.) N1=N1+1
  2130 IF (WG1A.EQ.0.) GO TO 2140
       IF (S1AEX(NA).GT.0.)  N2=N2+1
  2140 CONTINUE
       WEIGHT=WGTOT+WGEL+WG1+WGELA*FLOAT(N1)+WG1A*FLOAT(N2)
C
       READ (5,2210) FCHI,IQCONS,QCONST,BC,REBB,FNR,COMP
  2210 FORMAT (F6.0,I6,5F6.0)
       FNR2=FNR**2
C
       PLAMO=.031415927/FK(1)**2
       PLAM1=PLAMO/(SPIN(1)+.5)
       PLAMFL=2.5/FK(1)**2
       PLAM=PLAMFL/(SPIN(1)+.5)
       WRITE (6,3010) TITLE,DATE,NAME
  3010 FORMAT (1H1,4X,18A4,20X,6A4)
       WRITE (6,3020) FMASST,NOMASS,ELAB,ECM
  3020 FORMAT(/5X,30HMASS OF TARGET NUCLEUS........,F9.4,
      1         /5X,35HMASS NUMBER.......................,I4,
      2         /5X,30HENERGY IN LAB. SYSTEM.........,F9.4,4H MEV,
      3         /5X,30HENERGY IN C.M. SYSTEM.........,F9.4,4H MEV//)
       I2DJ=2.*DJ+.1
       SPIN2=HALF(I2DJ)

       LINE=(NLEV  +14)/15
       DO  3060 L=1,LINE
       N2=15*L
       N1=N2-14
       IF (L.EQ.LINE) N2=NLEV
       WRITE (6,3030) (LNAME(N),N=N1,N2)
  3030 FORMAT (11X,15A8)
       WRITE (6,3040) (EX(N),N=N1,N2)
  3040 FORMAT(7X,4HE    ,15F8.3)
       DO  3050 N=N1,N2
  3050 ISPIN(N)=2.*DJ*SPIN(N)+.1
  3060 WRITE(6,3070) (ISPIN(N),SPIN2,PARITY(N),N=N1,N2)
  3070 FORMAT (7X,4HSPIN,15(I5,A2,A1)/)
C
       WRITE (6,3100)
       WRITE(6,3110) (I,I=1,5),IFV,VO,(VE(I),I=1,5),IFW,WO,(WE(I),I=1,5),
      1      IFVSO,VSOO,(VSOE(I),I=1,5),IFRR,RRO,(RRE(I),I=1,5),
      2      IFRS,RSO,(RSE(I),I=1,5),IFA,AO,(AE(I),I=1,5),
      3      IFB,BO,(BE(I),I=1,5)
  3100 FORMAT ( //5X,28HINITIAL POTENTIAL PARAMETERS)
  3110 FORMAT                                       (//10X,18HPOWERS OF E
      1      0,5I8/14X,A1,2H V,3X,6F8.3/14X,A1,2H W,3X,6F8.3/14X,A1,4H VSO
      2,1X,6F8.3/14X,A1,3H RR,2X,6F8.3/14X,A1,3H RS,2X,6F8.3/14X,A1,2H A,
      33X,6F8.3/14X,A1,2H B,3X,6F8.3/10X,46H*'S INDICATE THE PARAMETERS T
      4O BE SEARCHED FOR/)
C
       IF (IFEXP.EQ.0) GO TO 4520
       WRITE (6,3210)
  3210 FORMAT(///5X,40HEXPERIMENTAL CROSS SECTIONS (AND ERRORS)/)
       IF (WGTOT.EQ.0.)GO TO 3230
       WRITE (6,3220) STOTEX,ERTOT,WGTOT
  3220 FORMAT(8X,26HTOTAL CROSS SECTION.......,F7.3,1H(,F6.3,6H) BARN,
      1         9X,11HWEIGHT.....,F7.3)
  3230 IF (WGEL.EQ.0.)GO TO 3250
       WRITE (6,3240) SELEX,EREL,WGEL
  3240 FORMAT(8X,26HELASTIC CROSS SECTION.....,F7.3,1H(,F6.3,6H) BARN,
      1         9X,11HWEIGHT.....,F7.3)
  3250 IF (WG1.EQ.0.)GO TO 3270
       WRITE (6,3260) S1STEX,ER1ST,WG1
  3260 FORMAT(8X,26H1ST LEVEL CROSS SECTION...,F7.3,1H(,F6.3,6H) BARN,
      1         9X,11HWEIGHT.....,F7.3)
  3270 IF (WGELA.EQ.0.)GO TO 3310
       WRITE (6,3280) WGELA
  3280 FORMAT(/8X,48HELASTIC ANGULAR DISTRIBUTION (MILLIBARN/STERAD.),
      1         7X,11HWEIGHT.....,F7.3/8X,
      2         4(5X,5HANGLE,2X,13HCROSS SECTION))
       LINE=(NANGL+3)/4
       DO  3290 L=1,LINE
       N2=4*L
       N1=N2-3
       N2=MINO(N2,NANGL)
  3290 WRITE (6,3300) (ANG(NA),SELAEX(NA),ERELA(NA),NA=N1,N2)
  3300 FORMAT (8X,4(F10.1,F7.1,1H(F6.1,1H)))
  3310 IF (WG1A.EQ.0.)GO TO 3400
       WRITE (6,3320) WG1A
  3320 FORMAT(/8X,50H1ST-LEVEL ANGULAR DISTRIBUTION (MILLIBARN/STERAD.),

      1         5X,11HWEIGHT.....,F7.3/
      2         8X,4(5X,5HANGLE,2X,13HCROSS SECTION))
       LINE=(NANGL+3)/4
       DO  3330 L=1,LINE
       N2=4*L
       N1=N2-3
       N2=MINO(N2,NANGL)
  3330 WRITE (6,3300) (ANG(NA),S1AEX(NA),ER1A(NA),NA=N1,N2,LINE)
  3400 IF (NSRCHO.EQ.0.AND.NSRCH.EQ.0) GO TO 4520
       NLO=1
       IF (WG1.NE.0..OR.WG1A.NE.0.) NLO=2
       NLD=0
       IF (WGELA.NE.0.) NLD=1
       IF (WG1A.NE.0.) NLD=2
C
       DO  4260 I=1,7
  4260 PARA1(I)=PARA(I)
C
       CALL   OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98766)
 98766 FORMAT (/////5X,15H*****MAIN    3 ////)
       CALL   SEARCH(NSRCH,NSRCHO,NLO,NLD,ITEST,TEND)
       CALL   OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98704)
 98704 FORMAT (/////5X,15H*****MAIN     4////)
C
C
C
  4500 DO  4510 I=1,7
  4510 PARA(I)=PARA1(I)
  4520 CALL   XSECT(NLOUT,NLOUT,PARA,SQCHIO,1,2)
C
  4610 WRITE (6,3010) TITLE,DATE,NAME
       LINE=1
       IF (NSRCH.EQ.0.AND.NSRCHO.EQ.0) GO TO 4613
       WRITE (6,4611)
  4611 FORMAT (/5X,26HFINAL POTENTIAL PARAMETERS)
       WRITE (6,3110) (I,I=1,5),IFV,VO,VE,IFW,WO,WE,IFVSO,VSOO,VSOE,
      1                IFRR,RRO,RRE,IFRS,RSO,RSE,IFA,AO,AE,IFB,BO,BE
       LINE=LINE+14
  4613 WRITE (6,4614)
  4614 FORMAT (//)
       WRITE (6,4620) STOT,SABS,SSEL
  4620 FORMAT (/5X,29HTOTAL CROSS SECTION...........,F7.3,5H BARN,
      1          /5X,29HABSORPTION CROSS SECTION.....,F7.3,5H BARN,
      2          /5X,29HSHAPE ELASTIC CROSS SECTION...,F7.3,5H BARN)
       LINE=LINE+8
       IF (IFEXP.EQ.0) GO TO 4640
       WRITE (6,4630) SQCHIO
  4630 FORMAT (5X,29HCHI-SQUARE VALUE..............,F12.3)
       LINE=LINE+1
  4640 WRITE (6,4650)
  4650 FORMAT (//3X,25HTRANSMISSION COEFFICIENTS)
       MG=(NLEV+9)/10
       LINE=LINE+3
       DO  4830 NG=1,MG
```

```
      N2=10*NG
      N1=N2-9
      N2=MIN0(N2,NLEV)
      LINE=LINE+5+2*NLMAXA
      IF (LINE.LE.58) GO TO 4730
      LINE=2*NLMAXA+8
      WRITE (6,3010) TITLE,DATE,NAME
      WRITE (6,4720)
4720 FORMAT (/3X,24HTRANSMISSION COEFFICIENT/)
      GO TO 4750
4730 WRITE (6,4740)
4740 FORMAT (/)
4750 WRITE (6,4760) (LNAME(N),N=N1,N2)
4760 FORMAT (5X,5HLEVEL,8X,10A11)
      WRITE (6,4770) (EN(N),N=N1,N2)
4770 FORMAT (5X,10HECM (FX1T),3X,10F11.3)
      WRITE (6,4780) (DHN(N),N=N1,N2)
4780 FORMAT (5X,4HMESH,9X,10F11.3)
      WRITE (6,4790) (RMATN(N),N=N1,N2)
4790 FORMAT (5X,13HMATCH. RADIUS,10F11.3)
      WRITE (6,4800)
4800 FORMAT (11X,1HL,2X,3HL-S)
      DO  4830 NL=1,NLMAXA
      J1=1
      IF(NL.EQ.1) J1=2
      L=NL-1
      DO  4830 J=J1,2
4830 WRITE (6,4840)  L,SIGLS(J),(T(NL,J,N),N=N1,N2)
4840 FORMAT (9X,I3,3X,A1,2X,1P10E11.4)
      LIN1=NLMAX(1)+7
      IF (FCHI.EQ.0..AND.COMP.NE.0.) LIN1=LIN1+4
      LINE=LINE+LIN1
      IF (LINE.LE.58) GO TO 4850
      WRITE (6,3010) TITLE,DATE,NAME
      LINE=LIN1+1
4850 WRITE (6,4860)
4860 FORMAT (///3X,42HS-MATRIX ELEMENTS FOR THE ELASTIC CHANNELS//
     1        26X,5HL=S =,28X,5HL=S +/10X,1HL,2(6X,9HREAL PART,4X,
     2        14HIMAGENARY PART))
      NL1=NLMAX(1)
      WRITE (6,4870) YETA(1,2)
4870 FORMAT (10X,1H0,35X,1P2E15.5)
      DO  4880 NL=2,NL1
      L=NL-1
4880 WRITE (6,4890) L,(YETA(NL,J),J=1,2)
4890 FORMAT (8X,I3,2(2X,1P2E15.5,1X))
      IF (COMP.EQ.0.) GO TO 5410
      LINE=LINE+6
      IF (FCHI.EQ.0.) GO TO 5010
      LINE=LINE+2*(NJMAX-NJMIN)+12
5010 IF (LINE.LE.58) GO TO 5050
      WRITE (6,3010) TITLE,DATE,NAME
5050 IF (FCHI.EQ.0.) GO TO 5080
      WRITE (6,5060)
5060 FORMAT (///3X,30HVARIOUS STATISTICAL QUANTITIES//10X,68HCALCULATIO
     1N OF COMPOUND PROCESS WAS CARRIED OUT BY USING MOLDAUER'S , 6HTHEO

