Lawrence Livermore Laboratory

MASTER

D⁺ PRODUCTION BY MULTIPLE CHARGE-TRANSFER COLLISIONS OF LOW-ENERGY
D IONS AND ATOMS IN CESIUM VAPOR

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ABSTRACT

The production of D⁻ by multiple charge-transfer collisions of a D⁺ beam in a cesium-vapor target is considered for D⁺ energies above 300 eV. The cross sections relevant to D⁻ formation are obtained by a least-squares fit of three-charge-state differential equations to experimental yield curves. Implications for production of intense negative-ion beams are discussed, and speculations are made about extrapolation to lower energies.

INTRODUCTION

A very promising technique for efficiently producing high energy (> 75 keV/nucleon) neutral beams for injection into fusion devices is acceleration and subsequent stripping of an intense beam of negative ions of hydrogen isotopes¹. Such beams are used for heating and fueling the plasma. One major method of producing intense negative hydrogen (or hydrogen isotope) ion beams is conversion of $H^+(D^+)$ ions to $H^-(D^-)$ ions in a suitable charge-transfer target, typically a metal vapor.

Metal-vapor targets are usually used as the charge-exchange medium for the conversion of $H^+(D^+)$ to $H^-(D^-)$ because the yield obtainable is an order of magnitude larger than in any known gas target at the optimum energy for each target. Metal vapors also are easily pumped and can also serve as a reflector for source gas, thus reducing pumping requirements. Current development efforts use cesium² and sodium³. Other metal vapors could also be used.

The D^- equilibrium fraction in cesium and rubidium vapors is very large at D energies of several hundred eV, reaching a value as large as 35% in cesium vapor at a D energy of 300-400 eV, the lowest energies at which these measurements have been made⁴. At these energies the possibility of obtaining the initial ions from beams of plasma offers an attractive means of obtaining high current densities⁵. Such a technique has several potential advantages. In particular, the plasma generator would be insensitive to small amounts of cesium, a very intense beam can be formed, and the initial beam is space-charge neutralized and can propagate to the charge-exchange cell without blowing up. The D^+ would then be converted to D^- in the target cell by charge-transfer collisions.

The present note considers the atomic physics in the target cell at low energies. Problems of production of the initial plasma or ion beam and its angular divergence, propagation of the negative ion beam, and so forth, are not analyzed here.

F_-^∞ and Charge-Transfer Cross Sections for D^-

The equilibrium fraction, F_-^∞ , of negative deuterium ions in cesium vapor is shown in Fig. 1 (taken from Ref. 4). All published results of which we are aware are shown. Schlachter⁴ discusses possible causes for the discrepancies among the data.

The results we consider to be the most reliable for F_-^∞ in cesium vapor are those of Schlachter et al.⁶, shown in detail in Fig. 2. The experimenters took into account corrections due to loss of beam scattered out of the solid angle seen by the detectors, used a heat-pipe target to be able to reach a target thickness sufficient for charge-state equilibrium, and used a pyroelectric detector to measure the flux of fast neutral atoms leaving the target. We consider these results to be more reliable than other recent measurements (see the discussion in Ref. 4).

These results for F_-^∞ in cesium vapor show a plateau at a D energy of 300-400 eV. Although it is expected that, at a sufficiently low energy, F_-^∞ will decrease with decreasing energy, there are at present no experimental data for D energies below 300 eV.

Yield curves, i.e., charge-state fractions as a function of target thickness, are uniquely determined by the charge-transfer cross sections. If the cross sections for all the relevant collisional processes are known, the charge-state fractions can be calculated. The inverse is almost true: if one can model the collisional interaction (determine the relevant charge

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Figure 1. Equilibrium fraction (F_{∞}) of D^{-} in Cs vapor, from Ref. 4. The numbers correspond to the references in this report.

