ELECTROEXCITATION OF GIANT RESONANCES BETWEEN 5 MeV AND 40 MeV EXCITATION ENERGY IN ^{197}Au

Kenneth Paul Ferlic

NAVAL POSTGRADUATE SCHOOL

Monterey, California

THESIS

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BETWEEN 5 MeV and 40 MeV
EXCITATION ENERGY IN ^{197}Au

by

Kenneth Paul Ferlic
and
Ronald Dallas Waddell

June 1974

Thesis Advisors: F.R. Buskirk
X.K. Maruyama

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ABSTRACT

Inelastic electron scattering from ^{197}Au between 5 MeV and 40 MeV excitation energy revealed giant multipole resonances. Angular distribution studies with incident 90 MeV electrons show evidence of previously unreported giant monopole states. Reduced matrix elements have been extracted and multipolarity assignments have been made. Seven states have been observed at excitations of 7.3 (undetermined magnetic), 9.2 (E0), 10.8 (E2), 14.0 (E1), 18.0 (undetermined), 22.5 (E2), and 33.5 MeV (E0 or E2).

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I. INTRODUCTION

Giant resonance investigations of heavy nuclei have been actively pursued at the Naval Postgraduate School electron linear accelerator since 1973. Initial studies by Warshawsky and Webber [Ref. 1] demonstrated the feasabiltiy of measuring inelastic electron spectra in the continuum region of ^{197}Au. They adapted analysis techniques developed at Darmstadt and measured cross sections for several known resonances. Warshawsky and Webber further suggested the existence of previously unreported resonances at about 9 MeV and 23 MeV excitation energy, but their analysis did not conclusively identify the multipolarities.

The work described in this thesis completes the study of ^{197}Au discussed above and extends the excitation energy range to 40 MeV. Seven giant multipole resonances have been observed. Besides the previously reported 7.3, 10.8, and 14.0 states [Refs. 1-4, 18 and 19], the existence of resonances at 9.2 and 22.5 MeV are required to explain the observed electron spectra.

Experimental values of the inelastic scattering form factors were measured at scattering angles of 60^o, 75^o, 90^o, 105^o, and 120^o with incident electrons of 90 MeV energy. Transition multipolarities have been deduced and reduced transition probabilities have been extracted. Newly identified are resonances at excitation energies of 9.2 MeV (isoscalar E0), 22.5 MeV (isovector E2), and 33.5 MeV (isovector E0 or E2). Previously reported multipolarities for the 10.8 MeV (isoscalar E2) and 14.0 MeV (isovector E1) [Ref. 18] resonances have been confirmed. The analysis contained here is unable to uniquely assign transition multipolarities to the 7.3 MeV (magnetic) and 18.0 MeV structures.

II. THEORY

A. ELECTRON SCATTERING

The Mott cross section for an extremely relativistic electron which scatters elastically from a nucleus of point charge Ze is given by [Ref. 6]

$$\left(\frac{d\sigma}{d\Omega}\right)_{Mott} = \left(\frac{Ze^2}{2E_i}\right)^2 \frac{\cos^2\frac{\theta}{2}}{\sin^4\frac{\theta}{2}} \quad . \qquad \text{II-1}$$

The electron is assumed to have spin while the nucleus has neither spin nor magnetic moment. Nuclear charge structure in a nucleus of finite extent modifies the scattering cross section to [Ref. 6]

$$\left(\frac{d\sigma}{d\Omega}\right)_{Measured} = \left(\frac{d\sigma}{d\Omega}\right)_{Mott} \left| \int_{\substack{nuclear\\volume}} \rho(\vec{r})\, e^{i\vec{q}\cdot\vec{r}}\, d\tau \right|^2 . \qquad \text{II-2}$$

$\rho(\vec{r})$ is the charge density within the nucleus as a function of $\vec{r}$, the radius vector from the center of the nucleus, and $\vec{q}$ is the momentum transfer vector. The Born approximation has been assumed. The term describing the nuclear structure is called the square of the form factor,

$$\left|F(q^2)\right|^2 = \frac{\left(\frac{d\sigma}{d\Omega}\right)_{Measured}}{\left(\frac{d\sigma}{d\Omega}\right)_{Mott}} \quad . \qquad \text{II-3}$$

For inelastic scattering, the cross section may also be written as a modification to the Mott scattering cross section, but the form is more complex, with both transverse and longitudinal contributions which are described elsewhere [Ref. 7]. For inelastic longitudinal scattering the form factor is related to the matrix element of the charge

operator evaluated between initial and final nuclear states. Although transverse components require modification of the simple expression II-2, it is conventional to call the experimental form factor squared the ratio of measured to Mott cross sections as in II-3. This value is compared to theoretical calculations based on particular nuclear models.

For inelastic scattering, the Born approximation may be used to compute the theoretical form factor based on an assumed nuclear transition charge distribution. First attempts at a solution were made by describing the perturbing fields in terms of a multipole expansion, and assuming the incident and scattered electron wave functions to be plane waves. This so called plane wave Born approximation (PWBA) is satisfactory for light nuclei, but becomes less accurate as the number of protons in the nucleus increases. For heavy nuclei, the Coulomb field surrounding the nucleus distorts both the incident and scattered electron wave functions sufficiently that a plane wave solution no longer gives the correct results. Consequently, the plane wave solutions of the PWBA have to be replaced by phase shifted spherical waves. This method, termed the distorted wave Born approximation (DWBA), in practice requires computer computations to extract the form factors [Ref. 8]. Form factors thus calculated are plotted as a function of scattering angle for each desired electric and magnetic transition. Comparison of these plots with experimental results allows for the assignment of transition modes to the observed resonances.

B. GIANT RESONANCES

The term "giant resonance" has been used until recently to describe the giant electric dipole resonance (GDR). This resonance appears as a

well known feature in the nuclear excitation spectra produced by such photonuclear processes as photodisintegration, photon absorption, and inverse reactions such as the (p,γ) reaction. The presence of the GDR is characterized by a giant bump in photonuclear spectra at excitation energies from 10 to 25 MeV. It occurs throughout the periodic table and, according to the Goldhaber-Teller and to the Steinwedel-Jensen model, appears at excitation energies that are proportional to the inverse nuclear radius, $E_x = 80A^{-1/3}$ [Ref. 9].

This conspicuous resonance appears also in inelastic electron scattering spectra. The advantage of electron scattering experiments over the photonuclear processes for exploring the nature of the giant resonances lies in the variable momentum transfer, q. In the case of the photonuclear processes, the momentum transfer is determined uniquely by the excitation energy. The giant resonance in the electron scattering cross section can be measured at different values of q depending on the scattering angle, θ, and the incident electron energy, E_i; the dependence being given by

$$q^2 = 4 E_i E_f \sin^2 \frac{\theta}{2} , \qquad \text{II-4}$$

where E_f is the final electron energy. In addition, at values of q higher than is available from photonuclear work, excitation modes other than E1 become observable. Consequently, the term "giant resonance" now refers to all multipole excitation modes which exhibit strongly coherent properties.

Early attempts to explain the giant resonances were based mainly on collective models. The initial Goldhaber-Teller model assumed a rigid displacement of the protons as a whole against the neutrons as a whole, thus producing a large collective dipole moment. The

Generalized Goldhaber-Teller model assumes that nuclear matter consists of four interpenetrating fluids: neutrons with spin up (n↑), protons with spin up (p↑), neutrons with spin down (n↓), and protons with spin down (p↓). Any two of these fluids may oscillate 180° out of phase with the other two, giving rise to four possible collective modes. For example, nucleons with spin up could oscillate against nucleons with spin down producing a magnetic resonance [Ref. 5].

The Steinwedel-Jensen model or hydrodynamic model is based on the oscillation of neutron and proton fluids within a rigid nuclear surface. An extension of this model is the dynamic collective model [Ref. 9]. The dynamic collective model replaces the rigid nuclear surface of the Steinwedel-Jensen model by a surface that may vibrate. These surface vibrations, however, are much slower than the internal giant dipole oscillations so that the approximation can be made that the dipole oscillations take place in a deformed nucleus.

A different model of the dipole giant resonances, used mainly for light, closed-shell nuclei, is based on the shell model of the nucleus. This particle-hole (ph) or Brown model arises from the observation by Wilkinson [Ref. 10] that a 1p nucleon, promoted into the 2s-1d shell, will produce dipole strengths large enough to explain the observed giant resonance cross sections. The shell model description [Ref. 10] gave the strength of the absorption correctly, but the resonance energy was incorrect, and the effect of the particle-hole interaction was noted by Brown [Ref. 11].

It has been shown [Ref. 9] that such a shell model is separable in the relative co-ordinate of all the protons versus all the neutrons; and that, upon absorption of a dipole photon, a particular linear combination of single-particle excitations is produced which corresponds

to a motion of all the protons against all the neutrons; i.e., a Goldhaber-Teller collective vibration. Hence, the shell model and collective models are equivalent in their description of collective states.

Giants resonances, then, may be described as strongly collective modes of excitation in which a considerable number of nucleons take part. In the last several years, much progress has been made in the investigation of these states using models such as those described above. Several modes of excitation other than the GDR have been identified, including the giant electric quadrupole resonance (GQR) and the giant magnetic dipole resonance (GMDR). A short summary of some of these works follow.

Early electron scattering investigation of the giant resonance structure was carried out by Isabelle and Bishop on ^{16}O [Ref. 7]. By studying the angular dependence of cross sections, the giant dipole was observed. These experiments demonstrated the feasibility of systematic studies of the level schemes and transitions in light nuclei.

Yamaguchi et. al. [Ref. 12] have carried out extensive investigations of the fine structure in the giant resonance region of ^{12}C. By making measurements at both backward and forward angles while keeping the momentum transfer constant, they were able to extract the longitudinal and transverse form factors as functions of excitation energy. The resolution of the fine structure in this manner revealed seven peaks associated with the longitudinal form factors and nine with the transverse. The dipole strength is distributed among a number of states to produce this fine structure in the giant resonance region.

An investigation of the isotopic characteristics of the giant dipole resonance has been carried out by Carlos et. al. [Ref. 13]. The giant

dipole resonances for the Neodymium isotopes ^{142}Nd to ^{146}Nd, ^{148}Nd, and ^{150}Nd were studied with a monochromatic photon beam by measuring the partial photonuclear cross sections $\sigma(\gamma,n)$ $\sigma(\gamma, pn)$ and $\sigma(\gamma,2n)$. As the number of neutrons in the nucleus increased, the dipole resonance began to broaden. For ^{150}Nd, the resonance actually split into two distinct peaks. An interpretation is given by the dynamic collective model in which there is a coupling between dipole oscillations and surface vibrations. The splitting of the resonance in ^{150}Nd characterizes a deformed nucleus, and the experimental cross section was closely reproduced by superposition of two separate Lorentz lines whose centers are separated by four MeV. In the framework of the hydrodynamic model, one can assume for an axially deformed nucleus two modes of excitation at differing energies, equivalent to oscillations in the direction of the two axes.

Pitthan and Walcher [Ref. 14] did (e,e') investigations with Ce, La, and Pr. All three elements show distinct resonances at excitation energies of 9, 12, and 15 MeV. The resonance at 15 MeV was identified as the E1 giant resonance based on correlation of the excitation energy and strength with the GDR seen in photo-neutron experiments. The 12 MeV resonance exhibited longitudinal properties similar to the E1 but did not appear in (γ,n) studies. It was assigned an E2 or E0 excitation mode based on comparison to form factors developed from the hydrodynamic model. The 9 MeV resonance was found to be transverse and most likely an M1 transition.

Later, Lewis and Bertrand [Ref. 15] observed that the (p,p') spectra of ^{27}Al, ^{54}Fe, ^{120}Sn, and ^{209}Bi consistently produced enhancements at excitation energies slightly lower than those of the known giant

dipole resonance. Since the resonance energies of the giant dipole had been previously well measured, they concluded that it was unlikely that the giant dipole excitation was responsible for most of the observed enhancement. This apparent resonance shift was due to the presence of a giant isoscaler-quadrupole vibration located at $E_x = 63\ A^{-1/3}$ MeV.

In forward angle (e,e') experiments, Fukuda and Torizuka observed [Ref. 16] similar E1 and E2 resonances in ^{90}Zr. The usual dipole resonance was seen at 16.65 MeV and additional resonances were seen at 14 MeV and 28 MeV. Based on a prediction of the hydrodynamic model that a quadrupole giant resonance should appear at a position 1.6 times the peak energy of the usual giant dipole resonance [Ref. 17], the 28 MeV resonance was assigned an E2 transition. An assignment of either E0 or E2 was made for the 14 MeV peak. Based on similar results for ^{59}Fe, ^{116}Sn, and ^{208}Pb [Ref. 16] these new giant resonances seem to be universal features existing at excitation energies of 65 $A^{-1/3}$MeV and 130 $A^{-1/3}$MeV in all nuclei. Table I contains a listing of the $A^{-1/3}$ dependence of the resonances identified in this work and a list of references where others have seen or predicted corresponding resonances in ^{197}Au and other nuclei.

TABLE I

$A^{-1/3}$ Dependence of ^{197}Au Resonances

E_x (MeV)	E_x ($A^{-1/3}$-MeV)	References
9.2	53	t [Refs. 21 & 22] Ce, La, Pr [Ref. 23]
10.8	63	Au [Refs. 3 & 18]
14.0	81	Au [Refs. 3, 18, and 25]
18.0	105	Pb [Refs. 24 & 26]
22.5	130	Au [Ref. 3] Pb [Ref. 24]
33.5	195	t [Ref. 22] Pb [Ref. 26]

t = Theoretical Prediction

C. TRANSITION PROBABILITIES AND SUM RULES

The transverse-electric and magnetic form factors are given by [Ref. 27]

$$\left| F_{\substack{E\\M},L}(\vec{q}_I) \right|^2 = \frac{4\pi}{Z^2}\left(\frac{L+1}{L}\right)\left[\frac{q_I^L}{2(L+1)!!}\right]^2 B\left(\substack{E\\M}, L, \vec{q}_I, J_i \to J_f\right). \qquad \text{II-5}$$

The continuity equation provides similar relationships for the longitudinal form factor. The coefficients B are the reduced nuclear transition probabilities and, as such, contain all of the nuclear physics of the inelastic scattering problem. The theoretical form factors are calculated by the GBROW computer program as described by Ziegler [Ref. 27].

To determine whether or not the resonances observed are collective phenomena, comparison of experimental to single-particle reduced transition probabilities may be made. For a heavy nucleus, one would expect a strength greater than several times the single-particle value. Furthermore, a giant resonance should exhaust an appreciable fraction of the appropriate sum rule. If an observed resonance greatly exceeds the sum rule under the assumption of a particular transition multipolarity, it is unlikely that the multipolarity assignment is correct.

The single-particle reduced transition strengths are given by the Weisskopf unit [Ref. 28],

$$B(EL)_{SP} = \frac{e^2(2L+1)}{4\pi}\left(\frac{3}{L+3}\, R^L\right)^2 \qquad \text{II-6}$$

and

$$B(ML)_{SP} = \frac{e^2(2L+1)\cdot 10}{\pi}\left(\frac{3}{L+3}\right)^2 R^{2L-2}(0.0111), \qquad \text{II-7}$$

where $R = 1.2\ A^{-1/3} = 6.98$ fm for ^{197}Au. Table II provides values of the single-particle transition strengths for ^{197}Au.

Another, to some extent model-independent, evaluation of the transition strength of EL modes may be achieved by expressing the strength relative to the energy-weighted sum rule (EWSR). Sum rules for magnetic transitions are more dependent on the structure of the nucleus in question and, therefore, no comparisons to these have been made here. States at excitation energies less than 15 MeV appear to be $\Delta T = 0$ except for the EL mode which is $\Delta T = 1$. The sum rule for isoscalar ($\Delta T = 0$) excitation modes with $L > 1$ is given by [Ref. 29]

$$S(EL, \Delta T=0) = \sum_f (E_f - E_i) B(EL, i \rightarrow f) = \frac{Z^2 e^2 L(2L+1)^2 \hbar^2 \langle R^{2L-2} \rangle}{8\pi A M} . \qquad \text{II-8}$$

The isovector ($\Delta T = 1$) sum rule for $L > 1$ is related to the isoscalar sum rule by

$$S(EL, \Delta T=1) = S(EL, \Delta T=0) \frac{N}{Z} . \qquad \text{II-9}$$

The corresponding sum rule for an isoscalar monopole (E0) excitation is [Ref. 30]

$$S(E0) = \sum_f (E_f - E_i) \, | M_{fi} |^2 = \frac{\hbar^2 Z}{M} \langle R^2 \rangle , \qquad \text{II-10}$$

where M_{fi} is the monopole matrix element. The strength of E1 resonances can be expressed relative to the sum rule given by Warburton [Ref. 31]:

$$S(E1) = \frac{e^2 \hbar^2}{2 M_p} \left(\frac{9}{4\pi} \right) \frac{NZ}{A} . \qquad \text{II-11}$$

Table III gives values of these sums for ^{197}Au using weighted radii of the ground state charge distribution.

TABLE II

Weisskopf Units for ^{197}Au

L	$\frac{B(EL)}{e^2}$ *	$\frac{B(ML)}{e^2}$ *
1	6.6	.06
2	3.35×10^2	3.1
3	1.63×10^4	1.44×10^2

* Units are fm^{2L}

TABLE III

Sum of EWSR For ^{197}Au

EL	ΔT	Sum	Units
E0	0	9.2×10^4	MeV-fm^4
E1	1	7.04×10^2	e^2-MeV-fm^2
E2	0	7.4×10^4	e^2-MeV-fm^4
	1	1.1×10^5	e^2-MeV-fm^4
E3	0	6.15×10^6	e^2-MeV-fm^6
	1	9.16×10^6	e^2-MeV-fm^6

D. QUASI-ELASTIC SCATTERING

Electrons incident upon a nucleus may scatter elastically with individual nucleons within the nucleus. This process is called quasi-elastic scattering. If sufficient momentum is imparted to the nucleon, it will be knocked out of the nucleus with some kinetic energy. The simultaneous energy loss by the incident electron may result in a measurable quasi-elastic peak. It is of interest to see at which value of E_x this contribution appears on the spectrum of $\frac{d^2\sigma}{d\Omega dE_x}$, to see if it contributes to, and therefore must be subtracted from, the scattered electron spectrum in the region of the giant resonance.

The inelastic electron-nucleus cross section has been calculated in three energy-loss regions with the Fermi gas model for the nucleus [Ref. 32]: the quasi-elastic region; the threshold pion region with its pion electroproduction cross sections; and the region containing the 3-3 resonance of the proton. Pion production begins at 135 MeV and the 3-3 resonance is 298 MeV above the elastic peak, so these regions are not of interest in this work.

In the Fermi gas model, the electron scatters elastically from a single nucleon in the free Fermi sea, with the recoiling nucleon required to scatter out of the Fermi sphere. Because of the Pauli principle, the nucleon cannot scatter into an already occupied state. The final nucleon energy is given by

$$\epsilon_{kf} = \left[k^2 + M^2 \right]^{\frac{1}{2}}, \qquad \text{II-12}$$

where k is the nucleon momentum and M is the nucleon mass. The initial (bound) nucleon energy is

$$\epsilon_{ki} = \frac{k^2}{2M} + U(k^2) = \frac{k^2}{2M^*} + U(0) \,, \qquad \text{II-13}$$

where the effective nucleon mass, M^*, is given by [Ref. 33]

$$M^* = \frac{M}{1.4} \qquad \text{II-14}$$

and $U(k^2)$ is the effective single-particle potential in nuclear matter. This potential effectively shifts the electron energy loss, ω , to take into account the nuclear binding. Moni treats $U(k^2)$ as a constant, $\bar{\epsilon}$, equivalent to the average nucleon interaction energy. The quasi-elastic peak energy loss will increase with q and approach the effective free nucleon kinetic energy, $q^2 / (2M^*)$, at large values of q.

The magnitude of the above shift for the gold nucleus is of interest. The average nucleon interaction energy, $\bar{\epsilon}$, and the nuclear Fermi momentum, k_F , have been determined for nine elements from ^{6}Li to ^{208}Pb [Ref. 34] by a least squares fit of theory to quasi-elastic peak data. In the cross-section formula, an energy-conserving delta function appears, given by

$$\delta\left(\omega + \frac{k^2}{2M} - \bar{\epsilon} - \frac{(\vec{k} + \vec{q})^2}{2M}\right), \qquad \text{II-15}$$

which determines ω . The nucleon momentum is approximated by the Fermi momentum and is roughly constant at 260-265 MeV/c for heavy nuclei from nickel through lead. $\bar{\epsilon}_{Au}$ = 43 MeV [Ref. 34]. The energy-conserving delta function requires that

$$\omega = \bar{\epsilon} + \frac{kq}{M} + \frac{q^2}{2M} . \qquad \text{II-16}$$

For the smallest momentum transfer of these experiments, ω = 73 MeV. The threshold value is $\omega \cong \bar{\epsilon}_{Au}$ = 43 MeV. Thus explicit corrections for the quasi-elastic contribution need not be made for the spectra of this work.

III. DATA ANALYSIS

A. DATA REDUCTION

Five experiments were performed with an incident beam energy of 90 MeV and at scattering angles of 60°, 75°, 90°, 105°, and 120°. The experimental information is given in Table IV. In general the data analysis procedure described by Warshawsky and Webber [Ref. 1] was followed throughout this work. The initial choice of resonance energies was determined from known resonances [Refs. 1, 2, 3, and 4] and by visual inspection. Previously determined resonances occur at 7.3, 9.2, 11.0, and 14.0 MeV. Visual inspection of the background subtracted data revealed wide structures at 18.0, 22.5, and 33.5 MeV.

The fitted inelastic spectra extended from 4 to 40 MeV, except the 120° spectrum which extends only to 31.5 MeV. In some cases the data extends to 50 MeV but no structures were observed at this high excitation energy. Since the 120° data has different boundary conditions for matching the background at high excitation energies, only cross sections for resonances below 20 MeV were extracted at this angle.

Breit-Wigner resonance forms were assumed for each resonance and computer code NAW (see appendix) simultaneously fits the entire inelastic spectrum including the radiation tail and background. The new resonance positions and widths were manually varied while the NAW code varied the peak strengths and background parameters until a best fit was obtained.

The criteria used to determine a reasonable fit were as follows:

1. The data and calculated spectrum should coincide visually.

2. χ^2 per degree of freedom should be less than one. The data is not strictly statistical because the detector momentum interval is larger

than the momentum increment of the spectrometer field and hence correlations exist between energy bins.

3. The difference between the total χ^2 for successive computer iterations was $\Delta\chi^2 \lesssim 0.5$. Typically there were 300 degrees of freedom and a change of 0.5 in the total chi squared resulted in 1.7×10^{-3} per degree of freedom.

4. All observed resonances should consistently fit each of the five spectra. Table V lists the positions and widths of the resonances required.

Figures 1 - 5 present the experimental data corrected for spectrometer dispersion effects with the fitted total background and the individual resonances drawn. Figures 6 - 10 present these spectra with the total background subtracted, revealing the resonance structures of Table V.

The areas under the inelastic resonances were calculated from the Breit-Wigner resonance shapes and the ratio of each inelastic resonance area to the area under the elastic peak was calculated (A_i/A_e). The inelastic form factors squared are obtained by multiplying A_i/A_e by the square of the elastic scattering form factors (F_{el}^2). Table VII presents the experimental ratios of the inelastic to elastic areas and the square of the inelastic form factors. The elastic form factors were calculated using the program of Rawitscher and Fischer [Ref. 35]. The charge distribution parameters were c = 6.38 fm and t = 2.32 fm.

TABLE IV

Experimental Conditions

Angle	Target Thickness	Incident Energy	F_{el}^2
60	.048 g/cm^2	90.32 MeV	.1185
75	.096 g/cm^2	90.24 MeV	.0444
90	.096 g/cm^2	90.21 MeV	.0298
105	.144 g/cm^2	89.98 MeV	.0217
120	.240 g/cm^2	89.60 MeV	.0132

TABLE V

Observed Resonances

Excitation Energy MeV	Widths MeV
7.3 $\pm$ 0.3	2.8 $\pm$ 0.4
9.1 $\pm$ 0.4	2.3 $\pm$ 1.0
10.9 $\pm$ 0.4	2.8 $\pm$ 0.4
14.0 $\pm$ 0.4	4.4 $\pm$ 0.4
18.0 $\pm$ 0.6	5.1 $\pm$ 0.6
22.5 $\pm$ 0.6	7.2 $\pm$ 0.6
33.5 $\pm$ 1.4	10.5 $\pm$ 2.5

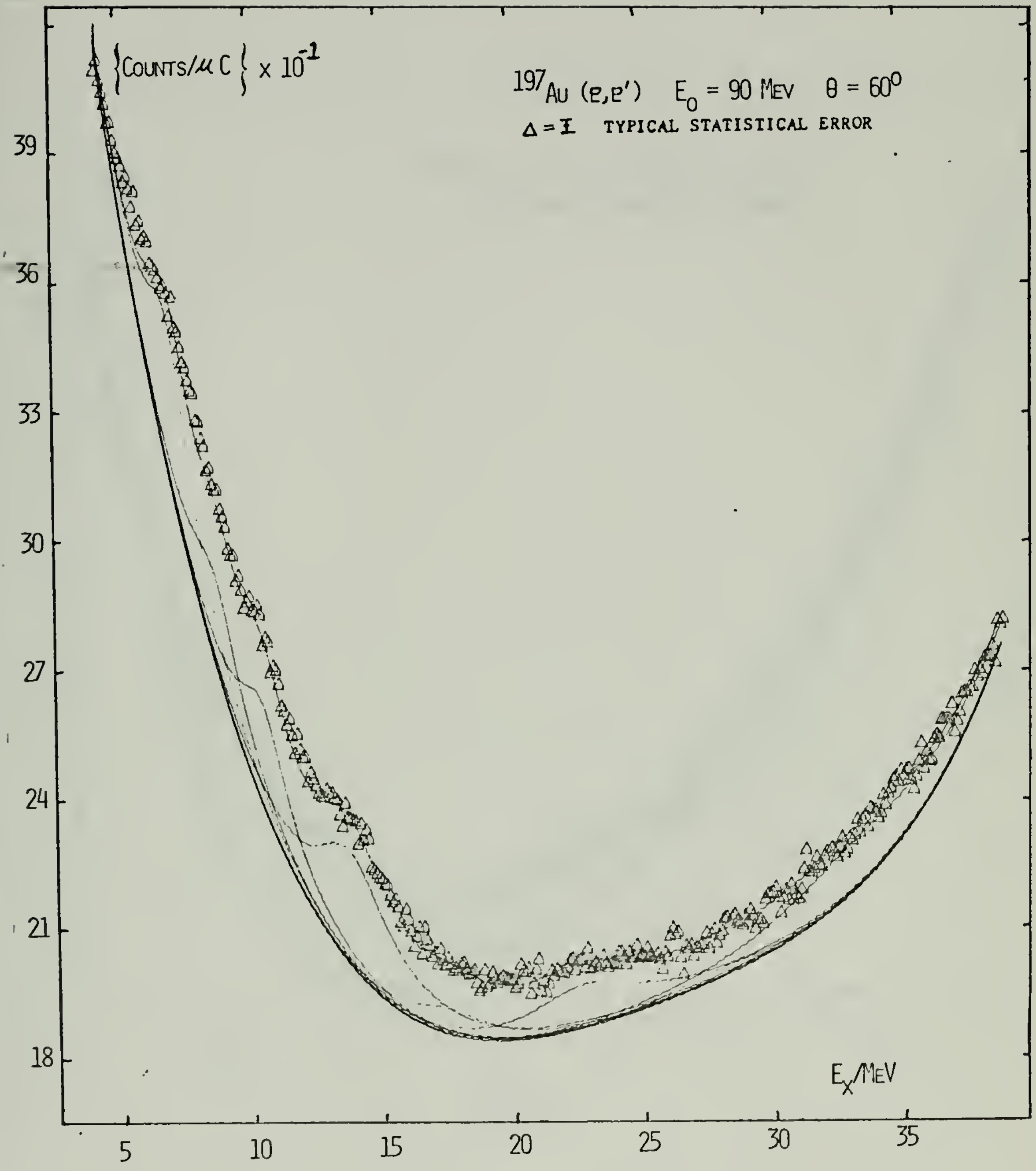

{Counts/μC} x 10^-1
197Au (e,e') E0 = 90 MeV θ = 60°
Δ = I TYPICAL STATISTICAL ERROR
39
36
33
30
27
24
21
18
Ex/MeV
5
10
15
20
25
30
35

FIGURE 1

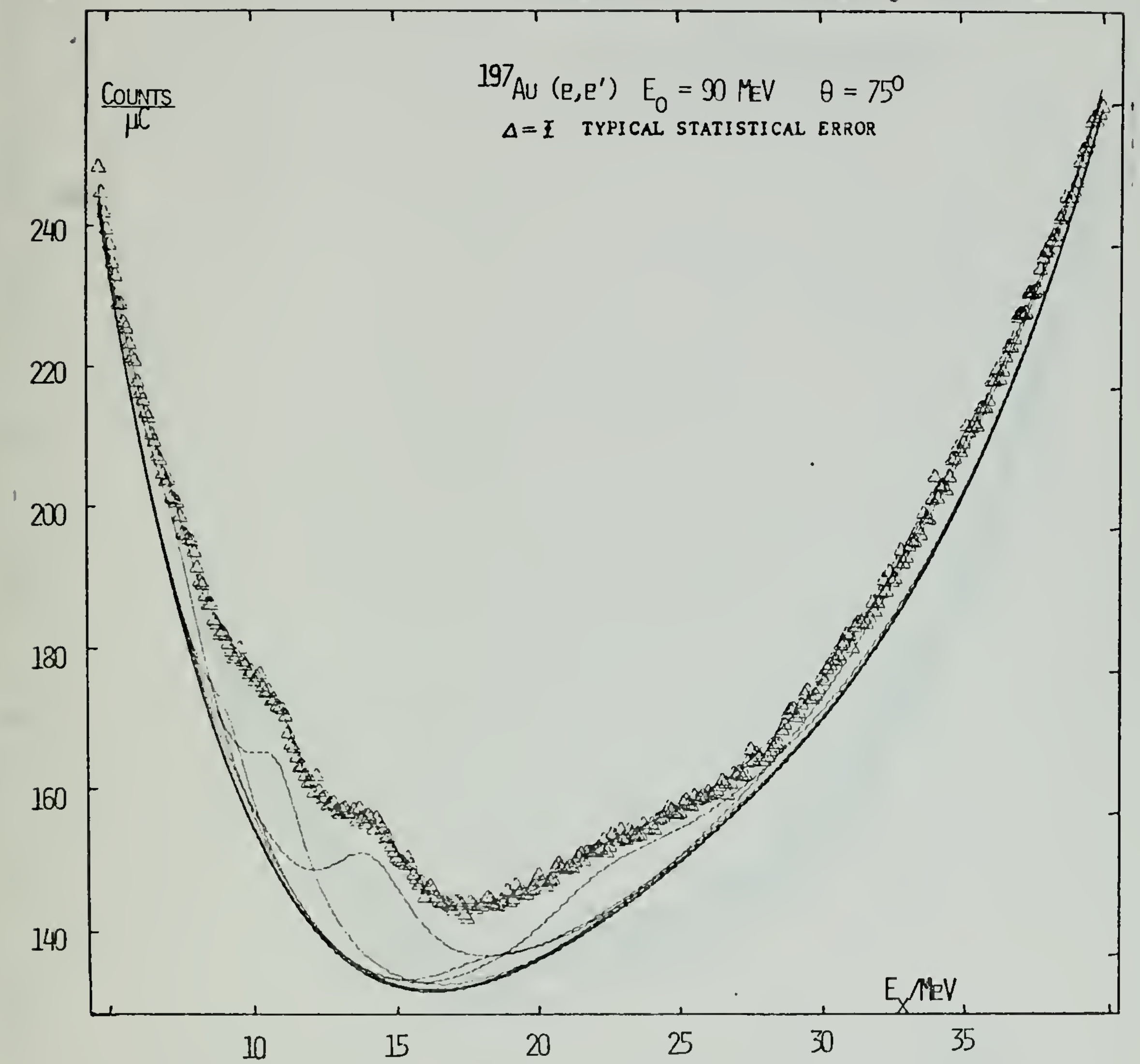

^{197}Au (e,e′) E_0 = 90 MeV θ = 75°
Δ = Ι TYPICAL STATISTICAL ERROR
Counts / μC
240
220
200
180
160
140
10
15
20
25
30
35
E_x/MeV