     2RY)
      WRITE (6,5070) FNR,RC,RFRB,FCHI
5070 FORMAT (/10X,3HN =,F6.3/10X,3HBC=,F6.3/10X,101HREAL PART OF THE RE
     1LATIVE PHASE OF SQUARES OF REDUCED WIDTH AMPLITUDES BETWEEN DIFFER
     2ENT CHANNELS....,F6.3/10X,101HDEGREE OF FREEDOM OF CHI-SQUARE DIST
     3RIBUTION FOR SQUARES OF REDUCED WIDTH AMPLITUDE..................
     4F6.3)
      GO TO 5110
5080 WRITE (6,5090)
5090 FORMAT (///10X,75HCALCULATION OF COMPOUND PROCESS WAS CARRIED OUT
     1BY USING HAUSER-FESHBACH'S ,6HTHEORY)
5110 IF (COMP.EQ.0.) GO TO 5130
      IF (COMP.EQ.1.0) GO TO 5130
      WRITE (6,5120) COMP
5120 FORMAT (10X,101HCOMPOUND CROSS SECTIONS WERE MULTIPLIED BY A FACTO
     1R..................................................,F6.3)
5130 IF (FCHI.EQ.0.) GO TO 5500
      WRITE (6,5150)
5150 FORMAT (//10X,6HTOTAL ,4X,8H TOTAL  ,4X,13H  COMPOUND   /
     1        10X,6H SPIN ,4X,8HSTRENGTH,4X,13H  FORMATION  /
     2        10X,6HPARITY,4X,8HFUNCTION,4X,13HCROSS SECTION,7X,1H0)
      NHF=3-1-2.*DJ
      DO  5240 NJ=NJMIN,NJMAX
      FJ=FLOAT(NJ)-DJ
      JOUT=FLOAT(NHF)*FJ+.1
      DO  5240 NOPAR=1,2
      SCOMP=0.
      NLMIN=1
      IF (2*NOPAR-3.NE.NPAR(1)) NLMIN=2
      DO  5230 J=1,2
      NL1=ABS(FJ-SPIN(1))-FLOAT(J)+2.6
      NL1=NL1+MOD(NL1+NLMIN,2)
      NL2=FJ+SPIN(1)-FLOAT(J)+2.6
      NL2=MIN0(NL2,NLMAX(1))
      IF (NL1.GT.NL2) GO TO 5230
      DO  5210 NL=NL1,NL2
5210 SCOMP=SCOMP+T(NL,J,1)
5230 CONTINUE
      SCOMP=SCOMP*(FJ+.5)/(2.*SPIN(1)+1.)*0.031415927/FK(1)**2
5240 WRITE (6,5250)  JOUT,HALF(NHF),SIGLS(NOPAR),THTOT(NJ,NOPAR),SCOMP,
     1               B(NJ,NOPAR)
5250 FORMAT (10X,I3,A2,A1,4X,F8.4,4X,F10.3,3X,F10.3)
      GO TO 5500
C
5410 WRITE (6,5420)
5420 FORMAT (3X,48HONLY SHAPE ELASTIC CROSS SECTION WAS CALCULATED.)
C
5500 WRITE (6,3010) TITLE,DATE,NAME
5710 WRITE (6,5720) LNAME(1),EX(1),ISPIN(1),SPIN2,PARITY(1)
5720 FORMAT (//5X,A6,F9.3,3H MEV,,I5,A2,A1)
5730 FORMAT            (/22X,4HLAB.,4X,4HLAB.,6X,4HC.M.,4X,4HC.M.,4X,8HCOM
     1POUND,4X,5HSHAPE,5X,5HTOTAL/21X,5HANGLE,3X,6HCOSINE,4X,5HANGLE,3X,
     26HCOSINE,4X,7HELASTIC,3X,7HELASTIC,3X,7HELASTIC)
      WRITE (6,5730)
      DO  5760 NA=1,NANGL
5760 WRITE (6,5770) ANGLAB(NA,1),COSLAB(NA,1),ANGCM(NA,1),COSCM(NA,1),

     1               SGA(NA,1),SSELA(NA),SELA(NA)
5770 FORMAT (20X,F7.2,F8.3,F10.2,F8.3,1X,3F10.2)
      WRITE (6,5780) SG(1),SSEL,SEL
5780 FORMAT (/20X,34HINTEGRATED CROSS SECTION..........,3F10.3)
      LINE=NANGL+9
      IF (NLOUT.EQ.1) GO TO 5980
      NANG2=(NANGL+1)/2
      DO  5900 N=2,NLOUT
      LINE=LINE+ 9+NANG2
      IF (N.EQ.NLOUT) LINE=LINE+2
      IF (LINE.LE.58) GO TO 5820
      LINE=NANG2+9
      WRITE (6,3010) TITLE,DATE,NAME
      GO TO 5840
5820 WRITE (6,5830)
5830 FORMAT (1H0)
5840 WRITE (6,5720) LNAME(N),EX(N),ISPIN(N),SPIN2,PARITY(N)
      WRITE (6,5850)
5850 FORMAT(/12X,2(10X,4HLAB.,4X,4HLAB.,6X,4HC.M.,4X,4HC.M.,5X,7H CROSS
     1 )/12X,2(9X,5HANGLE,3X,6HCOSINE,4X,5HANGLE,3X,6HCOSINE,4X,7HSECTIO
     2N))
      DO  5880 NA=1,NANG2
5880 WRITE (6,5890) (ANGLAB(NA,N),COSLAB(NA,N),ANGCM(NA,N),COSCM(NA,N),
     1               SGA(NA,N),NA=NA,NANGL,NANG2)
5890 FORMAT (12X,2(F15.2,F8.3,F10.2,F8.3,F11.2))
5900 WRITE (6,5780) SG(N)
5980 CALL  CLOCK(TIME2)
      TIME2=TIME2-TIME1
      WRITE (6,6000) TIME2
6000 FORMAT (/5X,29HTIME REQUIRED ..............,  I7,5H SEC.)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98705)
98705 FORMAT (/////5X,15H*****MAIN      5////)
7000 GO TO 10
      END
C  PARAMETER SEARCH
      SUBROUTINE    SEARCH(NSRCH,NSRCHO,NLO,NLD,ITEST,TEND)
C
      COMMON  /CCRS/NANGL,STOT,SABS,SEL,SSEL,SG(25),SELA(19),SSELA(19),
     1            SGA(19,25),PLAMEL
     2        /CSGT/STOTT,SABST,SELT,SCELT,SG2T,SELAT(19),SCELAT(19),
     3            SG2AT(19)
     4        /CDPR/CHIMIN,NPARA,PARA1(7),DPARA(7),DRPMAX(7),RAT(7),
     5            IDPAR(7),NPRE
     6        /CEXP/IFEXP,WEIGHT,WGTOT,WGEL,WG1,         WGELA,WG1A,
     7            STOTEX,ERTOT,SELEX,EREL,S1STEX,ER1ST,SELAEX(19),
     8            ERELA(19),S1AEX(19),ER1A(19)
     9        /CTDN/TDN(31),TIME1
C
      DIMENSION       DRP(7),DTOT(7),DEL(7),D2(7),DELA(7,19),D2A(7,19),
     1                AA(7,7),BB(7),DAA(7,7),U(7,7),UB(7),VB(7),DS(3)
C
      INTEGER         T1,TIME1,SEC,TEND
      DATA      DS/1H*,1H ,1HT/
C
      IGO=1
      IF (NSRCH.GE.0) GO TO 500
      NSRCH=-NSRCH
      IGO=2
 500 CALL   XSECT(NLO,NLD,PARA1,SQC,1,2)
      X=0.
      WRITE (6,600) TDN
 600 FORMAT(1H1,4X,18A4,20X,6A4//5X,16HPARAMETER SEARCH/59X,5HTOTAL,2X,
    1     10HCOMP.FORM.,5X,21HELASTIC CROSS SECTION,2X,9H1ST LEVEL/
    2     59X,5HCROSS,4X,5HCROSS,33X,5HCROSS/
    3     7X,3HNO.,6X,A1,1HV,5X,A1,1HW,3X,A1,3HVSO,3X,A1,2HRR,3X,A1,
    4     2HRS,4X,A1,1HA,4X,A1,1HB,2X,
    5               7HSECTION,2X,7HSECTION,7X,5HTOTAL,3X,5HSHAPE,1X,
    6   8HCOMPOUND,2X,7HSECTION,2X,10HCHI-SQUARE,2X,4HTIME)
      NS=0
      IDS=2
      MIN=1
      NGO=1
      LINE=6
C
 700 LINE=LINE+1
      CALL  CLOCK(T1)
      SEC=T1-TIME1
      IF (LINE.LE.58) GO TO 710
      WRITE (6,600) TDN
      LINE=7
 710 WRITE (6,720) NS ,DS(IDS),PARA1,STOT,SABS,SEL,SSEL,SG(1),SG(2),
    1                SQC,DS(MIN),SEC
 720 FORMAT (6X,I3,A1,F8.3,2F7.3,4F6.3,2F9.3,4X,3F8.3,F10.3,F12.3,A1,
    1        I6)
      IF (T1.GE.TEND) GO TO 2360
      GO TO (1010,2010,2150,2290         ),NGO
C
1010 STOTT=STOT
      SABST=SABS
      SELT=SEL
      IF (WGELA.EQ.0.)GO TO 1040
      DO  1030 NA=1,NANGL
      SELAT(NA)=SELA(NA)
1030 SCELAT(NA)=SGA(NA,1)
1040 SCELT=SG(1)
      SG2T=SG(2)
      IF (WG1A.EQ.0.) GO TO 1090
      DO  1050 NA=1,NANGL
1050 SG2AT(NA)=SGA(NA,2)
1090 IF (NS.EQ.0) GO TO 1120
      IF (SQC.LE.(.75*SQCHIO+.25*EXSQ)) GO TO 4000
1110 GO TO (1120,2020,2160,4000,4000,4000),NGO
1120 MNS=IABS(NSRCHO)
      IF (IGO.EQ.2) MNS=NSRCH
      NEND=0
1150 IF (MNS.EQ.0) GO TO 4100
      DO  4010 NS=1,MNS
      SQCHIO=SQC
      DO  1200 NP=1,NPARA
      I=IDPAR(NP)
      PARA1(I)=PARA1(I)+DPARA(I)