XBL 776-1108

Figure 2. Equilibrium fraction (F_{∞}) of D^- in cesium, from Ref. 6. These results were obtained from the data used in this report.

states), a consistent set of cross sections can be calculated by fitting the differential equations for the charge-state-components to experimental yield curves. Two potential pitfalls of this method of determining cross sections are (1) that it is a priori very difficult to ascertain the correctness of the model, that is, to incorporate in the model all the relevant particle states (excited states of the neutral atom are actually independent states), and (2) uniqueness of the set of cross sections found by this fitting technique is not guaranteed, and indeed must be shown, because the solution of the charge-transfer differential equations depends nonlinearly on the cross sections.¹⁵

The model used for the present note assumes only three relevant charge-state components: D^+ , D^0 in the ground state, and D^- . The state D^+ is, of course, unique; D^- is believed to have only one state. The D^0 atom can exist in many excited states, some of which are metastable and are therefore long-lived. However, it is known that the metastable $2s$ state plays almost no role in D^- formation in cesium vapor at low energies¹⁶ because $D(2s)$ is collisionally de-excited by collisions in cesium vapor. The present model does neglect effects due to higher long-lived excited states of D^0 . This three-component model is, however, expected to uniquely determine those cross sections which dominate the D^- formation. As excited states are not included there is no possibility of incorrect results due to too many degrees of freedom for fitting the data. This prevents the problem of strong correlations among calculated cross sections and hence a nonunique fit.

Experimental measurements of charge-state fractions (D^+ , D^0 , and D^-) from Schlachter et al. (unpublished) have been used to determine the charge-transfer cross sections. The thick-target part of these same data have

already been shown as F_{c}^{∞} (Fig. 1 and also References 4 and 6). The cross sections were found by a least-squares fit to the data, as described in Appendix I.

The experiment of Schlachter et al. was designed to measure thick-target yields rather than cross sections, so there are some uncertainties in the yield curves which should be mentioned:

(1) although target density can be determined from the target temperature by use of vapor-pressure data, the effective target length is not easily measurable, and has to be inferred by normalization (see next paragraph);

(2) the target was not always in thermodynamic equilibrium, hence the measured temperature did not always correspond precisely to the temperature of the cesium reservoir;

(3) it is assumed that a global scattering correction can be made. This will result if all charge-state components scatter through equal angles in a single collision or if all scattering angles are small compared to the acceptance angle of the detector¹⁷. With these reservations in mind, we nonetheless find that most of the cross sections determined by fitting the yield curves agree well with previous direct measurements. Thus, despite our caveats, the method is reasonably valid.

The absolute magnitude of the cross sections was determined by a one parameter fit to previous measurements of σ_{+0} at 1 keV. The parameter fitted corresponds to the length of the cesium cell used in the present experiment. An error in this normalization would change the magnitude of all the present cross sections by the same factor.

All known cross sections for charge-transfer of D ions and ground-state

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Figure 3. D - Cs cross sections, from Ref. 4. The points are the present results. The numbers correspond to the references in this report.

XBL779-2304

Figure 4. D - Cs cross sections, from Ref. 4. The points are the present results. The numbers correspond to the references in this report.

atoms in cesium vapor are shown in Figs. 3 and 4 (from Reference 4), along with the cross sections determined by the present method.

The cross section σ_{+0} has the same energy dependence as in previous direct measurements; the magnitude agrees because of our normalization. Our results are of insufficient accuracy to observe the maximum predicted by theory¹⁸. This is a matter of some interest because the charge-exchange neutralization of positive ions may be important at low energies for other purposes. Further measurements will be required to determine scaling at low energies.

As discussed in Appendix I, the value of σ_{+-} is not accurately determined in these experiments. The discrepancy (Fig. 3) between the present data and past results is consequently not significant.

There have been no direct measurements of σ_{-0} at low energies. The experimental results of Leslie et al.²⁰ as shown have been renormalized upward by a factor of 2 from their published values, to take advantage of more recent data (remeasurement of σ_{+0} at 30 keV; they had previously normalized to a σ_{+0} value now considered to be low by a factor of 2). Although this renormalization appears to make the agreement with the present results for σ_{-0} worse, it does bring their results at high energies into agreement with their own more recent measurements of σ_{-0} at high energies. Furthermore, this renormalization was done with the full agreement of one of the authors of the original paper (L. W. Anderson).

