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# ANALYSIS OF HEAVY ION ELASTIC SCATTERING DATA BY S-MATRIX PARAMETERIZATION

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### ABSTRACT

It is shown that the general features of the heavy ion elastic scattering data are reproduced by using a smooth cut-off model for the scattering matrix in which the real nuclear phase shift and the reflection coefficient are used as analytic functions and have a few adjustable parameters. A computer program is described for carrying out the calculations to fit the experimental ratio of elastic differential cross-sections to Rutherford cross-sections. The scattering of 10.375 MeV/ u  $^{12}$ C ions from Fe, Ag and Ta are considered as test cases. The absorption radii and reaction crosssections predicted by the theory are also calculated.

### INTRODUCTION

The subject of heavy ion interactions deals with the study of nuclear reactions/scattering of two atomic nuclei of mass number A > 4. There has been an ever increasing interest in this field since the availability of accelerators capable of imparting several MeV per nucleon (MeV/u) energies to nuclei heavier than alpha particles so that their Coulomb barriers could be overcome<sup>1)</sup>. At present this is one of the most active areas of Nuclear Physics research both theoretically and experimentally. The special interest in this field lies in the fact that one is capable of observing phenomena which were bitherto inaccessable to laboratory studies e.g. very high angular momentum states of nuclei, nuclear quasimolecules, deep inelastic reactions etc. For energies below 10 MeV/u one is interested in the processes like Coulomb excitation of the interacting nuclei, elastic scattering and quasi-elastic reactions. For higher energies, deep inelastic processes and the fusion reactions are of importance, giving rise to the possibility of the formation of Super Heavy Elements. At relativistic energies<sup>2)</sup>, (the Bevatron-Superhilac accelerator at Berkeley (BEVALAC) can impart energies upto 2 GeV/n to heavy ions), still different types of phenomena may occur e.g. the production of anamalons, pion condensate, or even quark plasma.

In the present report, we are interested in the elastic scattering of nuclei of A > 4 and energy  $E \sim 10$  MeV/u from heavy nuclear targets. The study of elastic scattering is important because the total reaction cross-section can be determined from it fairly accurately. This is necessary for taking into account all possible reaction channels, specially in a situation where new modes of reactions are possible<sup>3)</sup>.

A complete quantum mechanical description of the problem involves the use of ion-nucleus potential in the solution of Schrodinger equation. The scattering amplitude thus calculated is then used to find elastic differential cross-sections. Although this scheme has the advantage that the wave-functions can be used as input for the study of non-elastic processes, however, there

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are some difficulties. Firstly it has been found that the optical potential parameters are not uniquely determined from the comparison of theoretical and experimental differential cross-sections<sup>4</sup>. There may be different sets of parameters which produce quite different wave-functions, nevertheless the data is fitted well by all of them. Second difficulty which is of practical nature arising specially in heavy ion scattering is the large number of partial waves which contribute significantly towards scattering e.g. there are in excess of 700 partial waves which must be included in the scattering of <sup>238</sup>U from Gold at 10 MeV/u. Under these conditions, the optimization of optical potential parameters becomes excessively extravagent in computer CPU time. It has been, therefore, argued that the simpler methods of analysis<sup>5</sup> may be used by exploiting the special features of heavy-ion interaction viz;

- i. Large value of the Coulomb repulsion
- ii. Short wavelength of the relative motion of interacting nuclei.
- iii. Strong absorptions within nuclear range.

Thus there are various semi-classical approaches (6-9) and closed form experessions (10,11) for the scattering amplitude which have been successfully employed for the calculations of crosssections. The method adopted in this report avoids the necessity to solve the Schrodinger equation for the determination of S-matrix. Rather the S-matrix (see next section) is itself parameterized. This technique was first used by McIntyre et al<sup>5</sup>) for the analysis of  $\alpha$ -particle scattering and later extended to heavier ions by Alster et al<sup>12</sup>). The necessary mathematical formulation of this approach is described in the next section. The results obtained for the test cases are discussed in section 3. The program structure and the numerical aspects are described in section 4.

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### THEORY

### 2.1 Scattering Problem

The physical situation consists of the scattering of a projectile of mass  $M_p$  from a target nucleus of mass  $M_T$  at the laboratory energy  $E_{lab}$ . The Schrodinger equation for the relative motion of the projectile can be written as

$$\begin{bmatrix} -\frac{\hbar^2}{2\mu} \nabla^2 + V(\underline{1}) \end{bmatrix} \psi(\underline{1}) = E \psi(\underline{1})$$

where the reduced mass ' $\mu$ ' is

$$\mu = \frac{M_{\rm p} M_{\rm T}}{M_{\rm p} + M_{\rm T}}$$

and the centre-of-mass energy E is defined as

$$E = E_{lab.} \frac{M_T}{M_{p} + M_T}$$

These quantities can be written in terms of the reduced mass number

$$A_{red.} = \frac{A_p A_T}{A_p + A_T}$$

where  $A_p$  and  $A_T$  is the mass number of the projectile and the target respectively i.e.

where ' $\mathcal{E}$ ' is the laboratory energy per nucleon for the projectile and  $m_N = 931.5$  is the conversion factor for the units of mass 'a.m.u' to the units 'MeV/c<sup>2</sup>.' In eq. (1), V(<u>r</u>) is the assumed nucleus-nucleus potential. For a spherically symmetric potential, the boundary conditions at large 'r', (i.e. well outside the range of the potential) are represented by an incident plane wave moving along (say) 2-axis and the outgoing spherical wave i.e.

$$\Psi(\underline{r}) \xrightarrow{\tau \to \infty} \exp(ik3) + f(0) \tau' \exp(ikr)$$

Here  $f(\theta)$  is the relative scattering amplitude of the scattered wave and is related to the elastic differential cross-section as

$$\frac{d\sigma(\theta)}{d\Omega} = \left|f(\theta)\right|^2$$

For a short range potential (in general complex), the partial wave expansion for eq. (6) leads to the value of  $f(\theta)$  given by,

$$f(\theta) = \frac{i}{2h} \sum_{l=0}^{\infty} (2l+1) (1-S_l) P_l(\cos\theta)$$

where

$$\mathbf{k} = \frac{A_{\text{necl.}}}{ct} \int 2(m_N c^2) \varepsilon$$

 $P_1(\cos \theta)$  is the Legendre polynomial and S- is the S-matrix related to the complex nuclear phase shift  $\eta_s$  by

$$S_{l} = e^{2i\eta_{l}} = A_{l}e^{2i\delta_{l}}$$

In eq. (10),  $S_1$  is the real part of the nuclear phase-shift and  $A_1$  is the amplitude of 1-th partial wave. The quantity  $A_1'$ , also called the reflection co-efficient, represents the amount of absorption of the incident flux from elastic channel. Thus  $0 \le A_1 \le 1$ , with  $A_1 = 1$  corresponding to no absorption and  $A_1 = 0$  to complete absorption.