      CALL  XSECT(NLO,NLO,PARA1,SQC,0,IGO)
      IF  (WGTOT.NE.0.)DTOT(NP)=(STOT-STOTT)*RAT(I)
      IF  (WGEL.NE.0.)DEL(NP)=(SEL-SELT)*RAT(I)
      IF  (WG1.NE.0.)D2(NP)=(SG(2)-SG2T)*RAT(I)
      IF  (WGELA.EQ.0.)GO TO 1170
      DO   1160 NA=1,NANGL
 1160 DELA(NP,NA)=(SELA(NA)-SELAT(NA))*RAT(I)
 1170 IF (WG1A.EQ.0.)GO TO 1190
      DO   1180 NA=1,NANGL
 1180 D2A(NP,NA)=(SGA(NA,2)-SG2AT(NA))*RAT(I)
 1190 PARA1(I)=PARA1(I)-DPARA(I)
      CALL   CLOCK(T1)
      IF (T1.GE.TEND) RETURN
 1200 CONTINUE
C
      DO  1470 NP=1,NPARA
      BB(NP)=0.
      DO  1370 NP1=1,NP
      AA(NP,NP1)=0.
      IF (WGTOT.EQ.0.) GO TO 1310
      AA(NP,NP1)=AA(NP,NP1)+DTOT(NP)*DTOT(NP1)*WGTOT/ERTOT**2
 1310 IF (WGEL.EQ.0.) GO TO 1320
      AA(NP,NP1)=AA(NP,NP1)+DEL(NP)*DEL(NP1)*WGEL/EREL**2
 1320 IF (WG1.EQ.0.) GO TO 1330
      AA(NP,NP1)=AA(NP,NP1)+D2(NP)*D2(NP1)*WG1/ER1ST**2
 1330 IF (WGELA.EQ.0.) GO TO 1350
      DO  1340 NA=1,NANGL
      IF (SELAEX(NA).LE.0.) GO TO 1340
      AA(NP,NP1)=AA(NP,NP1)+DELA(NP,NA)*DELA(NP1,NA)*WGELA/ERELA(NA)**2
 1340 CONTINUE
 1350 IF (WG1A.EQ.0.) GO TO 1370
      DO  1360 NA=1,NANGL
      IF (S1AEX(NA) .LE.0.) GO TO 1360
      AA(NP,NP1)=AA(NP,NP1)+D2A(NP,NA)*D2A(NP1,NA)*WG1A/ER1A(NA)**2
 1360 CONTINUE
 1370 AA(NP1,NP)=AA(NP,NP1)
C
      IF (WGTOT.EQ.0.) GO TO 1410
      BB(NP)=BB(NP)+DTOT(NP)*(STOTEX-STOTT)
     1                                   *WGTOT/ERTOT**2
 1410 IF (WGEL.EQ.0.)GO TO 1420
      BB(NP)=BB(NP)+DEL(NP)*(SELEX-SELT)
     1                                *WGEL/EREL**2
 1420 IF (WG1.EQ.0.) GO TO 1430
      BB(NP)=BB(NP)+D2(NP)*(S1STEX-SG2T )*WG1/ER1ST**2
 1430 IF (WGELA.EQ.0.) GO TO 1450
      DO  1440 NA=1,NANGL
      IF (SELAEX(NA) .LE.0.) GO TO 1440
      BB(NP)=BB(NP)+DELA(NP,NA)*(SELAEX(NA)-SELAT(NA))
     1                                         *WGELA/ERELA(NA)**2
 1440 CONTINUE
 1450 IF (WG1A.EQ.0.) GO TO 1470
      DO  1460 NA=1,NANGL
      IF (S1AEX(NA) .LE.0.) GO TO 1460
      BB(NP)=BB(NP)+D2A(NP,NA)*(S1AEX(NA)-SG2AT(NA))
     1                                        *WG1A/ER1A(NA)**2

 1460 CONTINUE
 1470 CONTINUE
C
      F=0.
      DO  1510 NP=1,NPARA
 1510 F=F+AA(NP,NP)
      F=F/(10.**NPRE*FLOAT(NPARA))
      CALL  EIGEN(NPARA,AA,DAA,U,F,7)
      F=F*FLOAT(NPARA)*10.
      DO  1550 NP=1,NPARA
      UB(NP)=0.
      VB(NP)=0.
      IF (DAA(NP,NP).LT.      F) GO TO 1550
      DO  1540 N=1,NPARA
 1540 UB(NP)=UB(NP)+U(NP,N)*BB(N)
      VB(NP)=UB(NP)/DAA(NP,NP)
      IF (ABS(VB(NP)).GT.1.) VB(NP)=SIGN(1.,VB(NP))
 1550 CONTINUE
C
 1560 DO  1580 N=1,NPARA
      DRP(N)=0.
      DO  1570 K=1,NPARA
 1570 DRP(N)=DRP(N)+U(K,N)*VB(K)
      I=IDPAR(N)
      DRP(N)=DRP(N)*DRPMAX(I)
 1580 PARA1(I)=PARA1(I)+DRP(N)
      EXSQ=0.
      DO  1590 N=1,NPARA
 1590 EXSQ=EXSQ+DAA(N,N)*VB(N)**2
      EXSQ=SQCHIO-EXSQ/WEIGHT
      IF (ITEST.EQ.0) GO TO 1910
      LINE=LINE+2*NPARA+10
      IF (LINE.LE.58) GO TO 1600
      WRITE (6,600) TDN
      LINE=2*NPARA+17
 1600 WRITE (6,1610)
 1610 FORMAT (9X,2HAA)
      DO  1620 NP=1,NPARA
 1620 WRITE (6,1630) (AA(NP,NP1),NP1=1,NPARA)
 1630 FORMAT (12X,1P7E11.3)
      WRITE (6,1640)
 1640 FORMAT (9X,2HBB)
      WRITE (6,1630) (BB(N),N=1,NPARA)
      WRITE (6,1650)
 1650 FORMAT (9X,3HDAA)
      WRITE (6,1630) (DAA(N,N),N=1,NPARA)
      WRITE (6,1660)
 1660 FORMAT (9X,1HU)
      DO  1670 N=1,NPARA
 1670 WRITE (6,1630) (U(N,J),J=1,NPARA)
      WRITE (6,1680)
 1680 FORMAT (9X,2HUB)
      WRITE (6,1630) (UB(N),N=1,NPARA)
      WRITE (6,1690)
 1690 FORMAT (9X,2HVB)
      WRITE (6,1630) (VB(N),N=1,NPARA)
```

```
      LINE=LINE+1
      IF (LINE.LE.58) GO TO 1698
      WRITE (6,600) TDN
      LINE=7
 1698 WRITE (6,1700) EXSQ
 1700 FORMAT (9X,35HEXPECTED VALUE OF CHI-SQUARE .......,F12.1)
C
 1910 CALL  XSECT(NLO,NLD,PARA1,SQC,1,2)
 1920 NGO=2
      MIN=2
      IF (SQC.LT.SQCHI0) MIN=1
      X=MIN-1
      IDS=IGO
      GO TO 700
C
 2010 IF (MIN.EQ.1) GO TO 1010
 2020 GO TO (2050,2080),MIN
 2050 SQ0=SQC
      SQ2=SQCHI0
 2060 G=-0.5
      GO TO 2100
 2080 SQ0=SQCHI0
      SQ2=SQC
      G=0.5
 2100 LT=MIN-1
      DO  2110 N=1,NPARA
      I=IDPAR(N)
 2110 PARA1(I)=PARA1(I)-0.5*DRP(N)
      CALL  XSECT(NLO,NLD,PARA1,SQC,1,2)
      NGO=3
      MIN=2
      IF (SQC.LE.SQ0) MIN=1
      X=FLOAT(MIN-1)*G
      IDS=3
      GO TO 700
 2150 IF (MIN.EQ.1) GO TO 1010
C
 2160 SQ1=SQC
      A=0.5*(SQ2+SQ0)-SQ1
      B=0.5*(SQ2-SQ0)
      H=-G
      IF (B.LT.4.*A) H=(1.-0.5*B/A)*G
      DO  2200 N=1,NPARA
      I=IDPAR(N)
 2200 PARA1(I)=PARA1(I)-(G-H)*DRP(N)
      CALL  XSECT(NLO,NLD,PARA1,SQC,1,2)
      IF (ITEST.EQ.0) GO TO 2270
      LINE=LINE+1
      IF (LINE.LE.58) GO TO 2250
      WRITE (6,600) TDN
      LINE=7
 2250 WRITE (6,2260) A,B,H
 2260 FORMAT (9X,2HA=,1PE11.3,5X,2HB=,E11.3,5X,2HH=,E11.3)
 2270 NGO=4
      IDS=2
      IF (A.LE.0.) IDS=3