Our determination of σ_{-0} agrees well with the calculation of Olson¹⁸ at 10 keV, but diverges seriously with decreasing energy. Olson believes that further calculations are required.²⁴

Our determination of σ_{0-} is in excellent agreement with previous directly-measured results.^{9,13} We obtain a maximum in σ_{0-} between 500 eV and 1000 eV. It follows that increasingly large line densities of cesium will be required at low energies to obtain an equilibrium yield of D^- . On the other hand, between 300 eV and about 500 eV the energy dependence of σ_{0-} is almost the same as that of σ_{0+} , corresponding to the flat region of F_-^∞ shown in Fig. 2. It is thus quite possible that F_-^∞ remains large at low energies, despite the falloff in the cross sections.

Our determination of σ_{0+} is not in good agreement with the calculation of Olson¹⁸ (note that Olson's values as shown have been divided by a factor of 4 to correct for an error in the original publication). However, a translation in energy would improve the agreement. Olson²⁴ expects that a new calculation might bring theory into better agreement with experiment.

Our determination of σ_{-} gives results somewhat larger than previous direct measurements. Although our determination of this cross section is somewhat uncertain, especially at low energies where σ_{0+} is small, it is plausible that our values would be larger than direct measurements with a ground-state beam. The electron-loss cross section is known to be sensitive to an admixture of excited atoms in the incident beam. Since the electron-loss cross section can be much larger for atoms in an excited state than in the ground state, a small admixture of excited atoms in the beam can lead to a much larger effective electron-loss cross section than is found by direct measurement with a beam predominantly in the ground state²⁵. The electron-capture cross section, however, is probably relatively insensitive to an

admixture of excited states in the incident beam. It is expected that the electron-capture cross section is smaller for excited atoms than for ground-state atoms, as the only stable D^- state is the $1s^2$.

Angular Scattering During D^- Formation

Angular scattering of the beam becomes increasingly important as the particle energy is lowered. Hooper and Willmann¹⁷ have developed the theory of angular scattering in a charge-exchanging beam. However, the only differential cross section data available¹³ do not include the minus-neutral transition or elastic collisions. In the absence of these data, the theory cannot be applied to beams in which there is an appreciable negative ion fraction.

In the experiments by Schlachter et al.⁶ the total beam current to the detectors was measured. The detector half-angle acceptance was 1.9° , so these results provide a one-point measurement of the effects of angular scattering. Figure 5 shows f_- , the maximum negative-ion current to the detector, normalized to the initial positive-ion current into the charge-exchange target. Also shown is the cesium line density (target thickness), $n\lambda$, at which the maximum occurs. These results are subject to many of the same caveats discussed previously.

The figure also includes F_-^{∞} and the ratio f_-/F_-^{∞} . The latter, perhaps the best single measure of the importance of scattering, has dropped to 50% at 400 eV. It is clear that angular scattering effects will be important at low energies.

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Figure 5. Maximum negative current (f_-) collected on the detector (Ref. 6), normalized to the total current into the cesium cell. This is compared with F_∞ . Also plotted is the cesium line density at the maximum of f_- .

DISCUSSION

The equilibrium yield of D^- in cesium vapor, F_-^∞ , appears to reach a plateau value of 35% at the lowest D energies, 300-500 eV, used in the present experiment. Experimental difficulties (reliable measurement of the low intensity, low energy flux of D^0 atoms in the scattered beam) preclude extension of these measurements to lower energies without major redesign of the apparatus and techniques. It is thus of interest to extract cross sections for the individual collision processes in order to attempt to predict D^- formation at lower energies, at which no measurements are available.