In the above treatment, the long range Coulomb force has not been considered. It is, however, possible to include the Coulomb force and obtain a scattering amplitude similar to eq. (8) with a modified phase shift ( $\delta_{\ell} + \delta_{\ell}$ ), where  $\delta_1$  is the Coulomb phase shift. The eq. (8) can now be written as

$$f(\theta) = f_{c}(\theta) + \frac{1}{2k} \sum_{l=0}^{\infty} (2l+1)e^{2is_{e}} (1 - A_{e}e^{2is_{e}})f_{l}(s\theta)$$

where<sup>13)</sup>

$$f_{c}(\theta) = \frac{i}{2k} \sum_{l=0}^{\infty} (2l+1)(1-e^{2i\vartheta_{c}}) P_{l}(\cos\theta)$$
$$= \frac{-\eta}{2k} \cos(\theta/2) e^{-2i\eta \ln(\sin\theta/2) + 2i\vartheta_{0}}$$

and<sup>13)</sup>

$$\sigma_{l} = \arg \Gamma \left( 1 + l + in \right)$$
  
=  $\sigma_{l} + \sum_{l=1}^{l} \operatorname{are} \operatorname{tan} \left( n / l^{"} \right)$ 

In the above equation '  $\eta$  ' is Sommerfeld parameter which is defined as

$$\eta = \frac{z_1 z_2 e^2 \mu}{t^2 k}$$

The quantity  $S_1 = e^{2i\delta_1}$  is discussed in the next subsection. The final quantities of interest are calculated from  $f(\theta)$  and  $f_c(\theta)$  as described in section 3.

2.2 Treatment of S-matrix

The exact determination of the nuclear S-matrix involves the numerical solution of Schrodinger equation in the interaction region. However, an alternate way is to treat it phenomenologically. As an extreme case one may assume that it has a sharp boundary in the angular momentum space i.e. all the partial waves with values  $1 \leq l_c$  are fully absorbed whereas  $1 > l_c$  remain unaffected. Thus

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$$A_{\ell} = |S_{\ell}| = 1 \qquad \text{for } \ell > \ell_{c}$$
$$= 0 \qquad \text{for } \ell \leq \ell_{c}$$

The total reaction cross-section, then becomes

$$\sigma_{R}^{\prime} = \frac{\pi}{k^{2}} \left( L_{c} + 1 \right)^{2}$$

In classical terms this situation corresponds to the case where the nuclei with angular momentum 'L' moving along trajectoreic with  $r \leq R_c = L_c/k$  are fully absorbed whereas those with  $r > R_c$ undergo pure Goulomb scattering. This is called the shace cut-off model.

An improvement over this model can be achieved by asuming that the reflection coefficient  $A_1$  increases smoothly from zero to one over a definite ange of angular momenta. The variation of  $A_1$  with respect to 1, which is similar to nuclear Fermi distribution seems to be a natural choice. In this way one takes into account the nuclear diffuseness for defining the absorption region. It is usual to assume a similar shape for ' $\mathcal{E}_1$ ' although there is no a priori justification for such a choice. Following Methatyre et al<sup>5</sup>, we take

$$A_{l} = \left[\frac{-(l-l_{A})/\Delta l_{A}}{1+e}\right]^{-1}$$

and

 $S_{l} = S_{0} \left[ 1 + e^{(l-l_{s})/\Delta l_{s}} \right]^{-1}$ 

where 'l' is now a continuous variable and  $l_A$ ,  $\Delta l_A$ ,  $\kappa_0$ ,  $\Delta l_5$ ,  $l_8$ are the adjustable parameters. The physical significance of these parameters is discussed in the next section.  $\tau$ 

d.

# RESULTS AND DISCUSSION

## 3.1 Calculated Quantities

Using the expression for Coulomb scattering amplitude (eq. 12) one can find the Rutherford differential cross-section as,

$$\left(\frac{d\sigma(\theta)}{d\Lambda}\right)_{R} = \left|f_{c}(\theta)\right|^{2} = \frac{\eta^{2}}{4k^{2}} \cos^{2}(\theta/2)$$

Also from eq. (11) and (12), the ratio of elastic differential cross-section to Rutherford cross-section is determined to be

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$$\frac{d \sigma(0)/d \Omega}{(d \sigma(0)/d \Omega)_R} = \left| \begin{array}{c} -i \eta \ln \sin^2 \theta/2 \\ -i e & -\frac{\sin^2 (\theta/2)}{\eta} \end{array} \right|^{-1}$$

where

$$S = \sum_{\ell=0}^{\infty} \left(1 - A_{\ell} e^{2iS_{\ell}}\right) \left(2\ell+1\right) \hat{P}_{\ell}(\cos\theta) e^{2i(\sigma_{\ell} - \sigma_{\ell})}$$

The experimental values for the same quantity can be fitted to eq. (21) by varying the parameters of  $A_e$  and  $S_e$ . The subroutine used<sup>13)</sup> for the fitting minimizes the quantity,

$$\chi_{y}^{2} = \frac{1}{NP-N} \sum_{i=1}^{NP} \left[ \frac{d\sigma_{exp}^{i}(\theta) - d\sigma_{th}^{i}(\theta)}{\Delta \left( d\sigma_{exp}^{i}(\theta) \right)} \right]^{2}$$

where NP are the number of data points and N is the number of parameters. The fits obtained for the cases  ${}^{12}\text{C} + {}^{56}\text{Fe}$ ,  ${}^{12}\text{C} + {}^{107}\text{Ag}$ ,  ${}^{12}\text{C} + {}^{181}\text{Ta}$  are displayed in figs. 1-3 and the derived parameters are listed in table 1. The parameter  $1_A$  represents the value of '1' at which  $A_1 = 1/2$  or the absorption  $(1-A_L^2)$  is 75%. The variation of  $A_1$  with respect to 1 is given in fig. 4. Unlike the sharp cut-off model where the absorption radius corresponds to 100% absorption, we define a radius  $R_a$  which corresponds to 1 =  $1_A$ . By using the conservation of energy requirement

$$E = \frac{z_{1}z_{2}e^{2}}{r} + \frac{\ell(1+1)t^{2}}{2\mu t^{2}}$$

We find

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$$kr = \eta + \sqrt{\eta^2 + \ell(\ell+1)}$$

or

$$R_{a} = k^{-1} \left[ \eta + \sqrt{\eta^{2} + \ell_{A}(\ell_{A}^{+1})} \right]$$

Similarly from eq. (17), it can be seen that  $A_1$  goes from 0.9 to 0.1 over the range  $4.4 \Delta l_A$ . The corresponding region of space  $\Delta r=t$ , is similar to the nuclear surface thickness. For  $l \gg \eta$ , it is simply

$$t \simeq k' \Delta l_A$$

In table 2, the values of absorption radius parameter obtained from eq. (25) and the absorption surface thickness from eq. (26) are listed alongwith the total reaction cross-section which is given by 13)

$$\sigma_{R}^{\prime} = \frac{\pi}{k^{2}} \sum_{l=0}^{\infty} (2l+1)(1-A_{l}^{2})$$

In eq. (18) the parameter  $b_{1}$  gives the strength of the nuclear phase shift, however  $l_{6}$  and  $\Delta l_{5}$  do not have any apparent physical significance. The values given in table 2 under heading '1' have been obtained by using the central values of parameter of table 1. These are compared with the values obtained in ref. 12, where a number of different combinations of parameters with similar  $\lambda^{2}$ are used to obtain the uncertainties in the quantities  $r_{a}$ , t and  $r_{a}$ . Most of the values in the two calculations agree, however the small difference in some cases arises because of the restriction  $\Delta l_{A} = \Delta l_{5}$  and  $l_{A} = 1$  imposed in the present calculation. In view of the excellent fits obtained (Fig. 1-3) under this assumption, it is of no physical significance if this condition is relaxed. Another source of discrepancy is the different mass standards:  $l_{a}^{12}$  C in the present calculation and  $l_{b}^{16}$  O in reference 12.