FIGURE 2

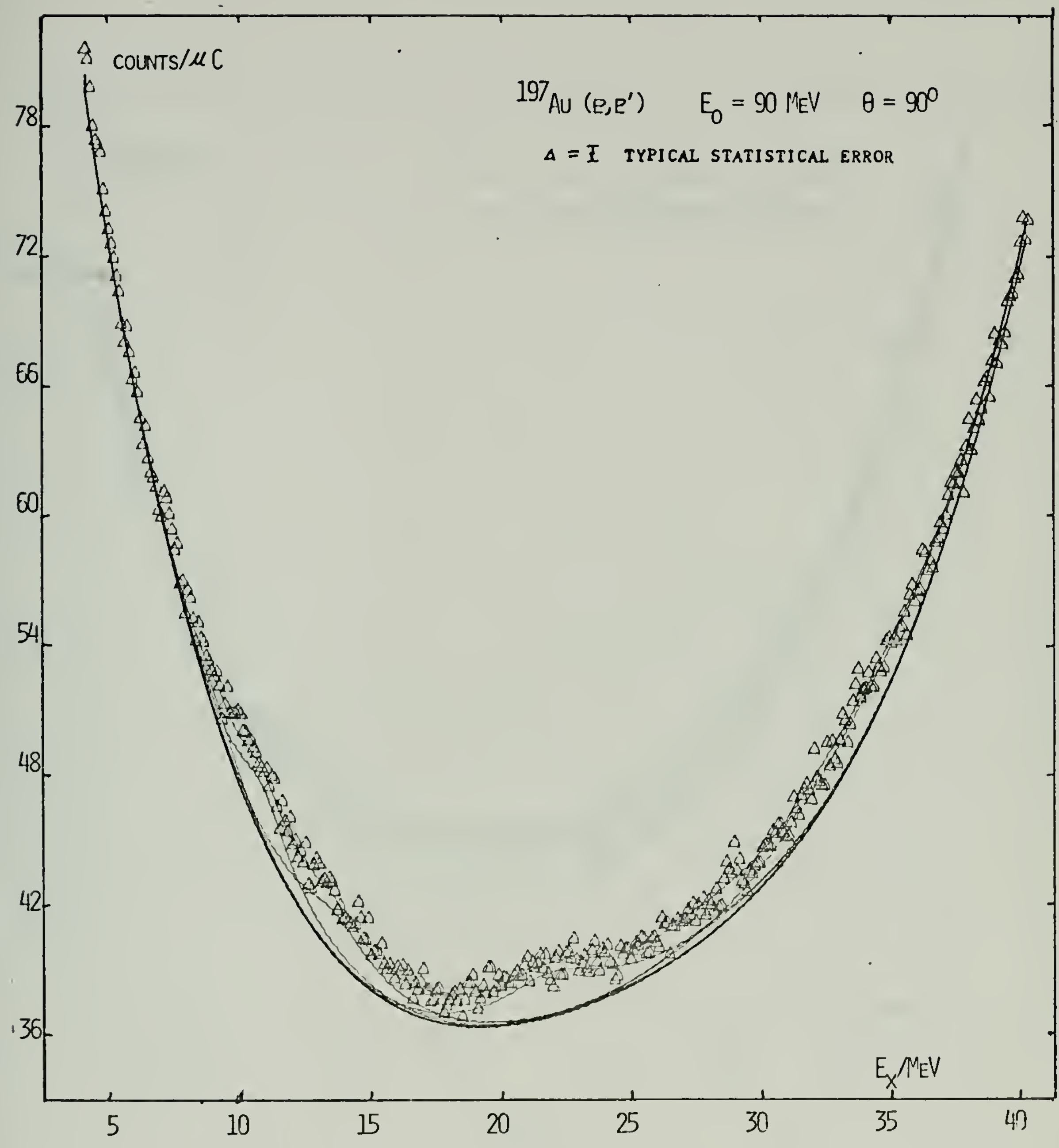

COUNTS/μC
^{197}Au (e,e′) E_0 = 90 MeV θ = 90°
Δ = Ī TYPICAL STATISTICAL ERROR
78
72
66
60
54
48
42
36
E_x/MeV
5
10
15
20
25
30
35
40

FIGURE 3

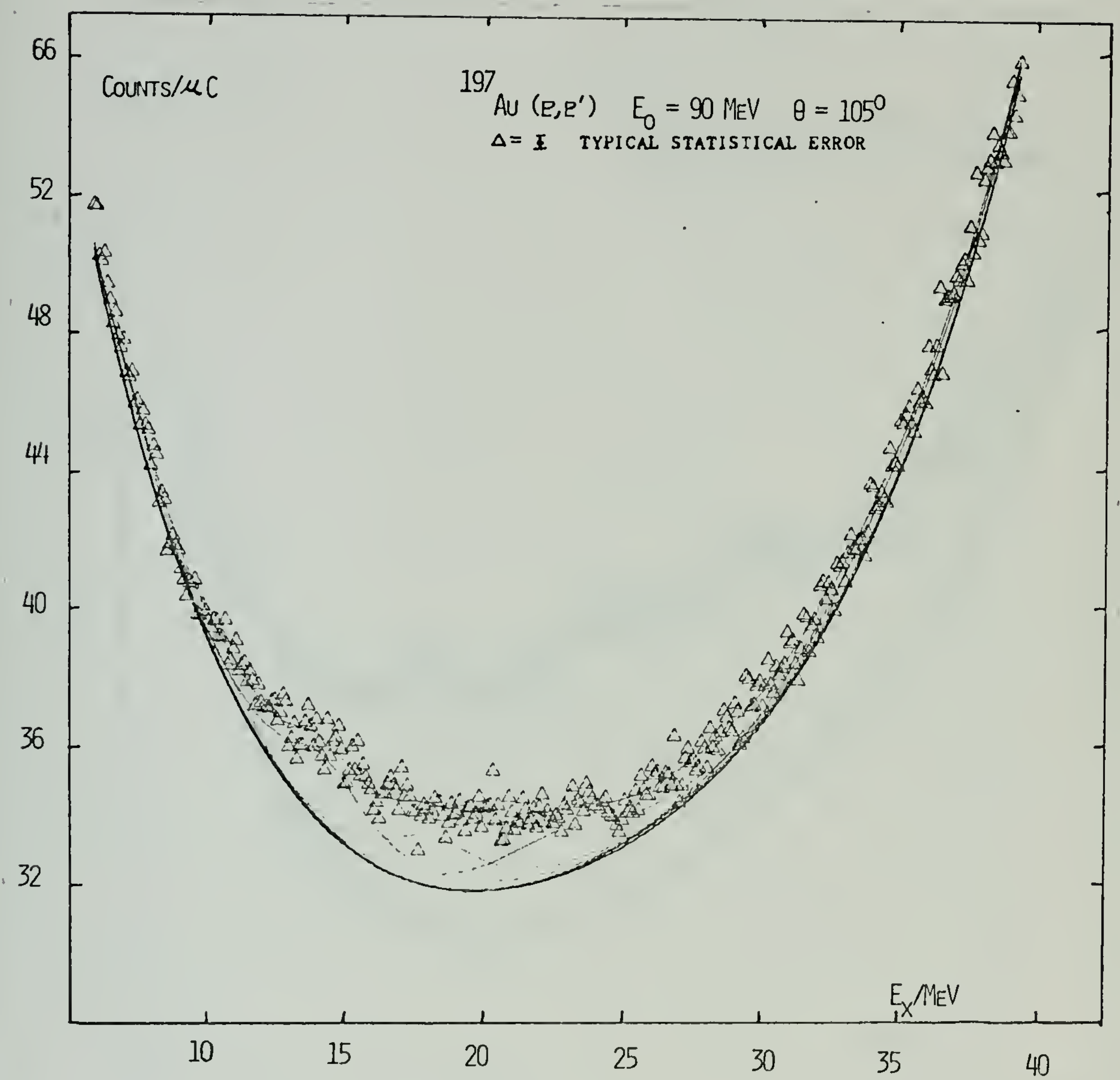
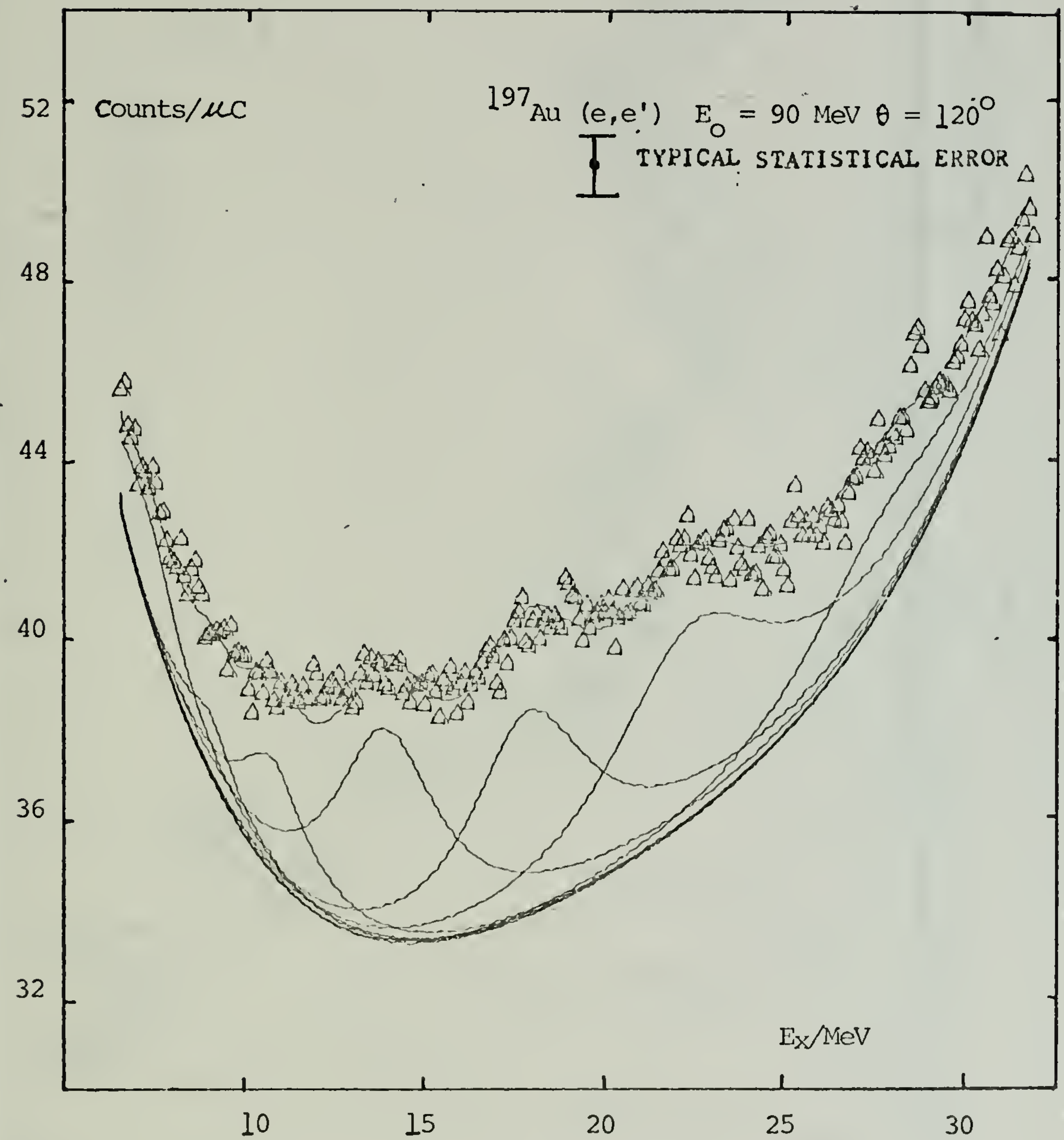

66
52
48
44
40
36
32
COUNTS/μC
197Au (e,e')   E0 = 90 MeV   θ = 105°
Δ = Ī   TYPICAL STATISTICAL ERROR
Ex/MeV
10
15
20
25
30
35
40

FIGURE 4



52
48
44
40
36
32
Counts/μC
^{197}Au (e,e') E$_0$ = 90 MeV θ = 120°
TYPICAL STATISTICAL ERROR
Ex/MeV
10
15
20
25
30

FIGURE 5

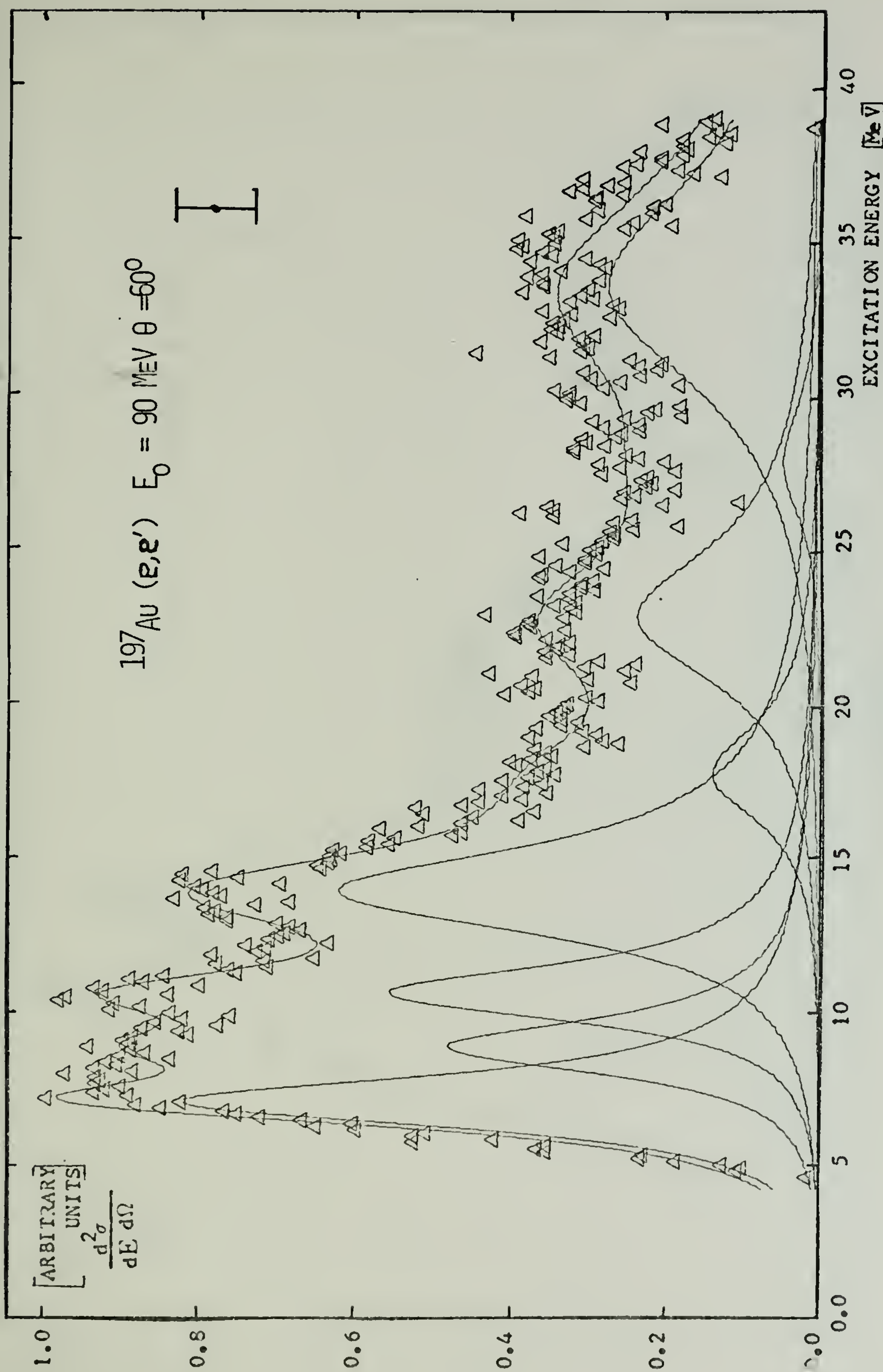
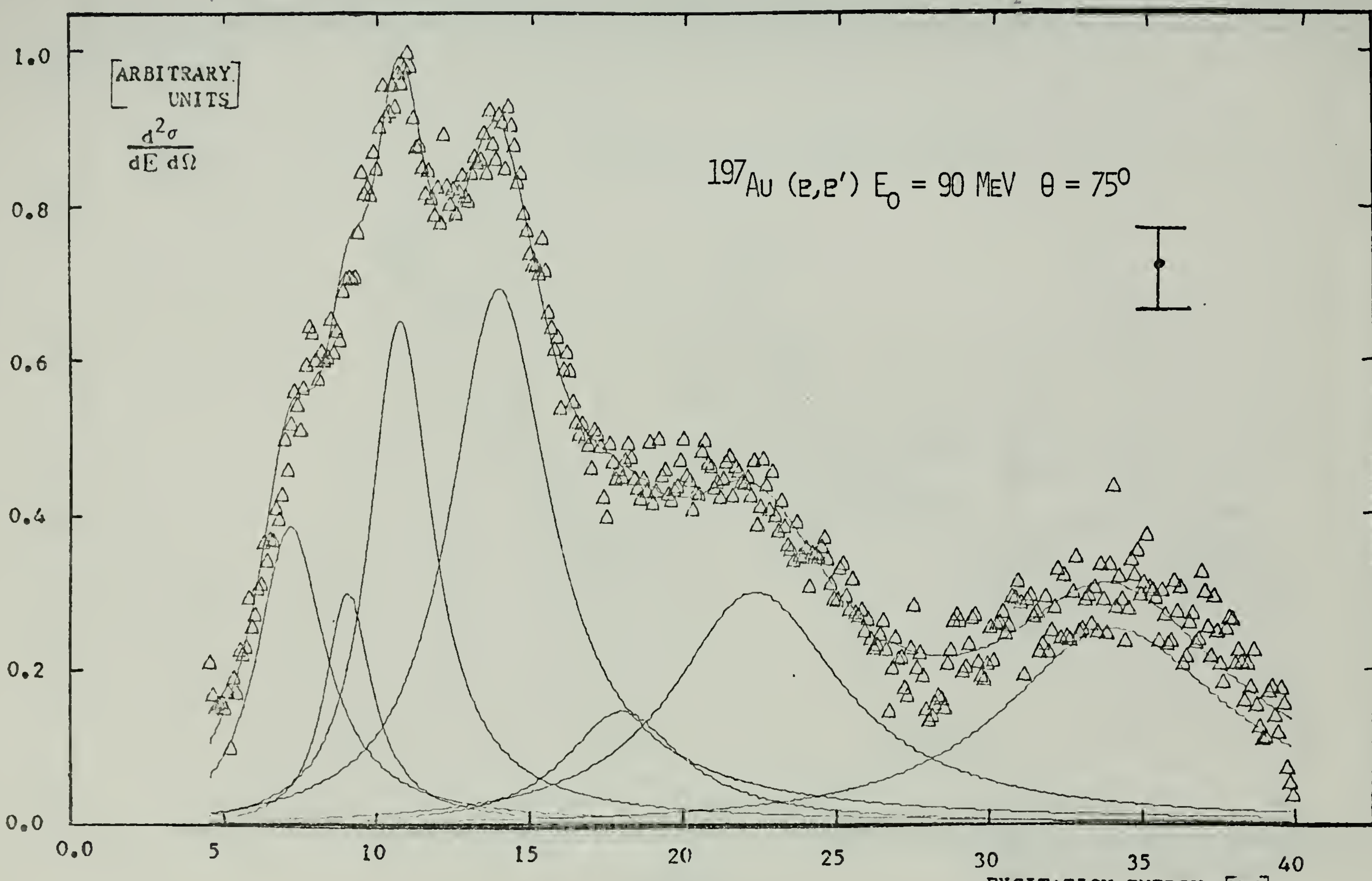
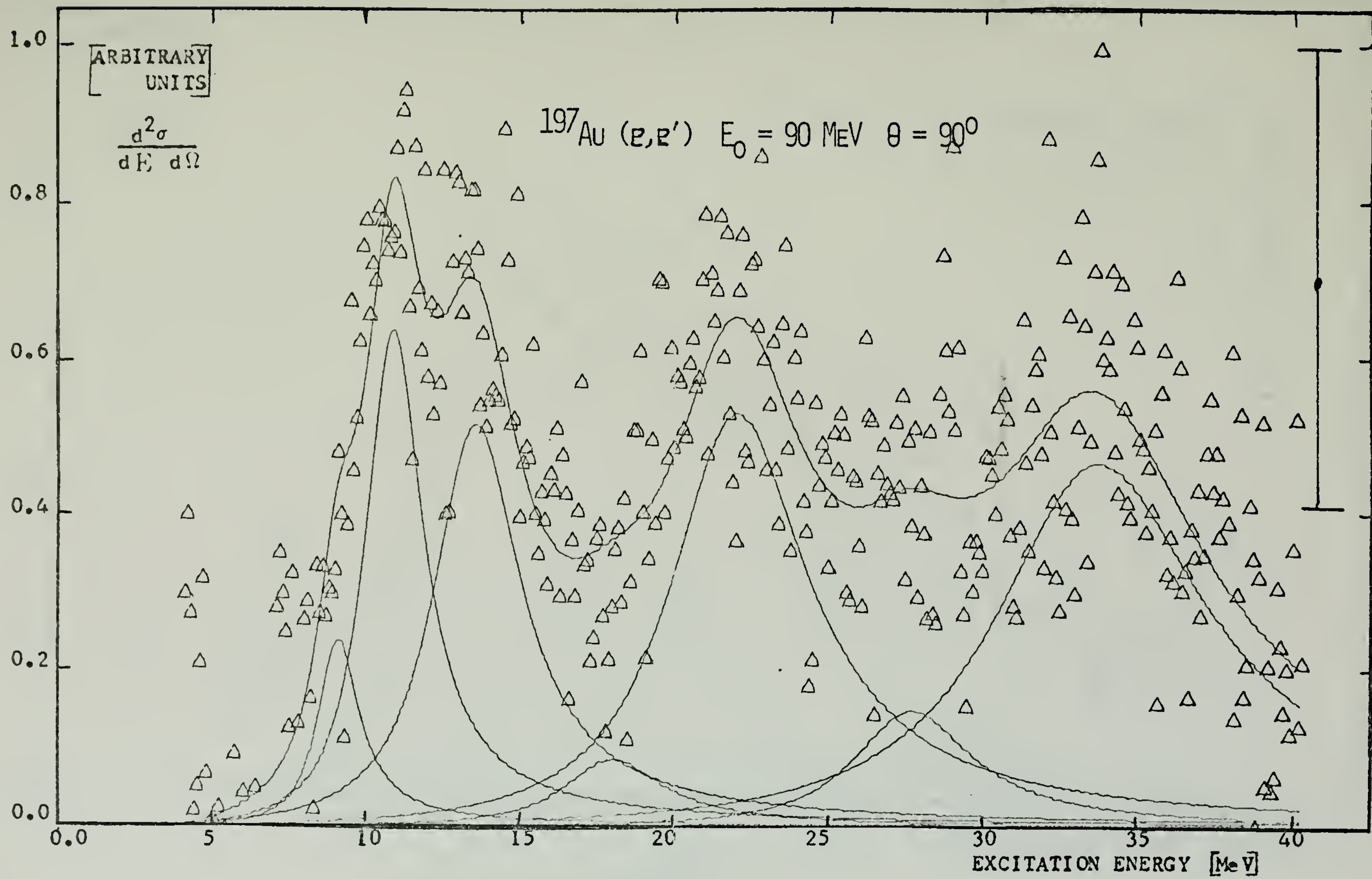

197AU (E,E') E0 = 90 MEV θ =60°
[ARBITRARY UNITS] d2σ/dE dΩ
1.0
0.8
0.6
0.4
0.2
0.0
0.0
5
10
15
20
25
30
35
40
EXCITATION ENERGY [MeV]

FIGURE 6



[ARBITRARY UNITS]
d²σ / dE dΩ
197Au (e,e') E0 = 90 MeV θ = 75°
1.0
0.8
0.6
0.4
0.2
0.0
0.0
5
10
15
20
25
30
35
40
EXCITATION ENERGY [MeV]

FIGURE 7



ARBITRARY UNITS
d²σ / dE dΩ
197Au (e,e') E0 = 90 MeV θ = 90°
1.0
0.8
0.6
0.4
0.2
0.0
0.0
5
10
15
20
25
30
35
40
EXCITATION ENERGY [MeV]

FIGURE 8

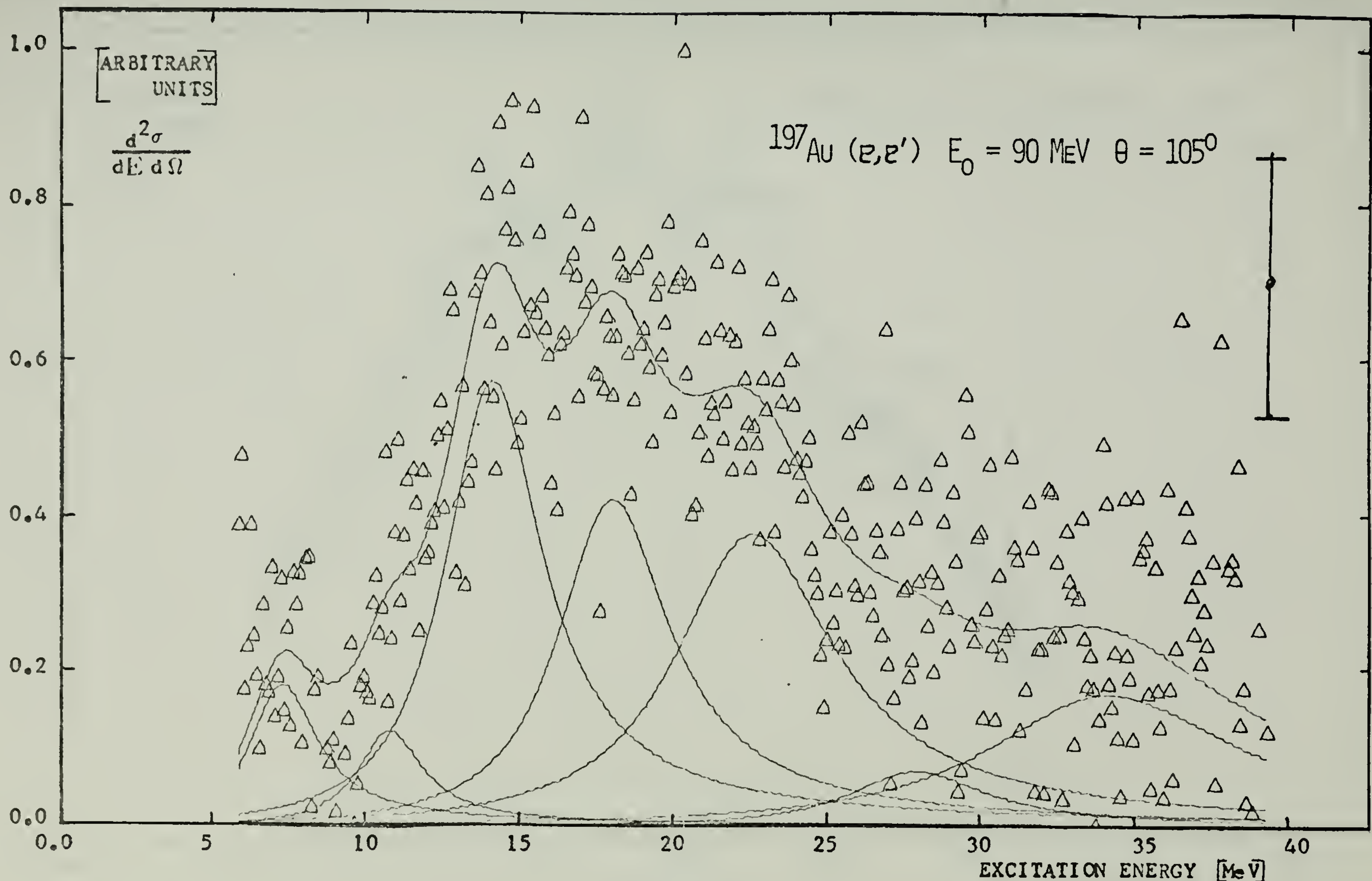
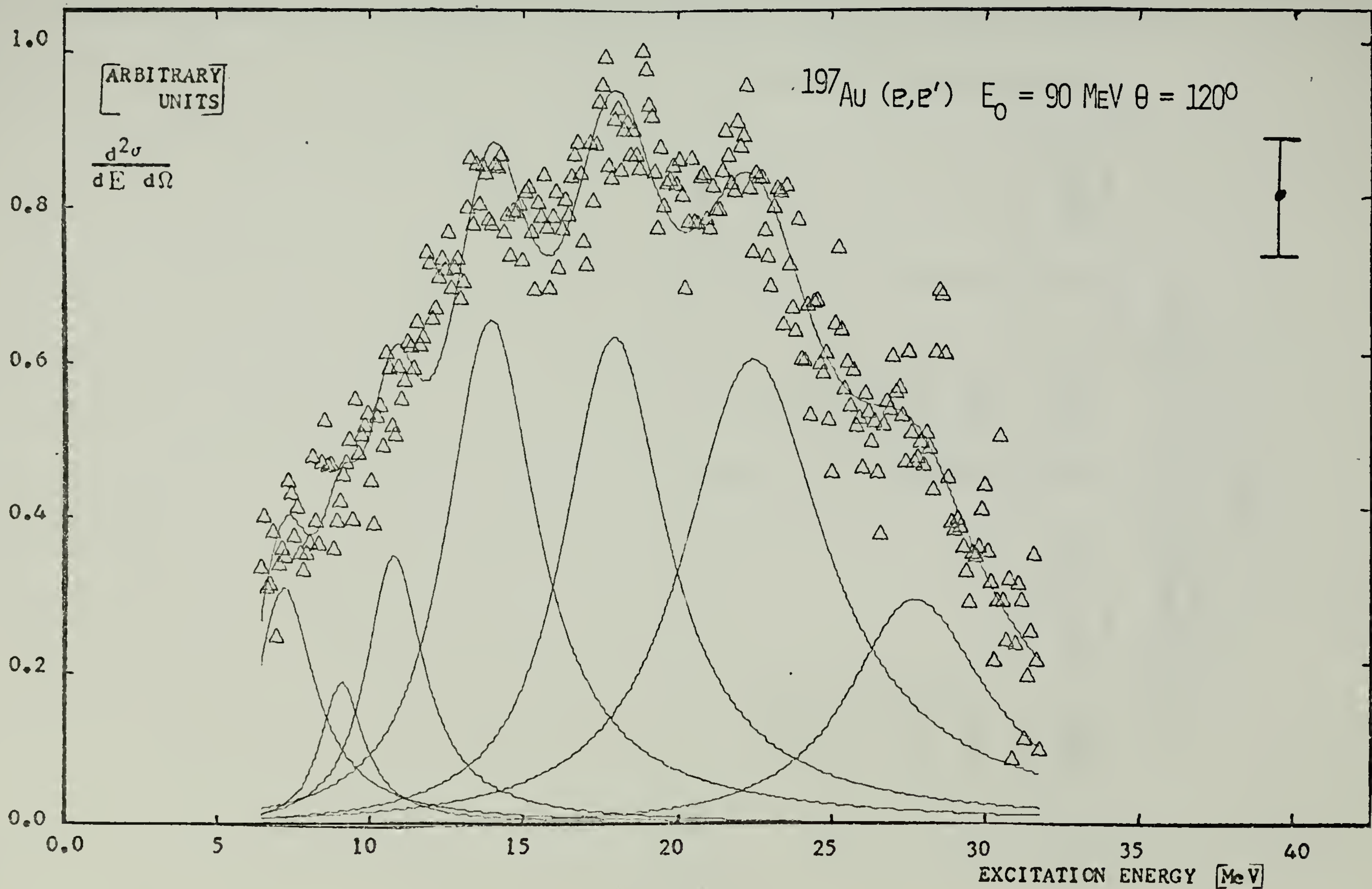