      MIN=2
      IF (SQC.LE.AMIN1(SQ0,SQ1)) MIN=1
      X=FLOAT(MIN-1)*(X-G+H)
      GO TO 700
 2290 IF (MIN.EQ.2) GO TO 2350
      GO TO 1010
C
 2350 SQC=AMIN1(SQ0,SQ1)
 2360 DO  2370 N=1,NPARA
      I=IDPAR(N)
 2370 PARA1(I)=PARA1(I)-X*DRP(N)
C
 4000 IF((SQC.LE.CHIMIN).OR.(SQCHI0-SQC.LE.CHIMIN*.01)) RETURN
      CALL  CLOCK(T1)
      IF (T1.GE.TEND) RETURN
 4010 CONTINUE
C
 4100 IF (NEND.EQ.1) RETURN
      NEND=1
      GO TO (4210,4310),IGO
 4210 IGO=2
      MNS=     NSRCH
      GO TO 1150
 4310 IGO=1
      MNS=IABS(NSRCH0)
      GO TO 1150
C
      END
C     EIGENVALUE
C
       SUBROUTINE    EIGEN(M,A,D,U,F,NDIM)
C
C    A...... MATRIX TO BE DIAGONALIZED (SYMMETRIC)
C    M...... ACTUAL DIMENSION OF THE MATRIX
C    D...... DIAGONALIZED MATRIX (DIAGONAL ELEMENTS ARE EIGENVALUES)
C    U(N,I). ORTHOGONAL MATRIX OF TRANSFORMATION ( UA=DU)
C            I-TH COMPONENT OF THE N-TH EIGENVECTOR
C    F...... UPPER LIMIT FOR THE OFF-DIAGONAL ELEMENTS)
C    NDIM.... MAXIMUM DIMENSION TAKEN IN THE MAIN PROGRAM
C
       DIMENSION     A(NDIM,NDIM),D(NDIM,NDIM),U(NDIM,NDIM)
C
      G=0.
      M1=M-1
      DO  1010 I=1,M
      DO  1010 J=1,M
      D(I,J)=A(I,J)
      U(I,J)=0.
      IF (I.EQ.J) U(I,J)=1.
 1010 CONTINUE
      IF (M.EQ.1) GO TO 3000
C
 2000 G=0.
      DO  2010 I=1,M1
      I1=I+1
      DO  2010 J=I1,M

       G1=ABS(D(I,J))
       IF (G.GE.G1) GO TO 2010
       K=I
       L=J
       G=G1
  2010 CONTINUE
       IF (G.LE.F) GO TO 3000
 C
       DD=D(L,L)-D(K,K)
       IF (2.*G.GT.ABS(DD)) GO TO 2110
       T=2.*D(K,L)/DD
       C=-T/(1.+SQRT(1.+T**2))
       GO TO 2120
  2110 T=DD/(2.*D(K,L))
       C=T-SQRT(1.+T**2)*SIGN(1.,T)
  2120 P=1./SQRT(1.+C**2)
       Q=C*P
 C
       DO  2210 I=1,M
       UK=P*U(K,I)+Q*U(L,I)
       UL=-Q*U(K,I)+P*U(L,I)
       U(K,I)=UK
  2210 U(L,I)=UL
 C
       DO  2310 I=1,M
       IF (I.EQ.K.OR.I.EQ.L) GO TO 2310
       DKI    =P*D(K,I)+Q*D(L,I)
       DLI   =-Q*D(K,I)+P*D(L,I)
       D(K,I)=DKI
       D(I,K)=DKI
       D(L,I)=DLI
       D(I,L)=DLI
  2310 CONTINUE
       DKK=D(K,K)+D(K,L)*C
       DLL=D(L,L)-D(K,L)*C
       D(K,K)=DKK
       D(L,L)=DLL
       D(K,L)=0.
       D(L,K)=0.
 C
       GO TO 2000
 C
  3000 F=G
       RETURN
       END
 C     CROSS SECTION
 C
       SUBROUTINE     XSECT(NLOUT,NLD,PAR,SQK,IX,IFC)
 C
       DIMENSION      BL(25,11),V(25),W(25),VSO(25),RR(25),RS(25),A(25),
      1               B(25),PAR(7),PL(11,19),PL1(11,19),PL2(11,19,3),
      3               TRMAT(25),TRPWR(25)
 C
       COMPLEX        WR,PHAIR(300),DPHAI,DL,YETA(11,2),YETAN,HI,HR
 C
       COMMON  /CLEV/NLEV,EX(25),SPIN(25),NPAR(25),NLMAX(25),DJ,NLMAXA
      1        /CSTA/T(11,2,25),TH(11,2,25),THTOT(21,2),Q(21,2),IQCONS,
      2             QCONST,FNR,BC,REBB,FCHI,COMP
      3        /CKIN/EN(25),FK(25),HM,PLAM,PLAM0,PLAM1,FNM13,COMPAI
      4        /CWAV/PHIPRE,DR,DRN(25),RMATN(25)
      5        /CPOT/PARA(7),VE(5),WE(5),VSOE(5),RRE(5),RSE(5),AE(5),
      6             BE(5)
      7        /CCRS/NANGL,STOT,SABS,SEL,SSEL,SG(25),SELA(19),SSELA(19),
      8             SGA(19,25),PLAMEL
      9        /CWEL/WR,VR,VSOR,RV,RW,AR,BR,ER,DR1,MESH,RPWR,RPWR1
       COMMON  /CFXP/IFEXP,WEIGHT,WGTOT,WGEL,WG1,
      1             WGELA,WG1A,STOTEX,ERTOT,SELEX,EREL,S1STEX,ER1ST,
      2             SELAEX(19),ERELA(19),S1AEX(19),ER1A(19)
       COMMON  /CYET/YETA/COMJ/NJMIN,NJMAX,NLMAXO(3),COSCM(19,25),IFFL
      3        /CSGT/STOTT,SABST,SELT,SCELT,SG2T,SELAT(19),SCELAT(19),
      4             SG2AT(19)
      5        /CCGW/CGL(11,11),WL(11,2,11)
 C
       CALL  OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98765)
 98765 FORMAT (/////5X,15H*****XSECT    1////)
       NLMAXA=0
       SG(2)=0.
       NLEV1=NLEV
       IF (IFC.EQ.1) NLEV1=1
       DO  2230 N=1,NLEV1
       ER=EN(N)*HM
       V(N)=PAR (1)
       W(N)=PAR (2)
       VSO(N)=PAR (3)
       RR(N)=PAR (4)
       RS(N)=PAR (5)
       A(N)=PAR (6)
       B(N)=PAR (7)
       FE=1.
       DO  2010 NE=1,5
       FE=FE*EN(N)
       V(N)=V(N)+FE*VE(NE)
       W(N)=W(N)+FE*WE(NE)
       VSO(N)=VSO(N)+FE*VSOE(NE)
       RR(N)=RR(N)+FE*RRE(NE)
       RS(N)=RS(N)+FE*RSE(NE)
       A(N)=A(N)+FE*AE(NE)
  2010 B(N)=B(N)+FF*BE(NF)
       VR=V(N)*HM
       WR=W(N)*HM*(0.,4.)
       VSOR=VSO(N)*HM*COMPAI/A(N)
       RV=RR(N)*FNM13
       RW=RS(N)*FNM13
       AR=A(N)
       BR=B(N)
       IF (IX.EQ.0) GO TO 2030
       VRX=AMAX1(ABS(V(N)*A(N)*FK(N)),ABS(VSO(N)*10.*COMPAI/RV))
       IF (VRX.EQ.0.) GO TO 2020
       R1=ALOG(VRX/(FN(N)*PHIPRE))*A(N)+RV
       GO To 2021
  2020 R1=0.

  2021 IF (W(N).EQ.0..OR.B(N).EQ.0.) GO TO 2022
       R2=ALOG(ABS(W(N)*B(N)*FK(N)*4./(FN(N)*PHIPRE)))*B(N)+RW
       GO TO 2023
  2022 R2=0.
  2023 RMATCH=AMAX1(R1,R2)
       RPWR=1.2/SQRT(ER+VR)
       TRMAT(N)=RMATCH
       TRPWR(N)=RPWR
       GO TO 2040
  2030 RMATCH=TRMAT(N)
       RPWR=TRPWR(N)
  2040 MESH=(RMATCH-RPWR)/DR+2.9999999
       IF (MESH.LE.300) GO TO 2050
       MESH=300
       DR1=(RMATCH-RPWR)/298.
       GO TO 2110
  2050 RMATCH=DR*FLOAT(MESH-2)+RPWR
       DR1=DR
  2110 ROH2   =RMATCH*FK(N)
       ROH1=ROH2-DR1*FK(N)
       RPWR1=RPWR-DR1
       NLC=ROH2+1.5
       RL=AMAX1(RV+4.6*AR,RW+4.6*BR)
       ZL=RL*FK(N)
       BL1=SIN(ZL)/ZL
       BLO=COS(ZL)/ZL
       BJMIN=0.1/(125.664*RL**2)
       DO  2112 NL=2,11
       BS=FLOAT(2*NL-3)*BL1/ZL-BLO
       IF (BS**2*FLOAT(2*NL-1).LE.BJMIN.AND.NL.GT.NLC) GO TO 2113
       BLO=BL1
  2112 BL1=BS
       NL=12
  2113 MNL=NL-1
       CALL  OVERFL(NOVFL)
 98766 FORMAT (/////5X,15H*****XSECT    2////)
       IF (NOVFL.EQ.1) WRITE (6,98766)
       NLMAX(N)=MNL
       T(1,1,N)=0.
       DO  2170 NL=1,MNL
       L=NL-1
       CALL  BESSE2(NL,BJ2,BN2,ROH2)
  2115 CALL  BESSEL(NL,BJ1,BN1,ROH1)
       LS=1
       IF (L.EQ.0) LS=2
  2120 CALL  DIFEQ(L,LS,PHAIR)
       DPHAI=PHAIR(MESH)*ROH1/(PHAIR(MESH-1)*ROH2)
       HR=BJ2-DPHAI*BJ1
       HI=(0.,1.)*(BN2-DPHAI*BN1)
       YETAN=(HI-HR)/(HI+HR)
       T(NL,LS,N)=1.-(CABS(YETAN))**2
       IF (N.EQ.1) YETA(NL,LS)=YETAN
       IF (LS.EQ.2) GO TO 2170
       LS=2
       GO TO 2120
  2170 CONTINUE

