NUMERICAL COMPUTATION OF IONIC CHARGE DISTRIBUTIONS AND THE ANALYSIS OF EXPERIMENTAL EQUILIBRIUM DISTRIBUTIONS

by

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B.S., Tunghai University, 1964

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

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KANSAS STATE UNIVERSITY
Manhattan, Kansas

1969

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CHAPTER I

INTRODUCTION

In recent years the investigation of the interaction of fast heavy ions passing through matter has received increased attention. The first studies of electron charge exchange processes began as early as 1922, but not until 1948, when accelerators were developed, were intensified studies begun. In particular the improved techniques for the acceleration of heavy ions, which are still being developed further, allow more specific experiments where the nuclear and ionic charge of the incident ions as well as the energy can be chosen and varied within wide limits. As not too many experiments with highly charged ions have been done in the past, this special field of heavy ion physics is potentially rich and may contribute not only to an improvement of future heavy ion accelerators, which are also of great use in many other fields, but in addition to a better understanding of the complicated charge exchange collisions, a many body problem which is difficult to describe by theoretical methods.

In this work, a few contributions of an auxiliary but basic character are presented. In part II, the process of electron loss and capture is described, the basic differential equations for the charge exchange collisions are discussed and the experimental and theoretical situation prior to 1969 is briefly summarized. Parts III and IV give two basic computer programs which are usually of great importance when

experimental data of heavy ion charge states are to be analyzed; in the program NEDT, methods for the numerical integration of the fundamental system of differential equations for ionic charge states are given, and in the routine EQUDIS, the equilibrium charge fractions are calculated. Both programs can be used for any sets of given ionic charge exchange cross sections. In order to use those routines for iteration procedures, special attention was given to keeping the computational execution time at a minimum. Finally, in part V, an analysis of the shape of equilibrium distributions is attempted. Experimental distributions, measured at Oak Ridge, have been fitted to Gaussian and more general distributions. Characteristic deviations from a Gaussian distribution as well as asymmetries have been found. Distributions of Br ions at 20 MeV and I ions at 15 and 60 MeV stripped in dilute gases of H_2, He, N_2, Ne, Ar and Kr have been analyzed in this work.

CHAPTER II

DESCRIPTION OF THE CHARGE EXCHANGE PROCESS

When ions enter into a gaseous or solid target, collisions take place between the ions and the target atoms. In such a collision, the incident ion may either capture or lose one or more electrons. Therefore, one can define a cross section σ_{ij}, which describes the probability that the charge i of an ion changes into j during an encounter. The cross sections are usually given in cm^2/atom, but sometimes the units cm^2/molecule are preferred, especially if the target consists of molecules.

We consider only those collisions in which the charge of the ions is actually changed. The cross sections introduced above do not take into account elastic collisions or encounters in which only excitation occurs. If we assume further, that the total energy loss of all ions in the target is negligible, the relative fractions, Y_i , of ions carrying a charge i in a beam, change with increased target thickness x, measured in atoms of molecules per cm^2 as follows:

$$\frac{dY_i}{dx} = \sum_j \sigma_{ji} Y_j \qquad \sigma_{ij} = - \sum_{j \neq i} \sigma_{ji} \cdot \tag{2.1}$$

In this system of equations all possible charge transfers are taken into account. If we neglect the probabilities for multiple electron exchange and consider only collisions in which

the charge of the ions charges by one unit of charge ($|j - i| = 1$), Eq. (1) reduces to

$$\frac{dY_i}{dx} = \sigma_L(i-1)Y_{i-1} - (\sigma_L(i) + \sigma_L(i)Y_i + \sigma_L(i+1)Y_{i+1} , \qquad (2.2)$$

where $\sigma_c(i) = \sigma_{i,i-1}$ and $\sigma_L(i) = \sigma_{i,i+1}$ are used for a better understanding of the influence of capture and loss processes on the charge state populations, as expressed in Eq. (2).

The reduced form in Eq. (2) may be used in connection with light ions stripped in light targets such as H_2 or He. In this case, the probabilities for multiple electron exchange are very small and can be neglected. But if the ions have a large atomic number, or if the target is heavy, simultaneous capture or loss of more than one electron in a single collision has an increased probability and cannot be neglected. Thus the system (1) is to be used. For example, if Br ions pass through an argon target, double loss is approximately half as likely as single loss. As the present work is mainly concerned with stripping of heavy ions, the complete system (1) will be considered in this and the following chapters.

The range of different charge states i in Eq. (1) should include all significant charge states. In principle, all charges ranging from i = -1 to i = Z, the nuclear charge of the ion in question, are possible. In practice, however, an ion beam shows only a limited number of charges even after

having passed through a thick target. For Br and I ions, usually 10 to 12 adjacent charge fractions can be observed.

If an incident beam consists of ions which carry the same charge i, a whole distribution of charge states will be produced according to the various charge changing probabilities σ_{ij}. Thus the various charge fractions Y_j will change with x, the thickness of the stripper. The corresponding distribution is called a non-equilibrium distribution, which is, of course, a solution of Eq. (1). An example for such a distribution is shown in Plates 1a through c and Table 1a through c. The distribution depends on the initial charge state of the incident ions. As the thickness of the stripper is increased more and more, all charge fractions approach a constant equilibrium value. These equilibrium fractions are no longer dependent on the special initial conditions or on the target thickness, as soon as the equilibrium thickness is reached. Examples for equilibrium distributions are discussed in part V. The equilibrium distribution is determined by the species of ions, their energy, and by the target material.

Experiments have shown that the energy loss is indeed very small, as long as x does not greatly exceed the equilibrium value. Therefore, one can assume that there is no energy dependence of the cross sections within a given system (1), and one then has constant coefficients. Another effect, however, can cause serious complications. If the target is very dense, excited ions will not have fallen back into the

EXPLANATION OF PLATE 1

Example for non-equilibrium charge distributions obtained with program NEDT. Initial pure charge states are 1+, 4+, and 6+ (Plates 1 a, b, c respectively).