ARBITRARY UNITS
$\frac{d^2\sigma}{dE\,d\Omega}$
$^{197}Au\ (e,e')\ \ E_0 = 90\ MeV\ \ \theta = 105^0$
1.0
0.8
0.6
0.4
0.2
0.0
0.0
5
10
15
20
25
30
35
40
EXCITATION ENERGY [MeV]

FIGURE 9



1.0
0.8
0.6
0.4
0.2
0.0
ARBITRARY UNITS
$\frac{d^2\sigma}{dE\ d\Omega}$
^{197}Au (e,e') E_0 = 90 MeV θ = 120°
0.0
5
10
15
20
25
30
35
40
EXCITATION ENERGY [MeV]

FIGURE 10

TABLE VI

Scale Factors for Converting
Arbitrary Units to Experimental Units

Figure	Angle	Scale Factor $\frac{fm^2}{MeV\text{-}sr}$ / Arb. units
6	60^o	9.9×10^{-4}
7	75^o	1.89×10^{-4}
8	90^o	2.99×10^{-5}
9	105^o	1.53×10^{-5}
10	120^o	1.47×10^{-5}

TABLE VII

Area Ratios and Inelastic Form Factors Squared

E_x	Angle	A_i/A_e	Total % Error	σ/σ_{Mott}
7.3	60	6.37×10^{-3}	21	7.75×10^{-4}
7.3	75	4.00×10^{-3}	25	1.78×10^{-4}
7.3	90	9.7×10^{-4}	--	2.9×10^{-5}
7.3	105	2.70×10^{-3}	85	6.03×10^{-5}
7.3	120	1.01×10^{-2}	50	1.34×10^{-4}
9.2	60	3.19×10^{-3}	60	3.78×10^{-4}
9.2	75	2.20×10^{-3}	60	9.78×10^{-5}
9.2	90	9.73×10^{-4}	85	2.91×10^{-5}
9.2	105	1.5×10^{-4}	--	3.2×10^{-6}
9.2	120	4.34×10^{-3}	75	5.73×10^{-5}
10.8	60	4.47×10^{-3}	25	5.30×10^{-4}
10.8	75	6.53×10^{-3}	20	2.86×10^{-4}
10.8	90	3.58×10^{-3}	30	1.07×10^{-4}
10.8	105	3.9×10^{-3}	--	8.40×10^{-5}
10.8	120	1.07×10^{-2}	35	1.41×10^{-4}

TABLE VII Continued

E_x	Angle	A_i/A_c	Total % Error	σ/σ_{Mott}
14.0	60	7.60×10^{-3}	18	9.02×10^{-4}
14.0	75	1.12×10^{-2}	16	4.98×10^{-4}
14.0	90	4.42×10^{-3}	30	1.32×10^{-4}
14.0	105	8.46×10^{-3}	35	1.84×10^{-4}
14.0	120	3.18×10^{-2}	20	4.2×10^{-4}
18.0	60	1.82×10^{-3}	40	2.16×10^{-4}
18.0	75	2.70×10^{-3}	35	1.20×10^{-4}
18.0	90	1.7×10^{-3}	--	5.10×10^{-5}
18.0	105	6.91×10^{-3}	40	1.50×10^{-4}
18.0	120	3.41×10^{-2}	22	4.50×10^{-4}
22.5	60	4.21×10^{-3}	30	5.00×10^{-4}
22.5	75	7.83×10^{-3}	20	3.47×10^{-4}
22.5	90	7.17×10^{-3}	25	2.14×10^{-4}
22.5	105	8.60×10^{-3}	45	6.02×10^{-4}
33.5	60	7.66×10^{-3}	50	9.09×10^{-4}
33.5	75	9.80×10^{-3}	50	4.35×10^{-4}
33.5	90	9.90×10^{-3}	60	2.48×10^{-4}
33.5	105	1.5×10^{-2}	--	3.2×10^{-4}

B. ERROR ANALYSIS

The procedure outlined in the previous section provides values of the ratios of A_i/A_e but the uncertainties attached to these ratios requires additional considerations. The program NAW computes only statistical errors. There are other errors, both systematic and random which are not strictly statistical. Some of these are the errors resulting from the instrumental effects and are outlined by Bernard and Traverso [Ref. 36].

To obtain a more realistic estimate of the errors in the ratios A_i/A_e, the non-statistical uncertainties are assumed to be those which arise from the uncertainties in locating the resonance positions and determining their respective widths. These arise from two sources: the overall instrumental uncertainty which is estimated to be 0.15 MeV, and the freedom allowed in the resonance peak positions and widths in fitting these spectra. The total uncertainty of the energy in this work is the sum of the fitting possibilities and instrumental errors.

The Breit-Wigner shape is then analysed to see how these variations in energy effect the area under the resonances. The Breit-Wigner shape is given by

$$\frac{d\sigma(E,E_R,\Gamma)}{dE} = \frac{A}{(E-E_R)^2 + (\Gamma/2)^2} \; ; \qquad \text{III-1}$$

where E_R is the resonance energy, Γ is the resonance width, A is the strength parameter, and E is the excitation energy. The resonance cross section is given by the integral of the Breit-Wigner form

$$\sigma(E_R, \Gamma) = \frac{A\pi}{\Gamma} + \frac{2A \tan^{-1}(E_R/\Gamma)}{\Gamma} . \qquad \text{III-2}$$

The variations in position and width introduce an uncertainty in the resonance cross section,

$$\Delta\sigma(E_R, \Gamma) = \left|\frac{\partial\sigma}{\partial E_R}\right| \Delta E_R + \left|\frac{\partial\sigma}{\partial\Gamma}\right| \Delta\Gamma . \qquad \text{III-3}$$

The absolute values of the partial derivatives are assumed since the peak position and width uncertainties may be correlated.

The fractional error in the resonance cross section is

$$\frac{\Delta\sigma}{\sigma} = \frac{\left[\frac{2}{\Gamma^2+E_R^2}\right]\Delta E_R + \left[\frac{\pi}{\Gamma^2} + \frac{2\tan^{-1}(E_R/\Gamma)}{\Gamma^2} + \frac{2E_R}{\Gamma^3+\Gamma E_R^2}\right]\Delta\Gamma}{\frac{\pi}{\Gamma} + \frac{2\tan^{-1}(E_R/\Gamma)}{\Gamma}} \qquad \text{III-4}$$

This uncertainty is then added to the statistical error to provide the total error. Table VIII lists the uncertainties from the two sources.

TABLE VIII

Fractional Error Contributions

E_r	$\frac{\Delta \sigma}{\sigma}$	Stastical Errors				
		60^o	75^o	90^o	105^o	120^o
7.2	.16	.05	.08	Upper Limit	.67	.32
9.2	.51	.08	.09	.35	Upper Limit	.27
10.8	.16	.07	.05	.34	Upper Limit	.17
14.0	.11	.07	.06	.20	.25	.10
18.0	.13	.27	.21	.10	.25	.08
22.5	.09	.20	.12	.16	.34	
33.5	.27	.25	.21	.30	Upper Limit	

IV. DISCUSSION

A. COLLECTIVITY

Data analysis techniques explained in Chapter III were used to subtract the background and extract the elastic and inelastic spectra of the scattered electrons. A least squares fit was used to evaluate these spectra and resulted in the identification of seven giant resonances at excitation energies of 7.3, 9.2, 10.8, 14.0, 18.0, 22.5, and 33.5 MeV. These resonances have strengths corresponding to an appreciable fraction of the appropriate sum rule as exhibited in Table IX. Additional support to their collective nature is given in Table X where it is seen that the transition strengths are greater than several Weisskopf units. True giant resonances are therefore being observed.

B. MULTIPOLARITY ASSIGNMENTS

7.3 MeV Resonance

The multipolarity assignment of the resonance at 7.3 MeV is uncertain. Buskirk et. al. [Ref. 18] and Lone et. al. [Ref. 19] have observed this structure in backward angle (e,e') experiments and indicate a transverse excitation. A comparison of the data with calculations using GBROW [Ref. 27] and a code by Drechsel [Ref. 37] is incapable of determining a definate multipolarity assignment. Among possible reasons for this situation are a multipolarity admixture, existence of unknown longitudinal resonances influencing the forward angle data, and experimental difficulties encountered by the high counting rate at forward scattering angles.

9.2 MeV Resonance

The analysis of the 9.2 MeV resonance (53 $A^{-1/3}$) favors an E0 multipolarity assignment. This resonance exhausts 38% and 18% respectively of the E0 and E2 energy-weighted sum rules and its strength corresponds to five Weisskopf units when an E2 assignment is made. However, the angular dependence of the experimental form factors favors E0 (Fig. 12). The result would be in agreement with the isoscalar giant monopole resonance predicted at 56 $A^{-1/3}$ MeV [Ref. 21] and at 58 $A^{-1/3}$ MeV [Ref. 22]. Resonances exhibiting the characteristics of E0 or E2 transitions were also seen at E_x = 53 $A^{-1/3}$ MeV in N = 82 nuclei [Ref. 23] and in ^{208}Pb [Ref. 24]. An E1 multipolarity assignment is ruled out by comparison with DWBA form factor calculations and furthermore by the fact that no resonance has been seen in γ - absorption measurements [Ref. 25] at this excitation energy.

10.8 MeV Resonance

The resonance at 10.8 MeV (63 $A^{-1/3}$) was seen previously in ^{197}Au [Refs. 3 and 18] and in many other nuclei (see e.g. [Ref. 5]). Generally an assignment of E2 was favored in these cases. In this experiment a transition strength of 14 Weisskopf units is obtained assuming an electric quadrupole excitation. Comparison of the experimental form factors to the angular distribution calculated from the DWBA form factors is inconclusive in distinguishing between an E0 and E2 modes (Fig. 13). However, the experimental strength corresponds to 113% and 68% of the E0 and E2 sum rules, respectively. Together with our results on the 9.2 MeV resonance, the E2 assignment is therefore favored. This resonance is thought to be the isoscalar quadrupole state predicted by the collective vibration model of Bohr and Mottelson [Ref. 38].

14.0 MeV Resonance

The 14 MeV (81 $A^{-1/3}$) giant dipole resonance was measured with monochromatic γ- experiments [Ref. 25] and has also been seen in other (e,e') experiments [Refs. 3 and 18]. For this experiment, form factor comparisons to DWBA calculations show reasonable agreement at forward angles, but exhibit deviations at backward angles. An attempt was made to further explore the nature of the giant dipole transition by assuming both volume and surface oscillations separately in the DWBA calculations (Fig. 14) [Ref. 23]. Transition strengths of six and eight Weisskopf units and 84% and 104% of the sum rule are obtained for the volume and surface oscillation modes respectively. However, neither model adequately describes the observed data. As suggested by Pitthan [Ref. 39], the discrepancy at backward angles might be explained by an electric spin flip contribution to the E1 resonance [Ref. 40]. Using only the forward angle data to extract the reduced matrix elements, the volume oscillation strength exhausts the sum rule (98%), whereas the surface oscillation exceeds the sum rule. Thus a volume oscillation is favored.

18.0 MeV Resonance

A resonance of undetermined multipolarity is observed at 18.0 MeV (105 $A^{-1/3}$) excitation energy. Nagao and Torizuka [Ref. 24] have observed E3 strength at the corresponding energy in ^{208}Pb, but the state in ^{197}Au does not conform to this multipolarity. E(0-3) and M (1-2) calculations have been compared to the data (Fig. 15), but no reasonable agreement is found. It appears that the cross-section at this excitation energy contains a mixture of various transitions.

22.5 MeV Resonance

Comparison of the experimental results for the 22.5 MeV ($130A^{-1/3}$) resonance with DWBA calculations (Fig. 16) gives support to an E2 assignment. At forward angles the data is indistinquishable between the E0 and E2 transitions, but the 105^{o} measurement is incompatable with the E0 assignment. The Sendai group has reported [Ref. 3] an electric monopole or quadrupole at this excitation energy in ^{197}Au and also at the corresponding energy in ^{208}Pb [Ref. 24]. Other multipolarity assignments are unsuccessful in predicting an angular distribution in agreement with the data. The 22.5 MeV state is thought to be the isovector quadrupole state predicted by the collective vibration model of Bohr and Mottelson [Ref. 38].

33.5 MeV Resonance

A new resonance, previously unreported in ^{197}Au, is observed at 33.5 MeV ($194\ A^{-1/3}$). This corresponds roughly to the isovector giant monopole resonance predicted by Suzuki [Ref. 22] through calculations based on the collective vibration model of Bohr and Mottelson. Both the E0 and E2 assignments exceed their respective energy-weighted sum rule prediction. However, our line shape fit, while very sensitive to any structure in the spectrum, may tend to over-estimate cross-sections for very wide resonances. For this reason, the B-values may be too large. Comparison of the experimental form factors to the DWBA calculations allow both E0 and E2 multipolarities to be possible. A similar new resonance was observed in ^{208}Pb at a corresponding energy of 32.5 MeV [Ref. 26] and tentatively given an E0 or E2 assignment. It is to be emphasized that consistent fits for all the spectra (^{197}Au) over the entire range from 5 MeV to 40 MeV excitation energy were only possible with the inclusion of this resonance at 33.5 MeV.

TABLE IX

Ratio of Resonance Strengths to Energy Weighted Sum Rules

E_r	Assumed Transition	ΔT	$B(\lambda L)$ e^2-fm^{2L} *	$E_x B(\lambda L)$	Sum	$\frac{E_x B(\lambda L)}{Sum}$
7.3	M_1	--	.35±.26	--	--	--
7.3	M_2	--	$(2.4\pm.8)\times10^3$	--	--	--
9.2	E_0	0	$(3.6\pm1.8)\times10^3$	3.4×10^4	9.3×10^4	.36
9.2	E_1	1	9.2±10.0	85	7.0×10^2	.10
9.2	E_2	0	$(1.5\pm.4)\times10^3$	1.4×10^4	7.4×10^4	.19
9.2	E_2	1	$(1.5\pm.9)\times10^3$	1.4×10^4	1.10×10^5	.13
10.8	E_0	0	$(9.2\pm1.9)\times10^3$	1×10^5	9.3×10^4	1.0
10.8	E_2	0	$(4.7\pm.8)\times10^3$	5.1×10^4	7.4×10^4	.68
10.8	E_2	1	$(4.7\pm.8)\times10^3$	5.1×10^4	1.1×10^5	.46

* For Monopole Matrix Elements are Given

TABLE IX Continued

E_r	Assumed Transition	ΔT	$B(\lambda L)$ e^2-fm^{2L}	$E_x B(\lambda L)$	Sum	$\frac{E_x B(\lambda L)}{Sum}$
14.0	$E_1[\rho_{tr} = \rho_0]$	--	$(4.9\pm.7)x10^1$	$6.9x10^2$	$7.0x10^2$	.98
14.0	$E_1[\rho_{tr} = \frac{d\rho_o}{dr}]$	--	$(8.6\pm1.1)x10^1$	$1.2x10^3$	$7.0x10^2$	.17
18.0	M_2	--	$(1.5\pm.8)x10^3$	--	--	--
18.0	E_0	0	$(5.0\pm1.5)x10^3$	$8.9x10^4$	$9.3x10^4$	.46
18.0	E_2	0	$(2.7\pm1.5)x10^3$	$4.8x10^4$	$7.4x10^4$	.65
18.0	E_2	1	$(2.7\pm1.5)x10^3$	$4.8x10^4$	$1.1x10^5$	.44
18.0	E_3	0	$(2.0\pm1.0)x10^5$	$3.6x10^6$	$6.2x10^6$	.58
18.0	E_3	1	$(2.0\pm1.0)x10^5$	$3.6x10^6$	$9.2x10^6$	.39

TABLE IX Continued

E_r	Assumed Transition	ΔT	$B(\lambda L)\ e^2\text{-}fm^{2L}$	$E_x B(\lambda L)$	Sum	$\frac{E_x B(\lambda L)}{Sum}$
22.5	E_0	0	$(2\pm.13)\times10^3$	4.3×10^4	9.3×10^4	.46
22.5	E_2	0	$(7.1\pm.5)\times10^3$	1.6×10^5	7.4×10^4	2.2
22.5	E_2	1	$(7.1\pm.5)\times10^3$	1.6×10^5	1.1×10^5	1.5
22.5	E_3	0	$(3.4\pm.8)\times10^5$	7.6×10^6	6.2×10^6	1.2
22.5	E_3	1	$(3.4\pm.8)\times10^5$	7.6×10^6	9.2×10^6	.83
33.5	E_0	0	$(1.4\pm.7)\times10^4$	8.2×10^5	9.3×10^4	5.0
33.5	E_2	0	$(6.3\pm2.2)\times10^3$	2.1×10^5	7.4×10^4	2.8
33.5	E_2	1	$(6.3\pm2.2)\times10^4$	2.1×10^5	1.1×10^5	1.9

TABLE X

Transitions Strengths in Weisskopf Units

E_r	Transition	$B(\lambda L)[e^2\text{-fm}^{2L}]$	$B_{sp}(EL/ML)/e^2$	$B(\lambda L)/B_{sp}$
7.3	M_1	.35 ± .26	.06	6
7.3	M_2	$(2.4\pm.8)\times10^3$	3.1	770
9.2	E_0	$(3.64\ \pm1.80)\times10^3$	--	--
9.2	E_1	$9.2\pm\ 10.0$	6.6	1
9.2	E_2	$(1.49\pm.92)\times10^3$	3.4×10^2	4
10.8	E_0	$(9.22\pm1.87)\times10^3$	--	--
10.8	E_2	$(4.68\pm.80)\times10^3$	3.4×10^2	14
14.0	$E_1[\rho_{tr}=\rho_0]$	$(4.9\pm7)\times10^1$	6.6	8
14.0	$E_1[\rho_{tr}=\frac{d\rho_0}{dR}]$	$(8.6\pm1.1)\times10^1$	6.6	13
18.0	M_2	$(1.48\pm.84)\times10^3$	3.1	480
18.0	E_0	$(4.96\pm24.4)\times10^3$	--	--
18.0	E_2	$(2.66\pm1.51)\times10^3$	3.4×10^2	8
18.0	E_3	$(1.97\pm.09)\times10^6$	1.6×10^4	12

TABLE X Continued

E_r	Transition	$B(\lambda L)$ $[e^2\text{-}fm^{2L}]$	$B_{sp}(EL/ML)/c^2$	$B(\lambda L)/B_{sp}$
22.5	E_0	$(1.90\pm.13)\times10^3$	--	--
22.5	E_2	$(7.10\pm.48)\times10^3$	3.4×10^2	22
22.5	E_3	$(3.39\pm.78)\times10^5$	1.63×10^4	21
33.5	E_0	$(1.40\pm.72)\times10^4$	--	--
33.5	E_2	$(6.25\pm2.15)\times10^3$	3.4×10^2	19

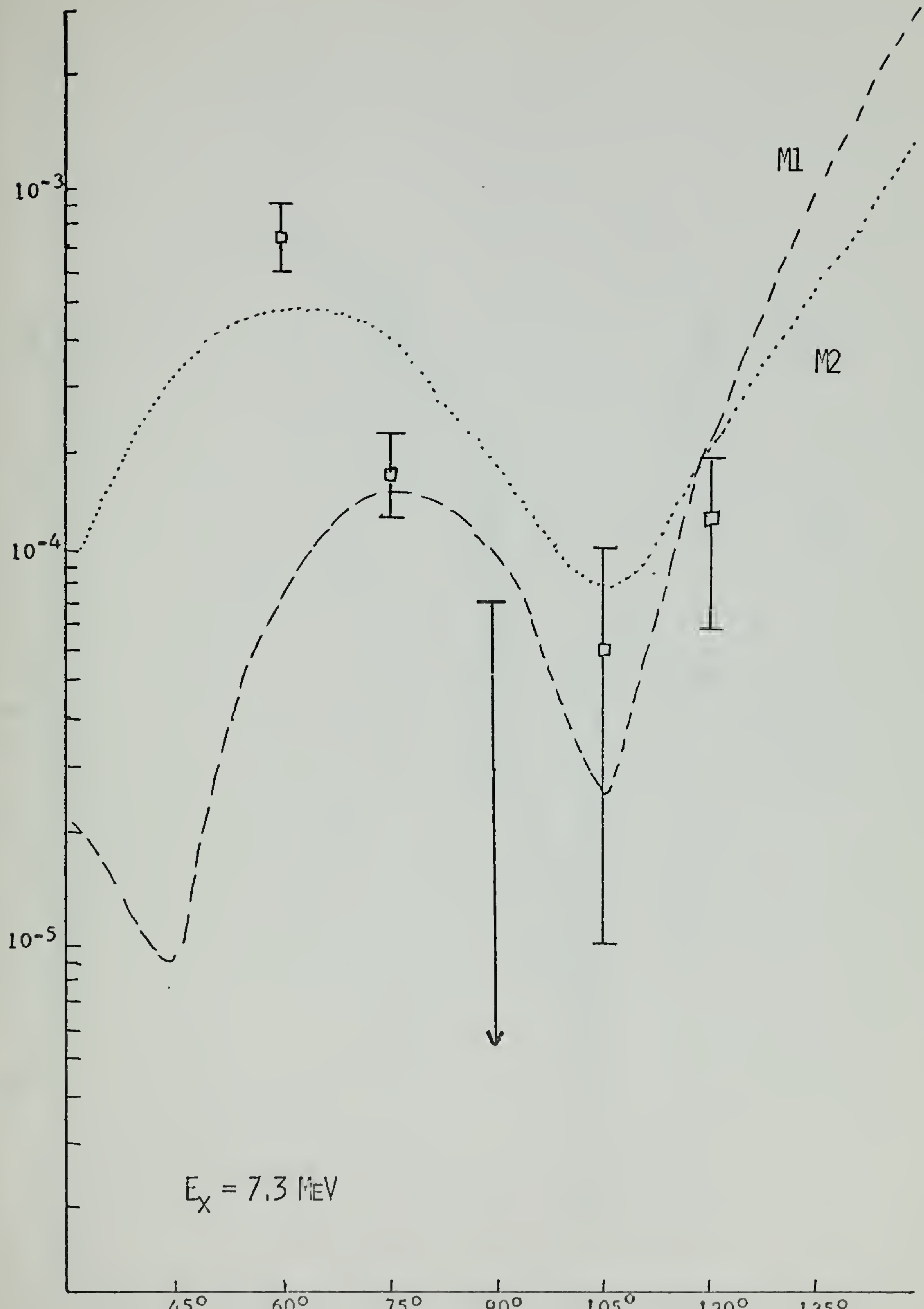


FIGURE 11

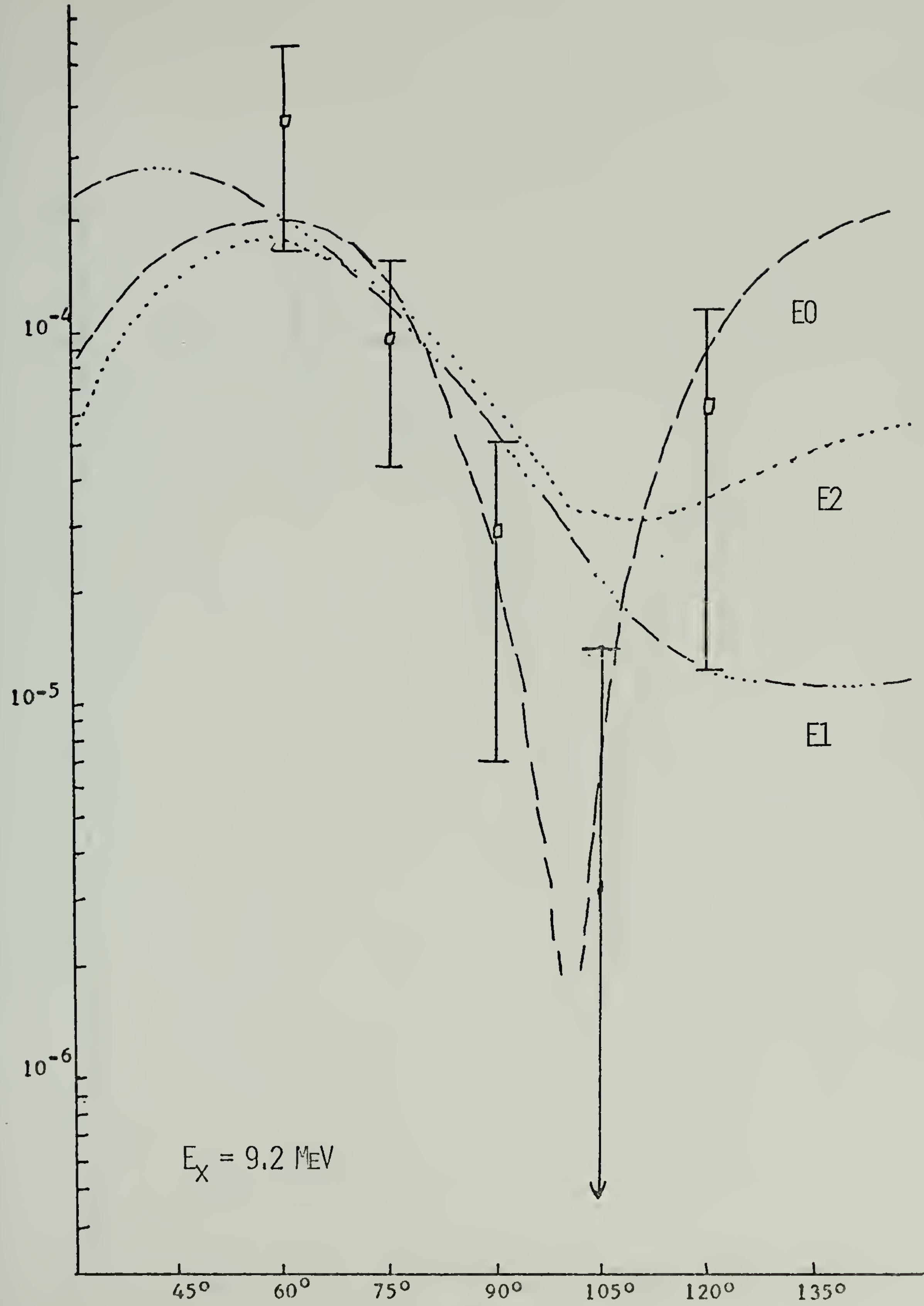


FIGURE 12

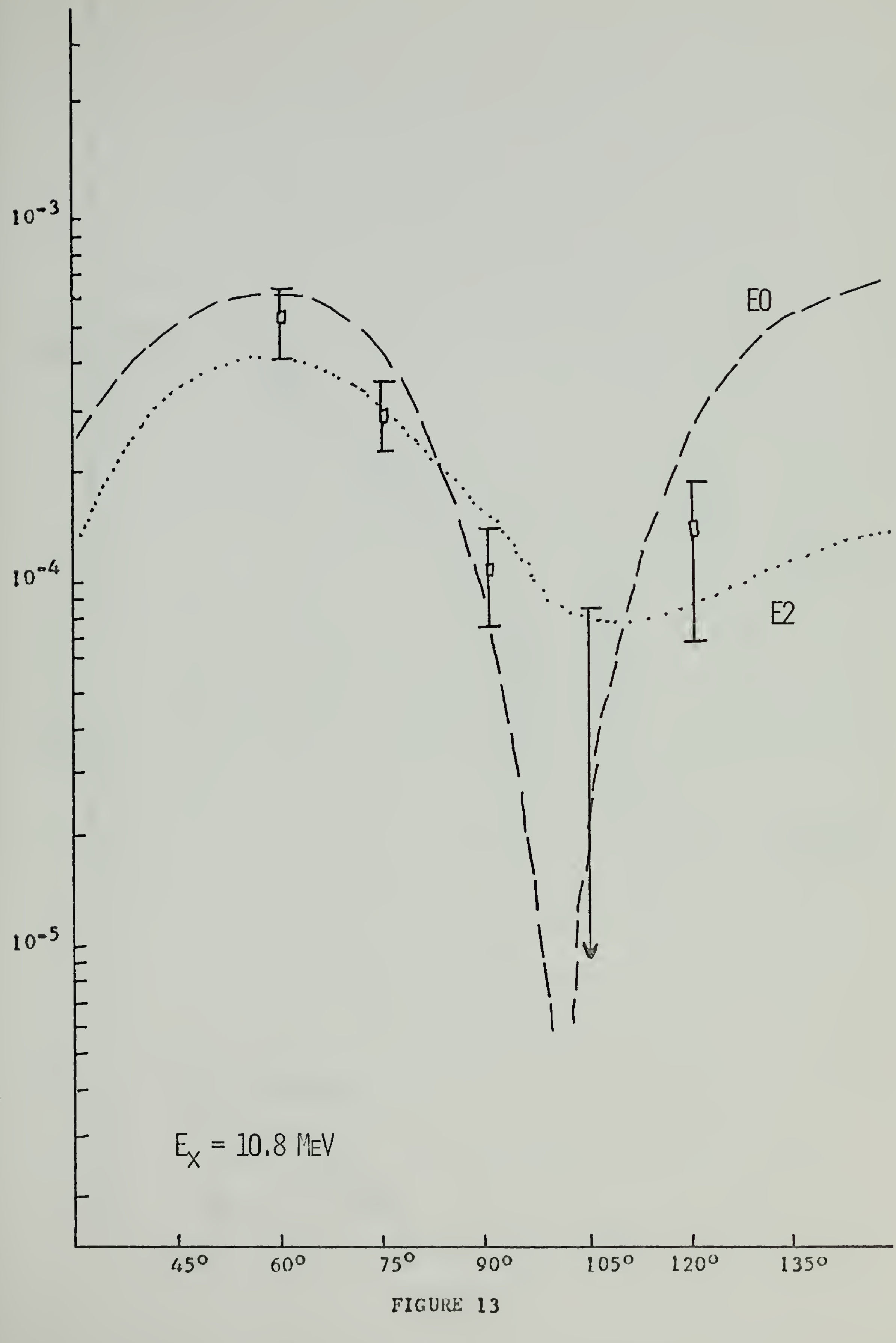
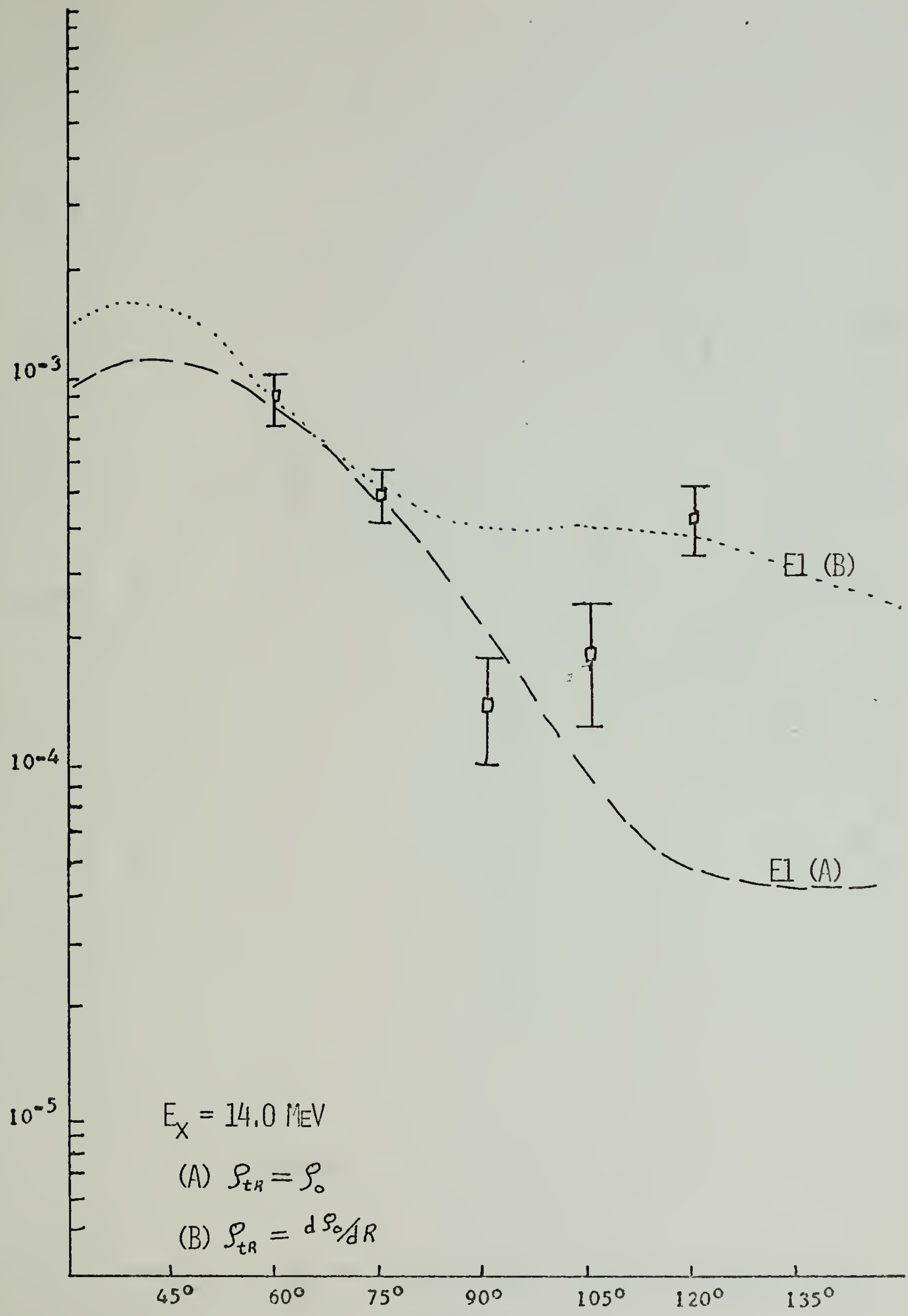