  2200 NLMAXA=MAX0(NLMAXA,NLMAX(N))
       IF (NLMAX(N).EQ.11) GO TO 2220
       N1=NLMAX(N)+1
       DO  2210 NL=N1,11
       T(NL,1,N)=0.
  2210 T(NL,2,N)=0.
  2220 RMATN(N)=RMATCH
       DRN(N)=DR1
  2230 CONTINUE
       CALL  OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98767)
 98767 FORMAT (/////5X,15H*****XSECT    3////)
 C
       IF (IFC.EQ.1) GO TO 3010
       DO  2340 NL=1,NLMAXA
       FNL=NL-1
       DO  2310 L=1,NL
       FL=2*(L-1)
  2310 CGL(NL,L)=CGO(FNL,FNL,FL)*(2.*FNL+1.)
       DO  2330 LS=1,2
       L1=NL+LS-2
       IF (L1.EQ.0) GO TO 2330
       FLS=FNL+FLOAT(LS)-1.5
       DO  2320 L=1,L1
       FL=2*(L-1)
  2320 WL(NL,LS,L)=WRAC(FNL,FLS,FNL,FLS,0.5,FL)
  2330 CONTINUE
  2340 CONTINUE
       CALL  OVERFL(NOVFL)
       IF (NOVFL.EQ.1) WRITE (6,98768)
 98768 FORMAT (/////5X,15H*****XSECT    4////)
 C
  3010 MAXL1=NLMAX(1)
       SABS=0.
       FNL=0.
       DO  3020 NL=1,MAXL1
       FNL1=FNL
       FNL=FNL+1.
  3020 SABS=SABS+FNL1*T(NL,1,1)+FNL*T(NL,2,1)
       SABS=SABS*PLAM0
 C
       IF (COMP.EQ.0.) GO TO 3700
       IF (IFC.EQ.1) GO TO 6010
       DO  3510 NF=1,NLOUT
       DO  3510 NL=1,MAXL1
  3510 BL(NF,NL)=0.
       NJMAX=MAXL1+INT(SPIN(1)-.4+DJ)
       FJ=FLOAT(MAXL1)-SPIN(1)-1.
       NJMIN=DJ-.4-FJ
       IF (NJMIN.LE.0) NJMIN=1
 C
       DO  3610 NJ=NJMIN,NJMAX
       CALL  OVERFL(NOVFL)
 98705 FORMAT (/////5X,15H*****XSECT    5////)
       IF (NOVFL.EQ.1) WRITE (6,98705)
       CALL  TRANS(IMAGRY,NJ,NNNNNN)
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      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98706)
98706 FORMAT (/////5X,15H*****XSECT    6////)
 3610 CALL  BLL(NLOUT,NLD,NJ,BL)
C
      DO  3670 N=1,NLOUT
      K=MINO(N,3)
      SG(N)=PLAM1*BL(N,1)*COMP
      IF (N.GT.NLD) GO TO 3670
      NL2=MINO(NLMAX(N),MAXL1)
      NL1=1
      IF (K.EQ.3) GO TO 3620
      IF (NL2.LE.NLMAXO(N)) GO TO 3640
      NL1=NLMAXO(N)+1
      IF (N.EQ.2) NLMAXO(2)=NL2
 3620 CALL  LEGND2(NL1,NL2,NANGL,PL2,COSCM,N,IFFL)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98707)
98707 FORMAT (/////5X,15H*****XSECT    7////)
 3640 DO  3660 NA=1,NANGL
      SGA(NA,N)=0.
      DO  3650 NL=1,NL2
 3650 SGA(NA,N)=SGA(NA,N)+BL(N,NL)*PL2(NL,NA,K)
 3660 SGA(NA,N)=SGA(NA,N)*PLAM*COMP
 3670 CONTINUE
C
 3700 IF (NLMAX(1).LE.NLMAXO(1)) GO TO 3701
      CALL  LEGND1(NLMAXO(1)+1,NLMAX(1),NANGL,PL,PL1,COSCM)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98708)
98708 FORMAT (/////5X,15H*****XSECT    8////)
      NLMAXO(1)=NLMAX(1)
 3701 CALL  SHAPE(FK(1),NANGL,MAXL1,YETA,SSELA,SSEL,PL,PL1,PLAMEL,PLAMO)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98709)
98709 FORMAT (/////5X,15H*****XSECT    9////)
      DO  3710 NA=1,NANGL
      IF (COMP.EQ.0.) SGA(NA,1)=0.
 3710 SELA(NA)=SSELA(NA)+SGA(NA,1)
      IF (COMP.EQ.0.) SG(1)=0.
      SEL=SSEL+SG(1)
      STOT=SABS+SSEL
C
      IF (IFEXP.EQ.0) RETURN
      SQK=0.
      IF (WGTOT.EQ.0.)GO TO 3810
      SQK=SQK+WGTOT*((STOT-STOTEX)/ERTOT)**2
 3810 IF (WGEL.EQ.0.)GO TO 3820
      SQK=SQK+WGEL*((SEL-SELEX)/EREL)**2
 3820 IF (WG1.EQ.0.)GO TO 3830
      SQK=SQK+WG1*((SG(2)-S1STEX)/ER1ST)**2
 3830 IF (WGELA.EQ.0.)GO TO 3850
      SQA=0.
      DO  3840 NA=1,NANGL
      IF (SELAEX(NA).LE.0.) GO TO 3840
      SQA=SQA+((SELA(NA)-SELAEX(NA))/ERELA(NA))**2

 3840 CONTINUE
      SQK=SQK+WGELA*SQA
 3850 IF (WG1A.EQ.0.)GO TO 3870
      SQA=0.
      DO  3860 NA=1,NANGL
      IF (S1AEX(NA).LE.0.) GO TO 3860
      SQA=SQA+((SGA(NA,2)-S1AEX(NA))/ER1A(NA))**2
 3860 CONTINUE
      SQK=SQK+WG1A*SQA
 3870 SQK=SQK/WEIGHT
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98710)
98710 FORMAT (/////5X,15H*****XSECT   10////)
 4100 RETURN
C
 6010 RATS=SABS/SABST
      SG(1)=SCELT*RATS
      SG(2)=SG2T*RATS
      IF (WGELA.EQ.0.) GO TO 6030
      DO  6020 NA=1,NANGL
 6020 SGA(NA,1)=SCELAT(NA)*RATS
 6030 IF (WG1A.EQ.0.) GO TO 3700
      DO  6040 NA=1,NANGL
 6040 SGA(NA,2)=SG2AT(NA)*RATS
      GO TO 3700
C
      END
C   SOLUTION OF SCHROEDINGER EQUATION
C
      SUBROUTINE    DIFEQ(L,LS,PHAIR)
C
      COMPLEX       PHAIR(300),WR,P(8), UO(8),FO(300),F(300),C(8)
C
      COMMON  /CWEL/WR,VR,VSOR,RR,RS,AR,B,ER,DR,MN,RPWR,RPWR1
C
      COMMON  /COUT/P
      DIMENSION     FSO(300),FR(10),G(8),FB(9),H(8)
      DOUBLE PRECISION   FR,G,FB,EV,EW,EA,EB,DE1,DE2
C
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98765)
98765 FORMAT (/////5X,15H*****DIFEQ    1////)
      GO TO (1010,1020),LS
 1010 FACL=-L-1
      RST1=RST1*RPWR1
      RST2=RST2*RPWR
      F2L2=F2L2+2.
      GO TO 1030
 1020 FACL=L
 1030 FLL=FACL*(FACL+1.)
      DR12=DR**2/12.
      FACL=FACL*VSOR
C
C  STARTING VALUES
C
      IF (L.NE.0) GO TO  1200