3.2 Conclusions

By utilizing an optimization routine from the CPC library<sup>13)</sup> and by writing a sub-program for calculating the function of eq. (21), we have obtained good fits to the elastic scattering data<sup>12)</sup> of <sup>12</sup>C + <sup>56</sup>Fe, <sup>12</sup>C + <sup>107</sup>Ag, <sup>12</sup>C + <sup>181</sup>Ta at 10.375 MeV/u. The total reaction cross-section obtained for the test cases agree with the previous calculations. The method described in detail in section 2 serves as a reliable and quick way of analysing elastic scattering data and therefore an operating program on PINSIECH'S local computer is useful for the experimentalists as well as theoretical physicists who wish to compare other elaborate calculations with this simplified approach.

### PROGRAM STRUCTURE

The computer program 'HISS' (<u>Heavy Ion Scattering by S-matrix</u> method) has been written in the standard FORTRAN IV language for the PINSTECH'S local computer. The program summary is given in the appendix I. For the purpose of least-square fitting, a subroutine from Computer Physics Communications library program ABMR UNIFIT2 is utilized. The R.H.S. of eq. (20) is calculated through the subprogram FNC(X) during optimization and for writing the final values with optimized parameters at the desired angles of scattering. A flow chart for the calculation done in the main and in FNC(X) is given in appendix II. The input data and output layout are described below while the complete program listing and specimen input/output appears in appendix III-V

4.1 Data Input.

Card A (1 card) FORMAT (1X, A1, 3X, 10A4)

KATCH - New case identifier : Must be 'Q' NTITI (1-10) - First title

Card B (1 card) FORMAT (5X, 10A4)

NTIT2 (1-10) - Second Title

Card C (1 card) FORMAT (15, F10.5, 15) NP ---Number of data points :  $2 \le NP \le 100$ DYSTD ---Default uncertainty If DELTY = 0.0 in Card D NTYPE ---If NTYPE  $\le 12$ , the input data is scaled. Different scalings may be done by different values of NTYPE. Present provision is for logarithmic transformation only.

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```
Card D (NP cards)
FORMAT (3G 15.5)
X(I) --- Values of scattering angles in C.M frame
Y(I) --- Values of d\sigma_{EXP}/d\sigma_R
DELTY(I) --- Uncertainties in Y(I) values
```

```
Card E (1 card)
FORMAT (15, F10.5, 15)
N ---No. of adjustable parameters : 1 \le N \le 20, N \le NP
EPSSTD --- Parameter increment ratio (Default 1. D-8)
M --- Total number of parameters : N \le M \le 20
```

Card F (1 card) FORMAT (512) 11, 12, 13, 14, 15 ----Sequence of parameters : Only the <u>first</u> M parameters are searched