FIGURE 13



10-3
10-4
10-5
E1 (B)
E1 (A)
Ex = 14.0 MeV
(A) ρtR = ρo
(B) ρtR = dρo/dR
45°
60°
75°
90°
105°
120°
135°

FIGURE 14

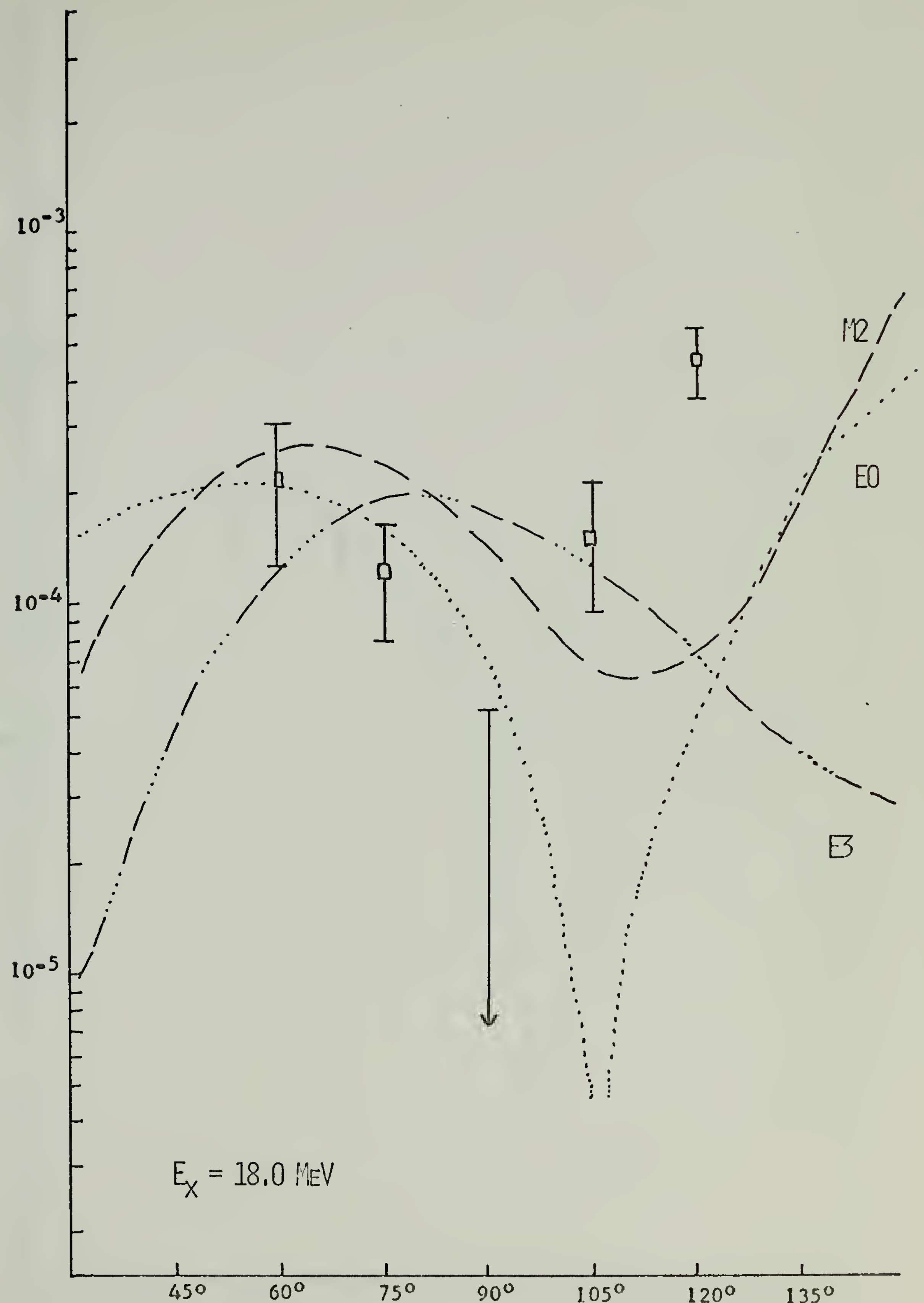


FIGURE 15

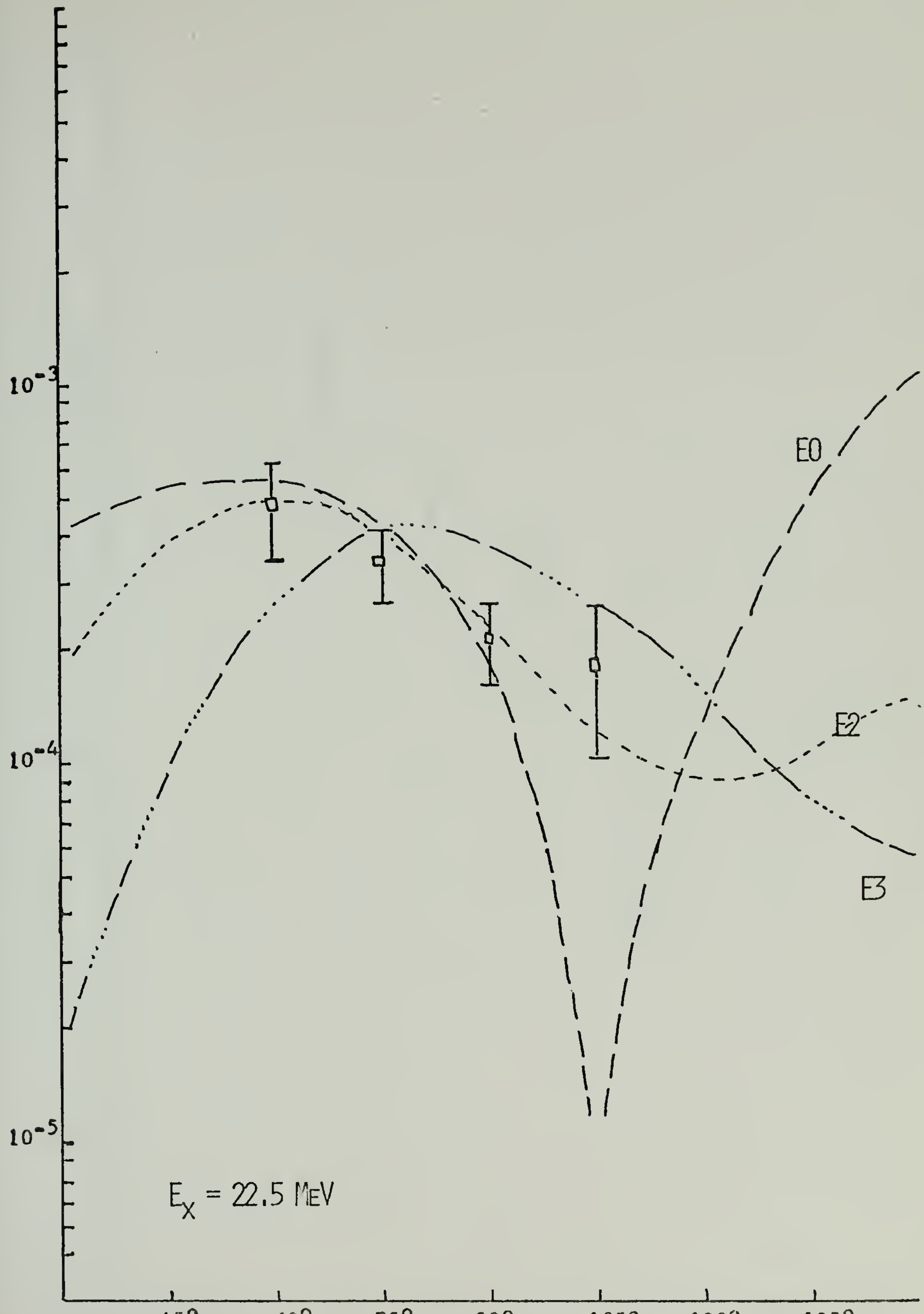


FIGURE 16

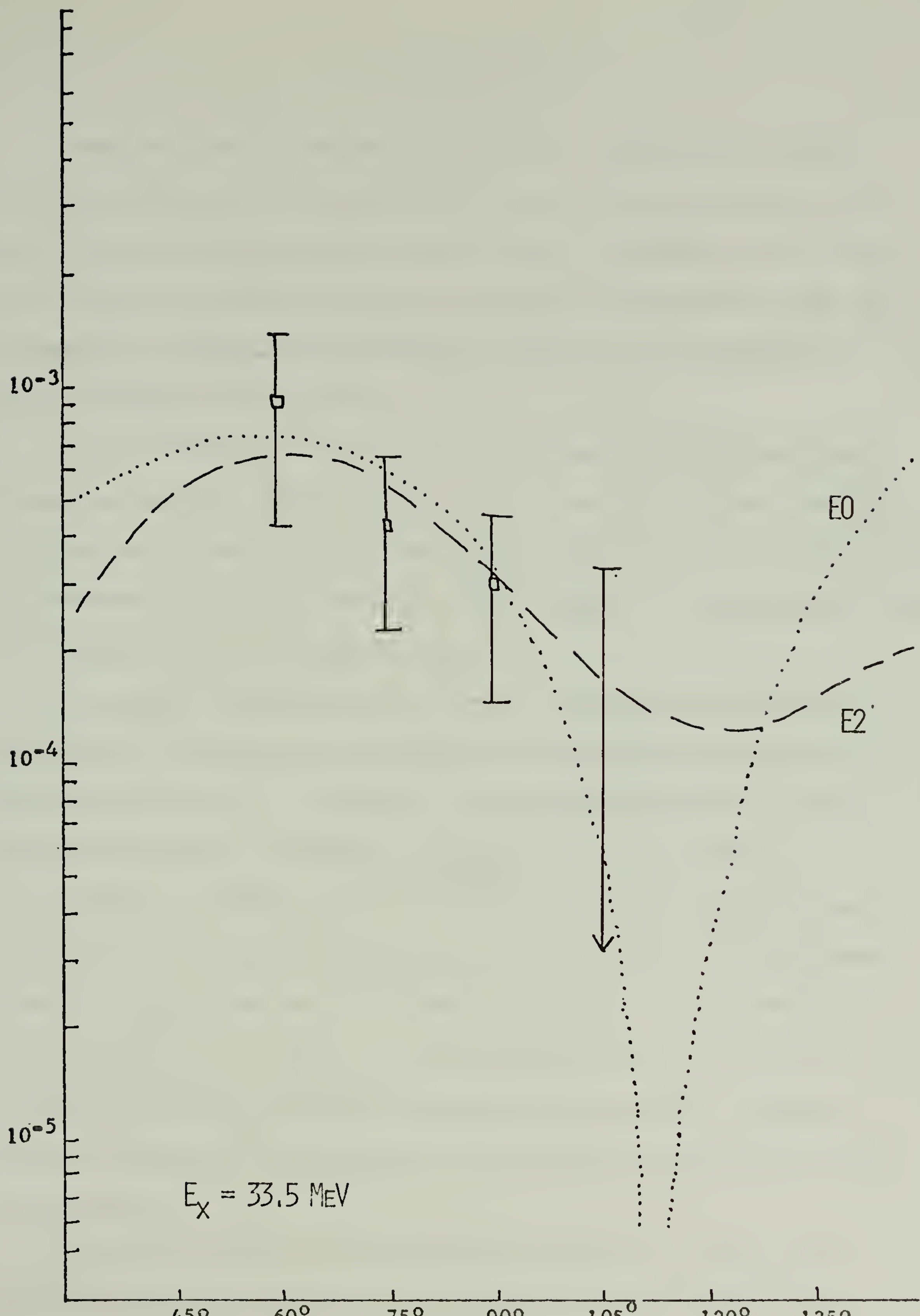


FIGURE 17

V. CONCLUSIONS

Giant multipole resonances in ^{197}Au were studied with inelastic electron scattering. Resonances at 7.3, 9.2, 10.8, 14.0, 18.0, 22.5, and 33.5 MeV excitation energy were observed. Of these, the 9.2, 18.0, 22.5, and 33.5 MeV states have not previously been reported in the open literature. Multipolarity assignments of these states were made as was discussed in section IV-B.

The 14.0 MeV state is identified as the much studied giant dipole resonance, see e.g. [Refs. 3, 5, & 25]. Our analysis suggests that this E1 state may be described by a volume oscillation of the charge distribution. Furthermore, the data is compatible with a suspected transverse spin flip contribution to the E1 cross section.

The angular distributions of the cross-sections for the 10.8 MeV and 22.5 MeV resonances are compatible with previous E2 multipolarity assignments [Ref. 3]. In addition, this investigation adds evidence for the exclusion of a monopole assignment for the 10.8 MeV state.

A state was found at 18 MeV in ^{197}Au. In ^{208}Pb a resonance was seen [Ref. 26] and cross-section analysis of another (e,e') experiment found E3 strength between 16 MeV and 22 MeV [Ref. 24]. The analysis of the experimental results for this energy region in ^{197}Au is not capable of assigning a definite transition multipolarity. The data suggests admixtures of longitudinal and transverse contributions to the cross-section.

The 7.3 MeV transition is known to be magnetic. However, this investigation, like others [Ref. 19], was not able to determine the transition mode.

Theoretical investigation concerning the existence and location of the giant monopole resonance is found in the literature [Refs. 21 and 22]. New resonances, discovered in this experiment at 9.2 MeV and 33.5 MeV, have angular distributions in agreement with monopole assignments. Their excitation energies are comparable to theoretical predictions [Ref. 22] of the location of the isoscalar and isovector monopole states. For the lower state, an E0 transition is favored over an E2 assignment. However, for the 33.5 MeV state, the transition multipolarity is inconclusive. The excitation energies and transition multipolarities are presented in Table XI.

TABLE XI

Multipolarity Assignments

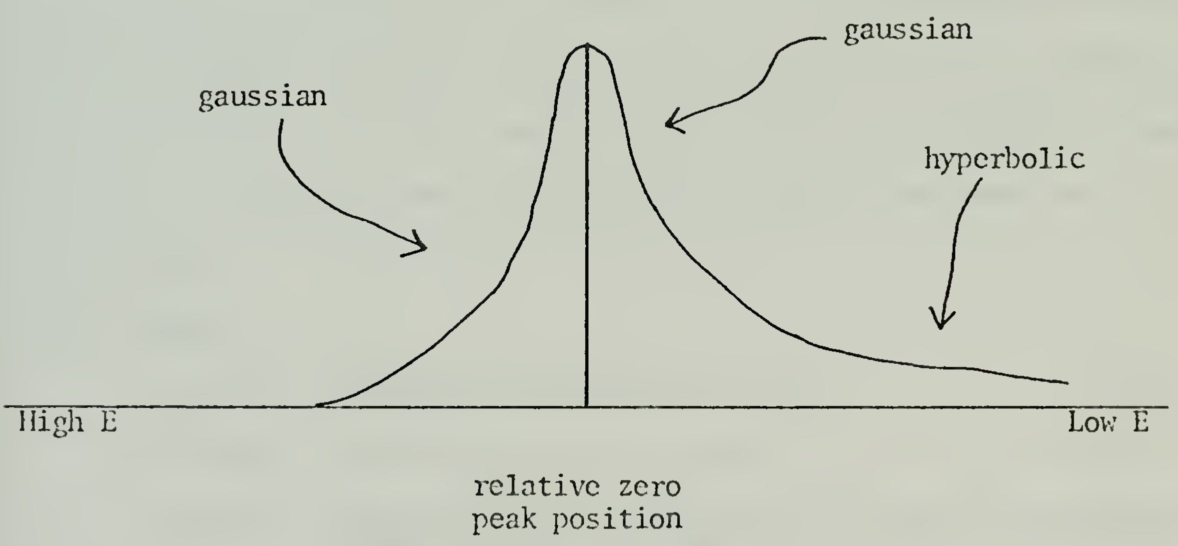
Excitation Energy (MeV)	Transition Multipolarity	Comments
7.3	undetermined	probable magnetic, mixture
9.2	E0	Isoscalar
10.8	E2	Isoscalar
14.0	E1	Isovector, volume oscillation
18.0	undetermined	
22.5	E2	Isovector
33.5	E0 or E2	Isovector

APPENDIX A

PROGRAM NAW, SPECTRUM FITTING CODE

A. GENERAL FEATURES

Naw is a Fortran program developed at Darmstadt [Refs. 41 & 43] which uses analytical expressions to approximate the inelastic and elastic line shapes and radiation tail to best fit the experimental spectra. The elastic line shape is assumed to be two half gaussians of differing half widths matched to a hyperbolic shape approximating the radiation tail. Work done by the experimenters at the Institut Für Technische Kernphysik at Darmstadt have found this parameterization to be an adequate estimate of the shape of the elastic peak (see Figure 18) [Ref. 41].



ASSUMED ELASTIC SPECTRUM SHAPE
FIGURE 18

The elastic radiation tail results from processes occurring during elastic scattering that produce lower energy electrons. The radiation tail is calculated from the theory [Ref. 43] at several designated energies

and these theoritical values are fitted with a polynomial of the fourth degree. The total background, which includes the radiation tail, is then simultaneously fit with a series of Breit-Wigner line shapes representing the nuclear excitation structure to reproduce the experimental spectrum. The positions and widths of the resonances are free parameters to be adjusted by best fit or to be assigned from known values. The areas under these resonances are then calculated from which the ratios A_i/A_e (inelastic peak area divided by the elastic peak area) are determined. The values A_i/A_e are then multiplied by the calculated scattering cross section resulting in the experimental inelastic cross section for each of the resonances.

B. CONTROL CARDS

NAW uses the output from program KIK as the input data. Since NAW's first use at the NPS IBM 360/67 [Ref.1] it has undergone various modifications. The present form is reproduced on the following pages, along with the control information. NAW accepts 200 elastic peak data points, 500 inelastic data points and 25 inelastic resonances per spectrum.

NAW CONTROL

1. TEXT Alphanumeric identifying remarks (20A4)

2. NORM, PN_2, PN_3, PN_4, PN_5, PN_6, PN_7 (7F10.5)

NORM Spectrometer energy normalization factor to change the origional energy units (OEU) to MeV: [MeV] = NORM*[OEU]

PN_i i=2-7, Starting values for the various parameters being used to fit the elastic spectrum with an analytical expression.

PN_2 Half-width of a gaussian to fit the high energy side of the elastic peak.

PN_3 Half-width of a gaussian to fit the low energy side of the elastic peak.

PN_4 Matching point for the low energy gaussian and the hyperbolic segment. PN_4 is specified in MeV from the position of the zero point and is a negative number.

PN_5 Dummy.

PN_6 $PN_6 \neq 0$, Height of a second elastic resonance peak if necessary.

PN_7 Position of a second elastic resonance peak if necessary, only with $PN_6 \neq 0$.

3. EE, THETA, D, UNT, (4F10.5)

EE Energy of the elastic peak in MeV. EE is used as a starting value in the elastic fit.

THETA Electron scattering angle in degrees.

D Target thickness in g/cm^2.

UNT Constant background at the high energy end of the elastic resonance spectrum in counts/μc.

4. EEL_u, EEL_l, $GSSW_u$, $GSSW_l$, DSSW, E_{ref} (6F10.5)

EEL_u High energy limit for fitting the elastic peak in OEU.

EEL_l Low energy limit for fitting the elastic peak in OEU.

$GSSW_u$ Upper limit for calculating the radiation tail in OEU.

$GSSW_l$ Lower limit for calculating the radiation tail in OEU.

DSSW Energy step to be used in calculating the radiation tail in OEU.

E_{ref} See card 7, L_2. If $E_{ref} = 0$, E_{ref} is calculated internally.

5. E_u, E_l (2F10.5)

E_u High electron energy limit for fitting the inelastic spectrum in excitation energy (MeV).

E_l Low electron energy limit for fitting the inelastic spectrum in excitation energy in (MeV).

6. GR^1_u, GR^1_l, GR^2_u, GR^2_l, GR^3_u, GR^3_l (6F10.5)

Regions where it is expected that only background contributes to the spectrum; i.e., between resonances in the inelastic spectrum. There must be at least one set of GR^1_u, GR^1_l input, with a maximum of three. It is recommended to set $GR^1_u \approx GSSW_l$ $GR^1_l \approx GSSW_u$ for giant resonances, energy in MeV.

7. L_i i=1 to 22 (22I3)

L_i

1 A continuous curve consisting of two gaussians and a segment of a hyperbolic is used for both elastic and inelastic fits.

2 The elastic resonance will be fit as if L_1=1 and the inelastic resonance will be fit using the Breit-Wigner formula. Each curve will be multiplied by a straight line with an equation $Y=1+P_i(E_x-E_x^{(i)})$. P_i will be specified on card #10, Ex is the excitation energy, and $E_x^{(i)}$ is the position of the maximum as specified on card #8.

3 The elastic resonance will be fit as if L_1=2 except that NAW will determine the values P_i and card #10 will be left blank.

L_2

Parameters which choose the analytical expression to fit the background due to the radiative and experimental processes, L_2 is a two digit number, the units give the order of a polynomial e.g. unit=3, $P_1+P_2A+P_3A^2$, the P_i's are free fitted paramters. The decades choose the function to be multiplied and the argument to be used.

$1 \leq L_2 < 10$ $\quad P_1+P_2A+P_3A^2+\ldots+P_{L2+1} \cdot FSSW$

$10 < L_2 < 20$ $\quad P_1+P_2A+P_3A^2+\ldots+ FSSW$

$20 < L_2 < 30$ $\quad \{P_1+P_2A+P_3A^2+\ldots+P_{L2+1} \cdot FSSW\} \exp\left[P_{L2+2}\left(\frac{E-E_e}{E}\right)\right]$

$30 < L_2 < 40$ $\quad \{P_1+P_2A+P_3A^2+\ldots+ FSSW\} \exp\left[P_{L2+1}\left(\frac{E-E_e}{E}\right)\right]$

FSSW is the calculated radiative tail, E is the energy of the outgoing electron, E_e, is the energy of the elastic peak. $A-(E-E_{ref})$ for $L_2 < 50$, E_{ref} is read in on card #7. If $50 < L_2 < 90$ the analytical form corresponding to $L_2=L_2-50$ is choosen, but A is replaced by 1/A.

L_3

The number of resonances with fixed energies. If $L_3 < 0$ then the resonance will be kept fixed relative to $E_x(1)$, but $E_x(1)$ will be fitted. See card #8.

L_4

The number of resonances with energies to be fitted. Note that $|L_3| + L_4$ must not exceed 25.

L_5 The number of lines widths to be fitted. >0 E.g. $=3$, means that three line widths are free and in fact are $E_x(1)$, $E_x(2)$, and $E_x(3)$. If there are more than three resonances, $E_x(3)$ through $E_x(N)$ will all be fitted with the same line widths.

L_6 For $L_1 \geq 2$ the first L_6 peaks will be fitted with Breit-Wigner forms, the remainders with gaussian shapes. For $L_6=0$, $L_6= |L_3| + L_4$

L_7 Target geometry:

=0 Transmission -normal thickness entered on card #3
=1 Reflection -normal thickness entered on card #3
=2 Effective thickness entered on card #3

L_8 Output control:

=0 Maximum output
=1 Minimal output-no tables and no intermediate calculations
=-1 Limited output-no tables

L_9 Plotting control:

=0 Results are not plotted.
=2 Results are plotted.

L_{10} Repetitions of NAW procedure.

=0 No repetitions are performed.
>0 In this case it is possible to evaluate the data with new parameters. The new parameters will be entered on additional cards placed after the control cards.

L_{11}-L_{14} Inelastic spectrum fit iteration control. Only override to the default options need be entered.

L_{11} Number of iterations where all energies are fixed, default $L_{11}=2$.

L_{12} Maximum number of iterations; default is $L_{12}=30$.

L_{13} Minimum number of iterations; default is $L_{13}=5$.

L_{14} Number of iterations where width are held constant in case $\chi^2_{actual} > 3\chi^2_{theory}$.

L_{15} =0 The radiation tail will be calculated using the Ginsber's method [Ref. 43].
<0 The radiation tail will be calculated using Schiff's method [Ref. 44].

L_{16}-L_{18} Radiation tail fit control. Only override options need be entered.

L_{16} Analytical representation of the theoretically calculated radiation tail; default is L_{16}=1.

=1 $SSW=P_1 + P_2A + P_3A^2 + P_4A^3 + P_5A^4$

=2 $SSW=P_1 + P_2A + P_3A^2 + P_4E + P_5E^2$

=3 $SSW=P_1 + P_2A + P_3E + P_4E^2 + P_5E^3$

=4 $SSW=P_1 + P_2E + P_3E^2 + P_4E^3 + P_5E^4$

=5 $SSW=P_1 + P_2U + P_3U^2 + P_4U^3 + P_5U^4$

P_i will be fitted internally by NAW
$A= 1/(E_{el} - E)$
$U=E - E_b$
$E_b= GSSW_1 + (GSSW_u - GSSW_1)/L_{18}$

<0 the radiation tail parameters P_i and E_b will be specified on card #15.

L_{17} The number of parameters for the radiation tail fit ($3 \leq L_{17} \leq 5$); default is L_{17} = 4.

L_{18} See L_{16}; default is L_{18} = 2.

L_{19} >0 Error ellipsoid control values will not be calculated.

L_{20} = 0

L_{21} >0 The calculation of the radiation tail will be modified by the factors entered on card #16.

L_{22} =3 Inelastic spectrum results. Card images will be written on file 7 and may be stored on the data cell for further handling.

8. $E_x(1), E_x(2), \ldots, E_x(i)$ (8F10.5)

Resonance excitation energies in MeV; enter those with variable positions first. $i = |L_3| + L_4 < 25$.

9. V(1), V(2), ..., V(i) (8F10.5)

Resonance line widths, $i = |L_3| + L_4 < 25$
If any V(i) = 0, the width of the elastic line will be assumed.

10. P(1), P(2), ..., P(i) (8F10.5)

The P_i factors when $L_1 = 2$ on card #7, $i = |L_3| + L_4 < 25$.

11. Z, A, XRAD, FIRA, C T (4F10.5, 20X,2F10.5)

Z Atomic number.

A Mass number.

XRAD Radiation length in g/cm^2.

FIRA Elastic form factor for E_E and THETA of the experiment.

C,T The fermi charge distribution parameters. Since these values are used as the parameters for the trapezoidal charge distribution potential used in the radiation tail calculations in Born Approximation, these values must be entered.

12. XMAS, H (2F10.5)

XMAS Nuclear mas equivalent in MeV.

H Isotope percentage (100% = 1.00).

13. A_i The A_i are the coefficients for the calculations of the elastic form factor using a power series expansion on q^2:

$$F_{el}^2 = \sum_{i=1}^{8} A_i q^{2(i-1)}$$

When $A_1 = 0$ the elastic form factor will be calculated using the Born Approximation.

14. U_i (8F10.5)

U_i may be used to get better starting values for the fit by taking the background parameters from a previous fit. If the $U_i = 0$, the starting values are chosen internally. See card #7.

15. P1, P2, P3, P4, P5, E_b (6F10.5)

This card is read only if $L_{16} < 0$.

P1-P5 Radiation tail parameters, see L_{16} for the expression.

E_b This value is read only when $L_{16} = -5$.

16. XSSW, XM, XB, (3F10.5)

This card is read only if $L_{21} > 0$.

XSSW Factor Multiplying the area under the elastic peak, A_e

XM Factor multiplying the Møller term.