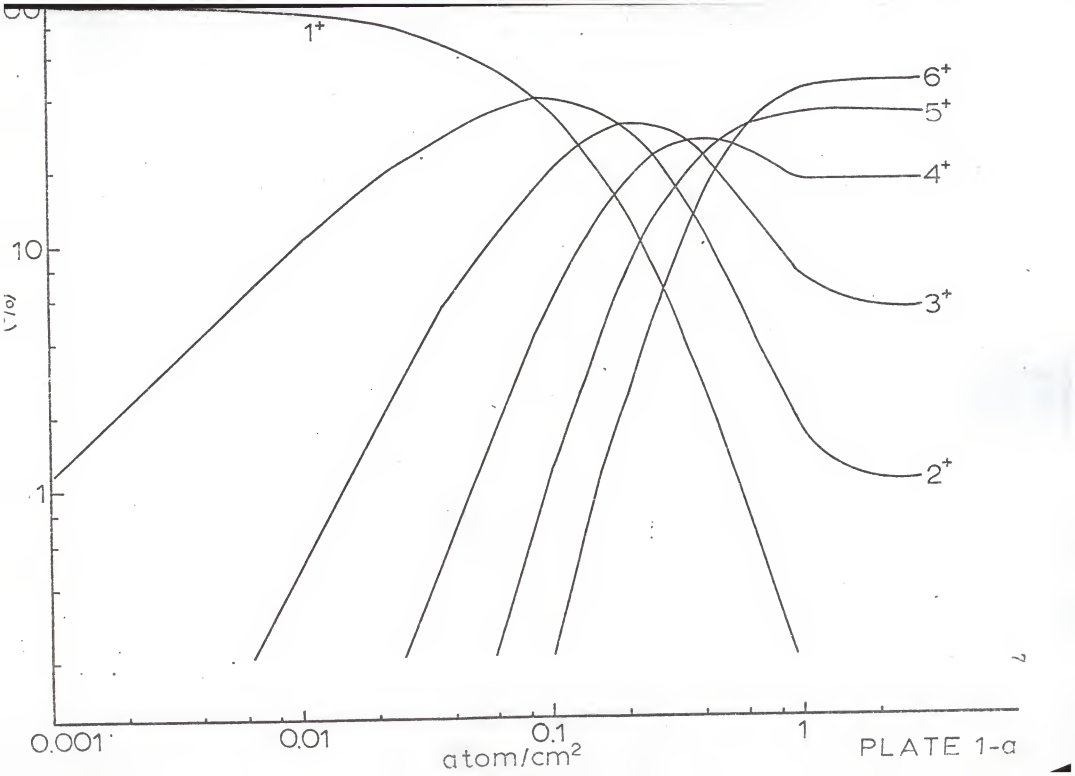


PLATE 1-a

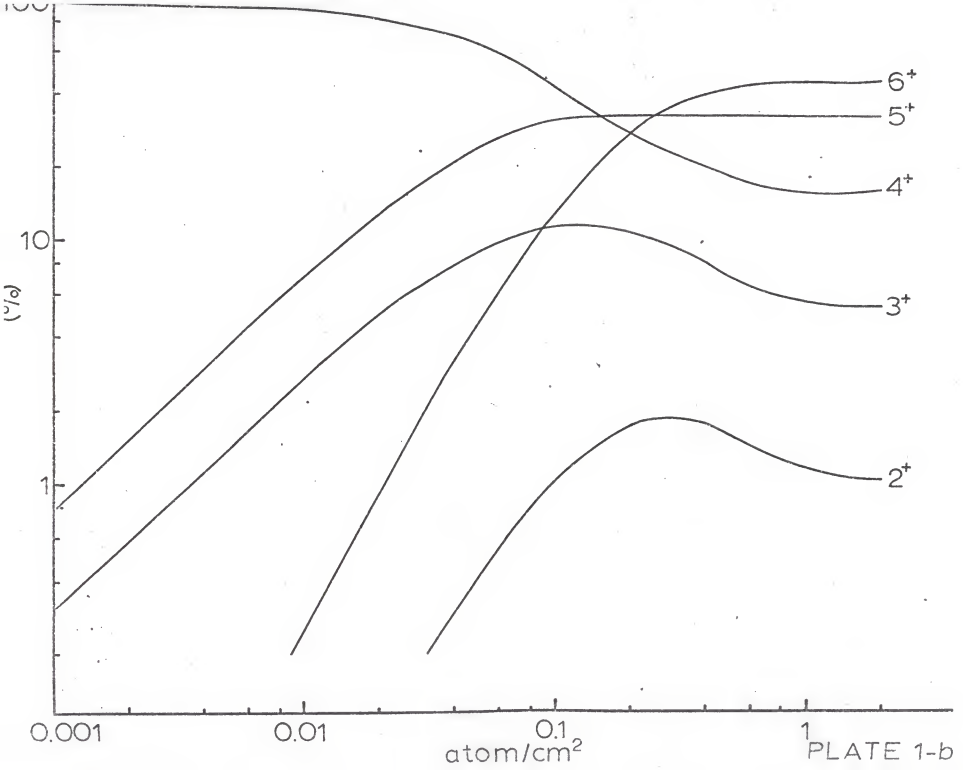


PLATE 1-b

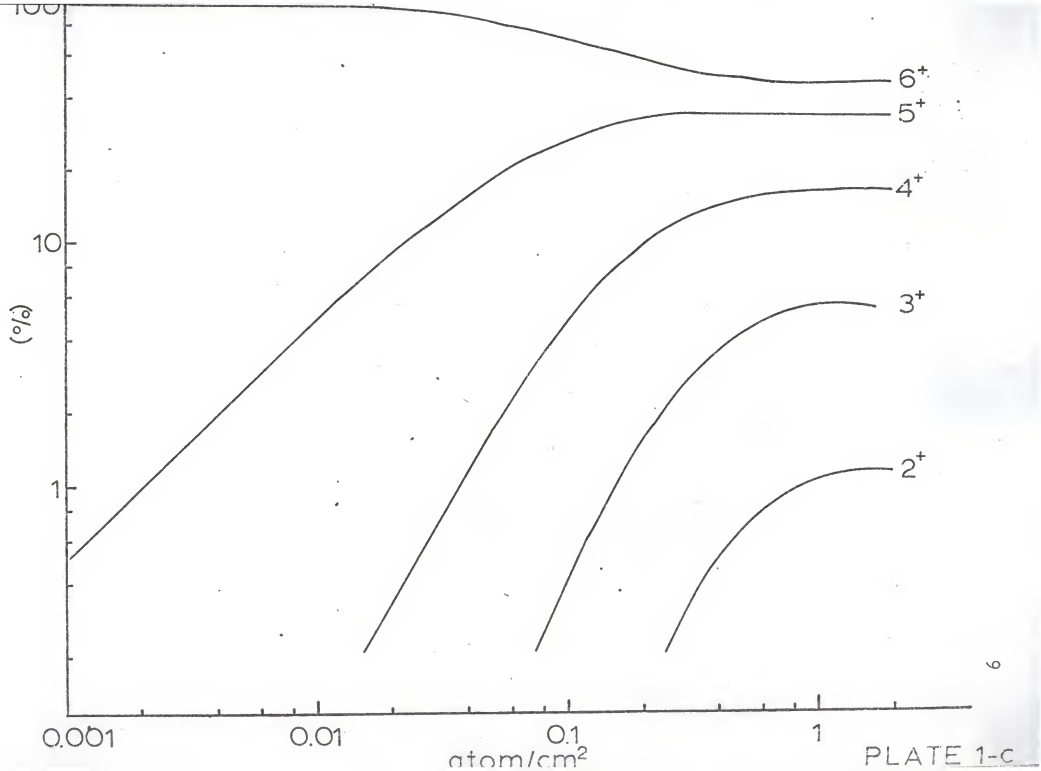


PLATE 1-c

Table 1-a Non-equilibrium charge distribution obtained with program NEDT. Initial charge state is 1+.

Ionic Charge Distribution		Non-equilibrium			Initial Charge 1+		
X	ZQX	Y(1)	Y(2)	Y(3)	Y(4)	Y(5)	Y(6)
0.0010	1.00	98.900	1.100	0.000	0.000	0.000	0.000
0.0020	1.02	97.819	2.165	0.016	0.000	0.000	0.000
0.0030	1.03	96.752	3.206	0.042	0.000	0.000	0.000
0.0040	1.04	95.696	4.224	0.078	0.001	0.000	0.000
0.0050	1.05	94.654	5.220	0.124	0.002	0.000	0.000
0.0060	1.07	93.623	6.194	0.179	0.003	0.000	0.000
0.0070	1.08	92.605	7.146	0.243	0.005	0.000	0.000
0.0080	1.09	91.559	8.078	0.316	0.007	0.000	0.000
0.0090	1.10	90.604	8.988	0.397	0.010	0.000	0.000
0.0100	1.11	89.621	9.879	0.485	0.014	0.000	0.000
0.0200	1.22	80.393	17.751	1.750	0.102	0.004	0.000
0.0300	1.32	72.192	23.923	3.553	0.312	0.018	0.001
0.0400	1.42	64.898	28.683	5.695	0.670	0.052	0.003
0.0500	1.52	58.402	32.270	8.021	1.184	0.115	0.008
0.0600	1.62	52.611	34.889	10.417	1.848	0.217	0.019
0.0700	1.72	47.443	36.710	12.795	2.652	0.363	0.037
0.0800	1.81	42.824	37.878	15.095	3.577	0.560	0.066
0.0900	1.91	38.689	38.515	17.272	4.605	0.812	0.108
0.1000	2.00	34.976	38.726	19.300	5.714	1.118	0.166
0.2000	2.81	13.417	29.926	29.902	17.670	6.903	2.182
0.3000	3.46	5.761	19.021	28.221	24.872	14.719	7.406
0.4000	3.95	2.751	11.841	22.973	26.643	21.188	14.605
0.5000	4.32	1.450	7.579	17.926	25.573	25.535	21.936
0.6000	4.58	0.836	5.077	14.018	23.594	28.203	28.273
0.7000	4.76	0.524	3.583	11.223	21.636	29.786	33.248
0.8000	4.89	0.353	2.670	9.291	20.027	30.724	36.934
0.9000	4.97	0.255	2.098	7.977	18.812	31.289	39.568
1.0000	5.03	0.196	1.732	7.086	17.934	31.637	41.414
2.0000	5.15	0.099	1.082	5.391	16.135	32.220	45.073
3.0000	5.15	0.098	1.074	5.371	16.114	32.226	45.117
Equilibrium Distribution							
3.3125	5.15	0.098	1.074	5.371	16.113	32.227	45.117
Exact Equilibrium Distribution as Follows							
	5.15	0.098	1.074	5.371	16.113	32.227	45.117

Table 1-b Non-equilibrium charge distributions obtained with program NEDT. Initial charge state is 4+.

Ionic Charge Distribution		Non-equilibrium Initial Charge 4+					
X	ZQX	Y(1)	Y(2)	Y(3)	Y(4)	Y(5)	Y(6)
0.0010	4.00	0.000	0.000	0.300	98.900	0.800	0.000
0.0020	4.01	0.000	0.001	0.590	97.826	1.574	0.008
0.0030	4.01	0.000	0.002	0.874	96.770	2.331	0.022
0.0040	4.02	0.000	0.004	1.152	95.731	3.072	0.040
0.0050	4.02	0.000	0.007	1.424	94.709	3.797	0.064
0.0060	4.03	0.000	0.010	1.689	93.703	4.506	0.093
0.0070	4.03	0.000	0.013	1.949	92.713	5.199	0.126
0.0080	4.04	0.000	0.017	2.204	91.738	5.877	0.164
0.0090	4.04	0.000	0.022	2.452	90.779	6.541	0.206
0.0100	4.05	0.000	0.027	2.696	89.835	7.190	0.253
0.0200	4.10	0.001	0.096	4.852	81.170	12.951	0.031
0.0300	4.14	0.002	0.195	6.563	73.768	17.544	1.929
0.0400	4.19	0.004	0.312	7.911	67.423	21.191	3.159
0.0500	4.23	0.007	0.440	8.964	61.963	24.073	4.552
0.0600	4.27	0.011	0.573	9.774	57.249	26.340	6.053
0.0700	4.31	0.016	0.707	10.388	53.162	28.110	7.618
0.0800	4.35	0.022	0.836	10.843	49.603	29.482	9.214
0.0900	4.39	0.028	0.961	11.168	46.491	30.536	10.816
0.1000	4.42	0.035	1.078	11.389	43.756	31.338	12.404
0.2000	4.70	0.107	1.792	10.858	28.566	33.007	25.669
0.3000	4.86	0.150	1.892	9.262	22.773	32.320	33.603
0.4000	4.96	0.161	1.766	8.001	19.975	31.988	38.108
0.5000	5.03	0.155	1.598	7.128	18.457	31.928	40.734
0.6000	5.07	0.143	1.450	6.541	17.578	31.968	42.321
0.7000	5.09	0.131	1.337	6.149	17.047	32.029	43.308
0.8000	5.11	0.122	1.254	5.888	16.716	32.084	43.937
0.9000	5.12	0.114	1.196	5.714	16.506	32.127	44.344
1.0000	5.13	0.109	1.156	5.597	16.369	32.159	44.610
2.0000	5.15	0.098	1.075	5.374	16.117	32.226	45.110
Equilibrium Distribution							
2.8889	5.15	0.098	1.074	5.371	16.113	32.227	45.117

Table 1-c Non-equilibrium charge distribution obtained with program NEDT. Initial charge state is 6+.

Ionic Charge Distribution			Non-equilibrium		Initial Charge 6+		
X	ZQX	Y(1)	Y(2)	Y(3)	Y(4)	Y(5)	Y(6)
0.0010	6.00	0.000	0.000	0.000	0.000	0.500	99.500
0.0020	5.99	0.000	0.000	0.000	0.008	0.988	99.009
0.0030	5.99	0.000	0.000	0.000	0.008	1.469	98.524
0.0040	5.98	0.000	0.000	0.000	0.014	1.942	98.044
0.0050	5.98	0.000	0.000	0.000	0.023	2.407	97.570
0.0060	5.97	0.000	0.000	0.000	0.033	2.865	97.102
0.0070	5.97	0.000	0.000	0.000	0.045	3.316	96.639
0.0080	5.96	0.000	0.000	0.000	0.058	3.760	96.181
0.0090	5.96	0.000	0.000	0.001	0.074	4.197	95.729
0.0100	5.95	0.000	0.000	0.001	0.090	4.627	95.282
0.0200	5.91	0.000	0.000	0.006	0.332	8.578	91.083
0.0300	5.87	0.000	0.000	0.020	0.689	11.953	87.338
0.0400	5.83	0.000	0.001	0.044	1.128	14.839	83.989
0.0500	5.79	0.000	0.002	0.078	1.626	17.309	80.985
0.0600	5.76	0.000	0.004	0.124	2.162	19.426	78.285
0.0700	5.73	0.000	0.006	0.180	2.721	21.244	75.849
0.0800	5.70	0.000	0.009	0.247	3.291	22.806	73.647
0.0900	5.67	0.000	0.014	0.324	3.863	24.150	71.649
0.1000	5.65	0.000	0.019	0.409	4.430	25.311	69.830
0.2000	5.46	0.005	0.134	1.526	9.168	30.947	58.221
0.3000	5.34	0.016	0.319	2.652	12.001	32.235	52.777
0.4000	5.28	0.032	0.510	3.518	13.610	32.492	49.839
0.5000	5.23	0.047	0.670	4.127	14.548	32.492	48.116
0.6000	5.20	0.061	0.793	4.540	15.114	32.436	47.056
0.7000	5.18	0.072	0.881	4.818	15.467	32.379	46.383
0.8000	5.17	0.080	0.943	5.003	15.692	32.333	45.949
0.9000	5.16	0.085	0.986	5.127	15.837	32.300	45.665
1.0000	5.16	0.089	1.016	5.210	15.932	32.276	45.477
2.0000	5.15	0.098	1.073	5.369	16.111	32.227	45.122
Equilibrium Distribution							
2.8148	5.15	0.098	1.074	5.371	16.113	32.227	45.117

Cross-sections for Capture (IN 10E-16 CM2/MOL)

N	SC(1)	SC(2)	SC(3)	SC(4)	SC(5)	SC(6)	SC(7)
1	0.0	1.000	2.000	3.000	4.000	5.000	

Cross-sections for Loss (IN 10E-16 CM2/MOL)

N	SL(1)	SL(2)	SL(3)	SL(4)	SL(5)	SL(6)	SL(7)
1	11.000	10.000	9.000	8.000	7.000		

ground state when they undergo the next collision, and the probabilities for charge exchange from and into excited states differ considerably from those for the ground state. Then the form of Eq. (1) cannot be used. In this work attention is confined to very dilute gaseous strippers, where excitations are believed to have no significant influence.