```
Card G 'M cards)
FORMAT (3G15.5)
P(J) --- Parameter values
EPS (J) ---Fractional parameter increment for gradient
calculation:
If other than EPSSTD
DP2(J) ---Uncertainty in P(J): May be omitted.
```

Card H (one card) FORMAT (13, 5F10.3)

LL ---1 in the summation over 1 in eq. (21): If LL is too small, the program increases LL in steps of 10 to reach the correct value.

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·曹代提下,1996年9月,1997年1月,1997年9月。

Zl ---Atomic number of the projectile nucleus
Z2 ---Atomic number of the target nucleus
Al ---Mass number of the projectile nucleus
A2 ---Mass number of the target nucleus
EPN ---Energy per nucleon for the projectile

Card I (One Card) FORMAT (13, 3F 10.3) MM ----Print option for the reflection co-eff. A<sub>1</sub>: MM=0 no printing. MM = 1; 100 values around 1 =  $1_A$  are printed. XF ---First angle at which the  $d\sigma/d\sigma_R$  is required XL ---Last angle at which the  $d\sigma/d\sigma_R$  is required XD ---Angular increment

### 4.2 Output

First Page: The first page of the output gives the heading comprising of the identification of heavy ion pair interacting at a specified energy alongwith the source of data and the desired data transformation. The initial and optimized  $\chi^2$  alongwith the list of all input parameter guesses and optimized parameters are written. The error code '0' appears when a successful convergence is obtained. The error code '1' shows that the convergence was not obtained in the permitted number of iterations.

Second Page: The angles at which the data is given are written under the heading "Independent" while the <u>transformed</u> data values appear under "Dependent". The "Optimized dependent" are the values obtained by using the model function with fitted parameters. The individual for each data point is also printed.

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Third Page: This page is an optional output (If MM = 1). It gives the value of  $A_1$  for different '1' in the vicinity of  $l_A$ . For 1 : 0-1<sub>max</sub>, the  $A_1$  should increase from zero to one.

Fourth Page: Here the final quantities of interest, i.e. the ratio of elastic to Rutherford differential cross-sections and the total reaction cross-section (in Fermi squared units) are printed. The former may be written for any desired range of angles and angle increments (see Input Data).

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Table 1. Parameter of  ${}^{12}$ C scattering at 10,375 MeV/u for the data ${}^{12}$  displayed in Figs. 1-3.

Parameter Target	k (fm <sup>-1</sup> )	η	$l_{A} = l_{E}$	$ \begin{vmatrix} \Delta \ell_A \\ = \Delta \ell_S \end{vmatrix} $	6,	$\chi^2_{\nu}$
56 <sub>Fe</sub> 26	6.963	7.627	52.571 ± 0.188	3.147 ± 0.080	0.467 ± 0.029	0.49
107 <sub>Ag</sub> . 47	7.602	13.788	60.538 ± 0.180	2.570 ± 0.071	0.586 ± 0.043	0.38
181 Ta 73	7.929	21.415	64.111 ± 0.159	2.573 ± 0.155	0.585 ± 0.036	0.03

Table 2. Values of the absorption radius parameter  $r_a$ , absorption thickness  $t_a$  and the total reaction cross-section  $\sigma_R$  derived from the central values of the parameters given in table 1. 1: This calculation 2: From ref. 12

Quantity	$r_{a} = R_{a} / (A_{p}^{13} + A_{T}^{13}) f_{m}$		t (•	fm)	6 <sub>R</sub> (mb)	
Target	1	2	1	2	1	2
56 <sub>3</sub> 26	1.438	1.42 ± 0.02	0.452	0.43 ± 0.05	2.061	1.96 ± 0.10
107 ~ 47	1.427	1.44 ± 0.02	U.414	0.31 ± 0.05	2.208	2.23 ± 0.07
181 70 <sup>Ta</sup>	1,420	1.45 ± 0.02	0.324	0.37 = 0.09	2.263	2.43 ± 0.03

### FIGURE CAPTIONS

- 1- The scattering angle in the centre-of-mass frame  $\Theta$  (C.M.) vs the ratio of elastic differential cross-section to the Rutherford cross-section using the logarithmic scale; for  $^{12}$ C +  $^{56}$ Fe at  $^{E}$ lab = 124.5 MeV.
- 2- Ibid; for  ${}^{12}C + {}^{107}Ag$
- 3- Ibid; for  ${}^{12}C + {}^{181}Ta$
- 4- Variation of the parameterized reflection co-efficient  $A_1'$ with respect to the angular momentum '1' for the three cases of fig. 1,2 and 3. The  $1_A$  and  $\Delta 1_A$  are the fitted parameters.

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Fig. 2.



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# Appendix 1

## PROGRAM SUMMARY

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Title of Program	:	HISS
Directory	:	DRA1: [INTINAN]
Program Obtainable from	:	T.P.G. of N.P.D.
Computer	:	VAX 11/780 Installation PINSTECH
Operating System	:	VMS/MOS
Programming Language	:	FORTRAN IV (G)
High Speed Storage Required	:	94 K Bytes
Number of bits in a word	:	32
Overlay Structure	:	None
Tape Code	:	F.BCDIC
Nature of Physical Problem	:	Calculation of d <b>6</b> /d6 <sub>R</sub> for heavy ions
		and fitting the parameters of S-
		matrix.
Method of Solution	:	Davidson's non-linear minimization
		technique programmed by E. von-
		Heerwall <sup>13)</sup>
Typical Running Time	:	6-10 min. for fitting 3-5 parameters
Program Features	:	1- Upto 100 data points with uncer-
		tainities can be read.
		2- The number of parameters should
		be less than 20.
		3- Only first H parameters out of N
		are fitted. $(M \leq N)$
		4- The parameter guesser may be given
		alongwith their ranges.



# APPENDIX II



	APP	ENDIX	111						
<del>,</del>	PROG	RAH 1.1	sting			· ••			
	****	(*****	****						
	*		*						
	*	HISS	*						
	*		*						
	****	<b>(**</b> *****	****						
THIS PROGRAM	UTILIZE	S AN A	DAPTED	SUBRO	UTINE	FROM	CPC I	LIBRAR	Y
PROGRAM *	UNIFIT2	: • B	Y 'E	. VON	MEERW	ALL ?	(CF°C	11(197	6)211
TO FIT THE DA	ATA ON H	IEAVY I	ON ELA	STIC D	IFFER	ENTIAL	CROS	S-SECT	IONS
WITH THE HELD	P OF THE	E EXPRE	SSION	DEFINE	DINI	EQ. 13:	20 1	21 OF	THE
N.P.D INTERN	AL REPOR	RT .	ANALYS	IS OF	HEAVY	ION EL	ASTI	C SCAT	TERING
DATA BY S-MA	TRIX PAP	AHETER	IZATIO	N ".					

I.E.QURESHI 25-10-1984

IMPLICIT REAL\*8(A-H,D-Z) COMMON XK,A,X,Y,DELTY,W,P,EPS,GRAD,CH2,NP,N,NTYPE COMMON/INP/LL, Z1, Z2, A1, A2, EPN COMMON/II/I1,I2,I3,I4,I5 DIMENSION A (1000), X (100), Y (100), W (100), EPS (20), P (20), GRAD (20), \* DELTY(100).DP(20),NTIT1(10),NTIT2(10),LABELX(5),LABELY(5),

\* DP2(20),KE(2),KV(2),FCTR(9),SRT(100),XX(100) DATA FCTR/1.D2,1.D-4,1.D6,1.D-8,1.D9,1.D-10,1.D11,1.D-12,1.D6/ DATA IRD/1/.IWT/2/.KUE/1H0/.KE/4H EPS.4HILON/.KV/4H +/-.4H DP /

```
2 FORMAT (15,F10,5,I5)
```

5 FORMAT (3G15.5)

- 11 FORMAT (1X,A1,3X,10A4)
- 12 FURMAT (5X,10A4)
- 13 FORNAT (45X,10A4/)
- 14 FORMAT (/10X.26HABORT THIS CASE SINCE NP =, 13.5H, N =, 13)
- 16 FORMAT (//15X,23HINITIAL CHI-SQUARE (PER,I3,
- \* 20H DEGREES OF FREEDOM),//)
- 17 FORMAT (23X.F20.5)

18 FORMAT <///15X,13HPARAMETER NO.,14X,15HPARAMETER VALUE,15X,2A4, \* 18X.8HGRADIENT./

19 FORMAT (/34X.14HRESULTS OF FIT)

```
20 FORMAT (///15X,23HNO, (MAX) OF ITERATIONS,16X,
```

ERROR CODE, 16X, 20HOPTIMIZED CHI-SQUARE) \* 16H

- 21 FORMAT (/24X, I2, 1H(, I2, 1H), 30X, I2, 23X, F20.6)
- 22 FORMAT (/20X, 35HTHERE WILL BE NO FIT FOR PARAMETERS, I3. \* 8H THROUGH, I3/)
- 23 FCRMAT (21X, 12, 15X, F20, 10, 13X, D12, 5, 13X, D12, 5)

```
26 FORMAT (/10X, 19HMULTIPLY ALL EPS BY, 1PD8, 1)
28 FORMAT (3X, I3, 4X, F10, 5, 6X, F10, 6, 5X, D12, 4, 10X,
```

```
* F10.6,9X,D13.5,7X,D13.6)
```

```
29 FORMAT (1H1,////10X,11HINDEPENDENT,6X,9HDEPENDENT,7X,6HWEIGHT,
```

- # 7X,19H0PTIMIZED DEPENDENT,5X,15HFNC(P(OPT),X)-Y,4X,
- \$ 22HCONTRIB, TO CHI-SQUARE,//)

INITIALIZATION OF PROGRAM

NCASE=0

```
INPUT OF CASE INFORMATION: TITLES AND LABELS
```

```
1 READ(IRD, 11, END=39) KATCH, (HTIT1(I), I=1, 10)
  IF (KATCH.NE.KUE) GO TO 1
  READ(IRD,12) (NTIT2(I),I=1,10)
  NCASE=NCASE+1
  Q=-1.137
```