XB factor multiplying the B
The equation for the radiation tail is now given by
$SSW = \frac{MAXI}{F^2 \sigma_{Mott}} + XM(\text{Møller term}) + XB(\text{Brems. term}) \cdot (XSSW)A_e$
MAXI are form factors as described by Maximon and Isabelle.

The data are assigned to file #4. The elastic and the inelastic data must be followed by one card image having the data energy step width entered beginning in column 72. Repeated evaluations of the same set of data (i.e. $L_{10} = 0$) must have the following set of cards placed after the 14 to 16 control cards as described above; one set for each repetition to be performed.

1) $L_1 \ldots L_{10}$ see card #7

2) E_u, E_1 see card #5

3) $E_x(1)$ ..., $E_x(i)$ see card #8

4) V(1), ..., V(i) see card #9

5) P(1), ..., P(i) see card #10

NAW LISTING

```
      DIMENSION DUM1(600),          LPAR(100),PAR(300)
      DIMENSION WORD(20),LP(25),PR(50),FFF(200),BR(25)
      DIMENSION BVAR(25) , PVAR(25)                                     EING0040
      COMMON PAR,LPAR,DUM1,      WORD,FFF
      COMMON /BVAR1/ BVAR /BVAR2/ PVAR                                  EING0070
      COMMON/SSWD/ACO(25)
      COMMON /USTART/UPAR(10)
      CALL ERRSET(208,300,-1,1,0,207)                                   EING0090
C   EINLESEN ZUSATZDATEN                                                EING0110
C     ZWEITE ELASTISCHE LINIE, LORENTZKURVE FUER UNELSTISCHEN FIT       EING0120
C     EINGEFUEGT   JAN 72  PITTHAN                                      EING0130
C    UMGESCHRIEBEN FUER TR-440 IM FEBRUAR 1971                          EING0140
      DATA WIED/4HWIED/,ERHL/4HERHL/                                    EING0170
      CALL SETIME
      PAR(39)=.0
      PAR(40)=0.0                                                       EING0190
    1 READ(5,1000) (WORD(I),I=1,20)
      DO  99 I=1,600                                                    EING0210
      DUM1(I)=0.                                                        EING0220
      IF(I.LE.100)  LPAR(I)=0                                           EING0240
      IF(I.LE.300)  PAR(I)=0.                                           EING0250
      IF(I.LE.200) FFF(I)=.0                                            EING0260
      IF(I.LE.50) PR(I)=0.                                              EING0270
      IF(I.GT.25)  GO TO 99                                             EING0290
      ACO(I)=.0
      PVAR(I)=0.                                                        EING0300
      LP(I)=0                                                           EING0310
      BVAR(I)=0.                                                        EING0320
      BR(I)=0.                                                          EING0330
      IF(I.LE.10) UPAR(I)=.0
   99 CONTINUE                                                          EING0340
      READ(5,1001) (PAR(I),I=1,5),(PAR(I),I=62,63),(PAR(I),I=6,12)      EING0350
     1  ,(PAR(J),J=21,24),(PAR(I),I=13,14),(PAR(I),I=64,68),(PAR(I),    EING0360
     1 I=15,20)                                                         EING0370
      READ(5,1002) (LPAR(I),I=1,20) ,LPAR(40),LPAR(38)                  EING0380
      IF(LPAR(1).EQ.2) PAR(64)=1.                                       EING0390
      IF(LPAR(1).EQ.3) PAR(64)=2.                                       EING0400
      IF(LPAR(1).GE.2) LPAR(1)=1                                        EING0410
      IM=IABS(LPAR(3))+LPAR(4)
      IF(LPAR(6).EQ.0) LPAR(6)=IM
      IM100=IM+100
    5 READ(5,1005) (PAR(I),I=101,IM100)
      READ(5,1005) (BR(I),I=1,IM)
      READ(5,1005) (BVAR(I),I=1,IM)
      IF(NWDH.EQ.1) GOTO 980                                            EING0600
      READ(5,1005) (PAR(I),I=51,58)                                     EING0610
      READ(5,1005) PAR(59),PAR(61)                                      EING0620
C    EINLESEN DER KOEFFIZIENTEN FUER FORMFAKTOR(Q**N)                   EING0630
```

```
   98 READ(5,1100)(ACO(I),I=1,8)
      READ (5,1002) (LPAR(I),I=41,50)                                   EING0740
      READ(5,1100)(UPAR(I),I=1,8)
      IF(LPAR(16).LT.0) READ(5,1007) (PAR(2*N+89),N=1,5),PAR(81)        EING0750
      IF(LPAR(40).GT.0) READ(5,1008) PAR(90),PAR(89),PAR(88),LPAR(39)   EING0760
 1000 FORMAT(20A4)
 1001 FORMAT(7F10.5/5F10.5/6F10.5/7F10.5/6F10.5)                        EING0780
 1002 FORMAT(22I3)                                                      EING0790
 1003 FORMAT(7F10.5,I10)                                                EING0800
 1004 FORMAT(7F10.5,I10)                                                EING0810
 1005 FORMAT(8F10.5)                                                    EING0820
      DOUBLE PRECISION ABCDE                                            EING0830
      IM=IABS(LPAR(3))+LPAR(4)                                          EING0840
      LPAR(21)=IM                                                       EING0850
      LPAR(25)=0                                                        EING0860
      WRITE (6,1006) (WORD(I),I=1,18)                                   EING0870
 1006 FORMAT(1H0,18A4)                                                  EING0880
 1007 FORMAT(6F10.5)                                                    EING0890
 1008 FORMAT(3F10.5,I3)                                                 EING0900
 1100 FORMAT(8F10.5)                                                    EING0910
C   BERECHNUNG HILFSGROESSEN                                            EING0930
      ILA=0                                                             EING0950
      EOO=PAR(6)*PAR(1)                                                 EING0960
      THETA=PAR(7)*0.0174533                                            EING0970
      CU2=COS(THETA/2.)                                                 EING0980
      SU2=SIN(THETA/2.)                                                 EING0990
      DEFF=PAR(8)                                                       EING1000
      IF(LPAR(7).EQ.0) DEFF=DEFF/CU2                                    EING1010
      IF(LPAR(7).GT.0) DEFF=DEFF/SU2                                    EING1020
      PAR(41)=DEFF                                                      EING1030
      PAR(46)=DEFF*1.4                                                  EING1040
   10 EOO=EOO+PAR(46)/2.                                                EING1050
      PAR(47)=1.+2.*EOO*SU2**2/PAR(59)                                  EING1060
      EOO=EQO*PAR(47)                                                   EING1070
      PAR(47)=1.+2.*EOO*SU2**2/PAR(59)                                  EING1080
C   AUSGABE DER EINGABEDATEN                                            EING1110
 9001 FORMAT(3X,20I6)                                                   EING1120
 9000 FORMAT(3X,10F12.3)                                                EING1130
C   CATENEINGABE,AUSWERTUNG ELASTISCH                                   EING1160
      IF(LPAR(20).GT.1)  CALL ZETKO                                     EING1180
      REWIND 1                                                          EING1200
      REWIND 3
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1230
       CALL       EGB                                                   EING1240
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1250
  105 REWIND L                                                          EING1260
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1270
       CALL       ELST                                                  EING1280
```

```
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1290
      LWD=0                                                             EING1300
C  BERECHNEN EPS,BREITEN                                                EING1320
  110 EE00=PAR(31)*PAR(1)+PAR(46)/2.                                    EING1340
      EE0=EE00                                                          EING1350
      PAR(47)=1.+2.*EE0*SU2**2/PAR(59)                                  EING1360
      EE0=EE0*PAR(47)                                                   EING1370
      PAR(47)=1.+2.*EE0*SU2**2/PAR(59)                                  EING1380
      EE0=EE00*PAR(47)                                                  EING1390
      PAR(36)=EE0                                                       EING1400
  112 XBR=(2.6*PAR(31) /(1000.*PAR(34)))**2                             EING1410
      DO 120 I=1,IM                                                     EING1420
      PAR(I+150)=PAR(I+100)/PAR(1)*(1.0+PAR(I+100)/2./PAR(59))/PAR(47)  EING1430
      PAR(I+125)=SQRT(1.-XBR*PAR(I+150)/PAR(31)*(2.-PAR(I+150)/PAR(31)))EING1440
      IF(PAR(64).GE.1.) BR(I)=BR(I)/PAR(34)/PAR(1)
      IF(BR(I).NE.0.) PAR(I+125)=BR(I)
  120 CONTINUE                                                          EING1470
C  UNELASTISCH,PLOTT,WIEDERHOLUNG                                       EING1490
      IF(LWD.GT.0) REWIND 3                                             EING1510
      DO 130 J=1,20                                                     EING1520
      LP(J)=0                                                           EING1530
  130 PR(J)=0.0                                                         EING1540
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1550
       CALL       UNST                                                  EING1560
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1570
      WRITE(6,9000)(PAR(I),I=1,300)                                     EING1580
      WRITE(6,9001)(LPAR(I),I=1,50)                                     EING1590
      WRITE(6,9000) (BVAR(I),I=1,25)                                    EING1600
      WRITE(6,9000) (PVAR(I),I=1,25)                                    EING1610
       CALL       AUSG                                                  EING1620
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1630
      IF(LPAR(9).GT.0) CALL DRUCK                                       EING1640
      IF(LPAR(20).GT.0)  CALL ZETKO                                     EING1650
      LWD=1                                                             EING1660
      IF(LPAR(10).EQ.0) GO TO 1                                         EING1670
C   EINLESEN DER WIEDERHOLUNGSDATEN                                    -(EING1680
                                                                        EING1690
      READ(5,1002,END=1050) (LP(I),I=1,20)                              EING1700
      IF(LP(1).NE.LPAR(1)) LWD=0                                        EING1710
      READ(5,1001) PAR(13),PAR(14),PR64                                 EING1720
      IF(PR64.GT.0.) PAR(64)=PR64                                       EING1730
      NWDH=1                                                            EING1740
      GOTO5                                                             EING1750
  980 NWDH=0                                                            EING1760
      DO 150 I=1,25                                                     EING1770
      IF(LP(I).EQ.0.AND.I.GT.10) GO TO 140                              EING1780
      LPAR(I)=LP(I)                                                     EING1790
  140 IF(PR(I).NE.0.0) PAR(I+100)=PR(I)                                 EING1800
```

```
      IF(PR(I+25).NE..0) BR(I)=PR(I+25)                                 EING1810
  150 CONTINUE                                                          EING1820
      IM=IABS(LPAR(3))+LPAR(4)                                          EING1830
      LPAR(21)=IM                                                       EING1840
      IMP=100+IM                                                        EING1850
      IMB=125+IM                                                        EING1860
      WORD(17)=WIED                                                     EING1870
      WORD(18)=ERHL                                                     EING1880
      WRITE(6,2070) (WORD(I),I=1,18)                                    EING1890
      WRITE (6,1002) (LPAR(I),I=1,20)                                   EING1900
      WRITE (6,2075) PAR(13),PAR(14)                                    EING1910
      WRITE (6,2080) (PAR(I),I=101,IMP)                                 EING1920
      WRITE(6,2085) (BR(I),I=1,IM)                                      EING1930
 2070 FORMAT(1H1,18A4//10X,      13H EINGABEDATEN      /   )            EING1940
 2075 FORMAT(1H0,13HNEUE GRENZEN      2F10.4)                           EING1950
 2080 FORMAT(1H0, 19HANREGUNGSENERGIEN    /2(10F10.4/))                 EING1960
 2085 FORMAT(1H0,'NEUE BREITEN:', /2(10F10.4/))                         EING1970
      LPAR(31)=0                                                        EING1980
      REWIND 1                                                          EING1990
      IF(LPAR(20).GT.1)  CALL ZETKO                                     EING2000
      IF(LWD.EQ.0) GO TO 105                                            EING2010
      GO TO 112                                                         EING2020
 1050 STOP                                                              EING2030
      END                                                               EING2040


      SUBROUTINE ZETKO                                                  EING2140
      DIMENSION PAR(300)
      COMMON PAR
      CALL GETIME(IET)
      Z0=FLOAT(IET)*.000026
      Z1=Z0-PAR(40)
      PAR(40)=Z0
      Z2=PAR(40)/60.0
      LZ2=INT(Z2)
      Z3=AMOD(PAR(40),60.0)
      Z4=AMOD(Z1,60.0)
      Z1=Z1/60.0
      LZ1=INT(Z1)
      WRITE (6,1000) LZ2,Z3,LZ1,Z4
 1000 FORMAT(1H ,5HZEIT  I4,5H MIN F 7.3,12H SEC, DIFF.   I3,5H MIN
     1    F7.3,5H SEC                )
      RETURN                                                            EING2300
      END                                                               EING2310

      SUBROUTINE INPUT(LB)                                              EING2330
      DIMENSION CO(500),HZ(500),FEH(500),PAR(300)                       EING2340
      COMMON PAR                                                        EING2350
```

```
      COMMON/DATA1/HZ,CO,FEH
      DO 10 I=1,250
      I1=2*I-1
      I2=2*I
      READ(4,100) (HZ(J),CO(J),FEH(J),J=I1,I2)
      CC(I1)=CO(I1)-PAR(9)
      CO(I2)=CC(I2)-PAR(9)
      IF(HZ(I1).EQ.0.)  GO TO 20
   10 CONTINUE
   20 IMAX=2*I
      IF(FEH(IMAX).GT.0.0)    PAR(LB+26)=FEH(IMAX)
      CALL SORT(HZ,CO,FEH,IMAX)
      WRITE(3) IMAX,LB
      DC  30 I=1,IMAX
   30 WRITE (3)  HZ(I),CO(I),FEH(I)
      IF(LB.EQ.0) GO TO 40
      PAR(49)= FLOAT(IFIX(50.*HZ(1)))/50.
      PAR(50)= FLOAT(IFIX(50.*HZ(IMAX-1)))/50.
   40 RETURN
  100 FCRMAT(2(F9.4,1X,F15.7,F13.7,2X))
      END

      SUBROUTINE  EGB
      DIMENSICN PAR(300),LPAR(100)
      CCMMON PAR,LPAR
      PAR(26)=0.0
      PAR(27)=0.0
      LB=0
      CALL INPUT(LB)
      LB1=1
      CALL INPUT(LB1)
      REWIND 3
      RETURN
      END

      SUBROUTINE SORT(HZ,CO,FEH,IMAX)
      DIMENSION HZ(500),CO(500),FEH(500)
      LA=1
    1 K=IMAX-1
      DC   10 L=LA,K
      HERZ=HZ(L)
      ZW=CO(L)
      ZF=FEH(L)
      M=L+1
      DC   9 I=M,IMAX
      IF(HZ(I).NE.0.)  GO TO 4
      IMAX=IMAX-1
```

```
      DO   3 LL=I,IMAX                                                  EING2840
      L2=LL+1                                                           EING2850
      HZ(LL)=HZ(L2)                                                     EING2860
      CO(LL)=CO(L2)                                                     EING2870
    3 FEH(LL)=FEH(L2)                                                   EING2880
      LA=L                                                              EING2890
      GO TO 1                                                           EING2900
    4 IF(HZ(L)-HZ(I))    5,9,9                                          EING2910
    5 HZ(L)=HZ(I)                                                       EING2920
      HZ(I)=HERZ                                                        EING2930
      CO(L)=CO(I)                                                       EING2940
      CC(I)=ZW                                                          EING2950
      FEH(L)=FEH(I)                                                     EING2960
      FEH(I)=ZF                                                         EING2970
      HERZ=HZ(L)                                                        EING2980
      ZW=CO(L)                                                          EING2990
      ZF=FEH(L)                                                         EING3000
    9 CONTINUE                                                          EING3010
   10 CONTINUE                                                          EING3020
      RETURN                                                            EING3030
      END                                                               EING3040

      SUBROUTINE ELST                                                   EING3050
C         ELST
C    ELASTISCHER PEAK   UND  STRAHLUNGSSCHWANZ                          ELST0010
      DIMENSION PAR(300),LPAR(100),FREQ(200),ZAEH(200),FEH(200),FF(200) ELST0020
      DIMENSION           WORD(20),XX(500),ERR(500),YY(500),P(25),DY(25)
      COMMON PAR,LPAR,FREQ,ZAEH,FEH,      WORD,FF
      IF(LPAR(20).GT.1)  CALL ZETKO                                     ELST0060
      COMMON/DATA1/XX,YY,ERR
      ZMAX=0.0                                                          ELST0070
      LPAR(24)=0                                                        ELST0080
      GAMMA=1000.                                                       ELST0090
      LEO=0                                                             ELST0100
      READ (3) IEL,LB                                                   ELST0110
      LPAR(32)=IEL                                                      ELST0120
      DO   9 I=1,IEL                                                    ELST0130
      M=IEL-I+1                                                         ELST0140
      READ (3) HZ,CO,FEHEL                                              ELST0150
      ZAEH(M)=CO                                                        ELST0160
      FREQ(M)=HZ                                                        ELST0170
      FEH(M)=FEHEL                                                      ELST0180
      ZMAX=AMAX1(ZMAX,CO)                                               ELST0190
      IF(LPAR(1).EQ.0)  GO TO 8                                         ELST0200
      IF(HZ.GT.PAR(11).OR.HZ.LT.PAR(12))  GO TO 9                       ELST0210
    8 LEO=LEO+1                                                         ELST0220
      XX(LEO)=HZ                                                        ELST0230
      YY(LEO)=CO                                                        ELST0240
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```
      ERR(LEO)=FEHEL                                                    ELST0250
    9 CONTINUE                                                          ELST0260
      IF(LPAR(20).GT.2)  CALL ZETKO                                     ELST0270
      IF(LPAR(1).GT.0)  GO TO 91                                        ELST0280
C   FIT ELASTISCH                                                       ELST0650
   91 P(1)=ZMAX                                                         ELST0670
      P(2)=PAR(2)                                                       ELST0680
      P(3)=PAR(3)                                                       ELST0690
      P(4)=PAR(4)                                                       ELST0700
      P(5)=PAR(6)                                                       ELST0710
      P(6)=PAR(62)                                                      ELST0720
      P(7)=PAR(63)                                                      ELST0730
      ME=5                                                              ELST0740
      LPAR(28)=ME                                                       ELST0750
      NZEL=5                                                            ELST0760
      IF(PAR(62).NE..0)       NZEL=7                                    ELST0770
      CALL FIT(NZEL,P,LEO,XX,YY,ERR,0,GAMMA,1)                          ELST0780
      PAR(31)=PAR(79)                                                   ELST0790
C                                                                       ELST0820
C   HALBWERTSBREITEN,FLAECHEN BEI ARC4                                  ELST0850
      CALL HALBW(PAR(73),PAR(75),PAR(77),PAR(74), PAR(76),HW,DHW,FHW,WW)ELST0870
      PAR(34)=HW                                                        ELST0880
      PAR(33)=WW*PAR(71)                                                ELST0890
      PAR(35)=PAR(71)                                                   ELST0900
      PAR(31)=PAR(79)-DHW                                               ELST0910
      PAR(48)=DHW                                                       ELST0920
      DESCHW=2.0*PAR(34)*PAR(1)                                         ELST0930
   97 CONTINUE                                                          ELST0960
      IF(LPAR(20).GT.1)  CALL ZETKO                                     ELST0970
C   AUSDRUCK   HALBWERTSBREITEN                                         ELST0980
      IF(LPAR(16).LT.0) GO TO 40                                        ELST1000
C   STRAHLUNGSSCHWANZ                                                   ELST1020
      NA1=0                                                             ELST1040
      NSW=40                                                            ELST1050
      IF(LPAR(15).LT.0)  NA1=1                                          ELST1060
      DOUBLE PRECISION U                                                ELST1070
      U=PAR(7)                                                          ELST1080
      EI=PAR(31)*PAR(1)                                                 ELST1090
      R=PAR(57)                                                         ELST1100
      T=PAR(58)                                                         ELST1110
      IF(LPAR(49).EQ.3)  R=PAR(55)                                      ELST1120
      IF(LPAR(49).EQ.3)  T=PAR(56)                                      ELST1130
      ATW=PAR(52)                                                       ELST1140
      XRAD=PAR(53)                                                      ELST1150
      Z=PAR(51)                                                         ELST1160
      FLAE=PAR(33)*PAR(1)                                               ELST1170
      DES=PAR(34)*2.                                                    ELST1180
      XGO=PAR(49)+0.3                                                   ELST1190
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      XGOB=(PAR(31)-DES     )*50.                                      ELST1200
      IF(XGO.GT.(PAR(31)-DES))  XGO=FLOAT(IFIX(XGCB))/50.              ELST1210
      XGU=PAR(50)-0.3                                                  ELST1220
      DIFF=XGO-XGU                                                     ELST1230
      DES=PAR(34)*2.*PAR(1)                                            ELST1240
      ABST=0.02                                                        ELST1250
      IF(DIFF.GT.1.2)  ABST=0.03                                       ELST1260
      IF(DIFF.GT.1.6)  ABST=0.04                                       ELST1270
      IF(LPAR(20).GT.1)  CALL ZETKO                                    ELST1280
C  DIREKT EINGABE STUETZSTELLEN                                        ELST1300
      IF(PAR(21).GT.0.)  XGO=PAR(21)                                   ELST1320
      IF(PAR(22).GT.0.)  XGU=PAR(22)                                   ELST1330
      IF(PAR(23).GT.0.)  ABST=PAR(23)                                  ELST1340
C                                                                      ELST1350
      DO   20 I=1,500                                                  ELST1360
      XX(I)=XGO-ABST*FLOAT(I-1)                                        ELST1370
      IF(XX(I).LT.XGU)  GO TO 25                                       ELST1380
      E=XX(I)*PAR(1)                                                   ELST1390
      CALL RADTL(U,YY(I),EI,E,R,T,ATW,Z,XRAD,DESCHW,FLAE,PAR(41),NA1,  ELST1400
     1  .02)                                                           ELST1410
      ADISP=E/EI                                                       ELST1420
      IF(PAR(64).EQ.0.) YY(I)=YY(I)*ADISP                              ELST1430
      IF(LPAR(40).EQ.0)  PAR(90)=1.                                    ELST1460
      YY(I)=YY(I)*PAR(90)                                              ELST1470
   20 ERR(I)=0.01*ABS(YY(I))
   25 NSW1=I-1                                                         ELST1490
      IF(LPAR(39).NE.1)  GO TO 31                                      ELST1500
      XX(NSW1+1)=0.                                                    ELST1510
      YY(NSW1+1)=0.                                                    ELST1520
      ERR(NSW1+1)=0.                                                   ELST1530
      WRITE(7,501)  (WORD(I),I=1,20)
  501 FORMAT (1H1,20A4)
      DO 30  I=1,NSW1,2                                                ELST1560
  500 FORMAT  (2(F9.4,1X,F15.7,F13.7,2X))                              ELST1570
   30 WRITE(7,500) XX(I),YY(I),ERR(I),XX(I+1),YY(I+1),ERR(I+1)         ELST1580
      CONTINUE                                                         ELST1590
C                                                                      ELST1600
   31 IF(LPAR(20).GT.1)  CALL ZETKO                                    ELST1620
      DO   26 J=91,100                                                 ELST1630
   26 PAR(J)=0.0                                                       ELST1640
   28 LPAR(24)=1                                                       ELST1670
      NPSW=LPAR(17)                                                    ELST1680
      IF(LPAR(17).EQ.0) NPSW=4                                         ELST1690
      IF(LPAR(16).EQ.0) LPAR(16)=1                                     ELST1700
      J1=IABS(LPAR(16))                                                ELST1710
      J=J1+1                                                           ELST1720
      P(1)=0.                                                          ELST1750
      P(4)=0.                                                          ELST1760
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      P(5)=0.                                                           ELST1770
      X1=1./(PAR(31)-XX(1))                                             ELST1790
      X2=1./(PAR(31)-XX(NSW1))                                          ELST1800
      Y2=YY(NSW1)                                                       ELST1810
      GC TO (50,50,53,53,55) ,J1                                        ELST1830
C                                                                       ELST1840
   50 P(3)=(YY(1)/X1-Y2/X2)/(X1-X2)                                     ELST1850
      P(2)=Y2/X2-P(3)*X2                                                ELST1860
      GO TO 32                                                          ELST1870
   53 P(2)=(YY(1)*XX(NSW1)-Y2*XX(1))/(XX(NSW1)*X1-XX(1)*X2)             ELST1890
      P(3)=YY(1)/XX(1)-(X1/XX(1))*P(2)                                  ELST1900
      IF(J1.EQ.4) GO TO 54                                              ELST1920
      GO TO 32                                                          ELST1930
   54 P(1)=P(2)                                                         ELST1960
      P(2)=P(3)                                                         ELST1970
      P(3)=0.                                                           ELST1980
      GO TO 32                                                          ELST1990
   55 IF(LPAR(18).EQ.0) LPAR(18)=2                                      ELST2020
      PAR(81)=(XGO-XGU)/FLOAT(LPAR(18))+XGU                             ELST2030
      XK1=XX(1)-PAR(81)                                                 ELST2040
      XK2=XX(NSW1)-PAR(81)                                              ELST2050
      P(3)=(YY(1)/XK1-Y2/XK2)/(XK1-XK2)                                 ELST2060
      P(2)=YY(1)/XK1-P(3)*XK1                                           ELST2070
C                                                                       ELST2080
   32 CALL FIT(NPSW,P,NSW1,XX,YY,ERR,0,GAMMA,J)                         ELST2090
      IF(LPAR(20).GT.1)  CALL ZETKO                                     ELST2100
   40 RETURN                                                            ELST2130
      END                                                               ELST2140

C SSWF  STRAHLENSCHWANZFIT                                              ELST2160
      SUBROUTINE SSWF(Y,X)                                              ELST2170
      DIMENSION PAR(300),LPAR(100)                                      ELST2180
      COMMON PAR,LPAR                                                   ELST2190
      J=IABS(LPAR(16))                                                  ELST2200
      IF(J.EQ.5) GO TO 50                                               ELST2210
      A=1./(PAR(31)-X)                                                  ELST2220
      Y=PAR(91)+PAR(93)*A                                               ELST2230
      GO TO (10,20,30,40),J                                             ELST2240
   10 Y=Y+PAR(95)*A**2+PAR(97)*A**3+PAR(99)*A**4                        ELST2250
      RETURN                                                            ELST2260
   20 Y=Y+PAR(95)*A**2+PAR(97)*X+PAR(99)*X**2                           ELST2270
      RETURN                                                            ELST2280
   30 Y=Y+PAR(95)*X+PAR(97)*X**2+PAR(99)*X**3                           ELST2290
      RETURN                                                            ELST2300
   40 Y=PAR(91)*A+PAR(93)*X+PAR(95)*X**2+PAR(97)*A**2+PAR(99)*X**3      ELST2310
      RETURN                                                            ELST2320
   5C A=X-PAR(81)                                                       ELST2330
      Y=PAR(91)+PAR(93)*A+PAR(95)*A**2+PAR(97)*A**3+PAR(99)*A**4        ELST2340
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      RETURN                                                            ELST2350
      END                                                               ELST2360
C     ANPASSUNG NACH DER METHODE DER KLEINSTEN QUADRATE                 ELST5430
      SUBROUTINE    FIT(MZ,P,N,X,Y,DY,NRM,DELTA,NUM)                    ELST5460
C     NRM = 0 FALLS DIE MESSFEHLER ABSOLUT SIND                         ELST5480
      DIMENSION PAR(300),LPAR(100),DUM(600),             WORD(20)
      DIMENSION  X( 500),  Y( 500), DY( 500), V1(25), V2(25),           ELST5520
     1    P(25), DP(25), DF(25), DZ(25), D2Z(50,50), U(50,50)
      DIMENSION            JOTA(10)                                     ELST5540
      DIMENSION ZWP(25),PNB(25)                                         ELST5550
      COMMON PAR,LPAR,DUM,      WORD
      REAL*8 TEXT,NAME1,NAME2,NAME3                                     ELST5580
      COMMON/SSWD/ACO(25)
      COMMON /LING1/ D2Z,U
      DATA TEXT/'          '/                                           ELST5600
      DATA V1,V2,DP,DF,DZ,ZWP,PNB /175*.0/
      DATA NAME3 /'.  GRD'/                                             ELST5610
      GAM1=.0                                                           ELST5620
      NORM = NRM                                                        ELST5630
      GAMMA=DELTA                                                       ELST5640
      M=MZ                                                              ELST5650
      MY=5                                                              ELST5660
      JC06=6                                                            ELST5670
      MC0Z=20                                                           ELST5680
      M001=5                                                            ELST5690
      DO 11 K=1,50
      DO 11 L=1,50
      D2Z(K,L)=.0
   11 U(K,L)=.0
C     DIAGNOSTIK                                                        ELST5750
      I1=1                                                              ELST5770
   13 IF(M) 16,16,15                                                    ELST5780
   15 IF(M-25)  17,17,16                                                ELST5790
   16 WRITE (6,997)M                                                    ELST5800
  997 FORMAT (40H1 NUR 1 BIS 25 PARAMETER ERLAUBT STATT    ,I7)         ELST5810
      RETURN                                                            ELST5820
   17 IF(N-500)   20,20,18                                              ELST5830
   18 WRITE (6,998)N                                                    ELST5840
  998 FORMAT (42H1 NUR 1 BIS 500  MESSPUNKTE ERLAUBT STATT      ,I7  )  ELST5850
      RETURN                                                            ELST5860
   20 ZSOLL = N - M                                                     ELST5870
      IF(ZSOLL)   24,25,26                                              ELST5880
   24 WRITE (6,999)M,N                                                  ELST5890
  999 FORMAT (19H1 MEHR PARAMETER  (, I2, 20H)  ALS MESSPUNKTE  (,  I2, ELST5900
     1     1H)  )                                                       ELST5910
      RETURN                                                            ELST5920
   25 NORM = 0                                                          ELST5930
```

```
   26 DO 27    I = 1,N                                                      ELST5940
      IF(DY(I))    28,28,27                                                 ELST5950
   27 CONTINUE                                                              ELST5960
      GO TO 14                                                              ELST5970
   28 WRITE (6,1000)I                                                       ELST5980
 1000 FORMAT (49H1 MESSFEHLER DY(I) IST NULL ODER NEGATIV FUER I = , I4)ELST5990
      RETURN                                                                ELST6000
   14 FEH=1.0                                                               ELST6020
      IF(NORM)    29,30,30                                                  ELST6030
   29 FEH=DY(1)**2                                                          ELST6040
   30 J = 0                                                                 ELST6050
C     BEGINN DER ITERATION ZUR LOESUNG DER NORMAL - GLEICHUNGEN             ELST6070
      IF(LPAR(8))     31,31,32                                              ELST6090
   31 WRITE (6,1002)                                                        ELST6100
 1002 FORMAT (1H1,17X,18HZWISCHENERGEBNISSE,                                ELST6110
     1    /85H NAEHERUNG          ZWANG          1.PARAMETER    2.PARAMETER ELST6120
     2  3.PARAMETER    USW......        //)                                 ELST6130
   32 G = 1.0                                                               ELST6140
      DATA NAME1/'.       '/                                                ELST6150
      TEXT=NAME1                                                            ELST6160
C                                                                           ELST6170
   50 Z = 0.0                                                               ELST6180
      DO 60    K = 1,M                                                      ELST6190
      DZ(K) = 0.0                                                           ELST6200
      DO 60    L = 1,M                                                      ELST6210
   60 D2Z(K,L) = 0.0                                                        ELST6220
      DO 70    I = 1,N                                                      ELST6230
      CALL THEORY  (NUM,X(I),P,F,DF)                                        ELST6240
      H1 = DY(I)**(-2)*FEH                                                  ELST6250
      H2 = Y(I) - F                                                         ELST6260
      Z = Z + H1*H2*H2                                                      ELST6270
      DO 70    K = 1,M                                                      ELST6280
      DZ(K) = DZ(K) - H1*H2*DF(K)                                           ELST6290
      DO 70    L = 1,M                                                      ELST6300
   70 D2Z(K,L) = D2Z(K,L) + H1*DF(K)*DF(L)                                  ELST6310
   71 ZY=Z/FEH                                                              ELST6320
      IF(NORM)    72,73,72                                                  ELST6330
   72 G=Z/ZSOLL                                                             ELST6340
   73 IF(LPAR(8))     74,74,78                                              ELST6350
   74 IF (NORM) 77,77,75                                                    ELST6360
   75 WRITE (6,1003)J, TEXT, Z, (P(K), K = 1,M)                             ELST6370
 1003 FORMAT (1X,I3,A6,1PE14.6,3X,7E15.6/(27X,7E15.6))                      ELST6380
      GO TO 78                                                              ELST6390
   77 WRITE (6,1004)J, TEXT,ZY, (P(K), K = 1,M)                             ELST6400
 1004 FORMAT (1X,I3,A6,F14.4,3X,1P7E15.6/(27X,7E15.6))                      ELST6410
C     PRUEFUNG AUF ITERATIONSSTOP                                           ELST6430
   78 IF(J-MY)  100, 80, 80                                                 ELST6450
   80 IF (ABS(Z-ZALT)-1.0E-02)  140,140,79
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   79 IF (Z-ZALT)  90,102,102                                         ELST6470
  102 DO    103 K=1,M                                                ELST6480
  103 P(K)=ZWP(K)                                                    ELST6490
      GAMMA=0.8*GAM1                                                 ELST6500
      WRITE (6,1040)GAMMA                                            ELST6510
 1040 FORMAT(13X,10H  GAMMA  =  F13.6)                               ELST6520
   90 IF(J-MOOZ)    100,130,130                                      ELST6530
C     DURCHFUEHRUNG DER ITERATION                                    ELST6550
  100 DO 104    K = 1,M                                              ELST6570
      DP(K) = - DZ(K)                                                ELST6580
      DO 104    L = 1,M                                              ELST6590
  104 U(K,L) = D2Z(K,L)                                              ELST6600
      CALL LINGL (U,DP,M,1)                                          ELST6610
  105 H1 = 0.0                                                       ELST6620
      DO 106    K = 1,M                                              ELST6630
  106 H1 = H1 + DP(K)*DP(K)*D2Z(K,K)                                 ELST6640
      DATA NAME2/'.  NWT'/                                           ELST6650
      TEXT=NAME2                                                     ELST6660
      GAM1=SQRT(H1)                                                  ELST6670
      IF(GAM1-GAMMA)    113,113,107                                  ELST6680
C     GRADIENTEN METHODE STATT NEWTON                                ELST67C0
  107 TEXT=NAME3                                                     ELST6720
      H1 = 0.0                                                       ELST6730
      H2 = 0.0                                                       ELST6740
      DO 109    K = 1,M                                              ELST6750
      H3 = DZ(K)                                                     ELST6760
      DZ(K) = H3/D2Z(K,K)                                            ELST6770
  109 H1 = H1 + H3*DZ(K)                                             ELST6780
      DO 110    K = 1,M                                              ELST6790
      DO 110    L = 1,M                                              ELST6800
  110 H2 = H2 + DZ(K)*D2Z(K,L)*DZ(L)                                 ELST6810
      H3= AMIN1(H1/H2,GAMMA/SQRT(H1))                                ELST6820
      DO 112    K = 1,M                                              ELST6830
  112 DP(K) = - H3*DZ(K)                                             ELST6840
  113 ZALT = Z                                                       ELST6860
      IF(J.LE.MQ01)  GO TO 114                                       ELST6870
      I1=I1+2                                                        ELST6880
  114 DO 120    K = 1,M                                              ELST6890
      ZWP(K)=P(K)                                                    ELST6900
  120 P(K) = P(K) + DP(K)                                            ELST6910
  124 J=J+1                                                          ELST6920
      GO TO 50                                                       ELST6930
C                                                                    ELST6940
C     AUSDRUCK FALLS NOCH KEINE KONVERGENZ NACH 20 ITERATIONEN        ELST6950
  130 WRITE (6,1005) MOOZ                                            ELST6960
 1005 FORMAT (24H  (KEINE KONVERGENZ NACH I3,15H ITERATIONEN)   )    ELST6970
  140 WRITE (6,1030)(WORD(I),I=1,20)
 1030 FORMAT(1H0,20A4//)
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      IF(LPAR(24))   131,131,132                                          ELST7020
  131 WRITE (6,1031)                                                      ELST7030
 1031 FORMAT(27H FITERGEBNISSE ELAST. PEAK      )                         ELST7040
      GO TO 133                                                           ELST7050
  132 WRITE (6,1032)                                                      ELST7060
 1032 FORMAT(20H FITERGEBNISSE SSW      )                                 ELST7070
      IF(ACO(1).NE.0.)WRITE(6,502)                                        ELST7080
  502  FORMAT( 1X,'SSW MIT PHASENANALYSE WQ BERECHNET' )                  ELST7090
  133 IF(NORM) 35,35,40                                                   ELST7100
C                                                                         ELST7110
C     ERWARTUNGSWERT VON Z IST ZSOLL = N - M FALLS DIE MESSFEHLER DY(I)   ELST7120
C     ABSOLUT SIND. STREUUNG IST SQRT (2*ZSOLL)                           ELST7130
C                                                                         ELST7140
   35 H1 = SQRT(2.0*ZSOLL)                                                ELST7150
      A012=H1                                                             ELST7160
      B012=ZY                                                             ELST7170
      WRITE (6,1007)ZSOLL, H1, ZY                                         ELST7180
 1007 FORMAT (9H    ZWANG, 9X, 8HSOLLWERT, F8.1, 3H +-, F5.1              ELST7190
    1   /18X,7HISTWERT ,F9.1)                                             ELST7200
   40 WRITE (6,1008)                                                      ELST7210
 1008 FORMAT (1H ,32X,7HOPTIMAL,13X,6HFEHLER,                             ELST7220
    1     28X,27HKONTROLLE  (SOLLWERT IST 1) //)                          ELST7230
      DO 160   K = 1,M                                                    ELST7240
      DO 150   L = 1,M                                                    ELST7250
  150 U(K,L) = 0.0                                                        ELST7260
  160 U(K,K) = G                                                          ELST7270
      CALL LINGL (D2Z, U, M, M)                                           ELST7280
  170 DO 180 K = 1,M                                                      ELST7290
  180 DP(K) = SQRT(ABS(U(K,K)))                                           ELST7300
C                                                                         ELST7310
C     KONTROLLE DURCH BERECHNUNG DES ZWANGES  AN DEN EXTREMPUNKTEN        ELST7320
C     DES FEHLERELLIPSOIDS                                                ELST7330
      DO 205   K = 1,M                                                    ELST7350
      DO 190   L = 1,M                                                    ELST7360
      U(K,L) = U(K,L)/DP(K)                                               ELST7370
      V1(L) = P(L) - U(K,L)                                               ELST7380
      V2(L) = P(L) + U(K,L)                                               ELST7390
  190 U(K,L) = U(K,L)/DP(L)                                               ELST7400
      J = J+1                                                             ELST7410
      H1 = 0.0                                                            ELST7420
      DO 195     I = 1,N                                                  ELST7430
      CALL THEORY (NUM,X(I),V1,F,DF)                                      ELST7440
  195 H1 = H1 + ((Y(I) - F)/DY(I))**2*FEH                                 ELST7450
      H1 = (H1 - Z)/G                                                     ELST7460
      J = J+1                                                             ELST7470
      H2 = 0.0                                                            ELST7480
      DO 200   I = 1,N                                                    ELST7490
      CALL THEORY( NUM,X(I),V2,F,DF)                                      ELST7500
```

```
  200 H2 = H2 + ((Y(I) - F)/DY(I))**2*FEH                                  ELST7510
      H2 = (H2 - Z)/G                                                      ELST7520
  205 WRITE (6,1009)K, P(K), DP(K), H1, H2                                 ELST7530
 1009 FORMAT (1X,I2,10H.PARAMETER,15X,1PE15.6,5H   +-,E15.6,11X,0P2F20.5ELST7540
     1   )                                                                 ELST7550
      WRITE (6,1010)                                                       ELST7560
 1010 FORMAT (40H KORRELATIONEN ZWISCHEN DEN PARAMETERN                    ELST7570
     1   //12X,31H1.PA     2.PA     3.PA     USW....     //)               ELST7580
      DO 185   K = 1,M                                                     ELST7590
  185 WRITE (6,1011)K,(U(K,L), L = 1,M)                                    ELST7600
 1011 FORMAT (1X,I2,6H.PA    ,15F8.3/9X,10F8.3)                            ELST7610
C                                                                          ELST7620
C     TABELLIERUNG DER ANGEPASSTEN FUNKTION                                ELST7630
      IF(LPAR(8))    181,186,181                                           ELST7660
  181 IF(LPAR(9))    216,216,182                                           ELST7670
  186 WRITE (6,1015)                                                       ELST7680
 1015 FORMAT(1H0,54X,13HT A B E L L E ////56X,8HORDINATE/                  ELST7690
     1   114H   NR.              ABSZISSE                        GEMESSEN  ELST7700
     2 BERECHNET                      DIFFERENZ        MESSFEHLER  //)     ELST7710
  182 IF(LPAR(9).LE.0.OR.LPAR(24).GT.0) GO TO 188                          ELST7720
  187 WRITE ( 1)           LPAR(24),          M,N,ZSOLL,A012,B012          ELST7730
      LPAR(25)=LPAR(25)+1                                                  ELST7740
  188 DO 213  I = 1,N                                                      ELST7750
      CALL THEORY (NUM ,X(I),P,F,DF)                                       ELST7760
      H1 = Y(I) - F                                                        ELST7770
      H14=H1/DY(I)                                                         ELST7780
      IF(LPAR(9).EQ.0.OR.LPAR(24).GT.0)  GO TO 215                         ELST7790
  197 UNT=0.0                                                              ELST7800
      WRITE ( 1)X(I),Y(I),F,H14,UNT,UNT
  215 IF(LPAR(8).NE.0)   GO TO 213                                         ELST7820
  214 WRITE (6,1016)I,X(I),Y(I),F,H1,DY(I)                                 ELST7830
 1016 FORMAT (I5,F19.4,3X,1P2(E27.6,E17.6))                                ELST7840
  213 CONTINUE                                                             ELST7850
C                                                                          ELST7860
  216 NO=70                                                                ELST7870
      IF(LPAR(24).GT.0)  NO=90                                             ELST7880
 1021 DO   1022 I=1,M                                                      ELST7890
      NON=NO+2*I                                                           ELST7900
      PAR(NON-1)=P(I)                                                      ELST7910
 1022 PAR(NON)=DP(I)                                                       ELST7920
      RETURN                                                               ELST7930
      END                                                                  ELST7940

      SUBROUTINE THEORY(J,X,P,Y,DA)                                        ELST8510
C     THEORY            ELAST                                              ELST8520
      DIMENSION P(25),DA(25),PAR(300),LPAR(100)                            ELST8530
      COMMON PAR,LPAR                                                      ELST8540
      GO TO (10,20,30,40,50,60) ,J                                         ELST8550
```

```
10 CALL ARC4(X,P,Y,DA)                                        ELST8560
   RETURN                                                     ELST8570
20 A=1./(PAR(31)-X)                                           ELST8580
   Y=P(1)+P(2)*A+P(3)*A**2+P(4)*A**3                          ELST8590
   IF(LPAR(33).EQ.5)  Y=Y+P(5)*A**4                           ELST8600
   DA(1)=1                                                    ELST8610
   DA(2)=A                                                    ELST8620
   DA(3)=A**2                                                 ELST8630
   DA(4)=A**3                                                 ELST8640
   DA(5)=A**4                                                 ELST8650
   RETURN                                                     ELST8660
30 A=1./(PAR(31)-X)                                           ELST8670
   Y=P(1)+P(2)*A+P(3)*A**2+P(4)*X+P(5)*X**2                   ELST8680
   DA(1)=1.                                                   ELST8690
   DA(2)=A                                                    ELST8700
   DA(3)=A**2                                                 ELST8710
   DA(4)=X                                                    ELST8720
   DA(5)=X**2                                                 ELST8730
   RETURN                                                     ELST8740
40 A=1./(PAR(31)-X)                                           ELST8750
   Y=P(1)+P(2)*A+P(3)*X+P(4)*X**2+P(5)*X**3                   ELST8760
   DA(1)=1.                                                   ELST8770
   DA(2)=A                                                    ELST8780
   DA(3)=X                                                    ELST8790
   DA(4)=X**2                                                 ELST8800
   DA(5)=X**3                                                 ELST8810
   RETURN                                                     ELST8820
50 A=1./(PAR(31)-X)                                           ELST8830
   Y=P(1)*A+P(2)*X+P(3)*X**2+P(4)*A**2+P(5)*X**3              ELST8840
   DA(1)=A                                                    ELST8850
   DA(2)=X                                                    ELST8860
   DA(3)=X**2                                                 ELST8870
   DA(4)=A**2                                                 ELST8880
   DA(5)=X**3                                                 ELST8890
   RETURN                                                     ELST8900
6C A=X-PAR(81)                                                ELST8910
   Y=P(1)+P(2)*A+P(3)*A**2+P(4)*A**3+P(5)*A**4                ELST8920
   DA(1)=1.                                                   ELST8930
   DA(2)=A                                                    ELST8940
   DA(3)=A**2                                                 ELST8950
   DA(4)=A**3                                                 ELST8960
   DA(5)=A**4                                                 ELST8970
   RETURN                                                     ELST8980
   END                                                        ELST8990


   SUBROUTINE ARC4(X,P,Y,DY)                                  ELST9400
```

```
      DIMENSION P(25),DY(25)                                             ELST9410
      BT=1.44269505                                                      ELST9420
C     DEZ'71: ZWEITE EL LINIE MIT HOEHE=P(6), LAGE=P(7)                 ELST9430
    6 U=(X-P(5))                                                         ELST9440
      V=(X-P(7))                                                         ELST9450
      IF(U)  20,10,10                                                    ELST9460
   10 CONTINUE                                                           ELST9470
      ALPHA=(U/P(2))**2/BT                                               ELST9480
  100 FORMAT( 5E15.4)                                                    ELST9490
   11 Y=P(1)*EXP(-ALPHA)                                                 ELST9500
      DY(1)=Y/P(1)                                                       ELST9510
      DY(2)=2.0*Y*U**2/(BT*P(2)**3)                                      ELST9520
      DY(3)=0.0                                                          ELST9530
      DY(4)=0.0                                                          ELST9540
      DY(5)=2.0*U*Y/(BT*P(2)**2)                                         ELST9550
      IF(P(6).EQ..0) RETURN                                              ELST9560
   60 Y6=P(6)*EXP(-(V/P(2))**2/BT)                                       ELST9570
      DY(6)=Y6/P(6)                                                      ELST9580
      DY(7)=2.0*V*Y6/(BT*P(2)**2)                                        ELST9590
      Y=Y+Y6                                                             ELST9600
      DY(2)=DY(2)+ 2.*Y6*V**2/(BT*P(2)**3)                               ELST9610
      RETURN                                                             ELST9620
   20 YP=P(1)*EXP(-(P(4)/P(3))**2/BT)                                    ELST9630
      IF(U-P(4))    42,30,30                                             ELST9640
   30 Y=P(1)*EXP(-(U/P(3))**2/BT)                                        ELST9650
      DY(1)=Y/P(1)                                                       ELST9660
      DY(2)=0.0                                                          ELST9670
      DY(5)=2.0*Y*U/(BT*P(3)**2)                                         ELST9680
      DY(4)=0.0                                                          ELST9690
      DY(3)=DY(5)*U/P(3)                                                 ELST9700
       IF(P(6).EQ..0) RETURN                                             ELST9710
      IF(X.GE.P(7)) GOTO 60                                              ELST9720
   61 Y6=P(6)*EXP(-(V/P(3))**2/BT)                                       ELST9730
      DY(6)=Y6/P(6)                                                      ELST9740
      DY(7)=2.0*V*Y6/(BT*P(3)**2)                                        ELST9750
      Y=Y+Y6                                                             ELST9760
      DY(3)= DY(3)+2.*Y6*V**2/(BT*P(3)**3)                               ELST9770
      RETURN                                                             ELST9780
   42 PP=2.0*(P(4)/P(3))**2/BT                                           ELST9790
      K6=0                                                               ELST9800
   62 IF(K6.EQ.1) YP=YP6                                                 ELST9810
      C=YP*P(4)*(2.0-PP)                                                 ELST9820
      D=YP*P(4)**2*(PP-1.0)                                              ELST9830
      PPP=YP*PP                                                          ELST9840
      CP3=PPP*P(4)*(4.0-PP)/P(3)                                         ELST9850
      DP3=PPP*PP*(P(4)**2/P(3)-3.0*BT*P(3)/2.0)                          ELST9860
      CP4=PPP*(2.0/PP-5.0+PP)                                            ELST9870
      DP4=PPP*P(4)*(5.0-PP-2.0/PP)                                       ELST9880
```

```
      IF(K6.EQ.1) GOTO 63                                       ELST9890
      Y=C/U+D/U**2                                              ELST9900
      DY(1)=Y/P(1)                                              ELST9910
      DY(2)=0.0                                                 ELST9920
      DY(3)=CP3/U+DP3/U**2                                      ELST9930
      DY(4)=CP4/U+DP4/U**2                                      ELST9940
      DY(5)=C/U**2+2.0*D/U**3                                   ELST9950
      IF(P(6).EQ..0)RETURN                                      ELST9960
      IF(X.GE.P(7))  GOTO60                                     ELST9970
      IF(X.LT.P(7)   .AND.   X.GE.P(4))  GOTO 61                ELST9980
      K6=1                                                      ELST9990
      YP6=P(6)*EXP(-P(4)/P(3))**2/BT                            ELST0010
      GOTO 62                                                   ELST0020
   63 Y6=C/V+D/V**2                                             ELST0030
      DY(6)=Y6/P(6)                                             ELST0040
      Y=Y+Y6                                                    ELST0050
      DY(7)=C/V**2+2.0*D/V**3                                   ELST0060
      DY(4)=DY(4)+CP4/V  +  DP4/V**2                            ELST0070
      DY(3)=DY(3)+CP3/V  +  DP3/V**2                            ELST0080
      RETURN                                                    ELST0090
      END                                                       ELST0100

      SUBROUTINE HALBW(P2,P3,P4,DP2,DP3,HWB,DHWB,FHW,W)         ELST0130
      IF(P2)    1,1,2                                           ELST0140
    1 HWB=0.0                                                   ELST0150
      DHWB=0.0                                                  ELST0160
      FHW=0.0                                                   ELST0170
      W=0.0                                                     ELST0180
      RETURN                                                    ELST0190
    2 PVP=P4/P3                                                 ELST0200
      BT=1.44269505                                             ELST0210
      YP=EXP(-PVP**2/BT)                                        ELST0220
      HWB=P2+P3                                                 ELST0230
      DHWB=(P3-P2)/2.0                                          ELST0240
      PP=2.0*PVP**2/BT                                          ELST0250
      C=YP*P4*(2.0-PP)                                          ELST0260
      D=YP*P4**2*(PP-1.0)                                       ELST0270
      X=-PVP/SQRT(BT)                                           ELST0280
      W=ERF(X)                                                  ELST0290
      W0= P2*SQRT(BT*3.14159265)*.5*(1.0+W*P3/P2)               ELST0300
      ZA=2.                                                     ELST0310
      GRENZ=ZA*HWB+.5*DHWB                                      ELST0320
      W2=C*ALOG(-P4/GRENZ)-D/P4-D/GRENZ                         ELST0330
      W=W0+W2                                                   ELST0340
      FHW=1.0                                                   ELST0360
      RETURN                                                    ELST0370
      END                                                       ELST0380
```

```
      SUBROUTINE RADTL(U1,SW,EIMEV,EMMV,R,T,ATW,Z,XRAD,DES,DS,D,NA1,ERR)ELST0410
      DIMENSION PAR(300),LPAR(100)                                      ELST0420
      COMMON PAR,LPAR                                                   ELST0430
      DOUBLE PRECISION  U      , DCOS    , W       , EI      , EF       ELST0440
      DOUBLE PRECISION  PI     , DSQRT   , PF      , A       , B        ELST0450
      DOUBLE PRECISION  XA     , XB      , XMIN    , XMAX    , X2       ELST0460
      DOUBLE PRECISION  X3     , X1      , X4   ,U1                     ELST0470
      U=U1                                                              ELST0480
      ERROR=ERR                                                         ELST0490
      EI=EIMEV/.5109                                                    ELST0510
      DESCHW=DES                                                        ELST0520
      DSMOT=DS                                                          ELST0530
      EMIN=EMMV/.5109                                                   ELST0540
      CU2=COS(.0174533*SNGL(U)/2.0)                                     ELST0550
      SU2=SIN(.0174533*SNGL(U)/2.0)                                     ELST0560
      U=DCOS(.0174533D0*U)                                              ELST0570
      DEFF=D/(2.0*XRAD)                                                 ELST0580
      REFF=(D*Z)/(ATW     )*.047829*.5                                  ELST0590
  302 Z13=EXP(-.3333*ALOG(Z))                                           ELST0600
      GZ13=ALOG(183.0*Z13)                                              ELST0610
      XO=2.0*(SNGL(EI)*SU2)**2                                          ELST0620
  282 CALL FORM(FO,XO,R,T)                                              ELST0750
      CALL DMOTT(DM,CU2,SU2,Z,EI)                                       ELST0760
  312 CALL DELTA(DELT,SU2,DESCHW,EI)                                    ELST0770
  322 SIGMA=DM*              FO**2                                      ELST0780
      ES   =EMIN                                                        ELST0790
      EF   =                 ES                                         ELST0800
      W=EI-EF                                                           ELST0810
      PI=DSQRT(EI**2-1.D0)                                              ELST0820
      PF=DSQRT(EF**2-1.D0)                                              ELST0830
      A=DSQRT(PI**2-2.D0*PI*PF*U+PF**2)                                 ELST0840
      B= EI*EF-PI*PF*U-1.D0                                             ELST0850
      DSIGMA    =0.0                                                    ELST0860
      IF(NA1)   303,303,304                                             ELST0870
  303 XA=B+W*(W+PF-PI*U)                                                ELST0880
      XB=W*(W-PI+PF*U)+B                                                ELST0890
      XMIN=.5D0*(A-W)**2                                                ELST0900
      XMAX=.5D0*(A+W)**2                                                ELST0910
      IF(SNGL(XA)-SNGL(XB)-15.0*SNGL(W)*(SNGL(EF)/SNGL(EI)+SNGL(EI)/SNGLELST0920
     1(EF))) 5,6,6                                                      ELST0930
    5 X2=XB                                                             ELST0940
      X3=XA                                                             ELST0950
      GO TO 7                                                           ELST0960
    6 X2=XB+10.D0*W*EF/EI                                               ELST0970
      X3=XA-10.D0*W*EI/EF                                               ELST0980
    7 IF(SNGL(XB)-15.0*SNGL(W)*SNGL(EF)/SNGL(EI)-SNGL(XMIN)) 8,9,9      ELST0990
    8 X1=XB                                                             ELST1000
      GO TO   10                                                        ELST1010
```

```
    9 X1=XB-10.DO*W*EF/EI                                                          ELST1020
   10 IF(SNGL(XMAX)-SNGL(XA)-15.0*SNGL(W)*SNGL(EI)/SNGL(EF)) 11,12,12              ELST1030
   11 X4=XA                                                                        ELST1040
      GC TO 2                                                                      ELST1050
   12 X4=XA+10.DO*W*EI/EF                                                          ELST1060
    2 CONTINUE                                                                     ELST1070
      CALL WEDDLE(H1,XMIN,X1,ERROR,EI,EF,PI,PF,U,A,B,W,R,T)                        ELST1080
      CALL WEDDLE(H2,X1,X2,   ERROR,EI,EF,PI,PF,U,A,B,W,R,T)                       ELST1090
      CALL WEDDLE(H3,X2,X3,   ERROR,EI,EF,PI,PF,U,A,B,W,R,T)                       ELST1100
      CALL WEDDLE(H4,X3,X4,   ERROR,EI,EF,PI,PF,U,A,B,W,R,T)                       ELST1110
      CALL WEDDLE(H5,X4,XMAX,ERROR,EI,EF,PI,PF,U,A,B,W,R,T)                        ELST1120
      DSIGMA    =H1+H2+H3+H4+H5                                                    ELST1130
      DSIGMA    =DSIGMA    *90.2376*(SNGL(PF)/SNGL(PI))*Z**2                       ELST1140
  304 EFMEV    =.5109*ES                                                           ELST1150
      XEF=2.0*(SNGL(EF)*SU2)**2                                                    ELST1160
      CALL FORM(FE,XEF,R,T)                                                        ELST1210
      BRA    =(1.0+((SNGL(EI)*FE)/(SNGL(EF)*FO))**2 )                              ELST1220
      SCHIFR    =0.0                                                               ELST1230
      SCH= .0                                                                      ELST1240
      IF(NA1.GT.0)  CALL SCHIFC(SCH,SU2,EI,EF,W)                                   ELST1250
      SCHIFR    =BRA    *SCH*DSMOT                                                 ELST1260
      DSIGMA=DSIGMA*DSMOT/SIGMA                                                    ELST1270
  306 CALL HEIMOL(H,REFF,DEFF,GZ13,EI,EF)                                          ELST1280
      HEMO    =BRA    *H*DSMOT                                                     ELST1290
      SSW=DSIGMA+HEMO                                                              ELST1300
      IF(NA1.GT.0)  SSW=SCHIFR+HEMO                                                ELST1310
      SW=SSW*(1.+DELT)                                                             ELST1320
 1001 FCRMAT(5E15.6)                                                               ELST1340
      RETURN                                                                       ELST1350
      END                                                                          ELST1360

      SUBROUTINE CAPR(Z,Y,EI,EF,PI,PF,U,A,B,W,R,T)                                 ELST1390
CSUBO SUBROUTINEFOR CALCULATION OF R(X) FOR ELECTRON SPECTRUM                      ELST1380
      DOUBLE PRECISION  A      , D       , X       , EI      , EF                  ELST1400
      DOUBLE PRECISION  D1     , DSQRT   , B       , D2      , G1                  ELST1410
      DOUBLE PRECISION  G2     , G3,W,U,  PI, PF,  F .                             ELST1420
      X  =  Y                                                                      ELST1430
      B1=PI**2-PI*PF*U                                                             ELST1440
      B2=B1-A**2                                                                   ELST1450
      D=2.DO*X*((EI*EF-1.DO)*U-PI*PF)*PI*PF                                        ELST1460
      D1=DSQRT((PI*X)**2+D+(PF*B)**2)                                              ELST1470
      D2=DSQRT((PF*X)**2+D+(PI*B)**2)                                              ELST1480
      G1=(2.DO*EI**2-X)*(B*B1+X*B2)/D2**3                                          ELST1490
      G2=(2.DO*EF**2-X)*(B*B2+X*B1)/D1**3                                          ELST1500
      G3=2.DO*(EI**2+EF**2)+B-X-2.DO*((1.DO+B)*(2.DO*EI*EF-X)+B*W**2)/(BELST1510
     1-X)                                                                          ELST1520
      F=((1.DO/D2)-(1.DO/D1))*G3-G2-G1-(2.DO/A)                                    ELST1530
      Z=SNGL(F)/SNGL(X)**2                                                         ELST1540
```

```
      XX=SNGL(X)                                                            ELST1550
      CALL FORM(FOR,XX,R,T)                                                 ELST1560
      Z=Z*FOR**2                                                            ELST1570
      RETURN                                                                ELST1580
      END                                                                   ELST1590

      SUBROUTINE FORM(F,X,R,T)                                              ELST1630
C    WAHLWEISE TRAPEZ- ODER EXAKTER FORMFAKTOR  IN POTENZEN VON Q**2        ELST1610
C    EINGEFUEGT AUGUST 72 PITTHAN,WALCHER                                   ELST1620
      COMMON/SSWD/ACO(25)
      IF(ACO(1).EQ.0.) GOTO 5                                               ELST1650
      QQ=X*2./386.1**2                                                      ELST1660
      F=0.                                                                  ELST1670
      DO 4 I=1,12                                                           ELST1680