We find that σ_{0-} and σ_{-0} are both decreasing with decreasing beam energy below about 800 eV, but the two curves are parallel at the lowest energy at which we have data, 300 eV. In the model in which the only important states are D^- and ground-state D^0 , (the D^+ fraction is negligible in a thick Cs target at low energies), the equilibrium yield of D^- , F_-^∞ , is $\sigma_{0-}/(\sigma_{0-} + \sigma_{-0})$. That the two cross-section curves are parallel is the same as saying that F_-^∞ has a plateau with energy.

We cannot predict F_-^∞ at low energies from the present results. It is, however, encouraging that the curves for σ_{0-} and σ_{-0} are parallel. Although we eventually expect F_-^∞ to approach zero for a sufficiently low energy, the cross section behavior does not preclude F_-^∞ remaining usably high down in the 50-100eV region. This speculation is, of course, no substitute for a measurement of F_-^∞ down to these energies.

The binding energy of the electron on a D^- (or H^-) ion is 0.75 eV. Ionization by a free electron thus requires a minimum speed of 5.2×10^7 cm/sec,

corresponding to this energy, and a deuteron at this speed would have an energy of 2.75 keV. At energies below this, stripping of the attached electron involves the deuterium and cesium nuclei, so one would expect σ_{-0} to decrease with decreasing energy, as found in Fig. 4. The critical question is the relative scaling of σ_{-0} and σ_{0-} ; hence further experiments and calculations are required.

Angular scattering clearly must be considered at low energy. The result shown in Fig. 5 may, however, over-emphasize the effect upon producing a useful beam. The energy scattered into motion perpendicular to the beam is not significant. A scattering angle of 0.1 radian at 300 eV yields a perpendicular energy of 0.3 eV. This is sufficiently small to not seriously degrade the optics of a high-voltage accelerator, and is probably small compared to the perpendicular energy of the initial beam. Furthermore, the space-charge potential of a background plasma which neutralizes the beam will tend to focus the negative ions,^{26,27} thus alleviating somewhat the beam-spreading problem.

Angular scattering must thus be considered for any system operating at low energies. It will probably be essential to close-couple the cesium charge-exchange cell and the accelerator in order to take advantage of low-energy production.

A background plasma is required to space-charge neutralize the beam. The generation of this plasma²⁸ may require particular attention at low beam energies, as direct ionization by the beam will be weak. The problem of electrons accompanying the beam may be correspondingly reduced, thus simplifying electron suppression.^{26,27}

Finally, we note again that there are no experimental data for the D-Cs interaction below 300 eV and no believable calculations below several keV. This lack of information limits our ability to predict the characteristics of negative ion generation at low energy. Results for D^- production in the low-energy range are urgently required for use in the high-energy neutral-beam program. Furthermore, more insight into the atomic physics of the actual D^- -formation process could be gained by cross-section measurements from 10 keV down to the lowest energies attainable.

APPENDIX I. DETERMINATION OF CHARGE-TRANSFER CROSS SECTIONS

A set of experimental data⁶ consists of simultaneous measurements of the fractions of D^+ , D^0 , and D^- in a beam scattered in a cesium-vapor target of length l and vapor density n , for various values of n ranging from low (thin target, $nl \ll 1$) to high (thick target, i.e. charge-state equilibrium). Such a set of data is called three-charge-state-component yield curves. The D^+ and D^- fractions are measured as currents, while the D^0 fraction is measured by a calorimetric technique (pyroelectric detector). The vapor density n is inferred from the target temperature by use of vapor-pressure data, while the target length l is determined by normalization to published values of σ_{+0} . We find l to be 6.2 ± 0.6 cm. (Because of the design of the heat-pipe target, normalization is felt to be more accurate than directly measuring the geometric length with assumptions about end effects.) Although the charge-state-fraction measurements are only uncertain to a few percent, the density measurement uncertainties might be as large as 20-25%. All data were taken with the incident beam at least 95% in the D^+ state. An example of the data is shown as the dots in Fig. 6.

