

EMPIRICAL FORMULAS FOR IONIZATION CROSS SECTION OF

ATOMIC IONS FOR ELECTRON COLLISIONS

CRITICAL REVIEW WITH COMPILATION OF EXPERIMENTAL DATA

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EMPIRICAL FORMULAS FOR IONIZATION CROSS SECTION OF ATOMIC IONS FOR ELECTRON COLLISIONS

- Critical Review with Compilation of Experimental Data -

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Abstract

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Based on the comparison with experimental data a critical review is made in Part I on empirical cross-section formulas for electron-impact ionization of atomic ions. Most extensively studied are the formulas proposed by Lotz and by Golden and Sampson. Several conclusions are drawn about the validity of those formulas. A new type of scaling factor is proposed to improve the formula of Golden and Sampson. Part II presents a compilation of experimental data on electron-impact ionization of atomic ions with Z (atomic number) \leq 19. All the experimental data available are shown in a graphical form with the results of the empirical formulas of Lotz and of Golden and Sampson. Experimental data were surveyed through the end of 1980 and the data on multiple ionization have been omitted.

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I. Critical Review of Empirical Formulas

1. Introduction

Electron-impact ionization of atomic (positive) ions is a fundamental elementary process in laboratory and space plasmas.¹⁾ It determines the ionization stage of the plasmas and thereby affects their macroscopic properties such as electrical conductivity and radiative energy loss. Although a rather extensive effort has been made to produce the ionization cross sections, the total number of the data presently available is still limited. If we consider the number of different ionic species, it is virtually impossible to calculate or measure the cross section for all of them. Empirical formulas for the ionization cross section have been proposed to alleviate this difficulty.

Empirical formulas, if sufficiently reliable, are very useful even when experimental or theoretical cross sections are available. In a modelling calculation of plasmas, for instance, it is much easier to handle empirical formulas than original data themselves. Empirical formulas can be used for an interpolation or extrapolation of available data over a range of electron energy.

Various empirical formulas²⁻¹¹⁾ for the ionization cross section have been adopted by plasma physicists and astrophysicists in their studies. In many cases, however, they use them with no attention to their validity. They often employ empirical formulas simply bacause the formulas are very convenient to be incorporated in their studies. In the

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present report a critical evaluation is made on the empirical formulas widely used for the electron-impact ionization of ions. The validity of the formulas is judged on the comparison with experimental data. Such a comparative study has been made several times.¹²⁻¹⁵⁾ The present one is much more extensive than others: the comparison is made (i) for all the ionic species with $Z \leq 19$ for which experimental data are available, and (ii) over a wide range of electron energies.

Here we should make clear the stand points on which the present evaluation of empirical formulas is made:

(1) For the present comparative study, experimental data obtained by beam methods are taken as a standard. No evaluation of the experimental data is attempted here. (It is under planning separately.)

(2) We deal with only the direct ionization. When a contribution of autoionization is expected to be large, the contribution should be estimated separately. In such a case, therefore, a care has to be taken when a comparison is made with experimental data.

(3) No theoretical results are referred here, though some fairly reliable methods of calculation have been developed recently. Those calculations have been done so far only for a few specific ions.¹⁶)

(4) The present comparative study is restricted to the ions with Z(atomic number) \leq 19 and N(number of bound electrons) \leq 18. For the ions with larger Z, experimental data are

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sparse and only for singly ionized ions. For those species, somewhat more sophisticated formulas may be necessary due to the large number of electrons.

(5) Empirical formulas for an ionization rate are not concerned here. Once a reliable formula is established for ionization cross section, it is easy to calculate therefrom the corresponding rate.

The outline of the present report is as follows. The definition of empirical formula is made in § 2. Then three empirical formulas (two by Lotz and one by Golden and Sampson) are taken to be reviewed. After an introduction of the formulas (§ 3), they are compared with experimental data (§4). Conclusions about the comparative study are given in § 5. The validity of several other empirical formulas is discussed in the Appendix.

In Part II of the present report, all the experimental data available for the ions with $Z \leq 19$ are presented in a graphical form. Those data are taken from the Atomic and Molecular Data Retrival and Display System (AMRDS) at the Research Information Center, Institute of Plasma Physics, Nagoya. An extensive data compilation is under way there on electron-ion collision cross sections and other atomic processes. The compiled data are stored in a computer to form a computerized data base. The cross sections produced by the empirical formulas reviewed in Part I are also plotted on the graphs.