```
PI=3.141592654D0
```

25

C

C

C C

C

C C C

С INPUT OF DATA: X, Y, DELTY, AND DEFAULT VALUES С C READ(IRD,2) NP.DYSTD,NTYPE -DYSTD=DABS(DYSTD) NBAR=0 IF(DYSTD.GT.1.D-7) GO TO 3 DYSTD=1.D0 NBAR=1 3 DO 4 L=1,NP READ(IRD,5,END=39) X(L),Y(L),DELTY(L) IF(X(L).GT.Q) Q=X(L) DELTY(L)=DABS(DELTY(L)) IF (DELTY(L), EQ.0.D9.AND.NBAR, EQ.1) GO TO 6 IF (DELTY(L), EQ.0, D0) DELTY(L)=DYSTD W(L)=(1,D0/DELTY(L))\*\*2 GO TO 4 6 W(L)=1,D0 **4 CONTINUE** INPUT OF PARAMETERS, EPSILONS, PARAMETER ERRORS, AND DEFAULTS С READ(IRD,2) N,EPSSTD,M IF (M.LT.N.OR.M.GT.20) M=N IF(NP.LT.3, OR.NP.OT, 100) GO TO 35 IF (N.GE, 1. AND. N.LT. NP. AND. N.LE, 20) 60 TO 36 35 WRITE(IWT,14) NP,N GO TO 1 36 IF(EPSSTD.E0.0.D0) EPSSTD=1.D-8 READ(IRD, 60) 11, 12, 13, 14, 15 69 FORMAT (512) DO 9 L=1,4 READ(IRD, 5, END=39) P(L), EPS(L), DP2(L) IF (EPS(L), LT.1, D-10) EPS(L)=EPSSTD Q=DABS(F(L)) IF(0,NE,9,D0) EPS(L)=EPS(L)\*0 Q=1,D-3\*DABS(DP2(L)) IF (0,NE,0,D0) EPS(L)=DMIN1(EPS(L),0) IF(L.LE.N) GD TO 9 EPS(L)=0.00 DP(L) = 0, D0DF2(L)=0.D0 GRAD(L)=0.00 9 CONTINUE NPN=NP-N ANPN1=1.D0/NPN READ(IRD, 61) LL, 21, 22, A1, A2, EPN-61 FORMAT(13,5F10,3) READ (IRD, 62) MM, XF, XL, XD 62 FORMAT(I5,3F10,3) С С SOME ECHO OUTPUT С WRITE(IWT.13) (NTIT1(I).I=1.10) (HTIT2(I).I=1.10) C C FIT INITIALIZATION C IF (N) YPE.GE.10) CALL TRAFO. CALL FDEL WRITE(IWT,16) NPN WRITE(IWT,17) CH2 WRITE(INT,18) KE WRITE(1WT,23) (I,P(I),EPS(I),GRAD(I),I=1,M) IF (M.EQ.N) GO TO 10 N1 = N+1

26

С C

```
WRITE(INT,22) N1,M
   10 LIMIT=4*N+6
      IF(LIMIT.GT.60) LIMIT=30
C
C
    FIT, EPS ADJUSTMENT FOR GRADIENT TROUBLE, RESULTS
C
      NERR=0
   34 NERR=NERR+1
      DO 38 L=1,M,1
   38 DP(L)=DP2(L)
      CALL DAVID2(DP,1.D-8,KOUNT,LIMIT,IER)
      IF(IER.NE.-1) GO TO 31
      IF (NERR.GT.9) GO TO 31
      FM=FCTR (NERR)
      WRITE(IWT,26) FM
      D0_32 L=1,N,1
   22 EPS(L)=EPS(L)*FM
      GO TO 34
   31 WRITE(IWT,19)
      WRITE(IWT,20)
      WRITE(IWT,21) KOUNT,LIMIT, IER,CH2
      WRITE(IWT,18) KV
      WRITE(IWT,23) (I,P(I),DP(I),GRAD(I),I=1,N)
С
C
    TABLE OF VALUES AND FIT
С
      WRITE(IWT,29)
      D027 JN=1.NP
      R=X(JN)
      Z=FRU CD
      Q=Y(JN)-Z
      Q2=ANPN1*Q*Q*V(JN)
      WRITE(IWT,28) JN,X(JN),Y(JN),W(JN),Z,0,02
   27 CONTINUE
C
C
         PRINT RATID OF THE DIFFERENTIAL CROSS-SECTIONS AT DESIRED
C
         ANGLES BY USING THE OPTIMIZED PARAMETERS,
С
         J1=P(1)-50
         J2=P(1)+50
         XX(1)=XF
         NN=(XL-XF)/XD
         DO 50 J=1,NN
         SR=FNC(XX(J))
         SRT(J)=10.0**SR
50
         XX(J+1)=XX(J):XD
         IF (MM, EQ, 1) WRITE (2,53)
         IF (MM.EQ.1) WRITE(2,54) (J-1,A(J), J=J1, J2)
         WRITE(IWT,52)
         WRITE(IWT,51)(XX(J),SRI((J),J=1.NN)
         FORMAT(3(10X,F5.2,015.5,5X))
51
                                             ',16X),/10X,3('ANGLE',4X,
52
         FORMAT(1H1,//10X,3(9X,78ATI0 000
      Х
                'DIFF, X-SECS',15X),//)
53
         FORMAT(1H1,///5X,3(1X,1L1,10X,1A(L)1,6X),//)
54
         FORMAT(3(2X, 15, 015, 5))
C
С
         CALCULATION OF THE TOTAL REACTION X-SECTION.
C
         SIGR=0,D0
         DO 70 J=1,LL
         SIGR=SIGR+(2.*J-1)*(1.-A(J)**2)
70
         SIGR=SIGR*PI/XK**2
         WRITE(IWT,80)SIGR
         FORMAT(//10X,'TOTAL REACTION X-SEC =',015.5,'
                                                           F**21)
80
```

	GO TO 1
57	STUP
-	SUBROUTINE EDEL
	COMPUTES CHI-SQUARE AND GRADIENT VECTOR FOR DAVID2
•	IMPLICIT REAL*8 (A-H.O-Z)
	COMMON XK,XA,X,Y,DELTY,W,P,EPS,GRAD,CH2,NP,N,HIYPE
	COMMON/INP/ LL,Z1,Z2,A1,A2,EPH
	COMMON/11/11,12,13,14,15
	DIMENSION XA(1000),X(100),Y(100),DELTY(100),W(100),P(20),EFS(20) X ,GRAD(20)
	ANFNI=1,107(NF=N) AFFA=0 100/N=0 9900
2	CHI-SQUARE
2	
	CH=0.00
	DU 1 1=1,NP,1
	R=X(1)
	A=FNC(R)-Y(I)
	1 CH=CH+A%A*W(I)
-	CH2=CH*AMPN1
•	GRADIENT VECTOR
	DO 3 K=1.N.1
	P (K) =P (K) +ÉPS (K)
	C=0,D0
	DD 2 I=1,NP,1
	R=X(I)
	A=FNC(R)-Y(I)
	2 C=C+A*A*W(I)
	GRAD(K)=ANPN1*(C+CH)/EPS(K)
	P(K) = F(K) - EPS(K)
-	3 EPS (K) #EPS (K) #ALFA
	DE T11031
	PAR FURNING CONTRACTOR C
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## SUBROUTINE DAVID2 (DP, TERH.KOUNT, LIMIT, IER) VARIABLE METRIC NON-LINEAR MINIMIZATION OF FUNCTION UNCONSTRAINED SIMPLIFIED DAVIDON METHOD US AEC R AND D REPORT ANL 5990, APPENDIX (1959, REV.) NEEDS FDEL FOR CHI-SQUARE (F) AND GRADIENT (G) IMPLICIT REAL\*8 (A-H.0-Z) COMMON XK, XA, X9, Y9, Z9, W9, P, EPS, G, F, NP, N, NTYPE DIMENSION X0(100),Y0(100),Z0(100),W0(100),P(20),EPS(20),G(20) DIMENSION DP (20), PB (20), (B (20), HU (20), HV (20), H(20, 20), XA (1990) INITIALIZATION ANPN= (NP-N) \*9.500 T=5.00 KOUSES 3 IER=0 N1=9 N2=4 IF (N2.LE.N) N2=N+1 NS=0 IF (LIMIT.LE.N2) LIMIT=N2+1 CALL FDEL Ĉ PREPARATION OF ERROR MATRIX H DO 1 J=1,N,1 IF (N.E0.1) GO TO 3 DO 2 K=1,N,1 2 H(J,K)=1,D-10 3 H(J,J)=1,D-2IF (DP(J).NE.0.00) GO TO 7 IF(P(J).E0.0.D0) GO TO 9 DP(J)=P(J)\*3.D-2 7 A=ANPN\*(DP(J)\*#2) B=A IF (DABS(G(J)).GT.5.D-3) 9=0.3D0\*DABS(DP(J)/G(J)) H(J, J) =0.3D0\*DSORT (A\*B) 9 PB(J)=P(J) GB(J)=G(J)1 DF(J) = H(J,J)FB C C ITERATIVE FIT C 60 KOUNT=KOUNT+1 IF(KOUNT.GT.LIMIT) GO TO 50 C C GO TO NEW MENEMUM C DO 10 K=1,N,1 HV(K)=0,00 DO 11 J=1,N,1 11 HV(K)=HV(K)+H(K,J)\*G(J) 10 P(K)=P(K)-HV(K) U=0.D0 ¥≖0.D9

C C C

С C

C

C

С

С

C C

C

C

C

1-1