The data were fit to the model using two techniques. In the first, the data were analyzed by hand to obtain cross sections; the analysis was done over limited target-thickness ranges so that particular collisional processes could be essentially isolated and their cross sections determined. In the second technique a least-squares fit was made of all

Figure 6. Experimental data (dots) and best fit to the data (lines). The percentages F_+ , F_0 , and F_- are plotted as a function of cesium density (per cm^3). At low density the data range from F_+ (maximum value) to F_- (minimum value).

the data to the model. The cross sections determined by both of these methods agreed to within 10% to 20%. We give the results of the second technique here, because they are presumedly more accurate.

The model consists of the solution of the three-charge-state differential equations given by Allison.²⁹ In his notation, the fraction of the beam in the i^{th} state (positive, neutral, or negative) is given by

$$F_i(\pi) = F_{i\infty} + \sum_z F_{z0} [P(z,i) \exp(\pi q) + N(z,i) \exp(-\pi q)] \exp\left(\frac{1}{2} \pi \sum \sigma_{if}\right),$$

where F_{z0} is the initial fraction of beam in the z^{th} state, and π is the line density, i.e., the number of atoms of the target per cm^2 . Allison gives expressions for the other parameters in terms of the six cross sections σ_{+0} , σ_{+-} , σ_{0+} , σ_{0-} , σ_{-+} , and σ_{-0} . In addition, the F_{z0} are parameters; because of normalization only two are independent. In general, therefore, there are eight unknown parameters in the model. In the calculations presented here, σ_{-+} was excluded because the fit was very insensitive to it, so seven parameters are determined.

The cross sections were determined by minimizing the function

$$\chi^2 = \sum_i \sum_j \left(\frac{[y_i(\pi_j) - F_i(\pi_j, \sigma_k)]^2}{y_i(\pi_j) F_i(\pi_j, \sigma_k)} \right)$$

where $y_i(\pi_j)$ is the measured fraction of the i^{th} component at a cesium line density π_j . The cross sections, σ_k , were varied to yield the minimum. The normalization factor, $y_i F_i$, was chosen to provide equal weight to results which varied over several orders of magnitude. No attempt was made to include estimates of the accuracy of individual data points.

The program written for this calculation, "LSTSQ7", is listed in Appendix II. It utilizes the IMSL subroutine ZXSSQ which is a modified Levenberg-Marquardt algorithm for finding the minimum of the sum of squares of M functions of N variables. For our purposes, $N = 7$ and M is the number of data points. Convergence was assumed if $\Delta = .001$ which meant that the Euclidean Norm of the approximate gradient was less than .001. This gave a good balance between computational speed and accuracy.

LSTSQ7 reads in the data and checks for obvious data errors. After performing the least squares calculation, results are both printed and plotted. Figure 6 is a sample output, with the line showing the model fit to the data.

Results are listed in Table 1 and plotted in Figs. 3 and 4. The data were very insensitive to σ_{-+} , and the program did not converge if it was included.

To estimate the accuracy of the results, we have utilized two outputs from the program:

$$SSQ = x^2 \text{ at the minimum}$$

$$(XJTJ)_{ij} \approx \frac{1}{2} \frac{\partial^2 x^2}{\partial x_i \partial x_j}$$

where the x_i are the varied parameters. As we have assumed that all the data are equally accurate, we can estimate the standard deviation for each data point by Δ , where

$$\Delta^2 = \text{SSQ}/(M-N-1).$$

These values are given in Table 1; most are between 5% and 10% as one would estimate from the data.

The mean square accuracy of the cross section σ_i is then estimated by³⁰

$$\Delta_i^2 \approx \Delta^2 * [XJTJ^{-1}]_{ii}$$

where $XJTJ^{-1}$ is the inverse matrix to $XJTJ$. The Δ_i are also included in Table 1. The results must be used with care; in particular stars are used for several values of Δ_{-0} . In these cases $[HJTJ^{-1}]_{ii}$ is very small but negative due to correlation with σ_{0-} . Nevertheless, in all cases the magnitudes of the Δ_i 's are roughly the same size as the scatter in the corresponding (calculated) cross sections, confirming that this scatter is due to uncertainties in the data.