      EV=DEXP(DBLE(-RR/AR))
      EW=DEXP(DBLE(-RS/B))
      RST1=RPWR1
      RST2=RPWR
      F2L2=2.
      FR(1)=1./(1.+EV)
      FB(1)=1./(1.+EW)
      FN=0.
      DO  1120 N=2,9
      FN=FN+1.
      N1=N-1
      FR(N)=-FR(N1)
      G(N1)=FB(N1)
      DO  1110 M=1,N1
      NM=N-M
      FR(N)=FR(N)+FR(M)*FR(NM)
 1110 G(N1)=G(N1)-FB(M)*FB(NM)
      FR(N)=FR(N)/(AR*FN)
 1120 FB(N)=-G(N1)/(B*FN)
      FR(10)=-FR(9)
      DO  1130 M=1,9
      M10=10-M
 1130 FR(10)=FR(10)+FR(M)*FR(M10)
      FR(10)=FR(10)/(9.*AR)
      FN=1.
      DO  1140 N=1,8
      FN=FN+1.
      C(N)=VR*SNGL(FR(N))+WR*SNGL(G(N))
 1140 H(N)=AR*FN*SNGL(FR(N+2))
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98766)
98766 FORMAT (/////5X,15H*****DIFEQ    2////)
      C(1)=C(1)+ER
C
 1200 RESID=-FACL*FR(2)*AR
      DO  1210 N=1,8
 1210 UO(N)=C(N)+H(N)*FACL
C
      P(1)=1.
      P(2)=-RESID/F2L2
      FN=1.
      DO  1320 N=3,8
      P(N)=-RESID*P(N-1)
      FN=FN+1.
      N2=N-2
      DO  1310 M=1,N2
      NM=N-M-1
 1310 P(N)=P(N)-P(M)*UO(NM)
 1320 P(N)=P(N)/(FN*(F2L2+FN-1.))
C
      PHAIR(1)=P(1)*RST1
      PHAIR(2)=P(1)*RST2
      ST1=RST1
      ST2=RST2
      DO  1330 N=2,8
      ST1=ST1*RPWR1
      ST2=ST2*RPWR
      PHAIR(1)=PHAIR(1)+P(N)*ST1
 1330 PHAIR(2)=PHAIR(2)+P(N)*ST2
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98767)
98767 FORMAT (/////5X,15H*****DIFEQ    3////)
C
C  NOUMEROV
C
      IF (L.NE.0) GO TO 4000
      DE1=DEXP(DBLE(DR/AR))
      MNO=INT((RR-87.*AR-RPWR1)/DR)+1
      IF (MNO.LE.0) GO TO 2520
      DO  2510 N=1,MNO
      FO(N)=ER+VR
 2510 FSO(N)=0.
      MNO=MNO+1
      GO TO 2530
 2520 MNO=1
 2530 R=RPWR1+FLOAT(MNO-1)*DR
      EA=EXP((R-RR)/AR)
      MN1=(RR-RPWR1)/DR+1.
      DO  2540 N=MNO,MN1
      E1=EA
      FO(N)=ER+VR/(1.+E1)
      FSO(N)=E1/(R*(1.+E1)**2)
      EA=EA*DE1
 2540 R=R+DR
      DE1=1./DE1
      EA=1./EA
      MN1=MN1+1
      DO  2550 N=MN1,MN
      E1=EA
      FO(N)=ER+VR*E1/(1.+E1)
      FSO(N)=E1/(R*(1.+E1)**2)
      EA=EA*DE1
 2550 R=R+DR
      DE2=DEXP(DBLE(DR/B))
      MNO=INT((RS-87.*B-RPWR1)/DR)+2
      IF (MNO.LE.0) MNO=1
      R=RPWR1+FLOAT(MNO-1)*DR
      EB=EXP((R-RS)/B)
      MN1=(RS-RPWR1)/DR+1.
      DO  2560 N=MNO,MN1
      E2=EB
      FO(N)=FO(N)+WR*E2/(1.+F2)**2
 2560 EB=EB*DE2
      MN1=MN1+1
      DE2=1./DE2
      EB=1./EB
      DO  2570 N=MN1,MN
      E2=EB
      FO(N)=FO(N)+WR*E2/(1.+F2)**2
 2570 EB=EB*DE2
C
 4000 R=RPWR1

      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98768)
98768 FORMAT (/////5X,15H*****DIFEQ    4////)
      DO  4010 N=1,MN
      F(N)=(FLL/R**2-FO(N)-FACL*FSO(N))*DR12
 4010 R=R+DR
C
      PHAIR(1)=PHAIR(1)*(1.-F(1))
      PHAIR(2)=PHAIR(2)*(1.-F(2))
      DO  5010 N=3,MN
 5010 PHAIR(N)=(2.+12.*F(N-1)/(1.-F(N-1)))*PHAIR(N-1)-PHAIR(N-2)
      PHAIR(MN)=PHAIR(MN)/(1.-F(MN))
      PHAIR(MN-1)=PHAIR(MN-1)/(1.-F(MN-1))
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98769)
98769 FORMAT (/////5X,15H*****DIFEQ    5////)
C
      RETURN
      END
C   SPHERICAL BESSEL FUNCTION
C
      SUBROUTINE BESSEL(NL,BJ,BN,Z)
C
C
      IF (NL-2) 10,20,30
   10 BJ=SIN(Z)/Z
      BN=-COS(Z)/Z
      BDJ=-BN-BJ/Z
      BDN=BJ-BN/Z
      GO TO 50
C
   20 BJ=-BDJ
      BN=-BDN
      GO TO 40
C
   30 BJ= FLOAT(2*NL-3)*BJ1/Z-BJ0
      BN= FLOAT(2*NL-3)*BN1/Z-BN0
C
   40 BJ0=BJ1
      BN0=BN1
   50 BJ1=BJ
      BN1=BN
      RETURN
      END
C   SPHERICAL BESSEL FUNCTION
C
      SUBROUTINE BESSE2(NL,BJ,BN,Z)
C
C
      IF (NL-2) 10,20,30
   10 BJ=SIN(Z)/Z
      BN=-COS(Z)/Z
      BDJ=-BN-BJ/Z
      BDN=BJ-BN/Z
      GO TO 50
C

   20 BJ=-BDJ
      BN=-BDN
      GO TO 40
C
   30 BJ= FLOAT(2*NL-3)*BJ1/Z-BJ0
      BN= FLOAT(2*NL-3)*BN1/Z-BN0
C
   40 BJ0=BJ1
      BN0=BN1
   50 BJ1=BJ
      BN1=BN
      RETURN
      END
C   SHAPE ELASTIC SCATTERING CROSS SECTION
      SUBROUTINE    SHAPE(FK,NANGL,NLMAX,YETA,SIGSEL,SIG,PL,PL1,F1,F2)
      COMPLEX       C,C1,F(20),G(20),YETA(11,2)
C
      DIMENSION     SIGSEL(19),PL(11,19),PL1(11,19)
C
      YETA(1,1)=(1.,0.)
      DO  100 NA=1,NANGL
      F(NA)=0.
  100 G(NA)=0.
      SIG=0.
      FNL=0.
      DO  130 NL=1,NLMAX
      FNL1=FNL
      FNL=FNL+1.
      SIG=SIG+FNL1*(CABS(1.-YETA(NL,1)))**2+FNL*(CABS(1.-YETA(NL,2)))**2
      C=FNL*(1.-YETA(NL,2))+FNL1*(1.-YETA(NL,1))
      IF (NL.EQ.1) GO TO 120
      C1=YETA(NL,2)-YETA(NL,1)
  120 DO  130 NA=1,NANGL
      F(NA)=F(NA)+C*PL(NL,NA)
      IF (NL.EQ.1) GO TO 130
      G(NA)=G(NA)+C1*PL1(NL,NA)
  130 CONTINUE
      DO  200 NA=1,NANGL
  200 SIGSEL(NA)=((CABS(F(NA)))**2+(CABS(G(NA)))**2)*F1
      SIG=SIG*F2
C
      RETURN
      END
C  LEGENDRE FUNCTION FOR SHAPE ELASTIC SCATTERING
      SUBROUTINE    LEGND1(L1,L2,NANGL,PL,PL1,COSIN)
C
      DIMENSION     COSIN(19,25),PL(11,19),PL1(11,19),
     1              FL1(11),FL2(11),FL23(11)
      IF (L1.EQ.1) FL=0.
      DO  5 L=L1,L2
      FL1(L)=FL
      FL=FL+1.
      FL2(L)=FL-2.
    5 FL23(L)=FL1(L)+FL2(L)
      DO  11 N=1,NANGL
      X=COSIN(N,1)
```

```
      IF (L1.GT.1) GO TO 8
      PL(1,N)=1.
      PL(2,N)=X
    8 IF (L2.LE.2) GO TO 11
      L3=MAX0(3,L1)
      DO  10 NL=L3,L2
   10 PL(NL,N)=(FL23(NL)*X*PL(NL-1,N)-FL2(NL)*PL(NL-2,N))/FL1(NL)
   11 CONTINUE
      DO  20 N=1,NANGL
      X=COSIN(N,1)
      Y=SQRT(1.-X**2)
      W=0.
      IF (Y.NE.0.) W=1./Y
      DO  20 NL=L1,L2
   20 PL1(NL,N)=    FL1(NL)*(PL(NL-1,N)-X*PL(NL,N))*W
      RETURN
      END
C  LEGENDRE FUNCTION FOR COMPOUND PROCESS
      SUBROUTINE     LEGND2(L1,L2,NANGL,PL,COSCM,N,IFFL)
      DIMENSION      PL(11,19, 3),COSCM(19,25),P1(19,3),
     1               FL47(11),FL45(11),FL24(11),FL22(11),FL23(11)
      K=MIN0(N,3)
      IF (IFFL.GE.L2) GO TO 110
      L3=IFFL+1
      IF (IFFL.EQ.0) FL=0.
      DO  100 L=L3,L2
      FL22(L)=FL
      FL24(L)=FL-2.
      FL23(L)=FL-1.
      FL=FL+2.
      FL45(L)=FL23(L)+FL22(L)
  100 FL47(L)=FL45(L)-2.
      IFFL=L2
  110 DO  1010 NA=1,NANGL
      X=COSCM(NA,N)
      IF (L1.NE.1) GO TO 200
      PL(1,NA,K)=1.
      P1(NA,K)=0.
  200 IF (L2.EQ.1) GO TO 1010
      I=MAX0(2,L1)
      DO  1000 I=I,L2
      P1(NA,K)=(FL47(L)*X*PL(L-1,NA,K)-FL24(L)*P1(NA,K))/FL23(L)
      PL(L,NA,K)=(FL45(L) *X*P1(NA,K)-FL23(L)*PL(L-1,NA,K))/FL22(L)
 1000 CONTINUE
 1010 CONTINUE
      RETURN
      END
C     CALCULATE GAMMA/D FROM T
C
      SUBROUTINE     TRANS(IMAGRY,NJ,NNNNNN)
C
      COMMON  /CLEV/NLEV,EX(25),SPIN(25),NPAR(25),NLMAX(25),DJ,NLMAXA
     1        /CSTA/T(11,2,25),TH(11,2,25),THTOT(21,2),Q(21,2),IQCONS,
     2               QCONST,FNR,BC,REBB,FKAI,COMP
     3        /CETC/NLLOW(2,2,25),NLUPR(2,2,25),FJ,NOPAR
      IMAGRY=0