An interesting quantity is the mean ionic charge $\bar{I}$, the center of an equilibrium distribution. The usual definition is

$$\bar{I} = \sum_i i\, Y_i \,, \qquad (2.3)$$

where Y_i are normalized charge fractions ($\sum_i Y_i = 1$). On the other hand, highly asymmetrical charge distributions are very often observed; consequently the most probably charge i, which is the charge for which the smoothed distribution shows its maximum may be defined. For symmetrical distributions, $\bar{I}$ equals i, but for asymetrical distributions, differences $\bar{I} - i$ 0.6 can be found. Further details are discussed in part V.

Present Status of Experiments and Theories

A detailed review of the investigations of charge exchange collisions prior to 1965 can be found in an article by V. S. Nikolaev (1). Briefly, the development was as follows. Rutherford (2), one of the first investigators, examined the passage of protons and particles through

gases and determined charge fractions and cross sections. Later, Lassen (3, 4) used fission fragments to study charge exchange by heavy ions. These experiments were difficult to analyze because fission fragments show a spectrum of both masses and energies. Moreover, initial charge states could only be estimated. After the development of particle accelerators, intensified studies began with light ions up to argon inclusive (see Reference 1) In recent years the techniques for heavy ion acceleration have been improved and detailed experiments have been started for heavy ions up to uranium (5-10). This is of special interest in connection with the design of future heavy ion accelerators, where high ionic charge states are desired in order to obtain effective acceleration to very high energies. However, the necessity of avoiding collisions of accelerated ions with residual gas in the beam line requires a knowledge of charge exchange cross sections. Although much information is already known, many questions are still open and more heavy ion data must be obtained in order to gain a complete understanding of stripping phenomena.

Theoretical studies have been done extensively by Bohr (11) (1948), but at that time not much experimental data was available which could be used to test theoretical results. Further attempts have been made (12-16), but the situation turned out to be extremely difficult. Whereas the passage of protons and particles through H_2 and He can be described

very well, all predictions for heavier ions and heavier targets at high energies are very poor and can hardly be used for practical purposes. In all theories stationary models are assumed, as well as various approximations, such as the Thomas-Fermi model. It seems, however, that an adequate description can only result from a dynamical model which also takes into account the atomic shell structure of both the ions and the target atoms. The magnitude of the cross sections for heavy ions (10^{-16} cm^2/atom) indicates that average impact parameters are of the size of the ions and atoms.

Therefore, one should expect that during an encounter both the ion and the target atom suffer considerable disturbances in their electron shells. In addition, many shell effects have been found (7, 8) which indicate that statistical models are only of limited accuracy. Finally, none of the presently existing theories takes into account the important multiple electron loss cross sections. It is therefore obvious that improved models are necessary in order to allow reasonable predictions for the basic cross sections and quantities, such as mean ionic charges and charge fractions under given conditions.

CHAPTER III

METHODS FOR NUMERICAL INTEGRATION OF NON-EQUILIBRIUM CHARGE DISTRIBUTIONS

Whenever charge exchange cross sections σ_{ij} are to be determined from experimental non-equilibrium distributions, or where non-equilibrium distributions are to be calculated from given cross sections, numerical integration of the system of differential equations (1) becomes necessary. Although various standard techniques exist for the numerical solution of linear first order differential equations with constant coefficients, it seems advantegeous to develop special programs which satisfy all requirements in connection with heavy ion work. For example, the determination of cross sections from experimental charge distributions requires repeated evaluation of the system (1) with certain cross section sets; thus, the integration routine should be very fast with respect to the execution time, while the error of the calculated charge fractions must be within approximately 1%. Therefore, various integration techniques discussed below have been studied.

It can be assumed that initial conditions are given for all charge states $i_A . . . , i_E$:

$$Y(i) = Y_o(i) \quad \text{for } x = x_o \text{ and } i = i_A . . . i_E . \tag{3.1}$$

If Eq. (1) is used, ΔY_i can be calculated for a small increase in path length, Δx:

$$\Delta Y(i) = \sum_j \sigma_{ij} Y_j(x) \Delta x . \qquad (3.2)$$

As Eq. (3.2) can be applied to all charge states i, one can find all new components Y_i (x + x). If this procedure is repeated the distribution $Y_i(x)$ can be found for all target thicknesses x up to equilibrium. Though it is well known that this simple method is not very accurate, it can be shown that an appropriate choice of the step width x leads to errors δY which are acceptable for our purpose. Therefore, the step width is discussed in several aspects.

Constant Step Width

All cross sections may be arranged as a matrix $M = [\sigma_{ij}]$, and the charge fractions at a certain target thickness may be arranged as a vector Y. Then for a given $Y_o(x_o)$, $Y_1(x_o + \Delta x)$ can be calculated as follows:

$$Y_1(x_o + x) = (I + xM)\, Y_o(x_o) . \qquad (3.3)$$

If this procedure is repeated n times, one obtains the expression

$$Y_n(x) = (I + xM)^n Y_o ; \; x = x_o + n\, x . \qquad (3.4)$$

In order to derive a condition for Δx which guarantees

convergence, the matrix M is transformed to a diagonalized matrix D:

$$M = SDS^{-1}, \quad \text{and} \quad D = S^{-1}MS = [\lambda_m] . \tag{3.5}$$

This relation can be used to rewrite Eq. (3.4) in the following form:

$$Y_n = S(I+\Delta x D)^n S^{-1} Y_o . \tag{3.6}$$

In expression (3.6), $I + \Delta x D$ is also a diagonal from and one may write the nonvanishing elements as $1 + \Delta x \lambda_m$. It is obvious that convergence is only obtained if $(1+\Delta x \lambda_m)^n$ is limited. This is equivalent to the condition

$$|1+\Delta x\ \lambda_m| < 1 \qquad \Rightarrow \Delta x < \frac{2}{|\lambda_m|} \tag{3.7}$$

Condition (3.7) must be fulfilled for the smallest of all the negative eigenvalues λ_m. Unfortunately, these eigenvalues are usually unknown. But the fact that the relation causes one of the eigenvalues to assume the value zero allows one to estimate:

$$\left|\frac{\mathrm{Tr}D}{N}\right| \leq |\lambda_{max}| \leq |\mathrm{Tr}D| , \tag{3.8}$$

where N is the number of charge states and $\mathrm{Tr}D = \sum_m \lambda_m = -\sum_{i,j} \sigma_{ij}$. Eqs. (3.7) and (3.8) allow the estimation of Δx, because all

cross sections are given. Table 1 shows three non-equilibrium distributions which have been calculated for three different conditions. At $x = 0$, all charge states were assumed to be zero except Y_1, Y_4, and $Y_6 = 100\%$ for the three distributions, respectively. The logarithmic scale was chosen for a better demonstration of the range of Y and x. It can be seen that a very large number of steps is necessary because x has to be chosen small compared with $x = 1$. On the other hand, the distributions Y(x) are very smooth curves and change less and less if x increased, hence a variable step width should be employed.

Variable Step Width

The simplest method is to choose a logarithmic step width. Then, in the logarithmic plot (Plate 1) Δx would always be represented by a constant interval. Thus, the actual increment depends on x and can be defined as

$$x = x \cdot f \,, \tag{3.9}$$

where f is a constant fraction. Test runs have shown that values of $f = 0.03$ yield results which are of an accuracy better than 1%. In many cases the calculated fractions are to be calculated in regular intervals. In Appendix I, a source listing of a program which integrates system (1) with a logarithmic step width as described above is given. A minor modification of Δx was made in order to print the resulting

fractions ten times per cycle. In Appendix I, a flow chart of the basic integration routine NEDT is also given. In this program, the number of integration steps per cycle can be controlled by the input data. The required input information is also listed in Appendix I.

Accuracy and Execution Time

Various test runs have been made in order to find a suitable constant f as defined by Eq. (3.9). In general, if f is decreased, the accuracy will become better at the cost of execution time. On the other hand, for values of f smaller than a certain minimum, computational errors will not allow any improvement. In Plate 2, two charge states have been selected where the errors ΔY have a maximum. Due to the fact that both at small and large values of x the uncertainties become negligible (see part "Equilibrium" below), these maximum errors occur somewhere between. Plate 2 indicates that 300 steps/cycle gives an accuracy better than about 1%. This is acceptable in many cases where measured charge fractions with uncertainties of 5-10% are to be compared with calculated fractions. The exact values in Plate 2 have been determined by means of the Runge-Kutta method (see below).

Equilibrium

It can be shown, that the equilibrium distribution is unique for given cross sections. If the index n in Eq. (3.4)

EXPLANATION OF PLATE 2

Change of two selected charge fractions for varying number of intergration steps per cycle. The exact values are also shown (dashed line).

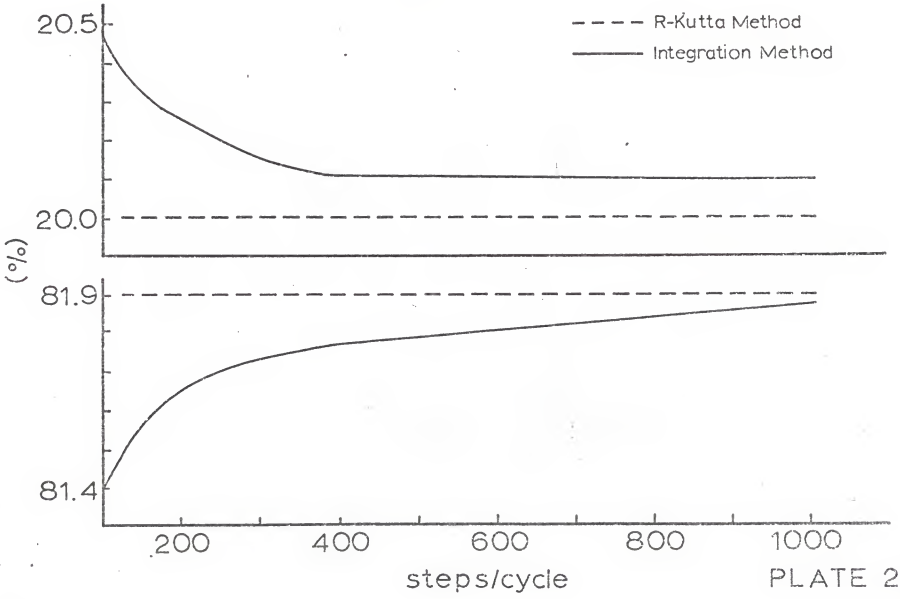

R-Kutta Method
Integration Method
20.5
20.0
81.9
81.4
(%)
200
400
600
800
1000
steps/cycle

PLATE 2

becomes infinitely large, which corresponds to equilibrium, obtains

$$Y_\infty = (I + xM)Y_\infty \Rightarrow MY_\infty = 0 \ . \tag{3.10}$$

If this result is compared with the differential Eq. (1), which can be written as $Y' = MY$, it is apparent that $Y' = 0$ is indeed the condition for equilibrium. Thus, whereever this integration method yields equilibrium it must be the correct one although charge fractions at smaller x may have large errors. It should be noted, however, that due to computational errors the condition $Y' = 0$ can not be fulfilled exactly. If the integration procedure is not interrupted, the fractions Y_i will not remain constant but will continue to change, and may assume unphysical values. In this program, a test for equilibrium is made. If the total change of all fractions becomes smaller than a certain minimum amount the integration procedure is stopped.