Systematic errors are probably more important than the statistical ones estimated above. The calculated value of σ_{0+} , for example, increases below 600 eV, almost certainly due to systematic effects; the value of Δ_{0+}/σ_{0+} is also relatively large there and these values have been omitted from the figure.

As an indication of the magnitude of systematic effects, two separate runs have been analyzed at 10 keV. The differences are substantial and range from 13% for σ_{-0} to 70% for σ_{+-} . These two runs were chosen because

they showed the worst agreement of any runs at one energy, results at one energy were generally in better agreement.

Table 1. Experimental Cross Sections and Uncertainties

Energy	Δ	σ_{+0}	Δ_{+0}	σ_{0+}	Δ_{+0}	σ_{0-}	Δ_{0-}	σ_{-0}	Δ_{-0}	σ_{+-}	Δ_{+-}
300 eV	0.152	9.0E-15	2.1E-16	5.9E-17	2.5E-17	3.6E-16	2.1E-17	6.4E-16	*	1.6E-17	7.9E-18
400	0.079	1.0E-14	9.9E-17	1.8E-17	5.9E-18	4.3E-16	1.2E-17	7.7E-16	3.3E-19	1.2E-17	2.9E-18
500	0.078	1.1E-14	9.5E-17	1.4E-17	4.9E-18	4.5E-16	1.3E-17	8.8E-16	3.4E-19	1.4E-17	3.4E-19
600	0.040	1.0E-14	3.6E-16	2.1E-17	7.9E-18	4.9E-16	2.0E-17	9.7E-16	1.8E-18	3.9E-17	1.2E-16
800	0.070	1.1E-14	1.1E-16	1.2E-17	5.1E-18	5.1E-16	1.7E-17	1.1E-15	*	2.2E-17	4.6E-18
1 keV	0.115	1.0E-14	6.8E-17	1.4E-17	3.4E-18	4.4E-16	1.0E-17	1.2E-15	*	1.4E-17	2.2E-18
1.5	0.067	7.4E-15	6.8E-17	1.8E-17	5.4E-18	3.2E-16	1.1E-17	1.3E-15	*	1.9E-17	2.2E-18
2.0	0.073	6.6E-15	5.7E-17	1.5E-17	3.1E-18	2.9E-16	9.3E-18	1.3E-15	*	1.5E-17	1.8E-18
2.5	0.068	6.3E-15	6.2E-17	2.7E-17	4.6E-18	2.1E-16	8.1E-18	1.4E-15	*	1.2E-17	2.5E-18
3.0	0.039	5.1E-15	4.4E-17	3.6E-17	3.9E-18	1.6E-16	4.4E-18	1.3E-15	*	4.1E-18	2.3E-18
5.0	0.095	5.1E-15	1.1E-16	5.4E-17	1.2E-17	1.1E-16	7.9E-18	1.6E-15	*	8.2E-18	1.3E-18
7.5	0.055	4.2E-15	4.1E-17	6.4E-17	5.7E-18	7.4E-17	3.0E-18	1.7E-15	*	1.5E-17	8.2E-18
10.**	0.081	4.3E-15	7.9E-17	1.3E-16	1.6E-17	5.1E-17	5.8E-18	2.2E-15	*	2.0E-17	1.7E-18
10.**	0.049	3.0E-15	4.5E-17	8.1E-17	8.2E-18	4.8E-17	3.3E-18	1.7E-15	*	9.7E-18	1.1E-18

* Δ_{-0} not determined (see text).