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For convenience, a nomenclature of the symbols used in the report is summarized in Table 1. Cross sections and energies are expressed in the units of cm² and eV, respectively.

2. Definition of empirical formula

Here an empirical formula is defined to be an analytical formula whose parameters are <u>empirically</u> related to physical properties so as to produce cross sections for any ionic species at any electron energies.

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It should be noticed that there are two other kinds of analytical formulas of cross sections.

(i) an approximate formula of cross section

It is derived in an approximate theory of cross section calculation. The parameters are determined ab initio in the theory. One example is the Bethe formula. This type of formula is applicable only within the range of the validity of the theory.

(ii) a formula analytically fitted to experimental data or theoretical results

Parameters in this formula are determined by the fitting procedure. This formula is, in principle, equivalent to the data originally chosen for the fit. This cannot be used to predict cross sections for other species than those which the original data are concerned with.

Though often called empirical formulas too, these two kinds of formulas are distinguished here from the empirical formula defined above. An approximate formula, however,

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becomes an empirical formula when applied to the case out of the validity range of the approximate theory. In such a case, some modification is ofen made in the formula. Sometimes an empirical formula is derived after an analytical fitting is made to a number of species and thereby an empirical relation is established between the parameters and physical properties of the ions.

3. The formulas proposed by Lotz and by Golden and Sampson Lotz^{5,6} proposed two empirical formulas for an ionization cross section of atomic ions: one for ions with q(ionic charge)
3 and the other for q > 3. Those formulas have been used very widely by plasma physicists and astrophysicists. Recently Golden and Sampson^{10,11} have provided another formula for the calculation of ionization cross section, which is based on the Coulomb-Born (with exchange) results for hydrogenic ions. This formula can be expected becoming more accurate with increasing net charge of ions. Thus that would be useful for highly charged ions which are of primary interest in the recent studies of fusion and interstellar hot plasmas.¹

In the following the definitions of the above three formulas are given with some remarks. The notation is somewhat different from the original one, but each formula is expressed in a unified manner (see, for the notation, Table 1). Several other empirical formulas are discussed in the Appendix.

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(1) Lotz (I)

$$\sum_{j=a_{j}}^{\ell} \frac{\xi_{j}}{\prod_{j=1}^{2}} \frac{\ell n X_{j}}{X_{j}} \{ 1-b_{j} \exp[-c_{j}(x_{j}-1)] \}$$
(3.1)

Lotz ^{5,6} determined first the X_j dependence at $X_j \longrightarrow \infty$ so as to coincide with the Bethe asymptote of the ionization cross section. Then he modified the form in the region of small X_j by introducing three adjustable parameters (a_j, b_j, c_j) . After fitting the resulting formula to experimental data then available, he gave in his papers^{6,17} the numerical values of the parameters for (He - Ga)⁺, (Li - Zn)⁺⁺ and (Be - Ga)³⁺. The parameters depend not only on the subshell, j, of the ejected electron but also on the ionic species (i,e, atomic number of the ion).

A few remarks would be necessary here. The parameter fitting was done over a finite range of electron energy. The values so determined do not necessarily give the correct high-energy limit in magnitude. The formula cannot be applied to any other ions than listed above, unless the determination of parameters is extended in some way.

(2) Lotz (II)

$$Q_{j} = 2.4 \times 10^{-16} \left(\frac{I^{H}}{I_{j}}\right)^{2} \xi_{j} \frac{\ln X_{j}}{X_{j}}.$$
 (3.2)

When we denote by Q_{j}^{H} an ionization cross section of a hydrogen-like ion with its electron in the subshell j, $Z^{4}Q_{j}^{H}$ has a finite value at $Z \rightarrow \infty$. Lot Z^{6} found that, when Q_{j}^{H} is calculated in the Coulomb-Born (with exchange) approximation,¹⁸) $[Z^{4}Q_{1s}^{H}]_{Z\rightarrow\infty} \infty$ can be fitted by an analytical function of X_{1s} in the following way in the range of $X_{1s}^{=}$ 1-10 (see Fig. 1):

$$[Z^{4}Q_{1s}^{H}]_{Z \to \infty} = 2.4 \times 10^{-16} \frac{\ln X_{1s}}{X_{1s}} . \qquad (3.3)$$

Taking into account the difference in an ionization energy and the number of electrons in a subshell, he proposed the formula (3.2) for an ionization cross section of any ions. His original proposal was restricted to the case which cannot be dealt with by the previous formula (3.1). Because of its simplicity, however, the formula (3.2) is used more widely.