      IF (FKAI.NE.0.) C=2.*BC/FNR
      FJ=FLOAT(NJ)-DJ
      DO  2300 NOPAR=1,2
      NJPAR=2*NOPAR-3
      THTOT(NJ,NOPAR)=0.
      DO  1120 N=1,NLEV
      NLMIN=1
      IF (NJPAR.NE.NPAR(N)) NLMIN=2
      DO  1120 J=1,2
      FLS=2.6-FLOAT(J)
      NL1=ABS(FJ-SPIN(N))+FLS
      NLLOW(NOPAR,J,N)=NL1+MOD(NL1+NLMIN,2)
      NL2=FJ+SPIN(N)+FLS
      NLUUU=MIN0(NL2,NLMAX(N))
      NLUPR(NOPAR,J,N)=NLUUU-MOD(NLUUU+NLMIN,2)
      IF (NLLOW(NOPAR,J,N).LE.NLUPR(NOPAR,J,N)) GO TO 1010
      NLUPR(NOPAR,J,N)=0
      GO TO 1120
 1010 NL1=NLLOW(NOPAR,J,N)
      NL2=NLUPR(NOPAR,J,N)
      DO  1110 NL=NL1,NL2,2
      THTOT(NJ,NOPAR)=THTOT(NJ,NOPAR)+T(NL,J,N)
 1110 TH(NL,J,N)=T(NL,J,N)
 1120 CONTINUE
      IF (FKAI.EQ.0.) GO TO 2300
      IF (IQCONS.EQ.0) GO TO 2130
      QJP=QCONST
      GO TO 2142
 2130 QJP=C*(1.-PHAI(THTOT(NJ,NOPAR)/(2.*FNR)))
 2142 SUM=0.
      DQ=0.
      INDEX=0
      IMNJ=0
      DO  2200 N=1,NLEV
      DO  2200 J=1,2
      NL2=NLUPR(NOPAR,J,N)
      IF (NL2.EQ.0) GO TO 2200
      NL1=NLLOW(NOPAR,J,N)
      DO  2190 NL=NL1,NL2,2
      DT=1.-QJP*T(NL,J,N)
      TO=TH(NL,J,N)
 2160 IF (DT.GT.0.0) GO TO 2170
      IMNJ=IMNJ+1
      QJP=0.99*QJP/(1.-DT)
      DT=0.01
 2170 SQDT=SQRT(DT)
      TN=2.*T(NL,J,N)/(1.+SQDT)
 2171 IF (ABS(TN-TO).GT.1.E-6.AND.IQCONS.EQ.0) INDEX=1
      TH(NL,J,N)=TN
      SUM=SUM+TN
      DQ=DQ+TN**2/SQDT
 2190 CONTINUE
 2200 CONTINUE
      IF (IQCONS.EQ.1.OR.INDEX.EQ.0) GO TO 2250
      S1=SUM/(2.*FNR)
      PH1=PHAI(S1)

      DPH=100.*(PHAI(S1+.01)-PH1)
      QN=C*(1.-PH1)
      QJP=QJP+(QN-QJP)/(1.+DQ*DPH*C/(8.*FNR))
      GO TO 2142
 2250 IMAGRY=IMAGRY+IMNJ
      Q(NJ,NOPAR)=QJP
 2290 THTOT(NJ,NOPAR)=SUM
 2300 CONTINUE
C
      RETURN
      END
C     PHAIO
      FUNCTION       PHAI(Y)
      IF (Y.LE.0.01) GO TO 100
      X=1./Y
      Z=(1.-EXP(-2.*Y))*.5
      PHAI=1.-X*(1.-X*Z-EI(Y)*(1.-Z-X*Z))
      RETURN
  100 IF (Y.LE.0.) GO TO  300
      A=-1.000617
      B=EI(Y)+1.000617
      Y2=-2.*Y
      PHAI=0.0
      F2=2.
      DO  200 I=1,6
      F1=F2
      F2=F2+1.
      A=A*Y2/F2
      B=B*Y2/F1
  200 PHAI=PHAI+A-B*(1.-2./F2)
      RETURN
  300 PHAI=0.
      RETURN
      END
C     INTEGRAL OF EXP(-T)/T (T=X,INFINITY   MULTPLIED BY EXP(X))
      FUNCTION       EI(X)
C
      DIMENSION      A(20)
      COMMON  /CINT/XI(8),WI(8),X1(8),X2(8),XL1(8),XL2(8),XD1(8),XD2(8)
C
      DATA           A/-.125,.125,-.11111111,.83333333E-1,-.53333333E-1,
     1               .29629630E-1,-.14512472E-1,.63492059E-2,-.25083282E-2,
     2               .90299982E-3,-.29851284E-3,.91208385E-4,-.25904663E
     3               E-4,.6878028E-5,-.1712810E-5,.396881E-6,-.87089E-7,
     4               .20424E-7,-.4451E-8,.416E-9/,C/.577215 66/
C
C
      IF (X.GE.4.) GO TO 3000
      EI=0.
      XN=1.
      X4=X/4.
      DO  2010 N=1,20
      XN=XN*X4
      EIN=XN*A(N)
      IF (ABS(EIN).LT.1.E-16) GO TO 2020
 2010 EI=EI-EIN
 2020 EI=(EI*32.-C-ALOG(X))*EXP(X)
      RETURN
C
 3000 EI=0.
      DO  3010 I=1,8
 3010 EI=EI+WI(I)*(X1(I)/(X-XL1(I))+X2(I)/(X-XL2(I)))
      EI=EI/1.0000098
      RETURN
C
      END
C     LEGENDRE COEFFICIENT
      SUBROUTINE     BLL(NLOUT,NLD,NJ,BL)
C
      COMMON  /CLEV/NLEV,EX(25),SPIN(25),NPAR(25),NLMAX(25),DJ,NLMAXA
     1        /CSTA/T(11,2,25),TH(11,2,25),THTOT(21,2),Q(21,2),IQCONS,
     2               QCONST,FNR,BC,REBB,FKAI,COMP
     3        /CETC/NLLOW(2,2,25),NLUPR(2,2,25),FJ,NOPAR
     4        /CCGW/CGL(11,11),WL(11,2,11)
C
      DIMENSION      BL(25,11),ZWN1(11,25,11),ZWN2(11,25,11),TZW(25)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98765)
98765 FORMAT (/////5X,15H*****BLL        1////)
      DO  150 N=1,NLOUT
      L2=MAX0(NLUPR(1,1,N),NLUPR(2,1,N))
      IF (L2.LE.1) GO TO 120
      L1=MIN0(NLLOW(1,1,N),NLLOW(2,1,N))
      DO  110 NL=L1,L2
      IF(NL.EQ.1) GO TO 110
      FLS=FLOAT(NL)-1.5
      LL=MIN0(NL-1,NJ)
      IF (N.GT.NLD) LL=1
      DO  100 L=1,LL
      FL=2*(L-1)
  100 ZWN1(NL,N,L)=(2.*FLS+1.)*CGL(NL,L)*WL(NL,1,L)
     1               *WRAC(FLS,FJ,FLS,FJ,SPIN(N),FL)
  110 CONTINUE
  120 L2=MAX0(NLUPR(1,2,N),NLUPR(2,2,N))
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98766)
98766 FORMAT (/////5X,15H*****BLL        2////)
      IF (L2.EQ.0) GO TO 150
      L1=MIN0(NLLOW(1,2,N),NLLOW(2,2,N))
      DO  130 NL=L1,L2
      FLS=FLOAT(NL)-0.5
      LL=MIN0(NL,NJ)
      IF (N.GT.NLD) LL=1
      DO  130 L=1,LL
      FL=2*(L-1)
  130 ZWN2(NL,N,L)=(2.*FLS+1.)*CGL(NL,L)*WL(NL,2,L)
     1               *WRAC(FLS,FJ,FLS,FJ,SPIN(N),FL)
  150 CONTINUE
      GJ=(FJ+0.5)**2
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98767)
98767 FORMAT (/////5X,15H*****BLL        3////)

      IF (FKAI.EQ.0) GO TO 3000
      DO  1270 NOPAR=1,2
      GJT=GJ/THTOT(NJ,NOPAR)
      DO  1270 JI=1,2
      ASSIGN 1167 TO NGO1
      IF (JI.EQ.1) ASSIGN 1165 TO NGO1
      NLI2=NLUPR(NOPAR,JI,1)
      IF (NLI2.EQ.0) GO TO 1270
      NLI1=NLLOW(NOPAR,JI,1)
      DO  1260 NLI=NLI1,NLI2,2
      TI=TH(NLI,JI,1)
 1110 IF (TI.LT.1.E-6) GO TO 1260
      FLI=NLI-1
      FJI=FLI+FLOAT(JI)-1.5
      DO  1250 NF=1,NLOUT
      IDS=ABS(SPIN(1)-SPIN(NF))+.1
      FSIGN=(-1)**IDS
      DO  1250 JF=1,2
      ASSIGN 1174 TO NGO2
      IF (JF.EQ.1) ASSIGN 1172 TO NGO2
      NLF2=NLUPR(NOPAR,JF,NF)
      IF (NLF2.EQ.0) GO TO 1250
      NLF1=NLLOW(NOPAR,JF,NF)
      IF (NF.EQ.1) NLF2=MIN0(NLI,NLF2)
      IF (NLF2.LT.NLF1) GO TO 1250
      DO  1240 NLF=NLF1,NLF2,2
      TF=TH(NLF,JF,NF)
      IF (TF.LT.1.E-6) GO TO  1240
      FLF=NLF-1
      FJF=FLF+FLOAT(JF)-1.5
      TT=GJT*TI*TF                 *S(NJ,NLI,JI,NF,NLF,JF)*FSIGN
      IF (NF.EQ.1.AND.NLF.NE.NLI) TT=2.*TT
      LL1=MIN0(NLI+JI-2,NLF+JF-2,NJ)
      IF (NF.EQ.1) GO TO 1150
      LL=LL1
      GO TO 1160
 1150 LL2=MAX0((NLI-NLF)/2+1,(IABS(NLI-NLF+JI-JF)+1)/2+1)
      LL3=MIN0(NJ,(NLI+NLF)/2,(NLI+NLF+JI+JF-3)/2)
      LL=MAX0(LL1,LL3)
 1160 DO  1230 L=1,LL
      IF (L.NE.1.AND.NF.GT.NLD) GO TO 1240
      FL=2*(L-1)
      IF (L.GT.LL1) GO TO 1200
      GO TO NGO1,(1165,1167)
 1165 ZWI=ZWN1(NLI,1,L)
      GO TO 1170
 1167 ZWI=ZWN2(NLI,1,L)
 1170 GO TO NGO2,(1172,1174)
 1172 ZWF=ZWN1(NLF,NF,L)
      GO TO 1180
 1174 ZWF=ZWN2(NLF,NF,L)
 1180 BL(NF,L)=BL(NF,L)+TT*ZWI*ZWF
 1200 IF (NF.NE.1) GO TO 1230
      IF (L.LT.LL2.OR.L.GT.LL3) GO TO 1230
      ZW2=(2.*FLI+1.)*(2.*FLF+1.)*(2.*FJI+1.)*(2.*FJF+1.)
     1    *(CGO(FLI,FLF,FL)*WRAC(FLI,FJI,FLF,FJF,0.5,FL)