Runge-Kutta Integration

Other methods, especially the Runge-Kutta integration techniques, have also been studied. Suitable application of the well known Runge-Kutta method gives extremely accurate results. In fact one could not produce fractions with observable errors without losing convergence. Therefore, the results obtained with this method could be used for a comparison

with the simple integration techniques described above. The only disadvantage is that the Runge-Kutta method requires much more execution time. Test runs indicated a time ratio of at least 1 : 4.

CHAPTER IV

DIRECT CALCULATION OF EQUILIBRIUM CHARGE DISTRIBUTION

It has been shown in Chapter III that a unique equilibrium distribution can be derived from a given set of cross sections. Although the integration programs described in Chapter III also give equilibrium, a more direct method can be of advantage for various reasons. Application of the integration technique requires the assumption of initial conditions for the charge states, which do not effect the equilibrium. In addition, the execution time is unnecessarily long if non-equilibrium fractions are calculated but not desired. The most direct way for a calculation of the equilibrium charge distribution is to solve the equation

$$MY_{\infty} = 0 \ . \tag{4.1}$$

In fact, the whole calculation then is reduced to solving a linear inhomogenous system of equations. Equation (4.1) turns out to be an inhomogeneous system because the relation $\sum Y_{\infty} = 1$ has to be used to reduce (4.1). Otherwise only trivial solutions would exist. If one eliminates, for example, $Y_{k\infty}$ by $Y_k = 1 - \sum_{i \neq k} Y_{i\infty}$, one gets the form

$$\tilde{M}Y_{\infty} = C \ , \tag{4.2}$$

with the elements

$$\tilde{M}_{ij} = M_{ij} - M_{ik} = \sigma_{ij} - \sigma_{ki} ,$$
$$\tilde{M}_{ii} = M_{ij} - M_{ij} = -\sum_{i \neq 1} \sigma_{jl} - \sigma_{ki} ,$$

and $C_i = -M_{ik} = \sigma_{kj}$.

The remaining problem is equivalent to finding the inverse matrix $\tilde{M}^{-1}$. Then the desired fractions are obtained by the products

$$Y = \tilde{M}^{-1} C . \tag{4.3}$$

The common standard technique is known as row operation. In this method, the diagonal elements of $\tilde{M}$ are successively changed to unity, whereas the off-diagonal elements become zero. Combininb $\tilde{M}$ and C in a partition matrix, the operations can be symbolized as follows:

$$[\tilde{M}, C] \Rightarrow [I, C'] , \tag{4.4}$$

where the elements of C' become the desired fractions Y . The remaining value $Y_{k\omega}$ is then obtained from $Y_{k\omega} = 1 - \sum_{i \neq k} Y_{i\omega}$. This technique is very effective and takes a minimum of computational time. As all diagonal elements of M are always different from zero, no complication can arise and no measures have to be taken in order to correct for an improper matrix.

The detailed source listing for the program EQUDIS is also given in Appendix I as a subroutine, including a brief flow chart. As can be seen from Table 1, there is perfect

agreement between the two equilibrium distributions calculated from the integration program NEDT and the routine EQUDIS.

CHAPTER V

ANALYSIS OF EQUILIBRIUM OF THE BR AND I ION METHOD

In this part, some of the equilibrium charge distributions are analyzed which have been measured at Oak Ridge (7). Our interest is not only in the mean ionic charge $\bar{I}$ but also in the shpae of the distribution; semi-empirical formulas for $\bar{I}$ can be tested as well as possible relations between asymmetries of the equilibrium distributions and multiple electron loss processes.

The distributions have been measured for Br ions at 20 MeV and for I ions at 15 and 60 MeV in dilute gases of H_2, He, N_2, Ne, Ar and Kr. A common test for a Gaussian distribution Y(i) is to plot the logarithim of the ratios Y(i)/Y(i+1) versus the charge i. A Gaussian shape will result in a straight line and deviations can be seen very easily (7). The advantage of this technique is that an incorrect normalization of the fractions, perhaps due to missing charge states, cannot cause errors since only ratios are decisive. On the other hand, all distributions are clearly asymmetrical and one may try to find a better approximation for Y(i) than is given by a Gaussian distribution. Therefore one tries to fit the equilibrium charge distribution to a generalized Gaussian,

$$Y_i = Y \exp\left(-\left(\frac{i-\bar{i}}{\gamma}\right)^n\right) , \qquad (5.1)$$

where $\hat{Y}$ is the maximum intensity of a smoothed distribution which occurs at the most probably charge $\hat{i}$. Of course, $\hat{i}$ need not necessarily be an integer. The assumption (5.1) is arbitrary and other functions could be used. But (5.1) implies a Gaussian for n = 2 and one can expect to obtain characteratic relations between the exponent n and the width parameter γ for the various fitted distributions.

Before one can find the best values of n and γ for the distributions in question by means of a least square technique, $\hat{Y}$ must be determined. As the fit does not depent too strongly on $\hat{Y}$, an approximation for $\hat{Y}$ is sufficient. Therefore, one defines $\hat{Y}$ as the maximum of a parabola, which is determined by the three largest charge fractions:

$$\hat{Y} - Y_1 = \frac{P}{2} (i - \hat{i})^2 . \qquad (5.2)$$

If the coordinates (i, Y_i) of the three largest charge fractions are inserted in Eq. (5.2), the three unknowns $\hat{Y}$, P and $\hat{i}$ are obtained:

$$\begin{aligned} \hat{Y} &= Y_1 + \frac{P}{2} (i_1 - \hat{i})^2 , \\ P &= 2Y_2 - Y_1 - Y_3 , \\ \hat{i} &= \frac{Y_2 - Y_1}{P} + i_1 + \tfrac{1}{2} . \end{aligned} \qquad (5.3)$$

In order to apply the least square methods for a straight line, Eq. (5.1) must be transformed into a linear equation:

$$Y = nx + a , \qquad (5.4)$$

where $Y = \ln(\ln(\hat{Y}/Y_i))$,

$x = \ln|\Delta i|$,

$a = -n\ln\gamma$.

Applying the standard formulas for the best fit of a straight line, one obtains for the best values $\bar{n}$ and $\bar{a}$:

$$\begin{aligned} \bar{n} &= (\Sigma x_i^2 \cdot \Sigma Y_i - \Sigma x_i \cdot \Sigma x_i Y_i)/D \ ; \\ \bar{a} &= (N\Sigma x_i Y_i - \Sigma x_i Y_i)/D \ ; \\ D &= N\Sigma x_i^2 - (\Sigma x_i)^2 \ , \end{aligned} \tag{5.5}$$

where all N experimental points are to be taken into account in the summation. The most probable error of $\bar{n}$ and $\bar{a}$ can also be derived as

$$\begin{aligned} \bar{n} &= (\Sigma x_i^2/D)^{\frac{1}{2}} \rho_o \ , \\ \bar{a} &= (\bar{n}/D)^{\frac{1}{2}} \rho_o \ , \end{aligned} \tag{5.6}$$

where N is the number of experimental points, and ρ_o is given by

$$\rho_o = [\Sigma(y_i - \bar{a} - \bar{n}x_i)^2/(n-2)]^{\frac{1}{2}} \tag{5.7}$$

Application of this method implies, that the two wings of the equilibrium distributions are examined separately. This procedure seems to be meaningful because of the asymmetries which will result in different values of $\bar{n}$ and $\bar{\bar{n}}$ for the left and the right sides.

Results and Discussion

The results of the various fits are shown in Plates 3 to 13 and in Table 2. Two different fits have always been attempted. First, $\bar{n}$ and $\bar{\delta}$ have been determined according to the method described above. Secondly, an independent determination of the width $\bar{\gamma}_2$ was made under the assumption of a Gaussian with n = 2.

Whenever one side contained more than three measured points, the fit was made. In most cases, where values of $\bar{n}$ and $\bar{\gamma}$ could be determined for the left side, the result of $\bar{n}$ was close to 2. This means, that the left sides of all equilibrium distributions are mostly Gaussians, independent of the ion and the stripper. Only for I at 60 MeV, somewhat larger values of $\bar{n}$ were found, indicating that the decrease Y_i to smaller charges i is steeper than for a Gaussian.

In all cases, the analysis of the right sides of the distributions resulted in values $\bar{n}$ smaller than 2, which indicates a less rapid decrease than Gaussian. In Br, n = 1.3 was found for all targets whereas in iodine $\bar{n}$ shows some dependence on the stripper (see Table 2). The width parameter for the right sides is smallest for Br, increases for I at 15 MeV, and is largest for I at 60 MeV. The width does not depend too much on the target except in the case of H_2, where smaller values of $\bar{\gamma}$ are always found. The results are given only for comparison. As the corresponding fit, especially for the right sides, is very bad under the

EXPLANATION OF PLATES 3 to 13

Equilibrium charge distributions for Br and I ions.

X -- experimental, O -- best fit, -- Gaussian fit.