```
С
    CLOSENESS TO MINIMUM
С
      CALL FUEL
      IF (F.GE.FB) GO TO 21
      IER=2
      N4=KOUNT
      N5=80+*
      FB=F
      DO 20 J=1,N,1
      DP(J) = H(J, J)
      IF (DP (J).LT.0.D0.AND.KOUNT.GE.M2) 60 TO 75
      PB(J) = P(J)
   20 GB(J) = G(J)
      IER=0
   21 DO 22 K=1.N.1
      HU (K) =9.09
      DO 23 J=1,N,1
   23 HU(K)=HU(K)+H(K,J)*G(J)
      V=V+G(K)*HV(K)
   22 U=U+G(K) *HU(K)
С
C
    RESCUE FROM BAD GUESSES AND/OR EARLY GRADIENT (ROUBLE
C
       IF (KOUNT.GT.3) GO TO 27
       A1=1.200%FB
       IF (F.LT.A1.AND.U.GT.0.D0) 60 TO 27
      DO 26 J=1,N,1
       IF(U,E0,0,D0) EPS(J)=1,D1*EPS(J)
      H(J,J) = 1, D - 1 + H(J,J)
   26 P(J)=PB(J)-5,D-2*H(J,J)*G(J)
      CALL FDEL
       GO TO 60
С
C
    TESTS OF CONVERGENCE AND STABLESY
С
   27 IF (KOUNT, LE, N2) GO TO 29
       IER=-1
       IF (U.EQ.V.OR.U.EQ.0.D9) GD TO 25
       IER=Ø
       IF(U,LE,TERM) GO TO 70
C
C
     COEFFICIENT FOR UPDATING H
C
   29 A1=-U/(T-1,D0)
       A2=U/(T+1.D0)
       A3=T*A2
       A4=-T*A1
       IF (V.GE.A1) GO TO AL
       ALFA=1,00/(V-U)
       GO TO 30
    41 IF(V.GE.A2) GO TO 42
       ALFA=1 (00/(T*U)-1,00/U
       60 TO 30
    42 IF(V.GE.A3) GO TO 43
       ALFA== (U-2,D0*V)/(U*(V-U))
       GO TO 30
    43 IF (V.GE.A4) GO TO 44
    44 ALFA=1,D0/(V-U)
```

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C
Ĉ
    UPDATE H, CYCLE
   30 DO 31 J=1,N,1
       J1=J
      DO 32 K=1, J1,1
      H(J,K)=H(K,J)+ALFA*HU(K)*HU(J)
   32 H(K, J) = H(J, K)
   31 CONTINUE
      GO TU 69
С
Ĉ
    TERMINATION
С
   50 N1=81+1
       IF (N1.GE.2) GD TO 69
      LIMIT=LIMIT+6
       60 TO 60
   69 IER=1
C
Ĉ
    COPY BEST RESULTS
   70 IF(N5.E0.0) IER=-1
       IF(IER.E0.-1.OR.IER.E0.2.OR.N4.LT.N) N1=-1
   75 F=FB
       DO 71 J=1,N,1
       IF (N1.E0.-1) DP (J) =0.00
       DP(J)=DSORT(DP(J)/ANPN)
       F(J) = FB(J)
   71 G(J)=GB(3)
       RETURN
       END
~
      - ----
```