    4 F=F+ACO(I)*QQ**(I-1)                                                  ELST1690
      RETURN                                                                ELST1700
C     TRAPEZFORMFAKTOR:                                                     ELST1710
    5 Q=(R+5.0*T/8.0)*SQRT(2.0*X)/386.154                                   ELST1720
      ETA=(R-5.0*T/8.0) /(R+5.0*T/8.0)                                      ELST1730
      QN=ETA*Q                                                              ELST1740
      F=12.0*(QN*SIN(QN)-Q*SIN(Q)+2.0*COS(QN)-2.0*COS(Q))/(Q**4-QN**4)      ELST1750
C     WRITE (6,10)                                                          ELST1760
   10 FORMAT (2F20.10)                                                      ELST1770
      RETURN                                                                ELST1780
      END                                                                   ELST1790

      SUBROUTINE DMOTT(X,CU2,SU2,Z,EI     )                                 ELST1820
      DOUBLE PRECISION  PI       , PF      , A       , B                    ELST1830
      DOUBLE PRECISION  U      , W       , EI      , EF                     ELST1840
      ANGL =CU2**2/(SU2**4)                                                 ELST1850
      X=ANGL*(Z/(2.0*EI))**2*79411.0                                        ELST1860
      RETURN                                                                ELST1870
      END                                                                   ELST1880

      SUBROUTINE SCHIFC(X,SU2,EI,EF,W)                                      ELST1910
CSCHIFF SUBROUTINE RADIATION TAIL DURING SCATTERING                         ELST1900
      DOUBLE PRECISION  PI       , PF      , A       , B                    ELST1920
      DOUBLE PRECISION  U      , W       , EI      , EF                     ELST1930
      X1=(1.0+(EF/EI)**2)*(DLOG(2.0*EI*SU2)-0.5)                            ELST1940
      X=.002323*X1/(W    *.5109)                                            ELST1950
      RETURN                                                                ELST1960
      END                                                                   ELST1970

CSUBD SUBROUTINE SCHWINGER CORRECTION                                       ELST1990
      SUBROUTINE DELTA(X,SU2,DESCHW,EI)                                     ELST2000
      DOUBLE PRECISION  U      , W       , EI      , EF                     ELST2010
      DOUBLE PRECISION  PI       , PF      , A       , B                    ELST2020
      R1=DLOG(2.0*EI    *SU2)-.5                                            ELST2030
```

```
      A1= DESCHW/.5109                                                  ELST2040
      R2=DLOG(EI    /A1)-1.0833                                         ELST2050
      X=.009236*(R1*R2+.2361)                                           ELST2060
      RETURN                                                            ELST2070
      END                                                               ELST2080

      SUBROUTINE WEDDLE(V,A,B,ERROR,EI,EF,PI,PF,U01,A01,B01,W01,R01,T01)ELST2110
CWEDDLE  EVALUATION OF QUADRATURES USING WEDDLE-S RULE                  ELST2100
      DIMENSION C(7),F(200)                                             ELST2120
C     DIMENSION C(7),F(200)                                             ELST2130
      DOUBLE PRECISION  U01   , W01    , EI    , EF  , A , B            ELST2140
      DOUBLE PRECISION  PI       , PF     , A01    , B01                ELST2150
  100 FORMAT(29H  **INTEGRAL NOT CONVERGENT**,  //)                     ELST2160
  101 FORMAT(8E14.6)                                                    ELST2170
  102 FORMAT(//17H   INTEGRAL FROM,E14.6,4H  TO,E14.6,10H  GIVES V=,    ELST2180
     1          E14.6,24H    (PREVIOUS VALUE - W=,E14.6,1H),//)         ELST2190
  103 FORMAT(21H  **A=B, INTEGRAL=0**,//)                               ELST2200
      IF(B-A)  2,3,2                                                    ELST2210
    3 WRITE (6,103)                                                     ELST2220
      V=0.0                                                             ELST2230
      GO TO 1                                                           ELST2240
    2 DO 10 I=1,7,2                                                     ELST2250
   10 C(I)=1.0                                                          ELST2260
      C(2)=5.0                                                          ELST2270
      C(4)=6.0                                                          ELST2280
      C(6)=5.0                                                          ELST2290
      DY=(B-A)/192.0                                                    ELST2300
      SUM=0.0                                                           ELST2310
      L=0                                                               ELST2320
      DO 20 I=1,193,32                                                  ELST2330
      L=L+1                                                             ELST2340
      Y=A+DY*FLOAT(I-1)                                                 ELST2350
      CALL CAPR(Z01,Y,EI,EF,PI,PF,U01,A01,B01,W01,R01,T01)              ELST2360
      F(I)=Z01                                                          ELST2370
   20 SUM=SUM+F(I)*C(L)                                                 ELST2380
      V=.3*SUM*DY*32.0                                                  ELST2390
      DO 50 N=1,5                                                       ELST2400
      W=V                                                               ELST2410
      K=2**(6-N)                                                        ELST2420
      M=K/2                                                             ELST2430
      K1=M+1                                                            ELST2440
      K2=193-M                                                          ELST2450
      DO 30 J=K1,K2,K                                                   ELST2460
      Y=A+DY*FLOAT(J-1)                                                 ELST2470
      CALL CAPR(Z01,Y,EI,EF,PI,PF,U01,A01,B01,W01,R01,T01)              ELST2480
   30 F(J)=Z01                                                          ELST2490
      K3=3*K                                                            ELST2500
      J1=193-K3                                                         ELST2510
```

```
      SUM=0.0                                                           ELST2520
      DC 40 J=1,J1,K3                                                   ELST2530
      J2=J+K3                                                           ELST2540
      L=0                                                               ELST2550
      DC 40 I=J,J2,M                                                    ELST2560
      L=L+1                                                             ELST2570
   40 SUM=SUM+F(I)*C(L)                                                 ELST2580
      V=.3*SUM*DY*FLOAT(M)                                              ELST2590
      IF(ABS((V-W)/V)-ERROR) 1,1,50                                     ELST2600
   50 CONTINUE                                                          ELST2610
      WRITE (6,100)                                                     ELST2620
    1 RETURN                                                            ELST2630
      END                                                               ELST2640

      SUBROUTINE HEIMOL(X,REFF,DEFF,GZ13,EI,EF)                         ELST2670
CHEMO SUBROUTINE HEITLER - MOELLER                                      ELST2660
      DIMENSICN  PAR(300),LPAR(100)                                     ELST2680
      CCMMON PAR,LPAR                                                   ELST2690
      DCUBLE PRECISION  U      , W         , EI       , EF              ELST2700
      DOUBLE PRECISION  PI        , PF        , A        , B            ELST2710
      W=EI-EF                                                           ELST2720
      BEOE=EF    /EI    *(((EI    **2+EF    **2)/(EI    *EF    )-.66667)+1.0/(ELST2730
     19.0*GZ13))                                                        ELST2740
      X1=BEOE*DEFF/W                                                    ELST2750
      IF(LPAR(40).EQ.0)  PAR(88)=1.                                     ELST2760
      X1=X1*PAR(88)                                                     ELST2770
      X21=6.28319*REFF                                                  ELST2780
      X22=1.0/EF    **2-(2.0*EI    +1.0)/(EF    *W    *(EI    +1.0)**2)+1.0/(ELST2790
     1W    **2)+1.0/(EI    +1.0)**2                                     ELST2800
      X2=X21*X22                                                        ELST2810
      IF(LPAR(40).EQ.0)  PAR(89)=1.                                     ELST2820
      X2=X2*PAR(89)                                                     ELST2830
      X=(X1+X2)/.5109                                                   ELST2840
      RETURN                                                            ELST2850
      END                                                               ELST2860

      SUBROUTINE   UNST                                                 ELST2880
C   UNELASTISCH                                                         ELST2890
      DIMENSION PAR(300),LPAR(100),FREQ(200),ZAEH(200),FEH(200)         ELST2900
      DIMENSION            WORD(20),XX(500),ERR(500),YY(500),P(50)
      DIMENSION IHO(25)                                                 ELST2920
      DIMENSION DUMMY(50)
      DIMENSION PVAR(25), BVAR(25)                                      ELST2930
      CCMMON PAR,LPAR,FREQ,ZAEH,FEH,      WORD
      CCMMON/BVAR1/BVAR                                                 ELST2950
      CCMMON/BVAR2/PVAR                                                 ELST2970
      COMMON/DATA1/XX,YY,ERR
      CCMMON /USTART/UPAR(10)
```

```
C
      IF(LPAR(20).GT.1)  CALL ZETKO
      IM=LPAR(21)
      IAN=15
      ISS=0
      LFE=IABS(LPAR(3))
      LVE=LPAR(4)
      LBV=LPAR(5)
      GAMMA=1000.
      UNAH=0.
      FNAH=0.
      DO 2 I=1,25
      IF(I.LE.LFE) PVAR(I)=BVAR(LVE+I)
      IF(I.GT.LFE .AND. I.LE.IM) PVAR(I)=BVAR(I-LFE)
    2 IHO(I)=0
C
C   EINLESEN UND HOEHEN-NAEHERUNGSWERTE
C
      LEO=0
    5 READ (3) IUN,LB
      IF(LB.GT.0)  GO TO 20
      DO   10 I=1,IUN
   10 READ (3) DMY1,DMY2,DMY3
      GO TO 5
   20 DO 30 I=1,IUN
      READ (3) HZ,CO,FEHEL
      IF(PAR(IAN).EQ.0.0.OR.IAN.GT.20)  GO TO 15
      IF(HZ-PAR(IAN))    12,12,15
   12 IF(HZ-PAR(IAN+1))    14,13,13
   13 CALL SSWF(FSSW,HZ)
      FNAH=FNAH+CO/FSSW
      IF(LPAR(2).GT.20) UNAH=UNAH+CO-FSSW
      ISS=ISS+1
      GO TO 15
   14 IAN=IAN+2
   15 CONTINUE
      IF(HZ.GT.PAR(13).OR.HZ.LT.PAR(14))  GO TO 30
      LEO=LEO+1
      XX(LEO)=HZ
C    DISPERSIONSKORREKTUR
      DISP=1.
      IF(PAR(64).GE.1.) DISP=PAR(31)/XX(LEO)
      YY(LEO)=CO*DISP
      ERR(LEO)=FEHEL*DISP
      DO   29 J=1,IM
      IF(HZ.LE.(PAR(31)-PAR(J+150)).AND.IHO(J).LE.0)  IHO(J)=LEO
   29 CONTINUE
   30 CONTINUE
```

```
      IF(LPAR(20).GT.1)  CALL ZETKO                                     ELST3460
C   NAEHERUNGSUNTERGRUND, HOEHENVERHAELTNISSE                           ELST3480
      DO   40 I=1,IM                                                    ELST3500
      IZ=IHO(I)                                                         ELST3510
      CALL SSWF(FSSW,XX(IZ))                                            ELST3520
      PAR(I+175)=(YY(IZ)-FNAH*FSSW/FLOAT(ISS))/PAR(35)
      IF(LPAR(2).GT.20)PAR(I+175)=(YY(IZ)-UNAH/FLOAT(ISS)-FSSW)/PAR(35)
      IF(PAR(I+175).LE.0.0)   PAR(I+175)=0.01*PAR(176)                  ELST3630
      IF(PAR(64).GT.1) PAR(I+175)=(YY(IZ)-FSSW)/PAR(35)
   40 CONTINUE                                                          ELST3640
C   NAEHERUNGSPARAMETER FUER FIT                                        ELST3660
      NPJ=INT(FLOAT(LPAR(2))/10.)
      NPA=LPAR(2)-10*NPJ
      LPAR2=LPAR(2)
      IF(LPAR2.GT.50) LPAR2=LPAR2-50
      NST=NPA+1
      IF(LPAR2.GT.10) NST=NPA
      IF(LPAR2.GT.20) NST=NPA+2
      IF(LPAR2.GT.30) NST=NPA+1
      DO 41 I=1,NST
   41 P(I)=UPAR(I)
      LBEZ=5.*(PAR(13)+PAR(14))                                         ELST3720
      PAR(45)=   0.1*FLOAT(LBEZ)                                        ELST3730
      IF(LPAR2.GT.10 .AND. LPAR2.LT.20) GO TO 45
      IF(LPAR2.GT.30 .AND. LPAR2.LT.40) GO TO 45
      IF(UPAR(NPA+1).EQ.0.) P(NPA+1)=FNAH/FLOAT(ISS)
      GO TO 46                                                          ELST3790
   45 CONTINUE                                                          ELST3800
      P(1)=UNAH/FLOAT(ISS)
   46 LPAR(22)=NST                                                      ELST3880
      IF(UPAR(1).EQ.0.) GOTO 44
      DO 43 I=1,IM
      IZ=IHO(I)
      CALL UNTF(XX(IZ),P,DUMMY,UNT,FSSW)
   43 PAR(I+175)=(YY(IZ)-UNT)/PAR(35)
   44 CONTINUE
C   ENERGIEN FEST,VARIABEL                                              ELST3890
      IF(LFE.EQ.0) LFE=1                                                ELST3900
      DO   50 I=1,LFE                                                   ELST3910
   49 NP=NST+I                                                          ELST3920
      NE=175+LVE+I                                                      ELST3930
   50 P(NP)=PAR(NE)                                                     ELST3940
   54  LFE=IABS(LPAR(3))                                                ELST3950
      IF(LVE.EQ.0) LVE=1                                                ELST3960
      DO   55 I=1,LVE                                                   ELST3970
   48 NP=NST+LFE+2*I-1                                                  ELST3980
      P(NP)=PAR(I+175)                                                  ELST3990
   55 P(NP+1)=PAR(I+150)                                                ELST4000
```

```
   56 LVE=LPAR(4)                                                      ELST4010
C     BREITEN                                                          ELST4020
      IF(LBV.EQ.0)  GO TO 61                                           ELST4030
      DO   60 I=1,LBV                                                  ELST4040
      NP=NST+LFE+2*LVE+I                                               ELST4050
   60 P(NP)=PAR(I+125)                                                 ELST4060
   61 M=NST+LFE+2*LVE+LBV                                              ELST4070
      LPAR(29)=M                                                       ELST4080
      LPAR(24)=1                                                       ELST4090
C                                                                      ELST4100
      NUM=LPAR(1)+1                                                    ELST4110
      IF(LPAR(20).GT.1)  CALL ZETKO                                    ELST4120
      CALL FITUN(M,P,LEO,XX,YY,ERR,-1,GAMMA,NUM,&80)                   ELST4130
      IF(LPAR(20).GT.1)  CALL ZETKO                                    ELST4140
C                                                                      ELST4150
      IF(LPAR(31).LE.0)  GO TO 75                                      ELST4160
      DO   70 J=1,IM                                                   ELST4170
      FEH(J)=PAR(31)-PAR(J+150)                                        ELST4180
      NP1=(NST+LFE)*2+200+1                                            ELST4190
      NP=NP1+4*J-2                                                     ELST4200
      IF(J.LE.LVE)  ZAEH(J)=PAR(31)-PAR(NP)                            ELST4210
      IF(J.GT.LVE.AND.LPAR(3).GT.0)  ZAEH(J)=FEH(J)                    ELST4220
   70 IF(J.GT.LVE.AND.LPAR(3).LT.0) ZAEH(J)=FEH(J)-PAR(NP1+2)+PAR(151) ELST4230
      WRITE (1) (FEH(J),J=1,IM)                                        ELST4240
      WRITE (1) (ZAEH(J),J=1,IM)                                       ELST4250
      IF(LPAR(20).GT.1)  CALL ZETKO                                    ELST4260
   75 CONTINUE                                                         ELST4270
      CONTINUE                                                         ELST4290
   80 RETURN                                                           ELST4300
      END                                                              ELST4310

      SUBROUTINE UNTF(X,P,DY,UNT,FSSW)
      DIMENSION P(50),DY(50)
      COMMON PAR(300),LPAR(100)
      IF(PAR(24).NE.0) PAR(45)=PAR(24)
      A=X-PAR(45)
      LPAR2=LPAR(2)
      IF(LPAR2.GT.50) LPAR2=LPAR2-50
      IF(LPAR(2).GT.50) A=1./(-A)
      CALL SSWF(FSSW,X)
      NPJ=INT(FLOAT(LPAR(2))/10.)
      NPA=LPAR(2)-NPJ*10
C
      UNT=.0
      DO 5 I=1,NPA
      UNT=UNT+P(I)*A**(I-1)
    5 DY(I)=A**(I-1)
      GO TO (10,20,10,20), NPJ
```

```
10 UNT=UNT+FSSW*P(NPA+1)
   DY(NPA+1)=FSSW
   IF(LPAR2.LE.10) RETURN
   GCTO 30
20 UNT=UNT+FSSW
   IF(LPAR2.LE.20) RETURN
30 UNT=UNT*EXP(-P(NPA+2)*(PAR(31)-X)/X)
   DY(NPA+2)=-UNT*(PAR(31)-X)/X
   RETURN
   END

      SUBROUTINE    FITUN(MZ,P,N,X,Y,DY,NRM,DELTA,NUM,*)                 UNST0030
C     NRM = 0 FALLS DIE MESSFEHLER ABSOLUT SIND                           UNST0050
      DIMENSION PAR(300),LPAR(100),DUM(600),              WORD(20)
      DIMENSION  X(500),Y(500),DY(500),V1(50),V2(50),                     UNST0090
     1   P(50), DP(50), DF(50), DZ(50), D2Z(50,50), U(50,50)              UNST0100
      DIMENSION JOTA(25)                                                  UNST0110
      DIMENSION ZWP(50),PNB(50)                                           UNST0120
      CCMMON PAR,LPAR,DUM,       WORD
      CCMMON/NZP/ LEO,LX,LV2                                              UNST0150
      CCMMON /XKURV/YKURV(10)
      CCMMON/LING1/D2Z,U
      REAL*8 TEXT,NAME1,NAME2,NAME3                                       UNST0160
      DATA TEXT /'        '/                                              UNST0170
      DATA NAME3 /'.  GRD'/                                               UNST0180
      GAM1=.0                                                             UNST0190
      NORM = NRM                                                          UNST0200
      GAMMA=DELTA                                                         UNST0210
      LEO=N                                                               UNST0220
      LV2=0                                                               UNST0230
      M=MZ                                                                UNST0240
      MY=5                                                                UNST0250
      J006=6                                                              UNST0260
      MOOZ=30                                                             UNST0270
      LFIT=IABS(LPAR(3))                                                  UNST0280
      LFIT1=LPAR(4)                                                       UNST0290
      NKURV=LFIT+LFIT1
      KC01=LPAR(22)+1                                                     UNST0300
      LPAR(31)=0                                                          UNST0310
      MG01=2                                                              UNST0320
      DC 5 K=1,50
      DC 5 L=1,50
      D2Z(K,L)=.0
    5 U(K,L)=.0
C     DIAGNOSTIK                                                          UNST0340
      I1=1                                                                UNST0360
      IF(NUM-4)   11,13,11                                                UNST0370
   11 LZ=M-LPAR(6)                                                        UNST0380
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```
      IF(LPAR(11).GT.0) M001=LPAR(11)                                  UNST0390
      IF(LPAR(12).GT.0)  M00Z=LPAR(12)                                 UNST0400
      IF(LPAR(13).GT.0)  MY=LPAR(13)                                   UNST0410
      IF(LPAR(14).GT.0)   J006=LPAR(14)                                UNST0420
      DO   8 I=1,LFIT1                                                 UNST0430
    8 JOTA(I)=LFIT+2*I+LPAR(22)                                        UNST0440
   13 IF(M) 16,16,15                                                   UNST0450
   15 IF(M-50)    17,17,16                                             UNST0460
   16 WRITE (6,997)M                                                   UNST0470
  997 FORMAT (40H1 NUR 1 BIS 50 PARAMETER ERLAUBT STATT    ,I7)        UNST0480
      RETURN                                                           UNST0490
   17 IF(N-500)    20,20,18                                            UNST0500
   18 WRITE (6,998)N                                                   UNST0510
  998 FORMAT (42H1 NUR 1 BIS 500  MESSPUNKTE ERLAUBT STATT    ,I7)     UNST0520
      RETURN                                                           UNST0530
   20 ZSOLL = N - M                                                    UNST0540
      IF(ZSOLL)    24,25,26                                            UNST0550
   24 WRITE (6,999)M,N                                                 UNST0560
  999 FORMAT (19H1 MEHR PARAMETER  (, I2, 20H)  ALS MESSPUNKTE  (,  I2, UNST0570
     1     1H)  )                                                      UNST0580
      RETURN                                                           UNST0590
   25 NORM = 0                                                         UNST0600
   26 DO 27    I = 1,N                                                 UNST0610
      IF(DY(I))    28,28,27                                            UNST0620
   27 CONTINUE                                                         UNST0630
      GO TO 14                                                         UNST0640
   28 WRITE (6,1000)I                                                  UNST0650
 1000 FORMAT (49H1 MESSFEHLER DY(I) IST NULL ODER NEGATIV FUER I = , I4)UNST0660
      RETURN                                                           UNST0670
   14 FEH=1.0                                                          UNST0690
      IF(NORM)    29,30,30                                             UNST0700
   29 FEH=DY(1)**2                                                     UNST0710
   30 J = 0                                                            UNST0720
C     BEGINN DER ITERATION ZUR LOESUNG DER NORMAL - GLEICHUNGEN        UNST0740
      IF(LPAR(8))    31,31,32                                          UNST0760
   31 WRITE (6,1002)                                                   UNST0770
 1002 FORMAT (1H1,17X,18HZWISCHENERGEBNISSE,                           UNST0780
     1    /85H NAEHERUNG          ZWANG          1.PARAMETER    2.PARAMETER  UNST0790
     2  3.PARAMETER    USW......       //)                             UNST0800
   32 G = 1.0                                                          UNST0810
      DATA NAME1/'.      '/                                            UNST0820
      TEXT=NAME1                                                       UNST0830
C                                                                      UNST0840
   50 Z = 0.0                                                          UNST0850
                                                                       UNST0860
      DO 60    K = 1,M                                                 UNST0870
      DZ(K) = 0.0                                                      UNST0880
      DO 60    L = 1,M                                                 UNST0890
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```
   60 D2Z(K,L) = 0.0                                                 UNST0900
      DO 70   I = 1,N                                                UNST0910
      CALL THEORU  (NUM,X(I),P,F,DF)                                 UNST0920
      H1 = DY(I)**(-2)*FEH                                           UNST0930
      H2 = Y(I) - F                                                  UNST0940
      Z = Z + H1*H2*H2                                               UNST0950
      DO 70   K = 1,M                                                UNST0960
      DZ(K) = DZ(K) - H1*H2*DF(K)                                    UNST0970
      DO 70   L = 1,M                                                UNST0980
   70 D2Z(K,L) = D2Z(K,L) + H1*DF(K)*DF(L)                           UNST0990
   71 ZY=Z/FEH                                                       UNST1000
      IF(NORM)   72,73,72                                            UNST1010
   72 G=Z/ZSOLL                                                      UNST1020
   73 IF(LPAR(8))   74,74,78                                         UNST1030
   74 IF (NORM) 77,77,75                                             UNST1040
   75 WRITE (6,1003)J, TEXT, Z, (P(K), K = 1,M)                      UNST1050
 1003 FORMAT (1X,I3,A6,1PE14.6,3X,7E15.6/(27X,7E15.6))               UNST1060
      GO TO 78                                                       UNST1070
   77 WRITE (6,1004)J, TEXT,ZY, (P(K), K = 1,M)                      UNST1080
 1004 FORMAT (1X,I3,A6,F14.4,3X,1P7E15.6/(27X,7E15.6))               UNST1090
C     PRUEFUNG AUF ITERATIONSSTOP                                    UNST1110
   78 IF(J-MY)  100, 80, 80                                          UNST1130
   80 IF (Z - ZALT)    90,101,101                                    UNST1140
  101 IF(Z-ZALT-1.0E-02)      91,102,102
   91 IF(NDUR)    140,140,102                                        UNST1160
  102 DO    103 K=1,M                                                UNST1170
  103 P(K)=ZWP(K)                                                    UNST1180
      GAMMA=0.8*GAM1                                                 UNST1190
      WRITE (6,1040)GAMMA                                            UNST1200
 1040 FORMAT(13X,10H  GAMMA  =  F13.6)                               UNST1210
   90 IF(J-MOOZ)    100,130,130                                      UNST1220
C     DURCHFUEHRUNG DER ITERATION                                    UNST1240
  100 DO 104   K = 1,M                                               UNST1260
      DP(K) = - DZ(K)                                                UNST1270
      DO 104   L = 1,M                                               UNST1280
  104 U(K,L) = D2Z(K,L)                                              UNST1290
      CALL LINGL (U,DP,M,1,DETERM)
      IF(LPAR(20).GT.2)  CALL ZETKO                                  UNST1310
      IF(DETERM)    105,107,105                                      UNST1320
  105 H1 = 0.0                                                       UNST1330
      DO 106   K = 1,M                                               UNST1340
  106 H1 = H1 + DP(K)*DP(K)*D2Z(K,K)                                 UNST1350
      DATA NAME2/'.  NWT'/                                           UNST1360
      TEXT=NAME2                                                     UNST1370
      GAM1=SQRT(H1)                                                  UNST1380
      IF(GAM1-GAMMA)    113,113,107                                  UNST1390
C     GRADIENTEN METHODE STATT NEWTON                                UNST1410
  107 TEXT=NAME3                                                     UNST1430
```

```
      H1 = 0.0                                                          UNST1440
      H2 = 0.0                                                          UNST1450
      DC 109   K = 1,M                                                  UNST1460
      H3 = DZ(K)                                                        UNST1470
      DZ(K) = H3/D2Z(K,K)                                               UNST1480
 109  H1 = H1 + H3*DZ(K)                                                UNST1490
      DC 110   K = 1,M                                                  UNST1500
      DC 110   L = 1,M                                                  UNST1510
 110  H2 = H2 + DZ(K)*D2Z(K,L)*DZ(L)                                    UNST1520
      H3= AMIN1(H1/H2,GAMMA/SQRT(H1))                                   UNST1530
      DC 112   K = 1,M                                                  UNST1540
 112  DP(K) = - H3*DZ(K)                                                UNST1550
 113  ZALT = Z                                                          UNST1570
      IF(J.LE.M001)  GO TO 114                                          UNST1580
      I1=I1+2                                                           UNST1590
 114  DC 120   K = 1,M                                                  UNST1600
      ZWP(K)=P(K)                                                       UNST1610
 120  P(K) = P(K) + DP(K)                                               UNST1620
 121  DC    123 K=K001,M                                                UNST1630
      IF(I1-25)    116,116,115                                          UNST1640
 116  NCUR=0                                                            UNST1650
      DC    118 KY=I1,25                                                UNST1660
      IF(K-JOTA(KY))    118,117,118                                     UNST1670
 117  NDUR=1                                                            UNST1680
      GO TO 119                                                         UNST1690
 118  CONTINUE                                                          UNST1700
 115  IF(K-(LPAR(22)+LFIT +2*LPAR(4)))    125,125,126                   UNST1710
 126  IF(Z-ZSOLL*FEH*3.0)    128,128,127                                UNST1720
 127  IF(J- J006)    119,119,128                                        UNST1730
 119  P(K)=ZWP(K)                                                       UNST1740
      NDUR=1                                                            UNST1750
      GC TO 123                                                         UNST1760
 128  IF(ABS(DP(K))-0.15*ZWP(K)) 125,125,129                            UNST1770
 129  P(K)=ZWP(K)+.10*DP(K)*ZWP(K)/ABS(DP(K))                           UNST1780
      WRITE (6,1042)K                                                   UNST1790
1042  FORMAT(14X,17HBREITE(PARAMETER I2,22H ) UM 10 PROZ. GEAEND.      )UNST1800
 125  IF(P(K))    122,122,123                                           UNST1810
 122  WRITE (6,1041)K,P(K)                                              UNST1820
1041  FORMAT(10X,I5,20H. PARAMETER NEGATIV(   E15.6,3H   ))             UNST1830
      P(K)=ZWP(K)                                                       UNST1840
 123  CONTINUE                                                          UNST1850
 124  J=J+1                                                             UNST1860
      GC TO 50                                                          UNST1870
 130  WRITE (6,1005) M00Z                                               UNST1900
1005  FORMAT (24H  (KEINE KCNVERGENZ NACH I3,15H ITERATIONEN)    )      UNST1910
 140  WRITE (6,1030)(WORD(I),I=1,18)                                    UNST1940
1030  FORMAT(1H1,18A4//)                                                UNST1950
 132  WRITE(6,1032)                                                     UNST1960
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 1032 FORMAT(23H FITERGEBNISSE SPEKTRUM )                                        UNST1970
  133 IF(NORM) 35,35,40                                                          UNST1980
C                                                                                UNST1990
C      ERWARTUNGSWERT VON Z IST ZSOLL = N - M FALLS DIE MESSFEHLER DY(I)         UNST2000
C      ABSOLUT SIND. STREUUNG IST SQRT (2*ZSOLL)                                 UNST2010
C                                                                                UNST2020
   35 H1 = SQRT(2.0*ZSOLL)                                                       UNST2030
      A012=H1                                                                    UNST2040
      B012=ZY                                                                    UNST2050
      PAR(42)=ZSOLL                                                              UNST2060
      PAR(43)=A012                                                               UNST2070
      PAR(44)=B012                                                               UNST2080
      IF(LPAR(20).GT.2)  CALL ZETKO                                              UNST2090
      WRITE (6,1007)ZSOLL, H1, ZY                                                UNST2100
 1007 FORMAT (9H    ZWANG, 9X, 8HSOLLWERT, F8.1, 3H +-, F5.1                     UNST2110
     1   /18X,7HISTWERT ,F9.1)                                                   UNST2120
   40 WRITE (6,1008)                                                             UNST2130
 1008 FORMAT (1H ,32X,7HOPTIMAL,13X,6HFEHLER,                                    UNST2140
     1      28X,27HKONTROLLE  (SOLLWERT IST 1) //)                               UNST2150
      DO 160   K = 1,M                                                           UNST2160
      DO 150   L = 1,M                                                           UNST2170
  150 U(K,L) = 0.0                                                               UNST2180
  160 U(K,K) = G                                                                 UNST2190
      CALL LINGL (D2Z, U, M, M, DETERM)
      IF(LPAR(20).GT.2)  CALL ZETKO                                              UNST2210
      IF(DETERM) 170, 210, 170                                                   UNST2220
  170 DO 180 K = 1,M                                                             UNST2230
  180 DP(K) = SQRT(ABS(U(K,K)))                                                  UNST2240
      DETERM = 1.0/DETERM                                                        UNST2250
C      KONTROLLE DURCH BERECHNUNG DES ZWANGES  AN DEN EXTREMPUNKTEN              UNST2270
C      DES FEHLERELLIPSOIDS                                                      UNST2280
      DO 205   K = 1,M                                                           UNST2300
      H1 = 0.0                                                                   UNST2310
      H2 = 0.0                                                                   UNST2320
      IF(LPAR(19).GT.0)  GO TO 205                                               UNST2330
      DO 190   L = 1,M                                                           UNST2340
      IF(DP(K).EQ.0.)  DP(K)=1. E-15
      U(K,L) = U(K,L)/DP(K)                                                      UNST2360
      V1(L) = P(L) - U(K,L)                                                      UNST2370
      V2(L) = P(L) + U(K,L)                                                      UNST2380
      IF(DP(L).EQ.0.) DP(L)=1. E-15
  190 U(K,L) = U(K,L)/DP(L)                                                      UNST2400
      DO 195    I = 1,N                                                          UNST2410
      CALL THEORU (NUM,X(I),V1,F,DF)                                             UNST2420
  195 H1 = H1 + ((Y(I) - F)/DY(I))**2*FEH                                        UNST2430
      H1 = (H1 - Z)/G                                                            UNST2440
      DO 200    I = 1,N                                                          UNST2450
      CALL THEORU( NUM,X(I),V2,F,DF)                                             UNST2460
```

```
 200 H2 = H2 + ((Y(I) - F)/DY(I))**2*FEH                          UNST2470
     H2 = (H2 - Z)/G                                              UNST2480
 205 WRITE (6,1009)K, P(K), DP(K), H1, H2                         UNST2490
1009 FORMAT (1X,I2,10H.PARAMETER,15X,1PE15.6,5H   +-,E15.6,11X,0P2F20.5UNST2500
    1   )                                                         UNST2510
     IF(LPAR(19).GT.0)  GO TO 333                                 UNST2520
     WRITE (6,1010)                                               UNST2530
1010 FORMAT (40H KORRELATIONEN ZWISCHEN DEN PARAMETERN            UNST2540
    1   //12X,31H1.PA     2.PA     3.PA     USW....     //)       UNST2550
     DO 185   K = 1,M                                             UNST2560
 185 WRITE (6,1011)K,(U(K,L), L = 1,M)                            UNST2570
1011 FORMAT (1X,I2,6H.PA    ,15F8.3,3(/9X,15F8.3) )               UNST2580
     WRITE (6,1014)DETERM                                         UNST2590
1014 FORMAT (1H0,11X,8HDETERM =,1PE11.3 ////)                     UNST2600
C    TABELLIERUNG DER ANGEPASSTEN FUNKTION                        UNST2620
     IF(LPAR(20).GT.2)  CALL ZETKO                                UNST2630
 333 LPAR(19)=0                                                   UNST2650
     IF(LPAR(8))   181,186,181                                    UNST2660
 181 IF(LPAR(9))   216,216,182                                    UNST2670
 186 WRITE (6,1015)                                               UNST2680
1015 FORMAT(1H0,54X,13HT A B E L L E ////29X,14HZAEHLRATE      /  UNST2690
    1  17H   NR.   FREQUENZ,7X,8HGEMESSEN,8X,9HBERECHNET,8X,      UNST2700
    2 7HY-UNT  ,8X,7HUNT    ,9X,7HSSW    ,8X,9HDIFFERENZ,7X,6HFEHLER//)UNST2710
     IF(PAR(64).GE.1.0)  WRITE(6,1019)
1019 FORMAT(1X,/' ZAEHLRATE AUF DISPERSION KORRIGIERT ')
 182 IF(LPAR(9))  2006,2006,187                                   UNST2740
 187 WRITE (1) LPAR(24),M,N,ZSOLL,A012,B012                       UNST2750
     LPAR(25)=LPAR(25)+1                                          UNST2760
     LPAR(31)=1                                                   UNST2770
2006 IF(LPAR(38).NE.1) GO TO 188
     WRITE(7,2001) (WORD(I),I=1,20)
     WRITE(7,2002) PAR(31),PAR(7),PAR(59),PAR(1)                  UNST2800
     WRITE(7,2003) (PAR(2*I+89),I=1,5),PAR(81),LPAR(16)           UNST2810
     WRITE(7,2004) (P(I),I=1,4),PAR(45),PAR(24),LPAR(2)           UNST2820
2001 FORMAT(20A4)
2002 FORMAT(4E12.4)                                               UNST2840
2003 FORMAT(6E12.4,I3)                                            UNST2850
2004 FORMAT(6E12.4,I3)                                            UNST2860
 188 LV2=1                                                        UNST2870
     DO 213  I = 1,N                                              UNST2880
     LX=I                                                         UNST2890
     CALL THEORU (NUM ,X(I),P,F,DF)                               UNST2900
     H1 = Y(I) - F                                                UNST2910
     H14=H1/DY(I)                                                 UNST2920
     CALL UNTF(X(I),P,DY,UNT,FSSW)
 197 H7=Y(I)-UNT                                                  UNST3150
     H21=Y(I)-FSSW                                                UNST3160
     H22=UNT-FSSW                                                 UNST3170
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      H13=F-UNT                                                          UNST3180
      IF(LPAR(9))   215,215,189                                          UNST3190
  189 WRITE ( 1)X(I),H7,H13,H14,UNT,(YKURV(K),K=1,NKURV),FSSW
  215 IF(LPAR(8))   213,214,213                                          UNST3210
  214 WRITE(6,1016)I,X(I),Y(I),F,H7,UNT,FSSW,H1,DY(I)                    UNST3220
 1016 FORMAT(I5,F12.4,2X,1P(2(E17.6,E15.6),E15.6,E17.6,E15.6))          UNST3230
      IF(LPAR(38).NE.2) GO TO 213                                        UNST3240
      H31=F-FSSW                                                         UNST3250
 2005 FORMAT(I5,6(1PE12.4))
      WRITE(7,2005) I,X(I),Y(I),DY(I),F,UNT,FSSW
  213 CONTINUE                                                           UNST3280
C                                                                        UNST3290
  216 DO  1022  I=1,M                                                    UNST3300
      PAR(2*I+199)=P(I)                                                  UNST3310
 1022 PAR(2*I+200)=DP(I)                                                 UNST3320
      IF(LPAR(20).GT.2)  CALL ZETKO                                      UNST3330
      RETURN                                                             UNST3340
C     FALLS SICH DAS LINEARE GLEICHUNGSSYSTEM NICHT AUFLOESEN LAESST     UNST3360
  210 WRITE (6,1012)                                                     UNST3380
 1012 FORMAT (42H0 NORMAL-GLEICHUNGEN SIND NICHT AUFLOESBAR    //)       UNST3390
      DO 220 K = 1,M                                                     UNST3400
  220 WRITE (6,1013)(U(K,L), L = 1,M)                                    UNST3410
 1013 FORMAT (1X,1P7E15.7)                                               UNST3420
  245 RETURN1                                                            UNST3430
      END                                                                UNST3450

      SUBROUTINE LINGL(A,B,N,M,DETERM)
C     AUFLOESUNG LINEARER GLEICHUNGSSYSTEME BIS ZUR ORDNUNG 25           UNST3490
      DIMENSION A(50,N),B(50,M)
   60 IF(N) 15,15,16                                                     UNST3510
   16 IF(M) 15,15,17                                                     UNST3520
   17 DETERM=1.0                                                         UNST3530
      DET=.0                                                             UNST3540
      AMAX=ABS(A(1,1))                                                   UNST3550
      LP = 1                                                             UNST3560
      DO 2 I=2,N                                                         UNST3570
      IF(ABS(A(I,1))-AMAX) 2,2,1                                         UNST3580
    1 AMAX = ABS(A(I,1))                                                 UNST3590
      LP = I                                                             UNST3600
    2 CONTINUE                                                           UNST3610
C                                                                        UNST3620
      DO 11 J=1,N                                                        UNST3630
      IP = LP                                                            UNST3640
      T = A(IP,J)                                                        UNST3650
   53 IF(T) 3,15,3                                                       UNST3660
    3 IF(J-N) 4,8,8                                                      UNST3670
    4 A(IP,J)=A(J,J)                                                     UNST3680
      JP1=J+1                                                            UNST3690
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```
      LP = JP1                                                           UNST3700
      AMAX = 0.0                                                         UNST3710
      DC 7 K=JP1,N                                                       UNST3720
      H = A(IP,K)/T                                                      UNST3730
      A(IP,K) = A(J,K)                                                   UNST3740
      A(J,K) = H                                                         UNST3750
      DO 7 I=JP1,N                                                       UNST3760
      A(I,K) = A(I,K) -A(I,J)*H                                          UNST3770
      IF(K-JP1) 5,5,7                                                    UNST3780
    5 IF(ABS(A(I,K))-AMAX) 7,7,6                                         UNST3790
    6 AMAX = ABS(A(I,K))                                                 UNST3800
      LP = I                                                             UNST3810
    7 CONTINUE                                                           UNST3820
C                                                                        UNST3830
    8 DC 11 K=1,M                                                        UNST3840
      H = B(IP,K)/T                                                      UNST3850
      B(IP,K) = B(J,K)                                                   UNST3860
      B(J,K) = H                                                         UNST3870
      IF(J-N) 9,11,11                                                    UNST3880
    9 DO 10 I=JP1,N                                                      UNST3890
   10 B(I,K) = B(I,K)-A(I,J)*H                                           UNST3900
   11 CONTINUE                                                           UNST3910
C                                                                        UNST3920
      IF(N-1)  15,15,12                                                  UNST3930
   12 DC 13  I = 2,N                                                     UNST3940
      IP=N-I+1                                                           UNST3950
      LP=IP+1                                                            UNST3960
      DC 13 J=1,M                                                        UNST3970
      DC 13 K=LP,N                                                       UNST3980
   13 B(IP,J) = B(IP,J)-A(IP,K)*B(K,J)                                   UNST3990
C                                                                        UNST4000
   15 RETURN                                                             UNST4010
      END                                                                UNST4020

      SUBROUTINE THEORU(J,X,P,Y,DA)                                      UNST4040
      DIMENSION P(50),DA(50)                                             UNST4060
   20 CALL ARC5(X,P,Y,DA)                                                UNST4100
      RETURN                                                             UNST4110
      END                                                                UNST4120

      SUBROUTINE ARC4U(X,P,Y,DY,I)                                       UNST5620
      DIMENSION P(25),DY(25),PVAR(25)                                    UNST5630
      CCMMON PAR(300),LPAR(100)                                          UNST5640
      CCMMON/BVAR2/PVAR                                                  UNST5650
      BT=1.44269505                                                      UNST5660
      IF(P(25)-1.0) 5,6,5                                                UNST5670
    5 P(6)=1.0                                                           UNST5680
    6 U=(X-P(5))/P(6)                                                    UNST5690
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      IF(PAR(64).GE.1. .AND. I.LE.LPAR(6)) GOTO 110                     UNST5700
      IF(U)  20,10,10                                                   UNST5710
   10 CONTINUE                                                          UNST5720
      ALPHA=(U/P(2))**2/BT                                              UNST5730
  100 FORMAT( 5E15.4)                                                   UNST5740
   11 Y=P(1)*EXP(-ALPHA)                                                UNST5750
      DY(1)=Y/P(1)                                                      UNST5760
      DY(2)=2.0*Y*U**2/(BT*P(2)**3)                                     UNST5770
      DY(3)=0.0                                                         UNST5780
      DY(4)=0.0                                                         UNST5790
      DY(5)=2.0*U*Y/(BT*P(2)**2)/P(6)                                   UNST5800
      DY(6)=U*DY(5)                                                     UNST5810
      RETURN                                                            UNST5820
   20 YP=P(1)*EXP(-(P(4)/P(3))**2/BT)                                   UNST5830
      IF(U-P(4))   42,30,30                                             UNST5840
   30 Y=P(1)*EXP(-(U/P(3))**2/BT)                                       UNST5850
      DY(1)=Y/P(1)                                                      UNST5860
      DY(2)=0.0                                                         UNST5870
      DY(5)=2.0*Y*U/(BT*P(3)**2)/P(6)                                   UNST5880
      DY(4)=0.0                                                         UNST5890
      DY(3)=DY(5)*U/P(3)*P(6)                                           UNST5900
      DY(6)=U*DY(5)                                                     UNST5910
      RETURN                                                            UNST5920
   42 PP=2.0*(P(4)/P(3))**2/BT                                          UNST5930
      C=YP*P(4)*(2.0-PP)                                                UNST5940
      D=YP*P(4)**2*(PP-1.0)                                             UNST5950
      PPP=YP*PP                                                         UNST5960
      CP3=PPP*P(4)*(4.0-PP)/P(3)                                        UNST5970
      DP3=PPP*PP*(P(4)**2/P(3)-3.0*BT*P(3)/2.0)                         UNST5980
      CP4=PPP*(2.0/PP-5.0+PP)                                           UNST5990
      DP4=PPP*P(4)*(5.0-PP-2.0/PP)                                      UNST6000
      Y=C/U+D/U**2                                                      UNST6010
      DY(1)=Y/P(1)                                                      UNST6020
      DY(2)=0.0                                                         UNST6030
      DY(3)=CP3/U+DP3/U**2                                              UNST6040
      DY(4)=CP4/U+DP4/U**2                                              UNST6050
      DY(5)=C/U**2+2.0*D/U**3/P(6)                                      UNST6060
      DY(6)=U*DY(5)                                                     UNST6070
      RETURN                                                            UNST6080
C     BREIT-WIGNER-KURVE MIT FESTEM P-FAKTOR (DISS PIT 72) AB 110       UNST6090
C     MIT GEFITTETEM P-FAKTOR AB 120                                    UNST6100
  110 C1=U/P(2)                                                         UNST6110
      C2=1.+C1**2                                                       UNST6120
      IF(PAR(64).GT.1.) GOTO 120                                        UNST6130
      Y=P(1)/C2                                                         UNST6140
      Y=Y*(1.+PVAR(I)*X-P(5))                                           UNST6150
      DY(1)=Y/P(1)                                                      UNST6160
      DY(2)=2.*P(1)*C1**2/P(2)/C2**2                                    UNST6170
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      DY(3)=2.*P(1)*C1**2/P(3)/C2**2                                  UNST6180
      DY(4)=.0                                                        UNST6190
      DY(5)=2.*DY(2)*C1/P(6)                                          UNST6200
      DY(6)=DY(5)*U                                                   UNST6210
      RETURN                                                          UNST6220
  120 IF(PAR(64) .GT.  2.) GOTO 130                                   UNST6230
      FLOR=P(1)/C2                                                    UNST6240
      Y=P(1)*(1+P(4)*U)/C2                                            UNST6250
      DY(1)=Y/P(1)                                                    UNST6260
      DY(2)=2.*FLOR*(1+P(4)*U)*C1**2/P(2)/C2                          UNST6270
      DY(3)=DY(2)*P(2)/P(3)                                           UNST6280
      DY(4)=FLOR*U                                                    UNST6290
      DY(5)=(-FLOR*P(4)+2.*DY(2)*C1)/P(6)                             UNST6300
      DY(6)=DY(5)*U                                                   UNST6310
      RETURN                                                          UNST6320
  130 CONTINUE                                                        UNST6330
      END                                                             UNST6340

      SUBROUTINE ARC5(X,P,Y,DY)                                       UNST6350
      DIMENSION P(50),DY(50),PAR(300),LPAR(100),DUM(600)              UNST6360
      DIMENSION PW(25),DYW(25)                                        UNST6380
      DIMENSION BVAR(25)                                              UNST6390
      COMMON PAR,LPAR,DUM
      COMMON /BVAR1/ BVAR                                             UNST6420
      COMMON/NZP/ LEO,LX,LV2                                          UNST6430
      COMMON /XKURV/YKURV(10)
C     UNTERGRUND                                                      UNST6460
      CALL UNTF(X,P,DY,UNT,FSSW)
   30 Y=UNT                                                           UNST6900
      MZH=LPAR(29)                                                    UNST6910
      LFIT=IABS(LPAR(3))                                              UNST6920
      LFIT1=LPAR(4)                                                   UNST6930
      L=LPAR(5)                                                       UNST6940
      ME=LPAR(28)                                                     UNST6950
      M=LFIT    +LPAR(4)                                              UNST6960
      KZ=M+LPAR(4)+L   +LPAR(22)                                      UNST6970
      PW(2)=PAR(73)                                                   UNST6980
      PW(3)=PAR(75)                                                   UNST6990
      PW(4)=PAR(77)                                                   UNST7000
      PW(25)=1.0                                                      UNST7010
      DY(KZ)=0.0                                                      UNST7020
      DPY=0.0                                                         UNST7030
      NP=LFIT+LPAR(22)+2                                              UNST7040
      DEPS=P(NP)-PAR(151)                                             UNST7050
      DO  120 I=1,M                                                   UNST7060
      K=150+LPAR(4)+I                                                 UNST7070
      INS=I+LPAR(22)                                                  UNST7080
      KB=M+LPAR(4)+LFIT1+INS                                          UNST7090
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      KC=2*I-LFIT   +LPAR(22)-1                                         UNST7100
      KD=M+LPAR(4) -LFIT+INS                                            UNST7110
      EPS=PAR(K)                                                        UNST7120
      IF(LPAR(3))    35,36,36                                           UNST7130
   35 EPS=PAR(K)+DEPS                                                   UNST7140
   36 PW(1)=P(INS)*PAR(71)                                              UNST7150
      PW(5)=PAR(79)-EPS                                                 UNST7160
      PW(6)=PAR(K- 25)                                                  UNST7170
   38 IF(LPAR(5))    55,55,40                                           UNST7180
   40 PW(6)=P(KZ)                                                       UNST7190
      IF(LFIT1+I-L)    45,45,55                                         UNST7200
   45 PW(6)=P(KB)                                                       UNST7210
   55 IF(I-LFIT)   80,80,60                                             UNST7220
   60 PW(1)=P(KC)*PAR(71)                                               UNST7230
      PW(5)=PAR(79)-P(KC+1)                                             UNST7240
      IF(LPAR(5))    75,75,65                                           UNST7250
   65 PW(6)=P(KZ)                                                       UNST7260
      IF(I-LFIT-L)    70,70,80                                          UNST7270
   70 PW(6)=P(KD)                                                       UNST7280
      GO TO 80                                                          UNST7290
   75 KW=I-LFIT+125                                                     UNST7300
      PW(6)=PAR(KW)                                                     UNST7310
C                                                                       UNST7320
   80 CALL ARC4U(X,PW,YK,DYW,I)                                         UNST7330
      IF(I.LE.10 .AND. LV2.EQ.1) YKURV(I)=YK
      Y=Y+YK                                                            UNST7370
      IF(I-LFIT)   84,84,85                                             UNST7380
   84 DY(INS)=DYW(1)*PAR(71)                                            UNST7390
      DPY=DPY-DYW(5)                                                    UNST7400
      GO TO 90                                                          UNST7410
   85 DY(KC)=DYW(1)*PAR(71)                                             UNST7420
      DPY=DPY+DYW(2)                                                    UNST7430
      DY(KC+1)=-DYW(5)                                                  UNST7440
   90 IF(LPAR(5))    120,120,95                                         UNST7450
   95 IF(I-LFIT)   100,100,130                                          UNST7460
  100 IF(L-LFIT1)   105,105,110                                         UNST7470
  105 DY(KZ)=DY(KZ)+DYW(6)                                              UNST7480
      GO TO 120                                                         UNST7490
  110 IF(I-L+LFIT1)    115,105,105                                      UNST7500
  115 DY(KB)=DYW(6)                                                     UNST7510
      GO TO 120                                                         UNST7520
  130 IF(I-LFIT-L)    135,140,140                                       UNST7530
  135 DY(KD)=DYW(6)                                                     UNST7540
      GO TO 120                                                         UNST7550
  140 DY(KZ)=DY(KZ)+DYW(6)                                              UNST7560
  120 CONTINUE                                                          UNST7570
      IF(LPAR(3))    150,160,160                                        UNST7580
  150 LJT=LFIT+LPAR(22)+2                                               UNST7590
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      DY(LJT)=DY(LJT)+DPY                                                UNST7600
  160 CONTINUE                                                           UNST7610
      RETURN                                                             UNST7620
      END                                                                UNST7630

      SUBROUTINE AUSG                                                    AUSG0020
      DIMENSION EPS(25),DEPS(25),BR(25),DBR(25),PIP(25),DPIP(25)         AUSG0050
      DIMENSION FIF(25),DFIF(25)                                         AUSG0060
      DIMENSION PAR(300),LPAR(100),DUM( 600),WORD(20)
      COMMON PAR,LPAR,DUM,WORD                                           AUSG0080
      DIMENSION BVAR(25)                                                 AUSG0090
      COMMON/BVAR1/BVAR                                                  AUSG0100
      COMMON/SSWD/ACO(25)
      DATA A001/4H    /                                                  AUSG0110
C                                                                        AUSG0120
C                                                                        AUSG0130
 1000 FORMAT(1H1,10HERGEBNISSE    /1H ,18A4,F8.0,2H /,F8.1,2H /,F9.1  ) AUSG0140
 1001 FORMAT(1H ,34HELASTISCH               (BERECHNET MIT    A4,4H   )     ) AUSG0150
 1002 FORMAT(1H ,20HENERGIE ELAST. PEAK 14X,F9.4,7H MHZ  = F13.4,4H MEV)AUSG0160
 1003 FORMAT(1H ,15HPRIMAERENERGIE ,19X,F9.4,7 H MHZ  = F13.4,4H MEV   )AUSG0170
 1004 FORMAT(1H ,23HHALBWERTSBREITE ELAST. ,11X,3PF9.4,7H KHZ  = F13.4, AUSG0180
     1   8H KEV   = F8.2,12H  PROMIL EE    )                             AUSG0190
 1005 FORMAT(1H ,7HFLAECHE,24X,F12.4,7H MHCO = F13.4,6H MEVCO    )      AUSG0200
 1006 FORMAT(1H ,9HPEAKHOEHE ,22X,F12.4,5H Z/AS   )                     AUSG0210
 1008 FORMAT(1H ,43HUNTERE INTEGRATIONSGRENZE BEI EE - 2*HWB      )     AUSG0230
 1009 FORMAT(1H ,12HUNELASTISCH //35H STRAHLUNGSSCHWANZ
     17H  SSW =1PE12.4,3H  +E11.4,5H*U  +E11.4,8H*U**2  +E11.4,8H*U**3  AUSG0250
     2+  E11.4,6H*U**4    )                                              AUSG0260
 1010 FORMAT(1H ,10HUNTERGRUND,I5,4X,12HMIT  X = E - F6.2,4H MHZ   )    AUSG0390
 1011 FORMAT(1X,' UNTERGRUNDSPARAMETER=',7(1PE12.2))
 1013 FORMAT(1H ,22HUNELASTISCHE LINIEN     /                            AUSG0430
     1113H (EPS0 VORGEGEBEN, EPSI BERECHNET, V VARIABEL, F FEST, FB ENERAUSG0440
     2GIEABSTAND ZU EPSI(1) FEST ---- BRV VORGEGEBENES,    /             AUSG0450
     3110H  BRB BERECHNETES BREITENVERHAELTNIS, U BREITE UNABHAENGIG, G AUSG0460
     4GEMEINSAM VARIIERT, F FEST ---- Z PEAKHOEHEN,      /              AUSG0470
     584H  P/P HOEHENVERHAELTNIS, F/F FLAECHENVERHAELTNIS -- IN KLAMMERNAUSG0480
     6  FEHLER IN PROZENT          ,5H    )      //                      AUSG0490
     76H  EPS0,7X,4HEPSI,17X,3HBRV,6X,3HBRB,16X,1HZ,10X,3HP/P,22X,3HF/F)AUSG0500
 1014 FORMAT(F7.3,F9.4,3H +-F7.4,A3,A2,F7.3,F8.3,3H +-F7.4,1PE11.2,      AUSG0510
     1  E13.4,3H +-E9.2,E13.4,3H +-E9.2, 2H (   2PF7.2 , 2H )    )       AUSG0520
C                                                                        AUSG0530
C                                                                        AUSG0540
      NST=LPAR(22)                                                       AUSG0550
      LF=IABS(LPAR(3))                                                   AUSG0560
      LF1=LPAR(4)                                                        AUSG0570
      LBV=LPAR(5)                                                        AUSG0580
      IM=LPAR(21)                                                        AUSG0590
      DHWB=PAR(48)                                                       AUSG0600
```

```
      WRITE (6,1000) (WORD(I),I=1,18),(PAR(I),I=42,44)                  AUSG0610
      DATA ARC3/4HARC3 /                                                AUSG0620
      DATA ARC4/4HARC4     /                                            AUSG0630
      DATA EFT/4H  F     /                                              AUSG0640
      DATA EVA/4H  V     /                                              AUSG0650
      DATA EFB/4H FB     /                                              AUSG0660
      DATA BUN/4H U      /                                              AUSG0670
      DATA BGE/4H G      /                                              AUSG0680
      DATA BFT/4H F      /                                              AUSG0690
      A001=ARC3                                                         AUSG0700
      IZT=PAR(51)                                                       AUSG0710
      WRITE (6,1015)  PAR(1),PAR(9)                                     AUSG0720
      WRITE (6,1016) IZT,(PAR(I),I=52,59)                               AUSG0730
      WRITE (6,1017) (PAR(I),I=11,14)                                   AUSG0740
      WRITE (6,1018) (PAR(I),I=15,20)                                   AUSG0750
 1017 FORMAT(22H FITGRENZEN    ELAST.    F8.4,2H - F8.4,5X,             AUSG0760
     1    9HUNELAST.    F8.4,2H - F8.4)                                 AUSG0770
 1015 FORMAT(1H ,13HEINGABEWERTE            // 12H EICHFAKTOR  F10.5, 5X AUSG0780
     1    32HUNTERGRUND OBERHALB ELAST. PEAK  F10.5,8H Z/MIKAS     )    AUSG0790
 1016 FORMAT(2H Z,I4,5H,ATW F7.2,6H,XRAD F7.3,4H,RM F6.3,3H,R F7.3,     AUSG0800
     1    3H,G F7.3,3H,C F8.4,3H,T F8.4,12H,MASSE(MEV)   F10.1)         AUSG0810
 1018 FORMAT(37H NAEHERUNGSUNTERGRUND ZWISCHEN (MHZ) ,3(F11.4,2H -F8.4))AUSG0820
      IF(LPAR(1).GT.0)  A001=ARC4                                       AUSG0830
      WRITE (6,1001) A001                                               AUSG0840
      EE=PAR(31)                                                        AUSG0850
      EEMEV=EE*PAR(1)                                                   AUSG0860
      EOMEV=PAR(36)                                                     AUSG0870
      EO=PAR(36)/PAR(1)                                                 AUSG0880
      HW=PAR(34)                                                        AUSG0890
      HWMEV=HW*PAR(1)                                                   AUSG0900
      HWPRO=HW/EE                                                       AUSG0910
      FL=PAR(33)                                                        AUSG0920
      FLMEV=FL*PAR(1)                                                   AUSG0930
      WRITE (6,1002) EE,EEMEV                                           AUSG0940
      WRITE (6,1003) EO,EOMEV                                           AUSG0950
      WRITE (6,1004) HW,HWMEV,HWPRO                                     AUSG0960
      WRITE (6,1005) FL,FLMEV                                           AUSG0970
      WRITE (6,1006) PAR(35)                                            AUSG0980
      IF(LPAR(1).GT.0)  WRITE (6,1008)                                  AUSG1000
      JO1=IABS(LPAR(16))                                                AUSG1010
      WRITE(6,1009) (PAR(2*I+89),I=1,5)
      WRITE(6,1010) LPAR(2),PAR(45)
      WRITE (6,1011) (PAR(2*I+199),I=1,NST)
      WRITE (6,1013)                                                    AUSG1110
      IF(PAR(64).GE.1.) WRITE(6,1035)                                   AUSG1120
 1035 FORMAT(1H ,'F/F FUER BREIT-WIGNER-FORM BERECHNETAUS PI*BRB*HWMEV*ZAUSG1130
     1 /FLMEV/2.  BREITEN ABSOLUT IN MEV ' /)                           AUSG1140
C                                                                       AUSG1150
```

```
C                                                                       AUSG1160
      DC    140 I=1,IM                                                  AUSG1170
      BR(I)=PAR(I+125)                                                  AUSG1180
      DBR(I)=0.0                                                        AUSG1190
      IF(LBV.EQ.0)  GO TO 100                                           AUSG1200
      MB=2*(NST+LF)+4*LF1+2*I-1                                         AUSG1210
      IF(I.GT.LBV)  MB=2*(NST+LF)+4*LF1+2*LBV-1                         AUSG1220
      BR(I)=PAR(MB+200)                                                 AUSG1230
      DBR(I)=PAR(MB+201)                                                AUSG1240
  100 IF(I.GT.LF1)  GO TO 110                                           AUSG1250
      MP=2*(NST+LF)+4*I-3+200                                           AUSG1260
      ME=MP+2                                                           AUSG1270
      EPS(I)=PAR(ME)                                                    AUSG1280
      IF(PAR(ME).EQ..0) GO TO 119                                       AUSG1290
      DEPS(I)=PAR(ME+1)/PAR(ME)                                         AUSG1300
      GC TO 120                                                         AUSG1310
  110 MP=2*NST+2*(I-LF1)+199                                            AUSG1320
      EPS(I)=PAR(I+150)                                                 AUSG1330
      DEPS(I)=0.0                                                       AUSG1340
C     IF(LPAR(3).LT.0)  EPS(I)=EPS(I)+DHWB*(BR(I)-1.0)                  AUSG1350
      NP1=(NST+LF)*2+203                                                AUSG1360
      IF(LPAR(3).LT.0)  EPS(I)=EPS(I)+PAR(NP1)-PAR(151)                 AUSG1370
      GC TO 120                                                         AUSG1380
  119 DEPS(I)=0.0                                                       AUSG1390
  120 PIP(I)=PAR(MP)                                                    AUSG1400
      IF(PAR(MP).EQ..0) GOTO 125                                        AUSG1410
      DPIP(I)=PAR(MP+1)/PAR(MP)                                         AUSG1420
      GC TO 126                                                         AUSG1430
  125 DPIP(I)=.0                                                        AUSG1440
  126 CONTINUE                                                          AUSG1450
      EPS(I)=EPS(I)*PAR(1)*PAR(47)                                      AUSG1460
      ILA=0                                                             AUSG1470
  130 EPSNH=EPS(I)                                                      AUSG1480
  131 EPS(I)=EPSNH /(1.+EPS(I)/(2.*PAR(59)))                            AUSG1490
      ILA=ILA+1                                                         AUSG1500
      IF(ILA.LE.3)  GO TO 131                                           AUSG1510
      FIF(I)=PIP(I)*BR(I)                                               AUSG1520
      DFIF(I)=SQRT(DPIP(I)**2+DBR(I)**2)                                AUSG1530
      DEP=EPS(I) *DEPS(I)                                               AUSG1540
      DFF=DFIF(I)*FIF(I)                                                AUSG1550
      DPP=DPIP(I)*PIP(I)                                                AUSG1560
      DBB=DBR(I)*BR(I)                                                  AUSG1570
      ZM=PIP(I)*PAR(35)                                                 AUSG1580
      TXE=EFT                                                           AUSG1620
      IF(I.LE.LF1)  TXE=EVA                                             AUSG1630
      IF(I.GT.LF1.AND.LPAR(3).LT.0)  TXE=EFB                            AUSG1640
      TXB=BFT                                                           AUSG1650
      IF(LBV.GT.0)  TXB=BUN                                             AUSG1660
```