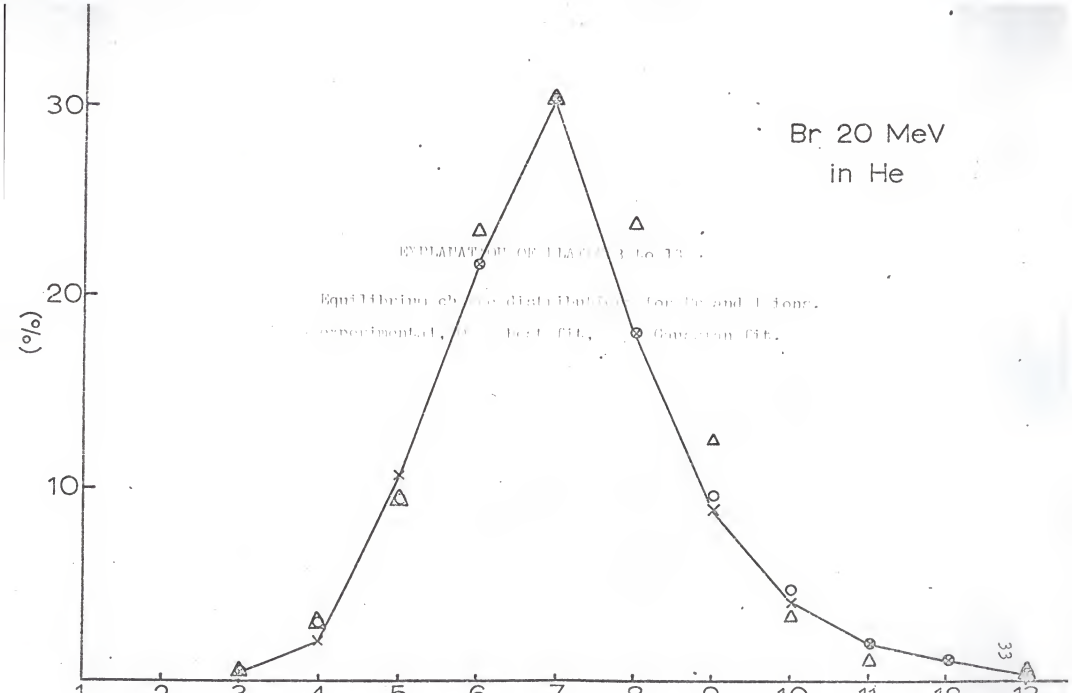
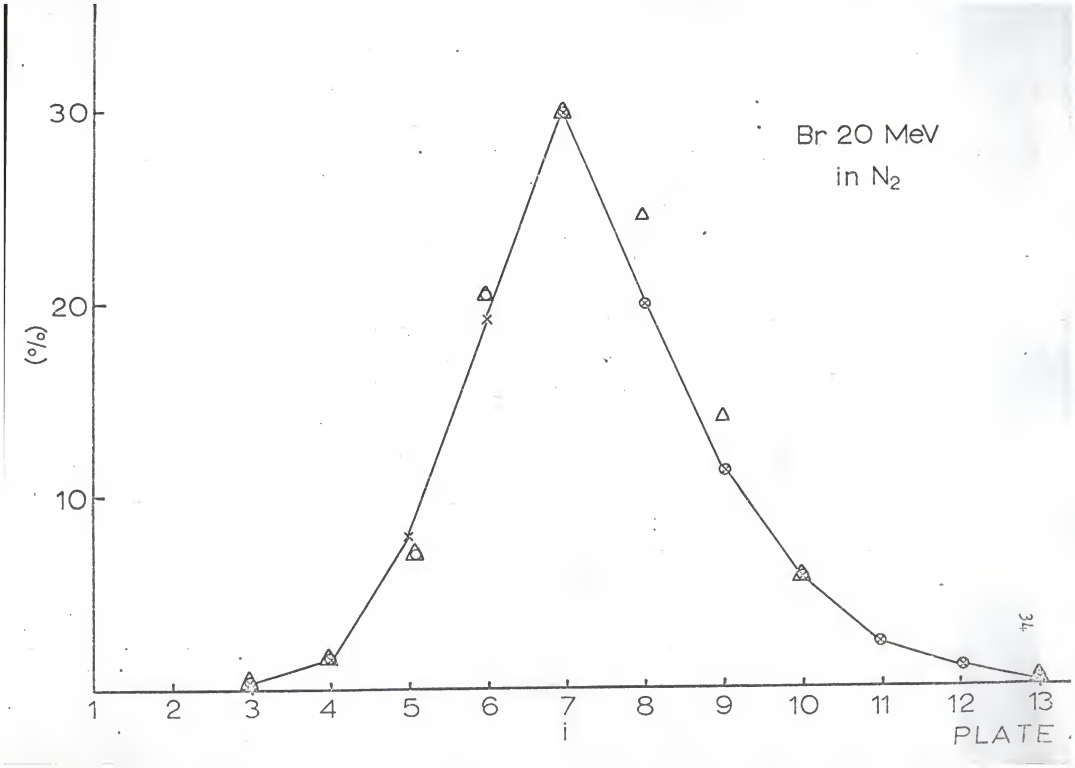