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544 <b>4</b> 4 6	<b>₽₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩</b>	6 <b>6</b> 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
с с	THIS CHROONGRAM FALCHEATER THE CHHETTOM DECTATION	*
c .	THE RATIO OF FLASTIC DIFFERENTIAL CROSS-SECTION	か 大
Ē	NTUTDED BY THE RUTHEREORD CROCK-SECTION	*
Ċ.		
	****	****
C		
•	FUNCTION FNC(X)	
	IMPLICIT REAL*8(A-H.O-Z)	
	REAL#4 UL	
	COMPLEX#16 XI,F1,F31,F32,F3,CHECL	
	COMMON/INP/ LL,Z1,Z2,A1,A2,EPM	
	COMMON/11/ 11,12,13,14,15	
	COMMON XK,A,01,02,03,04,P,05,96,07,NPO,N,NTYFE	
	DINENSION A(1999),D(1999),FF(1999),S(1999) DINENSION A(198) A7(198) A7(198) A(198) F(28) A5	(20) 04/20)
	PT=7 14159745A NG	(207,00(207
	CH=197.32892 D0	
	ALP=7.29735150-03	
	XM=731.5D0	
	XI=DCMPLX(0,D0 ,1,D0)	
	RC=1,4*((A1**0,3333300)+(A2**0,3333300))	
	ARED= (A1*A2)/(A1+A2)	
	XHU=XH#ARED	
	XK=DSQRT(2,*XMU*EPN*ARED)/SH	
	ETA=Z1#Z2*ALP*XMU/(CH*XK)	
	UL=SNGL(XK*RC)	
228	CALL AL(LL,P(II),P(IZ),A)	
	CHECL DEALL, FAIL), FAI2), FAID), D) CHECL-A/LL)+CDEYE/2, +YI+D/LL))	
	TE (BREAL (CHECL-1.).)E.1.D-A)GO TO 990	
	11 = 11 + 10	
	GO TO 998	
790	CALL SL(LL,ETA,S)	
	SINE=DSIN(X*PI/340.)	
	SING=SINE#SINE	
	F1=-XI*CDEXP(-XI*ETA*DLOG(SIR(S))	
	F2=SINS/ETA	
	CALL PL(LL,X,PP)	
	$F_3 = DCMF(1, X)(0, D0, D0)$	
	DU 30 LTI,LL Y) -DED DAT (1 - 1)	
	FR1=CDFYF(2,±X1*F(1))	
	F32=A(L) *CDEXP(2.*XI*D(L))	
	F3=F3+(1,-F32)*(2,*XL+1,D0)*PP(L)*F31	
30	CONTINUE	
	FNC=CDABS(F1-F2*F3)**2	
~ • •	FNC=DLOG10(FNC)	
C40	CONTINUE	
	RETURN	
	n nu servici de la casa	
	NUDRUULLNE ALVELANDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDULLIAUNDU	
	TITHENGTON A(())	
	10 10 T=1.11	
	XL=DFLOAT(L)	
	P=(XL-XLP)/DXL	
	1F(F,LT,-30,)00 TO 2 Tr/(P.GT.+30,)00 TO X	
	Q=DEXP(-P)	
	A(I)=1,D0/(1,D0+0)	
1	GO TO 10	
2	A(1)=0.	
i	- 32 -	
1		

•

7	50 TO 19 A(T)=1 D0
10	PONT 1NE
10	
	RETURN
	SUBRUUTINE UL(LL,XLU,UXL,ULD,D)
	IMPLICIT REAL*8(A-H,O-Z)
	DIMENSION D(LL)
	DO 10 I=1,LL
	L=I-1
	XL=DFLOAT(L)
	P=(XL-XLD)/DXL
	IF(P,LT,-50,)60 TO 2
	IF(P.GT.+50.)GO TO 3
	Q=DEXP(P)
	P(I) = DLD/(1, DQ+Q)
	GO TO 10
2	D(T) = D(D)
<b>.</b>	60 TO 10
7	D(T)-0 D0
10	D(1)-0,00
10	
	SUBRUULINE SEVEL, TH, SZ
	IMPLICIT KEAL#8(A-H,U-2)
	DIMENSIUN S(LL)
	SS=0,D0
	S(1)=SS
	DO 10 I=2,LL
	L=I-1
	THET=ETA/L
	SS=SS+DATAN(THET)
	S(1)=SS
10	CONTINUE
	RETURN
	END
	SUBROUTINE PL (LL_XC_P)
	IMPLICIT REAL*8(A-H.0-Z)
	DIMENSION P(LL)
	P(1)=1.00
	P(2) = f(2) S(2) S(2) S(2) S(2) S(2) S(2) S(2) S
	10 10 Terz II
	ν
	ハニールドニカリントフ やノビンティング サインド・ペードは入し、水やノベンルやノビニオン、ノンドニペードはシャレノレーペン
	F (1) = (2,4)(A1)22,00) F1,7 AF (2)AF (1) = (A12,007AF (1)27) F(1) - F(1) (A1)24 - A
10	P(L)=P(L)/(AL=1,) CONTINUE
16	CONTINUE
	RETURN
	END
	SUBROUTINE TRAFD
C	
C	PERFORMS INDICATED TRANSFORMATION ON THE DATA, AND/OR THE
C	PARAMETER GUESSES, FOR NTYPE.GE.10
C	
	IMPLICIT REAL*8(A-H,O-Z)
	COMMON XK,A,X,Y,DELTY,W,P,EPS,GRAD,CH2,NP,N,NTYPE
	DIMENSION $A(1000), X(100), Y(100), DELTY(100), W(100), F(20), EPS(20)$
	X ,GRAD(20)
-	DATA IWT/2/
C	

~ ~

•

3

•

IF (NTYPE,GT,12) G0 T0 10 D0 2 I=1,NP,1 C X(I)=2.09\*X(I) IF (Y(I).LT.1.D-5) G0 T0 3 IF (DELTY(I).LT.1.D-95)G0 T0 3 DELTY(I)=DELTY(I)/Y(I) W(I)=(1.D0/DELTY(I))\*\*2 Y(I)=DLOG10(Y(I)) G0 T0 2 3 Y(I)=-4.D9 DELTY(I)=9.D0 W(I)=0.D0 2 CONTINUE 10 RETURN

4

<u>\*</u>,

C

\$

C

END

- 34 -

## INPUT DATA

0 j2C + 1	BITA AT J	0.375 ME	ÚŽN T	• • •
ALSTER	AND CONZET	DATA (LO	G SCALE)	
31	10			
7.9	0.77		0.9977	
9.0	1.01		0.0101	
10,2	1.01		0.9101	
11.2	0.78		0.0078	
12.2	0.96		0.0076	
13.5	0.97		0,0097	
14,4	1.01		9.9101	
15.5	0.98		0.0078	
16,5	0.77		0,0099	
17.6	1.04		0.0104	
18.7	1.00		0.0105	
19.7	0.78		0.0098	
20.9	0,91		0.0001	
22.1	0,75		0.0076	
23,2	1,07		0.0107	
24.2	1 70		0.0117	
20.3 74 7	1 1		0,0127 0.0125	
20.3	1 77		0,0122	
28.5	1.09		0.0109	
29.5	0.94		0.0094	
30.6	0.81		0.0081	
31.6	0.57		0,9967	
33.3	0.46		0.0138	
34.3	0.39		0.0038	
34.9	0.31	2	0.00312	
35.8	0.25	-	0.0025	
37.6	0.16	5	0.00166	
33.7	0.12	2	0.00244	
39.6	0.10	3	0,00309	
41.2	0.06	3	0.00189	
3	5	-		
12453				
66.0				
3.0				
0.3				
66.0				
3.0				
120 6.0	73.9	12,0	181.0	10.375
1 10.0	50.0	1.0		

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### APPENDIX V

## OUTPUT PAGE(1)

12C + 181TA AT 10,375 MEV/N

### ALSTER AND CONZET DATA (LOG SCALE)

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1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 19

4

INITIAL CHI-SQUARE (PER 28 DEGREES OF FREEDOM)

### 7.83349

PARAHETER NO.	PARAMETER VALUE	EPSILON	GRADIENT
•	65.000000000	-0,624800-06	<b>0.91348D+01</b>
2	3,000000000	-0,294000-07	0.497210+01
3	0,300000000	-0,28400D-08	0.22873D+02
4	44,9000000000	0,000000+00	0.90000D+00
5	3,000000000	0,00000+00	0.000000+00