     2    *WRAC(FJI,FJ,FJF,FJ,SPIN(1),FL))**2
      IF (NLI.EQ.NLF.AND.JI.EQ.JF) GO TO 1220
      BL(1,L)=BL(1,I)+ZW2*(1.+BC     *REBB)*TT
      REBT=REBB
      GO TO 1221
 1220 REBT=1.
 1221 ZW2=ZW2*GJ*REBT*Q(NJ,NOPAR)*TI*TF/4.
      IF (NLF.NE.NLI) ZW2=2.*ZW2
      BL(1,L)=BL(1,L)-ZW2
 1230 CONTINUE
 1240 CONTINUE
 1250 CONTINUE
 1260 CONTINUE
 1270 CONTINUE
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98768)
98768 FORMAT (/////5X,15H*****BLL        4////)
      RETURN
 3000 DO  3310 NOPAR=1,2
      LL=MIN0(MAX0(NLUPR(NOPAR,1,1)-1,NLUPR(NOPAR,2,1)),NJ)
      GJT=GJ/THTOT(NJ,NOPAR)
      DO  3310 L=1,LL
      FL=2*(L-1)
      NNLL=NLOUT
      IF (L.GE.2) NNLL=NLD
      DO  3210 N=1,NNLL
      TZW(N)=0.
      DO  3210 LS=1,2
      ASSIGN 3118 TO NGO3
      IF (LS.EQ.1) ASSIGN 3116 TO NGO3
      L2=NLUPR(NOPAR,LS,N)
      IF  (L2.LT.L+2-LS) GO TO 3210
      L1=NLLOW(NOPAR,LS,N)
      IF (L1.GE.L+2-LS) GO TO 3110
      L3=L+2-LS
      L1=L3+MOD(L3-L1,2)
      IF (L2.LT.L1) GO TO 3210
 3110 DO  3120 NL=L1,L2,2
      GO TO NGO3,(3116,3118)
 3116 TZW(N)=TZW(N)+T(NL,1,N)*ZWN1(NL,N,L)
      GO TO 3120
 3118 TZW(N)=TZW(N)+T(NL,2,N)*ZWN2(NL,N,L)
 3120 CONTINUE
 3210 CONTINUE
      DO  3310 N=1,NNLL
 3310 BL(N,L)=BL(N,L)+FLOAT((-1)**INT(ABS(SPIN(1)-SPIN(N))+.1))*GJT
     1               *TZW(1)*TZW(N)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98705)
98705 FORMAT (/////5X,15H*****BLL        5////)
      RETURN
      END
C     WIDTH FLUCTUATION FACTOR
      FUNCTION       S(NJ,NLI,JI,NF,NLF,JF)
C
      DIMENSION      A(500)
```

```
C
      COMMON  /CINT/XI(8),WI(8),XA(8),XB(8),XL1(8),XL2(8),XD1(8),XD2(8)
     1        /CLEV/NLEV,FX(25),SPIN(25),NPAR(25),NLMAX(25),DJ,NLMAXA
     2        /CSTA/T(11,2,25),TH(11,2,25),THTOT(21,2),Q(21,2),Q@CONS,
     3             *CONST,FNR,BC,REBB,FKAI,COMP
     4        /CDEG/DEGO
     5        /CETC/NLLOW(2,2,25),NLUPR(2,2,25),FJ,NOPAR
C
 1000 S=0.
      A1=TH(NLI,JI,1)
 1020 IF (A1.LT.1.E-6) RETURN
      ALPHA=A1
      A2=TH(NLF,JF,NF)
 1040 IF (A2.LT.1.E-6) RETURN
      ALPHA=ALPHA+A2
C
      EP=FKAI*.5
      I=0
      DO  1142 N=1,NLEV
      DO  1141 J=1,2
      NL2=NLUPR(NOPAR,J,N)
      IF (NL2.EQ.0) GO TO 1141
      NL1=NLLOW(NOPAR,J,N)
      DO  1140 NL=NL1,NL2,2
      AO=TH(NL,J,N)
      IF (AO.LT.1.E-6) GO TO 1140
      I=I+1
      A(I)=AO
      ALPHA=ALPHA+AO*EP
 1140 CONTINUE
 1141 CONTINUE
 1142 CONTINUE
      IMAX=I
      IF (IMAX.EQ.0) RETURN
      DEG=2.+FLOAT(IMAX)*EP
      ALPHA=ALPHA/DEG
      DEG=DEGO/(DEG-1.)
      A1=A1/ALPHA
      A2=A2/ALPHA
      DO  1150 I=1,IMAX
 1150 A(I)=A(I)/ALPHA
C
      DO  2020 K=1,8
      X1=XA(K)**DEG
      X2=XB(K)**DEG
      DS1=XD1(K)                     /(((1.-A1)*X1+A1)*((1.-A2)*X1+A2))
      DS2=XD2(K)                     /(((1.-A1)*X2+A1)*((1.-A2)*X2+A2))
      DO  2010 I=1,IMAX
      DS1=DS1/((1.-A(I))*X1+A(I))**EP
 2010 DS2=DS2/((1.-A(I))*X2+A(I))**EP
 2020 S=WI(K)*(DS1+DS2)/2.+S
      S=S*DEG*EP*THTOT(NJ,NOPAR)/ALPHA
      IF (NF.EQ. 1.AND.NLI.EQ.NLF.AND.JI.EQ.JF) S=S*(1.+2./FKAI)
      RETURN
      END
C FACTORIAL

      SUBROUTINE    FACTRL
      COMMON  /CFAC/FAC0,FAC(100),EFAC0,EFAC(100)
      FAC0=1.0
      FACN=1.0
      EFAC0=0.
      EFACN=0.
      DO  10 N=1,100
      FACN=FACN*FLOAT(N)
    1 IF (FACN.LE.3.16) GO TO 5
      FACN=FACN/10.
      EFACN=EFACN+1.
      GO TO 1
    5 FAC(N)=FACN
   10 EFAC(N)=EFACN
      RETURN
      END
C  COUPLING CONDISIONS ARE ASSUMED TO BE SATISFIED
      FUNCTION      DELT(A,B,C)
      COMMON  /CFAC/FAC0,FAC(100),EFAC0,EFAC(100)
      I1=A+B-C+.1
      I2=B+C-A+.1
      I3=C+A-B+.1
      I4=A+B+C+1.1
      DELT=FAC(I1)*FAC(I2)*FAC(I3)/FAC(I4)
      RETURN
      END
C
      FUNCTION      EXDELT(A,B,C)
C
      COMMON  /CFAC/FAC0,FAC(100),EFAC0,EFAC(100)
C
      I1=A+B-C+.1
      I2=B+C-A+.1
      I3=C+A-B+.1
      I4=A+B+C+1.1
      EXDELT=EFAC(I1)+EFAC(I2)+EFAC(I3)-EFAC(I4)
      EXDELT=EXDELT/2.
      RETURN
      END
C     CLEBSCH-GORDAN COEFFICIENT
C  COUPLING CONDISIONS ARE ASSUMED TO BE SATISFIED
      FUNCTION      CGO(A,B,C)
C
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98765)
98765 FORMAT (/////5X,15H*****CGO        1////)
      D=(A+B+C)/2.
      CGO=FLOAT((-1)**INT(D-C+.1))
     1    *SQRT((2.*C+1.)*DELT(A,B,C))/((D+1.)*DELT(A/2.,B/2.,C/2.))
     2    *10.**(EXDELT(A,B,C)-2.*EXDELT(A/2.,B/2.,C/2.))
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98766)
98766 FORMAT (/////5X,15H*****CGO        2////)
      RETURN
      END
C     RACAH COEFFICIENT

C  COUPLING CONDISIONS ARE ASSUMED TO BE SATISFIED
      FUNCTION   WRAC(A,B,C,D,E,F)
C
      COMMON  /CFAC/FAC0,FAC(100),EFAC0,EFAC(100)
C
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98765)
98765 FORMAT (/////5X,15H*****WRAC       1////)
      W1=DELT(A,B,E)*DELT(C,D,E)*DELT(A,C,F)*DELT(B,D,F)
      I1=A+B+E+1.1
      I2=C+D+E+1.1
      I3=A+C+F+1.1
      I4=B+D+F+1.1
      J1=A+B+C+D+1.1
      J2=A+D+E+F+1.1
      J3=B+C+E+F+1.1
      N1=MAX0(I1,I2,I3,I4)
      N2=MIN0(J1,J2,J3)
      W2=0.
      EW=EXDELT(A,B,E)+EXDELT(C,D,E)+EXDELT(A,C,F)+EXDELT(B,D,F)
      DO  1000 N=N1,N2
      K1=N-I1
      K2=N-I2
      K3=N-I3
      K4=N-I4
      L1=J1-N
      L2=J2-N
      L3=J3-N
 1000 W2=W2+FLOAT((-1)**L1)    *FAC(N)/(FAC(K1)*FAC(K2)*FAC(K3)*FAC(K4)*
     1   FAC(L1)*FAC(L2)*FAC(L3))*10.**(EW+EFAC(N)-EFAC(K1)-EFAC(K2)-
     2   EFAC(K3)-EFAC(K4)-EFAC(L1)-EFAC(L2)-EFAC(L3))
      WRAC=W2*SQRT(W1)
      CALL  OVERFL(NOVFL)
      IF (NOVFL.EQ.1) WRITE (6,98766)
98766 FORMAT (/////5X,15H*****WRAC       2////)
      RETURN
      END
```