PLATE 3



PLATE

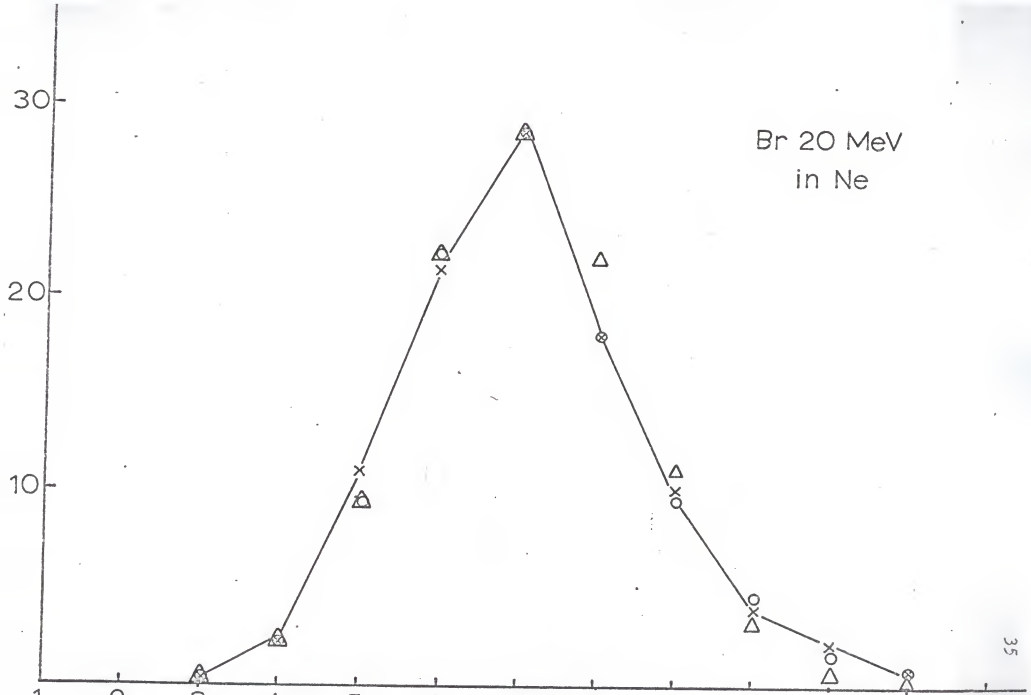


PLATE 5

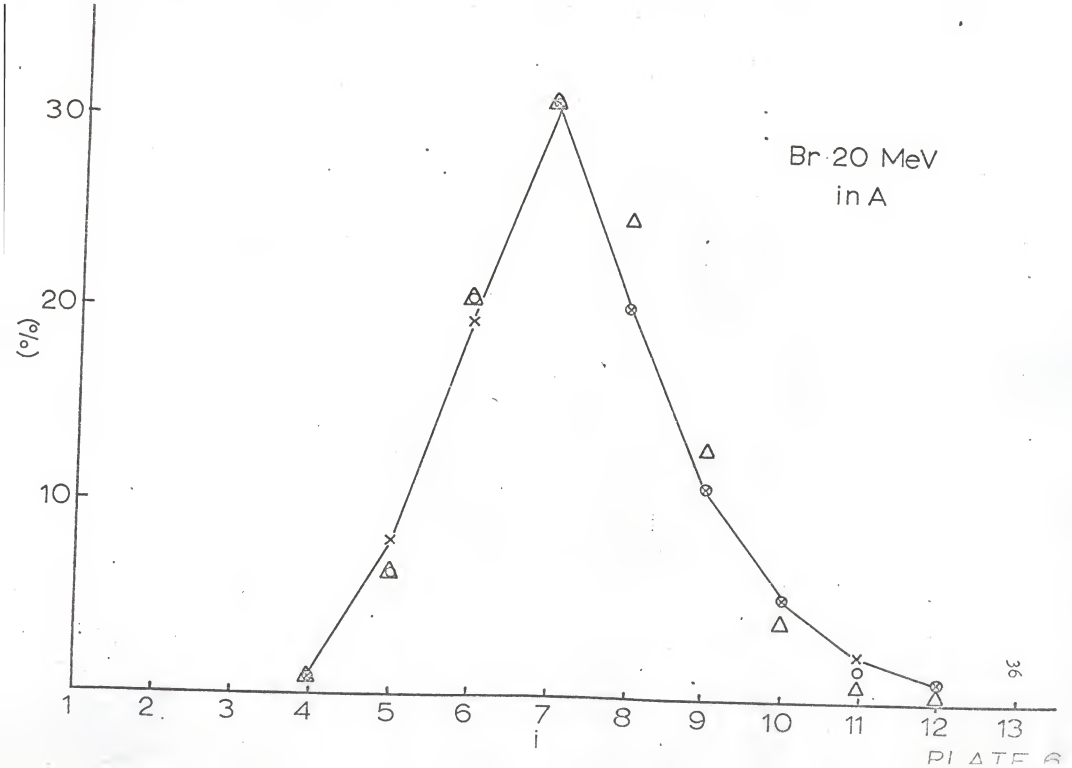


PLATE 6

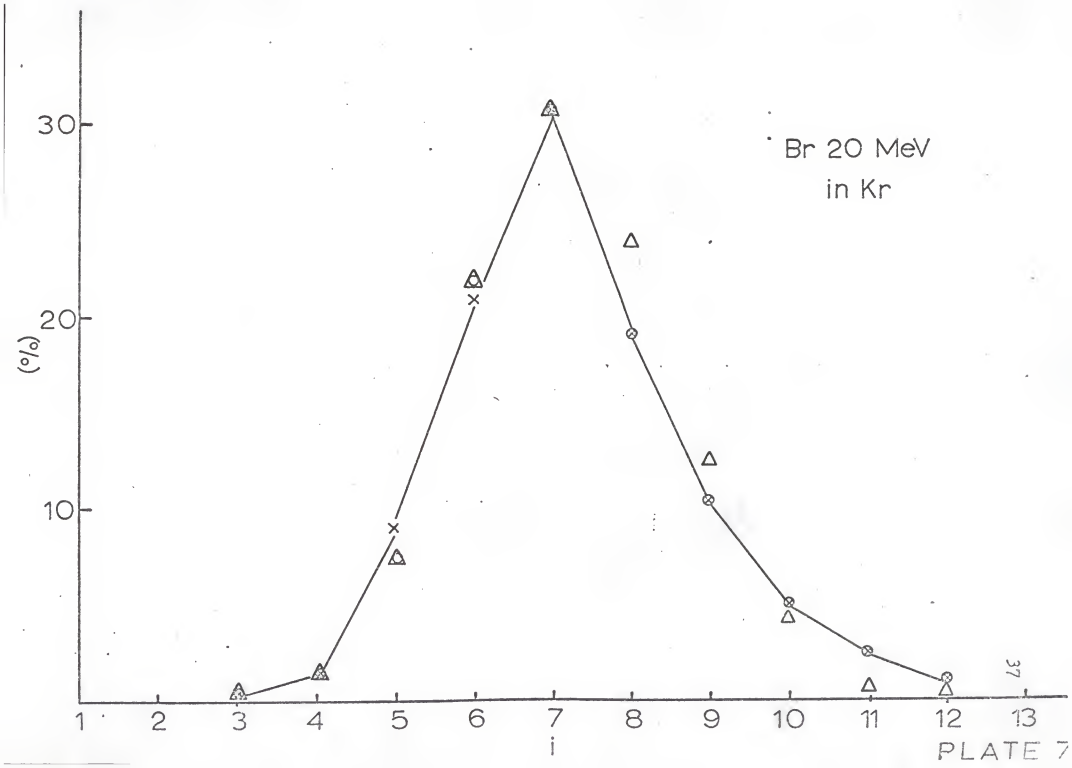


PLATE 7

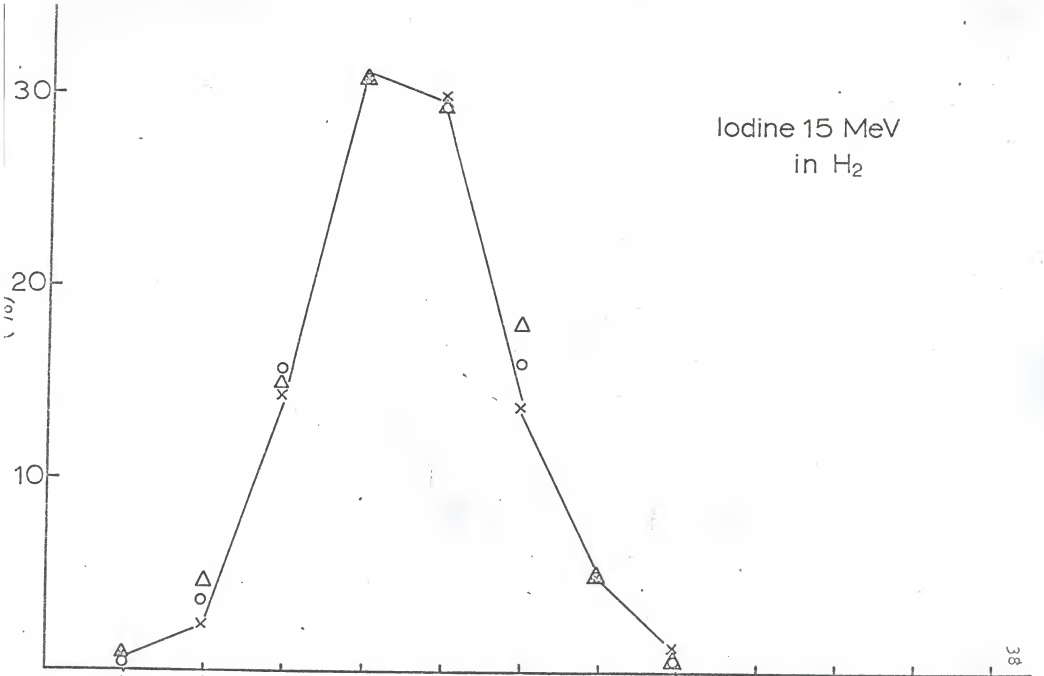


PLATE 8

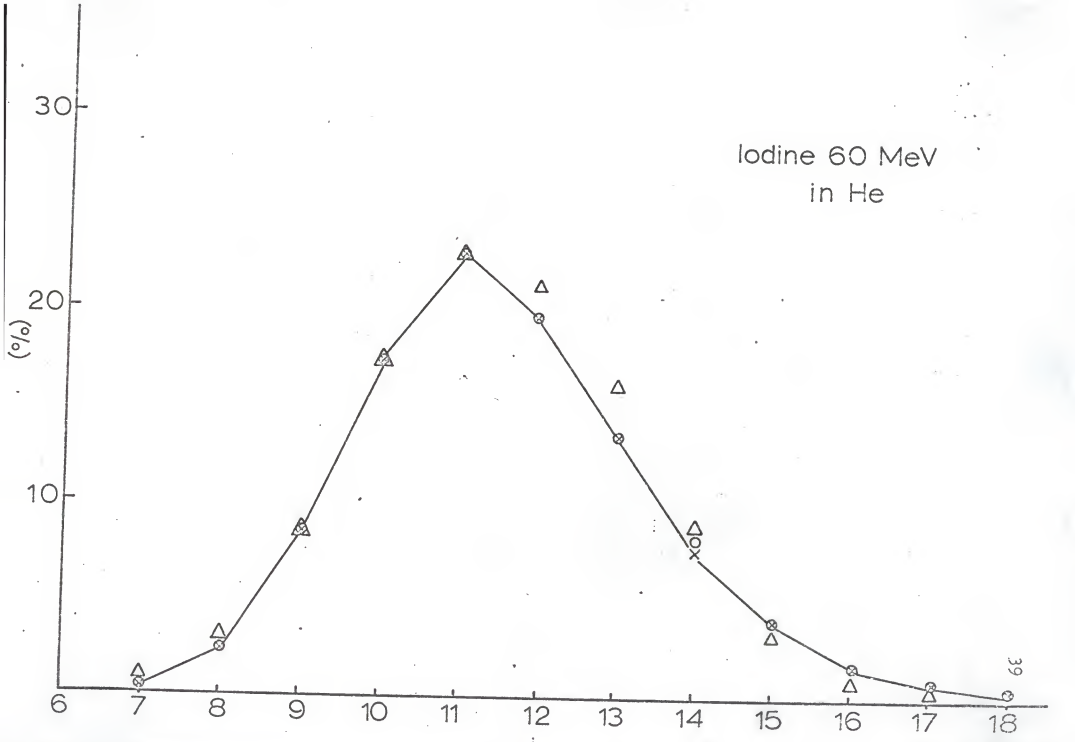


PLATE 9

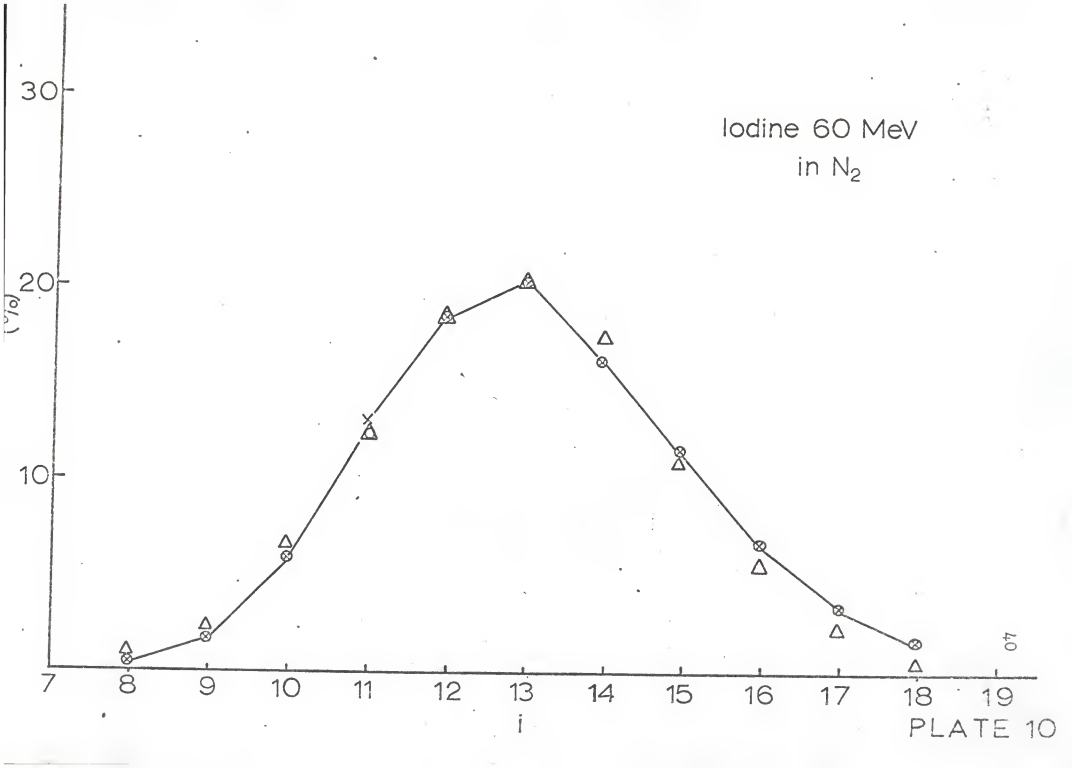


PLATE 10

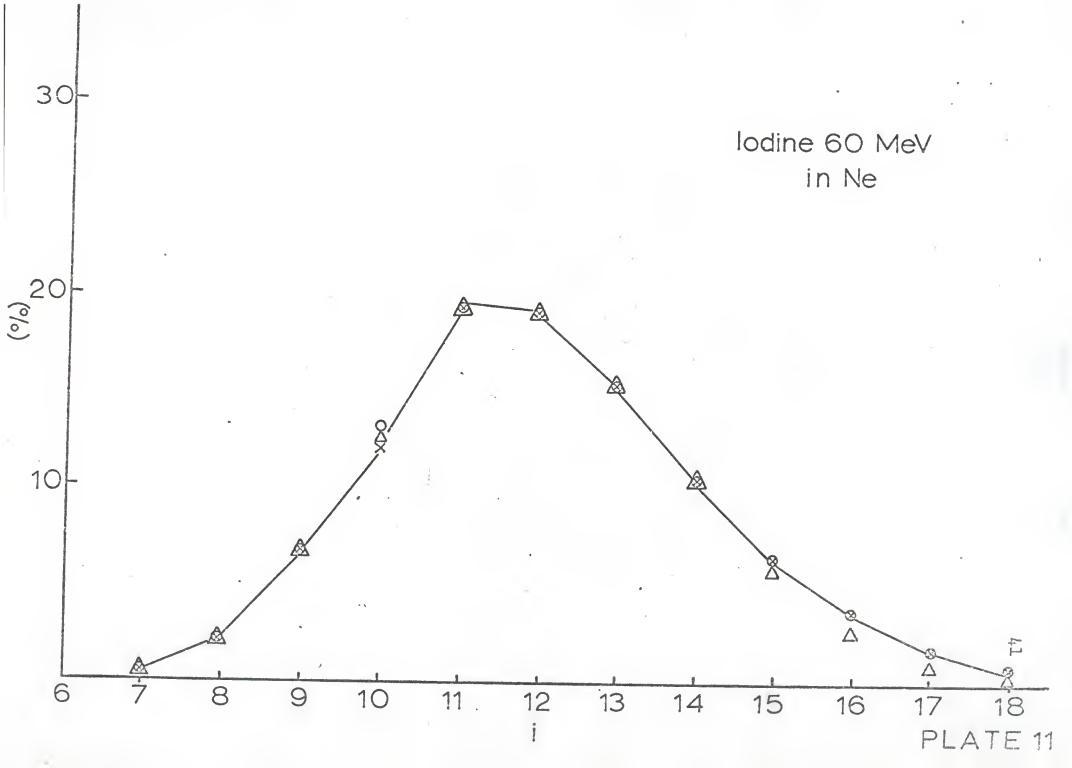


PLATE 11

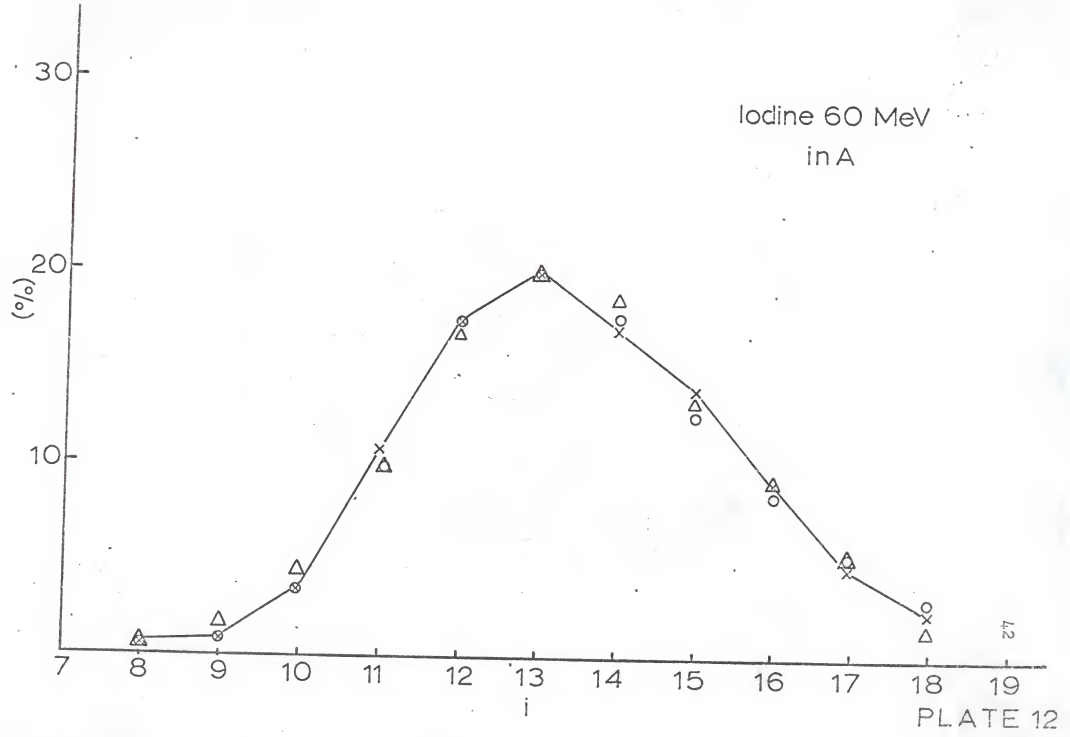


PLATE 12

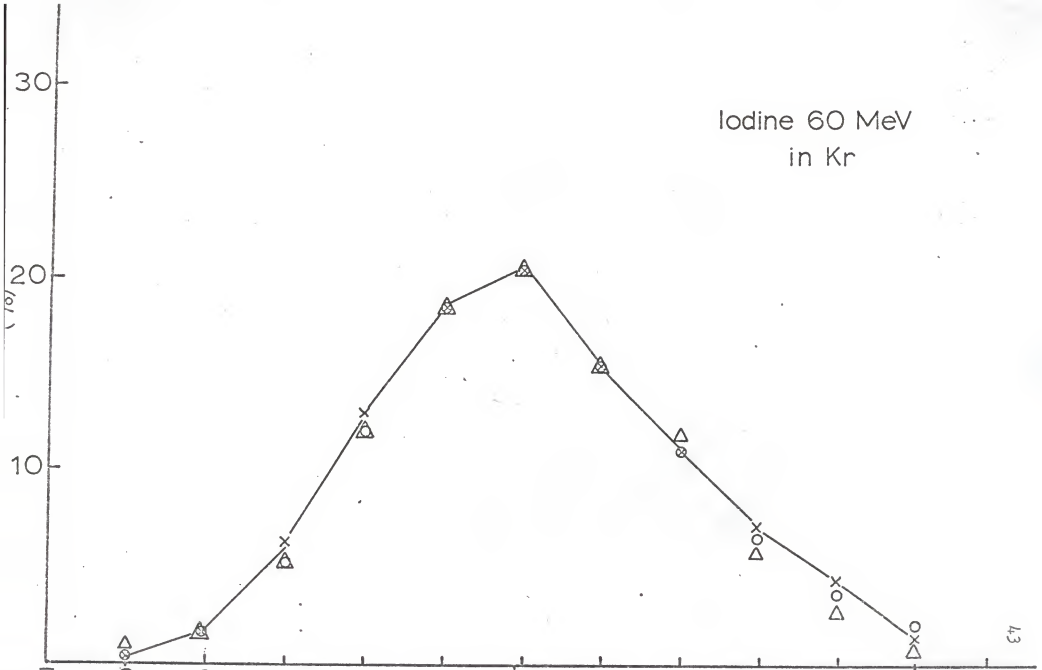


PLATE 13

Table 2 Distribution parameters and mean ionic charges for Br and I ions in various gases as obtained from the fit procedures.

		Left Side			Right Side				
		n			$\bar{n}$			$\bar{i}$	i
Br 20 MeV	H_2	2.38	1.66	1.78	1.96	1.82	1.81	6.17	6.20
	H_e	2.01	1.74	1.74	1.31	1.81	2.12	6.88	7.11
	N_2	2.01	1.68	1.70	1.26	1.99	2.30	7.02	7.37
	N_e	2.00	1.79	1.80	1.28	2.00	2.19	6.87	7.06
	A	2.00	1.73	1.71	1.33	1.93	2.00	6.92	7.14
	K_r	2.01	1.64	1.62	1.30	1.95	2.15	7.01	7.16
I 15 MeV	H_2	2.16	1.88	1.90	1.67	2.10	2.21	4.44	4.58
	H_e	---	---	---	1.36	2.46	2.65	4.93	5.54
	N_2	---	---	---	1.46	2.60	2.69	5.00	5.69
	N_e	---	---	---	1.40	2.61	2.68	5.04	5.76
	A	---	---	---	1.32	2.45	2.64	4.96	5.64
	K_r	---	---	---	1.24	2.34	2.68	4.77	5.45
I 60 MeV	H_e	2.06	2.14	2.18	1.682	3.20	2.72	11.15	11.58
	N_2	2.30	2.46	2.50	1.82	3.20	3.20	12.58	13.09
	N_e	2.17	2.45	2.65	1.58	3.10	3.32	11.54	12.07
	A	2.37	2.50	2.54	1.86	3.24	3.23	12.99	13.48
	K_r	2.35	2.50	2.53	1.86	3.30	3.30	12.77	13.13

assumption n = 2, $\bar{Y}_2$ should not be weighted too much. Plates 3 to 13 give a better idea about the quality of the various fits.

As only a few measurements have been done for heavy ions in that energy range, it is difficult to make a comparison with other results. In gaseous targets the trend seems to be as follows: for light ions, all measured charge distributions show a nearly perfect Gaussian shape (1) in all stripper gases. The heavier the ion, the greater the deviation from a Gaussian; in all cases the higher charge states have more intensity than compared with a Gaussian. The stripper apparently has some influence: in H_2 and He, the distributions are more symmetrical and in very heavy strippers the largest asymmetries can be found. This is also obvious from the differences $\hat{i} - \bar{i}$, as listed in Table 2.