** Separate data runs.

APPENDIX II. LSTSQ7, PROGRAM TO FIT DATA

```

1 $ ACHAT LSTSQ7 BLS NONE US0 L
2 $ ALOD BLS$ T, O, C, INSL, CLS+ + 1*
3 $ DESTROY ACHATDF ALODDF
4 $ CLS
5 C LSTSQ WRITTEN ON 11/11/77 DETERMINES BY LEAST SQUARES
6 C THE CROSS SECTIONS FOR A THREE COMPONENT CHARGE EXCHANGE BEAM.
7 C FOR A THREE COMPONENT CHARGE-EXCHANGING SYSTEM THE COMPONENT
8 C DENSITIES (IN PERCENT) VS. VAPER LINE DENSITY ARE PROGRAMMED USING
9 C EXPRESSIONS BY S.K. ALLISON. REVIEWS OF MODERN PHYSICS, 30, 1137 (1958).
10 C THESE ARE FIT TO DATA TO DETERMINE THE CROSS SECTIONS AND THE INITIAL
11 C PERCENTAGES OF EACH COMPONENT. THE 0-4 CROSS SECTION IS NEGLECTED.
12 PROGRAM LSTSQ(TAPE2=100, TAPE6=100)
13 COMMON X(400), Y(400), Z(400), M1, M2, EL, SSO, SUMR1, TITLE(6)
14 DIMENSION Q(7), R(400), XJAC(400,7), XJTJ(28), WORK(863)
15 , PARM(4), X1(200), FM(200), FP(200), F0(200), SIG(7)
16 EXTERNAL FUNC
17 100 FORMAT(16I5)
18 101 FORMAT(6F10.4)
19 102 FORMAT(" ERROR IN ZXSSO, IER = ", I5, " OR ERROR IN LIN2VP, JER = ", I5)
20 103 FORMAT(" DATA ERROR IN NEXT LINE")
21 104 FORMAT(1PE12.3, 3P3F10.5)
22 105 FORMAT(6A10)
23 106 FORMAT(" Q SIG"// (1P2E12.3))
24 107 FORMAT(" SSO=", 1PE12.4// " WORK=", 5F10.5)
25 DATA (IER=0), (INFER=0), (IOPT=0), (NSIG=10), (EPS=.000),
26 , (MAXFN=1000), (IXJAC=400), (DELTA=.001), (PARM(1)=0.), (JER=0)
27 , (D1=0.), (R(1)=0.), (XJAC(1,1)=0.), (XJTJ(1)=0.), (WORK(1)=0.)
28 , (SSO=0.), (Q(1)=0.), (EL=6.2), (YMIN=0.), (YMAX=0.), (D2=0.)
29 OPTIMIZE
30 C SET UP DROP FILE FOR DEBUGGING.
31 CALL CHANGE(6H+LSTSQ)
32 C INITIALIZE PLOTS.
33 CALL KEEP80(1)
34 CALL DDB0JD
35 C Q IS VECTOR OF N PARAMETERS.
36 READ (2,105) TITLE
37 WRITE (6,105) TITLE
38 READ (2,100) N
39 READ (2,101) (Q(I), I=1,N-2)
40 C SCALE CROSS SECTIONS.
41 DO 5 I = 1, N-2
42 5 Q(I) = 1.E+15*Q(I)
43 K = 1
44 DO 10 I = 1, 200
45 READ(2,101) X1(I), FM(I), FP(I), F0(I)
46 C CHECK FOR END OF DATA.
47 IF(X1(I).LT.0.) GO TO 15
48 C CHECK FOR DATA ERROR.
49 IF(ABS(FM(I)+FP(I)+F0(I)-100.).GT.101) WRITE(6,103)
50 WRITE (6,104) X1(I), FM(I), FP(I), F0(I)
51 10 CONTINUE
52 15 Q(6) = F0(1)
53 Q(7) = FM(1)
54 DO 20 J = 1, I-1
55 IF(FM(J).LE.0.0) GO TO 20
56 X(K) = X1(J)