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      IF(LBV.GT.O.AND.I.GE.LBV) TXB=BGE                                 AUSG1670
C     PAR(64)=BREIT-WIGNER-FORM                                         AUSG1590
      IF(PAR(64).GE.1. .AND. I.LE.LPAR(6)) GOTO 136
      GCTO 138
  136 CCNTINUE
      FIF(I)=ZM*3.1416*BR(I)*HWMEV/FLMEV/2.
      PAR(I+125)=PAR(I+125)*PAR(1)*PAR(34)
      IF(PIP(I).NE.0.) DFF=DFF*FIF(I)/(PIP(I)*BR(I))
      DBB=DBB*PAR(1)*PAR(34)
      BR(I)=BR(I)*PAR(1)*PAR(34)
      IF(I.EQ.LPAR(6)+1) WRITE(6,1036)
 1036 FCRMAT(1X,//'FOLGENDE LINIEN SIND GAUSSKURVEN:')
  138 IF(BVAR(I).NE.0.0)  WRITE(6,1037) BVAR(I)
 1037 FCRMAT(1H , '    FOLGENDE LINIE WURDE MIT DER GERADEN 1+X*',F10.3,'AUSG1720
     1MULTIPLIZIERT')                                                   AUSG1730
                                                                        AUSG1740
  140 WRITE (6,1014) PAR(I+100),EPS(I),DEP,TXE,TXB,PAR(I+125),BR(I),    AUSG1750
     1DBB,ZM,PIP(I),DPP,FIF(I),DFF,DFIF(I)
      CALL RESULT(EPS,DEPS,FIF,DFIF,BR)
      RETURN                                                            AUSG1780
      END                                                               AUSG1790