One could try to ascribe this asymmetry to the occurrence of multiple electron loss. In fact, if one increases multiple electron loss probabilities, the equilibrium fractions tend to shift to higher charge states. This is consistent with the result that multiple electron capture is very unlikely, and therefore no corresponding trend to smaller charge states exists. On the other hand, even for light ions such as argon, where Gaussian distributions have been measured, multiple electron loss can be significant. Obviously the equilibrium distribution is a result of the competing processes for electron capture and loss, σ_{ij}. But these cross sections

depend on the electronic shell structure of both the ion and the target. Therefore one must expect different shapes for the distributions, depending on the ion, their energy, and the target. Also, shell effects will occur (7). It is somewhat surprising that, nevertheless, very similar equilibrium distributions can be observed; for example, for one ion in one target in a very wide energy range. Although the cross sections which determine the distribution depend strongly on the energy, it seems as if the distribution did not change its shape but is simply shifted to higher charge states as the energy increases (7).

We conclude that empirical formulas for the equilibrium distributions of fast ions can be found, but due to the specific atomic structure of both ions and target, no simple relation Y(i) can be given which holds in a general sense.

ACKNOWLEDGEMENTS

The author wishes to thank Dr. Hans D. Betz for his guidance throughout the work. The author also wishes to thank Dr. L. D. Ellsworth and Dr. C. P. Bhalla for their helpful suggestions.

The author wishes also to thank Mr. Herbert R. Rosner for his assistance and encouragement in this work.

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Appendix I.