THERE WILL BE NO FIT FOR PARAMETERS 4 THROUGH 5

### RESULTS OF FIT

NO. (MAX) OF ITERATIONS ERROR CODE OPTIMIZED CHI-SQUARE 0.903868 20(24) Ø PARAMETER NO. PARAMETER VALUE +/- DP GRADIENT 64.1107382029 -3.449410-05 1 0.159140+00 -0.735370-07 2 2,5726808455 0.15531D+00 3 0.360750-01 -0.95264D-06 0,5847672986

APPENDIX V OUTPUT PAGE (2)

	INDEPENDENT	DEPENDENT	WEIGHT	OPTIMIZED DEPENDENT	FNC (P (0PT) , X) -Y	CONTRIB. TO CHI-SQUARE
•				000135	-8,44993D-82	8 . 723888D-82
- (					-0.640370-05	9.1557480-97
C1 P					8.85991D-82	8.244886D-01
ŋ (				0 007140	-0.159430-01	9.9977340-91
<del>,</del> 1					-0.880880-02	<b>9.</b> 277122D-81
0			001000100	0.004914	-0.181420-01	0.117551D+09
6 P				0.007957	-8.363520-82	0.4719510-02
× α			0.10001-05	018985	6.923120-62	0.384339D-91
) Ø		-0.004345	0.10091+05	-0.005954	9.159950-82	0.9137520-03
- C			0 10001-05	8.826475	-9.944150-02	g.319365D-01
1 <b>*</b>			8.1868D+65	0.018513	0.267630-92	9.2558820-92
		-9.988774	0.10001+05	-9,018921	8.18147D-91	0.3677360-01
1 P + +		0202020	8.1000D+05	-0.051893	8.189340-81	0.4269750-01
7 -			8 10900÷93	-9.829139	9.10410D-01	9.3378460-81
- 10 4 +		037425	9 . 19901+95	8,824545	0.108410-01	8,421302D-01
1 V 1 F		<b>9</b> , <b>9</b> 75547	8 19901+95	9.978915	0.463150-02	0.7451410-02
)		8 1 1 8 5 9 B	8.18980+85	9.09917	8.11573D-C1	g.478328D-01
		9,996919	8.18801+85	8.100658	-8.315880-82	9,3543960-92
) ( 1 <del>-</del>		871788 B		0.077266	8°99942D-82	8.295373D-81
- C			0.10000+05	8,832498	9,49283D-02	8.847417D-62
ŕ			8 10001+05	-9.824255	-8.24174D-82	0.244666D-02
: 6			0.1000105	-g. 699817	6 . 936230-00	<u>e.246172D-01</u>
1 C		506521-0-	9.10000+0S	54001°0-	8.48177D-82	6.129331D-01
) <b>4</b>		-9.337242	6.1111D+94	-0.332139	-0.51834D-00	
ŗ		-8.428216	e.16660+65	-0.430884	0.105880-01	8.466352D-01
) v   C		-9, 595845	9.10900+05	-8.491745	-0.14100D-01	0.7100270-01
2		-8.62948	9.19980+05	-0.584874	-0.159860-01	19-052216.8
ič	ADDA TT	-9.779892	8.1888D+85	-0.782403	9.551880-92	8.108462D-01
		-913640	8 2588D+84	-0.912160	-8.147990-82	<b>8.195539D-03</b>
- 3		- 8.987163	0.1111D+94	-1.019910	0.327470-01	6.422242D-81
Ē	41.2000	-1.288459	8,1111D+84	-1.215917	0.15258D-01	8.923797D-02
;				•		•

## APPENDIX V

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# OUTPUT PAGE (3)

L	A(L)	L	A(L)	L	A(L)
13	0.23550E-08	14	0.34738F-08	15	0.51240E-08
14	0,20000C 00	17	0 111A0C-07	10	0.144455-07
10	0 74758E-07	20	0 X57975-07	71	0,107700F-07
27	0 77254F-07	23	0 114845-04	24	0 14940E-04
25	0.24987E-04	26	0.348575-04	27	0.543676-06
28	0.24707E 00	29	9.118295-05	30	0.17449E-05
31	<b>9.25738E-05</b>	32	0.37965E-05	33	0.54000E-05
34	0.82604E-05	35	0.12185E-04	36	0.17973E-04
37	0.26511E-04	38	0.39105E-04	39	0.57680E-04
40	0.85080E-04	41	0.12549E-03	42	0.13510E-93
43	0.27301E-03	44	0.40265E-03	45	0,59382E-03
46	0.87568E-03	47	0,12911E-02	49	0,19033E-02
49	0,28050E-02	59	0.41321E-02	51	0.60831E-02
52	0,89471E-02	53	0,13142E-01	54	0.19264E-01
55	0.281595-01	56	0.40987E-01	57	0.39304E-01
58	0.85080E-01	59	0.12062	60	0.16829
61	0.22985	62	0.30567	63	0.37371
64	0,48924	65	0,58556	66	0.67576
67	0.75455	68	0.81932	67	0.86994
70	0,99797	71	0,93571	72	0.95549
73	0.96939	74	0.97904	75	0.98569
76	0,99026	77	0,99337	78	0.99550
79	0.99694	80	0,99793	81	0.99859
52	0,99905	83	0,99935	84	0,99956
85	0,99970	86	<b>0,777</b> 80	87	0,77986
88	0,99991	82	0,99994	90	0,99996
91	0,99997	92	0,99998	93	0.99799
94	0,99999	95	0,99999	96	1.0000
97	1,0000	78	1.0000	97	1,0000
100	1.0000	101	1,0000	102	1,0000
103	1,0000	104	1.0000	105	1,0000
106	1.0000	107	1,0000	108	1.0000
107	1.0000	110	1,0000	111	1,0000
417	1 0000	117	1 0000		

		TUATUO	PAGE (4)		
ANGLE	RATIO OF DIFF, X-SECS	ANGLE	RATID DF Diff. X-SECS	ANGLE	RATIO DF DIFF. X-SECS
	2 98857	11.60	1.0143	12,00	0,98604
		14.00	1.0307	15,80	0.97972
		17,00	1.0249	18,00	1,0692
		20.00	0.93030	21.00	0,88706
		23,69	1.0378	24.00	1.1570
01.00 01.00	1.2414	26.00	1.2654	27,80	1.2248
29, 90	1.1365	29,00	1,0130	30,60	0.87731
MI BB	8,73998	32.88	0,61089	33,89	0.49689
34.99	B. 39744	35,00	0,31476	36,00	0.24679
37, 88	9.15136	38,68	<b>B.</b> 14764	39,00	9.11277
49.99	0.95461E-91	41.80	0,644475-01	42.00	0.48026E-01
47.00	A. 355726-01	44.86	<b>G.</b> 26144E-01	45,00	0.18957E-01
46.00	0.13676E-01	47,00	0.975855-82	48.00	0.685905-02
49,00	<b>9.4</b> 8056E-02				•

F\*\*0

226.32

TOTAL REACTION X-SEC =

APPENDIX V

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