      SUBROUTINE RESULT(EPS,DEPS,FIF,DFIF,BR)                           AUSG1830
      DIMENSICN EPS(25),DEPS(25),FIF(25),DFIF(25),BR(25)                AUSG1840
      DIMENSICN DI(25)
      DIMENSION PAR(300),LPAR(100),DUMMY( 600),WORD(20)
      DIMENSION FKCR(25),FORF(25)
      CCMMON PAR,LPAR,DUMMY,WORD                                        AUSG1880
      CCMMON/SSWD/ACO(25)
      IF(PAR(61).EQ.0) PAR(61)=1.
      ZET=PAR(51)                                                       AUSG1940
      ATW=PAR(52)                                                       AUSG1950
      XO =PAR(53)                                                       AUSG1960
      FIRA=PAR(54)
      IF(FIRA.EQ.0) FIRA=1.
      DEFF=PAR(41)                                                      AUSG2020
      DEE=PAR(34)*PAR(1)                                                AUSG2030
      IM=LPAR(21)                                                       AUSG2050
      DC   2 I=1,IM                                                     AUSG2090
    2 DI(I)=BR(I)                                                       AUSG2100
      CC   6 I=1,IM                                                     AUSG2110
      IF(PAR(64).EQ.0.) DI(I)=DI(I)*DEE                                 AUSG2120
    6 CONTINUE                                                          AUSG2130
 1020 FCRMAT(F10.5)                                                     AUSG2140
 1102 FCPMAT(F10.4)                                                     AUSG2150
 1103 FORMAT(10I3)                                                      AUSG2160
 1104 FCRMAT(10F6.3)                                                    AUSG2170
 1105 FORMAT(10F5.3)                                                    AUSG2180
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Electroexcitation of giant resonances between 5 MeV and 40 MeV excitation energy in ^{197}Au.