Source listing of programs NEDT and EQUDIS, controlled by main routine, a list of input parameters and a brief flow chart.

```
      MAIN PROGRAM
      COMMON CS (30,30), JA(30),JE(30),ZF(9),IO,IA,IE,NC,NL,IPO,
     YP,XP,X,NP
    1 FORMAT(1H1,A6,4S,2CHNUCLEAR-CHARGE  Z = ,14,11X,17HAROMIC
     1MASS  M =,14,//,11X, 20HKIN. ENERGY  E =,F6.2,26H  MEV
     2VELOCITY V/VO =,F7.3,//,9H STRIPPER,A8,14H -GAS  IO =,13,
     31H+,11X,13HCHAR GE STATES,13,4H+ TO,13,1H+,//,31H MULTIPLE
     4STRIPPING NC =,I3,12X,4HNL =,12,///)
    2 FORMAT(1H-, 35HCROSS-SECTION FOR CAPTURE (IN 10E-,12,
     19H CM2/MOL))
    3 FORMAT (1HO,6X,13(6X,I2,1X))
    4 FORMAT(1H+,6H  N  ,13(3X,6HSC(  )),/)
    5 FORMAT  (10(F6.3,2X))
    6 FORMAT (1H ,13,3X,13F9.3)
    7 FORMAT(1H-,35HCROSS-SECTIONS FOR LOSS (IN 1oE-,12,9H
     1CM2/MOL))
    8 FORMAT(1H+,6N  N ,13(3X, 6HSL(  )),/)
    9 FORMAT (A4,12,13,F6.2,F6.3,A4,813,3F7.5)
   10 DATA IRE,IWR/1,3/
      DATA IST,IGO/4HSTOP,4HGO  /
   14 READ (IRE,9) IN,IZ,IB,E,V,STR,IA,IE,NP,IPO,NC,NL,LO,IQ,
     1X,YP,XP
      IF  (IPO.EQ.0) IPO=16
      IF (IN.EQ.IST) STOP
      IF (IN.EQ.IGO) GOTO 98
   15 WRITE (IWR,1) IN,IZ,IB,E,V,STR,IO,IA,IE,NC,NL
      WRITE(IWR,2) IPO
      WRITE(IWR,3) (I,I=IA,IE)
      WRITE(IWR,4)
      IF ((IE-IA).GT.L4)  STOP
      DO 16 I=IA,IE
      DO 16 J=IA,IE
   16 CS(I,J)=0.
      DO 18 N=L,NC
      K=N+LA
      I1=IE
      IF ((IE-IA).GT.9) I1=IA+9
      READ(IRE,5) (ZF(L),L=1,N),(CS(I,I-N),I=K,I1)
      IF ((IE-IA).LE.9) GOTO 18
      I2=I1+1
      READ  (IRE,5) (CS(I,I-N),I=I0,IE)
   18 WRITE(IWR,6) N,(ZF(L),L=1,N),(CS(I,I-N),I=K,IE)
      WRITE(IWR,7) IPO
      WRITE(IWR,3) (I,I=IA,IE)
      WRITE(IWR,8)
      DO 20 N=1,NL
      K=IE-N
      I1=K
```

```
      IF((K-IA).GY.9) I1=IA+9
      READ(IRE,5) (CS(I,I+N),I=IA,I1)
      IF ((K=IA).LE.9) GOTO 20
      I2=I1+1
      READ(IRE,5) (CS(I,I+N),I=I2,K)
 20   WRITE (IWR,6) N,(CS(I,I+N),I=IA,K)
      DO 25 I=IA,IE
      KA=MAO(I-NC,IA)
      IE=MINO(I+NL,IE)
         SUM=0.
         DO 24 K=KA,KE
 24      SUM=SUM-CS(I,K)
         CS(I,I)=SUM
      JA(I)=MAXO(I-NL,IA)
 25   JE(I)=MINO(I+NC,IE)
 98   IF (IO.NE.O) CALL NEDT
      IF (IQ.NE.O) CALL EQUDIS
      GOTO 14
 99   STOP
      END
      SUBROUTINE NEDT
      COMMON CS(30,30),JA(30),JE(30),ZF(9),IO,IA,IE,NE,NL,IPO,
      YP,XP,X,NP DIMENSION Y(30),YS(30)
  1   FORMAT(1H1,43HIONIC CHARGE DISTRIPUTION NON-EQUILIBRIUM,
     112X, 14HINITIAL CHARGE,13,1H+,9X,9HX IN IOE+,12,26H
     2MOL/CM2  Y IN PERCENT,17,6H STEPS)
  2   FORMAT (IH-,15X,13(6X,12,1X))
  3   FORMAT(IH+,4X,1HX,6X,4H ZQX,13(4X,5HY(  )),/)
  4   FORMAT (1H ,F8.4,F7.2,2PF9.3,12F9.3)
  5   FORMAT(1HO, 26HEQUILIBRIUM DISTRIBUTION  ,/)
  6   FORMAT(5X,F8.3,6X,6(3X,F7.3))
  7   FORMAT(8(3X,F7.3))
  8   FORMAT(IH-, 45HEQUILIBRIUM DISTRIBUTION COULD NOT BE REACHED)
      DATA IWR,IPU/3,2/
      IF (NP.EQ.O) NP=10
      PN=1./FLOAT(NP)
      IF (NP.EQ.10) PN=.1
      WRITE(IWR,1) IO,IPO,NP
      WRITE(IWR,2) (I,I=IA,IE)
      WRITE(IWR,3)
      IF (X.EQ.O.) X=.001
      DO 10 I=IA,IE
 10   Y(I)=X*CS(IO,I)
      Y(IO)=Y(IO)+1.
      ZQX=IO
      YM2=99.
      DO 16 NN=1,6
      DX=PN*X
      DO 16 N=1,9
      WRITE(IWR,4) X,ZQX,(Y(I),I=IA,IE)
      IF (YP.EQ.O.) GOTO 12
      IF (X.LT.XP) GOTO 12
      DO 11 I=IA,IE
      YS(I)=O.
```

```
      IF (Y(I).LT.YP) GOTO 11
      YS(I)=Y(I)*100.
11    CONTINUE
      I1=IA+5
      WRITE(IPU,6) X,(YS(I),I=IA,I1)
      IF (IE.LE.I1) GOTO 12
      I2=I1+1
      WRITE(IPU,7) (YS(I),I=I2,IE)
12    DO 16 M=1,NP
      X=X+DX
      ZQX=0.
      YM1=YM2
      YM2=0.
      DO 14 I=IA,IE
      YS(I)=0.
      JAA=JA(I)
      JEE=JE(I)
      DO 13 J=JAA,JEE
13    YS(I)=YS(I)+CS(J,I)*Y(J)
14    YM2=YM2+ABS(YS(I))
      DO 15 I=IA,IE
      Y(I)=Y(I)+YS(I)*DX
15    ZQX=ZQX+Y(I)*FLOAT(I)
      IF (YM2.GY.YM1) GOTO 17
16    CONTINUE
17    IF (YM2*DX.LE..01) GOTO 18
      WRITE(IWR,8)
      RETURN
18    WRITE(IWR,5)
      WRITE(IWR,4) X,ZQX,(Y(I),I=IA,IE)
      RETURN
      END
      SUBROUTINE EQUDIS
      DOMMON DS(30,30),JA(30),JE(30),ZF(9),IO,IA,IE,NC,NL,IPO,
     YP,XP,X,NP
      DIMENSION A(30,30)
1     FORMAT (1H-,rlHEXACT EQUILIBRIUM DISTRIBUTION AS FOLLOWS,/)
2     FORMAT(1H-,32HDIAGONAL-ELEMENT IS ZERO  STOP,/)
3     FORMAT (13X,3HZQX,13(6X,I2,1H+))
4     FORMAT (1H  )
5     FORMAT (9X,F7.2,PF9.3,12F9.3)
      DATA IWR/3/
      IEE=IE-1
      DO 11 I=IA,IEE
      A(I,IE)=CS(IE,I)
      DO 11 J=IA,IEE
11    A(I,J)=CS(J,I)-CS(IE,I)
      WRITE (IWR,1)
      DO 15 I=IA,IEE
      TEMP=A(I,I)
      IF(TEMP.NE.0) GOTO 12
      WRITE (IWR,2)
      STOP
```

```
12    DO 13 J=IA,IE
      IF(J.LT.I) GOTO 13
      A(I,J)=A(I,J)/TEMP
13    CONTINUE
      DO 15 K=IA,IEE
      TEMP=A(K,I)
      IF(K.EQ.I) GOTO 15
      DO 14 J=IA,IE
      IF(J.LT.I) GOTO 14
      A(K,J)=A(K,J)-TEMP*A(I,J)
14    CONTINUE
15    CONTINUE
      ZQ=0.
      A(IE,IE)=1.
      DO 16 I=IA,IEE
      A(I,IE)=-A(I,IE)
      ZQ=ZQ+A( I,IE*FLOAT( I)
16    A(IE,IE)=A(IE,IE)-A(I,IE)
      ZQ=ZQ+A(IE,IE*FLOAT(IE)
      WRITE (IWR,3) (I,I=IA,IE)
      WRITE (IWR,4)
      WRITE (IWR,5) ZQ,(A(I,IE),I_IA,IE)
      RETURN
      END
```

INPUT PARAMETERS

CONTROL CARD: (format 9)

IN	ion,#
IZ	nuclear charge
IB	mass
E	energy in MeV
V	velocity in V_o
STR	stripper
IA	smallest charge state 0
IE	highest charge state
NP	NP x 50 steps per cycle (if=0, NP = 2)
IPO	unit for CS and X, (if = 0, IPO = 16)
NC	maximum value of multiple capture (= 0)
NL	maximum value of multiple loss (= 0)
IO	initial charge (if = 0, no CALL NEDT)
IQ	= 0. = exact equilibrium charge dist. will be calculated.
	= 0. = no extra calculation equilibrium charge distribution.
X	starting target thickness (if 0, x = 0.001 x 10^{-IPO} atom/cm^2)
YP	= 0 = Y are punched
	= 0 Y are not punched
XP	if cards punched, then only if X XP

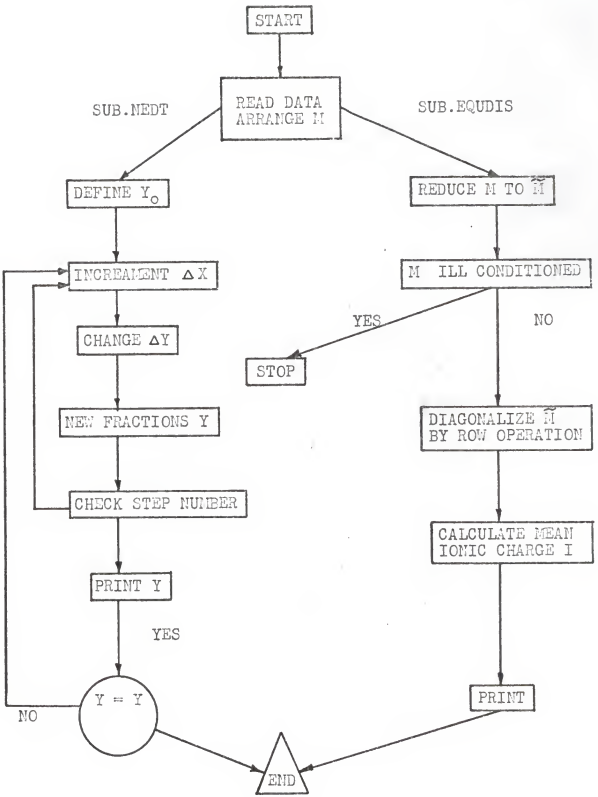
CONDITIONS:

1. IA 0
2. IE-IA 12
3. IA 10 IE

#IN = STOP program stop

IN = GO CALL NEDT for another initial charge state and same CS set

*not used for calculation


START
READ DATA
ARRANGE M
SUB.NEDT
SUB.EQUDIS
DEFINE Y_o
REDUCE M TO $\tilde{M}$
INCREAMENT ΔX
M ILL CONDITIONED
YES
NO
CHANGE ΔY
STOP
NEW FRACTIONS Y
DIAGONALIZE $\tilde{M}$
BY ROW OPERATION
CHECK STEP NUMBER
CALCULATE MEAN
IONIC CHARGE I
PRINT Y
YES
Y = Y
NO
PRINT
END

NUMERICAL COMPUTATION OF IONIC CHARGE DISTRIBUTION AND THE ANALYSIS OF EXPERIMENTAL EQUILIBRIUM DISTRIBUTIONS

by

TANG CHIAO

B. S., Tunghai University, 1964

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Physics

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1969

The processes of electron capture and loss of fast heavy ions passing through matter are described and the status of relevant experimental and theoretical work is reviewed. Programs for the numerical calculation of ionic charge states in non-equilibrium and equilibrium are presented, which can be used for given sets of charge exchange cross sections. Experimental equilibrium distributions of Br and I ions at 15, 20 and 60 MeV, stripped in various gases, are analyzed with respect to their form.