57 Y(K) = FM(J)
58 K = K + 1
59 20 CONTINUE
60 C M1 = NUMBER OF FUNCTIONAL VALUES FOR FIRST(F-) EQUATION.
61 M1 = K - 1
62 DO 30 J = 1, I-1

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119 C Q(1)=Q(4)+Q(2)+Q(3)+Q(4)+Q(5)+Q(6)+Q(7)+F-8
120 A = -(Q(2)+Q(3)+Q(4))
121 B = Q(1) - Q(4)
122 F = Q(2)
123 G = -Q(1) - F
124 S = F*(G-A)
125 A = A*(G-A)
126 F = -(G-A)
127 FPI = (F*(G-A))/D
128 FFI = (F*(G-A))/D
129 FFI = (F*(G-A))/D - F*(G-A)/D
130 QU = .5*(SORTI((G-A)/F)-1.0)
131 C IN FOLLOWING VECTORS + IN (1)*S. 0 IN (2)*S. - IN (3)*S.
132 F0(1) = 169. - G(7) - Q(4)
133 F0(2) = Q(6)
134 F0(3) = Q(7)
135 TUDD = 2.*QU
136 PP0(1) = (D*FPI+(B-G-QU)*FFI)/TUDD
137 PP0(2) = -(S-QU)*(1.-FFI)+B*FFI/TUDD
138 PP0(3) = ((S-QU)*FFI-D*FPI)/TUDD
139 ENP0(1) = -(B*FPI+(B-G-QU)*FFI)/TUDD
140 ENP0(2) = ((S-QU)*(1.-FFI)+B*FFI)/TUDD
141 ENP0(3) = -(S-QU)*FFI-B*FFI/TUDD
142 D0 5 J = 1, 3
143 PPP(1) = PP0(1)*(S+QU)/D
144 PPH(1) = -PP0(1)*(B-G-QU)/B
145 ENPP(1) = ENP0(1)*(S+QU)/B
146 ENPM(1) = -ENP0(1)*(B-G-QU)/B
147 5 CONTINUE
148 C WE MULTIPLIED THE Q'S BY 1.615 AT START TO MAKE THEM NEAR 1.
149 ARG1 = 1.6-15*QUML
150 ARG2 = .5E-15*TMEL
151 SUM1 = 0.
152 D0 10 I = 1, M
153 E1 = EXP1(ARG1*(X(I)))
154 E2 = EXP1(ARG1*(Y(I)))
155 E3 = EXP1(ARG2*(X(I)))
156 IF(1.GT.M1) GO TO 7
157 C CALCULATE THEORETICAL F'S.
158 FI = 100.*FPI
159 D0 6 J = 1, 3
160 FI = FI + F0(J)*E3*(PPM(J)*E1+ENPM(J)*E2)
161 6 CONTINUE
162 GO TO 11
163 7 IF(1.GT.M2) GO TO 9
164 C CALCULATE THEORETICAL F0'S.
165 FI = 100.*FFI
166 D0 8 J = 1, 3
167 FI = FI + F0(J)*E3*(PP0(J)*E1+ENP0(J)*E2)
168 8 CONTINUE
169 GO TO 11
170 C CALCULATE THEORETICAL F0'S.
171 FI = 100.*FBI
172 D0 10 J = 1, 3
173 FI = FI + F0(J)*E3*(PP0(J)*E1+ENP0(J)*E2)
174 10 CONTINUE
175 11 IF(FI.LT.8.) CALL QUIT(1)
176 R(I) = (Y(I)-FI)/SORTI(Y(I)*FI)
177 Z(I) = FI
178 IF(MOD(11,N+1),EQ.8) WRITE(6,101) 1,X(I),Y(I),FI,R(I)
179 SUM1 = SUM1 + R(I)**2
180 1C CONTINUE
181 I = I + 1
182 IF(11.GT.1) GO TO 20
183 C PLOT THEORETICAL CURVES USING STARTING APPROXIMATIONS.
184 CALL TRACE(X,Z,M1)
185 CALL TRACE(X,R1,M1),Z(M1+1),M2-M1)
186 CALL TRACE(X,Z(M2+1),M1)
187 CALL FRAME
188 20 RETURN
189 END

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