Hinnov's formula⁷⁾ is exactly the same as (3.2). Post's³⁾ is also the same as (3.2) but with a little different numerical factor $(1.9 \times 10^{-16} \text{ instead of } 2.4 \times 10^{-16})$. Post obtained his result from very limited number of experimental and theoretical cross sections available as of 1961.

It should be noted that, as in the case of Lotz (I), the formula (3.2) does not give a correct asymptotic value at $X_j \longrightarrow \infty$. The Bethe asymptote for a hydrogen-like ion with ls-electron gives¹⁹

$${}^{[Z^{4}Q_{1s}^{H}]_{Z} \longrightarrow \infty} \xrightarrow{X_{1s} \longrightarrow \infty} 0.99732 \times 10^{-16} \xrightarrow{ln X_{1s}} (3.4)$$

(3)' Golden and Sampson

$$Q_{j} = S_{j} \xi_{j} [0.880 \times 10^{-16} \frac{1}{X_{j}} \{A_{j} \ell n X_{j} + D_{j} (1 - \frac{1}{X_{j}})^{2} + (\frac{c_{j}}{X_{j}} + \frac{d_{j}}{X_{j}^{2}}) (1 - \frac{1}{X_{j}})\}], \qquad (3.5)$$

with

$$S_{j} = \left(\frac{n_{j}}{Z_{eff}}\right)^{4} \quad ---- \quad GS1$$
$$= \left(\frac{n_{j}}{Z_{eff}}\right)^{2} \left(\frac{I^{H}}{I_{j}}\right) \quad -----GS2$$

$$= \left(\frac{1}{1} \right)^{2}$$
 -----GS3

Golden and Sampson^{10,11)} use the relation

$$[z^{4}Q_{j}]_{Z \longrightarrow \infty} = \xi_{j} [z^{4}Q_{j}^{H}]_{Z \longrightarrow \infty}$$
(3.6)

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where Q_j^H is the ionization cross section of a hydrogenic ion with its electron in the subshell j. For an ion with finite Z, they adopt also the cross section on the right side of eq.(3.6) but with some modification. Actually they first calculate $[Z^A n_j^{-4} Q_j^H]_Z \longrightarrow \infty$ in the Coulom-Born

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(with exchange) approximation. They fit the result by an analytical formula to find the expression in the square brackets in (3.5). The parameters (A_j, D_j, c_j, d_j) are thus determined. Then, to scale the formula to the non-hydrogenic ions with finite Z, they multiply $[Z^4n_j^{-4} Q_j^H]_{Z \rightarrow \infty}$ by a factor S_j . Taking into account the relation

$$\frac{z^4}{n_1^4} = \left(\frac{z_1^H}{z_1^H}\right)^2, \qquad (3.7)$$

they propose the two kinds of the factors, GSl and GS2, with an ⇒ffective nuclear charge, Z_{eff}. The third factor, GS3, is proposed here for the first time by the present authors. It will be shown in the next section that GS3 is much better than GSl or GS2, when compared with experimental data.

The parameters (A_j, D_j, c_j, d_j) depend only on the subshell of the ejected electron. The numerical values have been determined so far for $j = 1s \sim 4f$.^{10,11,20,21,22)} Among the parameters, A_j is chosen in such a way that the correct Bethe asymptote (for the hydrogenic ion) is reproduced at $X_j \rightarrow \infty$. The effective nuclear charge is also given by Golden and Sampson.^{10,20,21,22)} This quantity depends on the isoelectronic sequence, as well as on the subshell.

4. Comparison with experimental data

The three empirical formulas introduced in the previous section are compared with all the experimental data available

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for the ions with $Z \leq 19$. The graphs showing the comparison are given in Part II of the present report. (1) Lotz (I)

To determine the parameters in this formula, use has been made of the experimental data for He^+ , Li^+ , N^+ , Ne^+ , Na^+ and K^+ . Those species, therefore, should be excluded from the comparative study. As is mentioned in §3 (1), this formula cannot be applied to the ions with q > 3.

A graphical comparison for all the ions other than those excluded above shows that the cross section calculated with this formula is in quite good agreement (within about 20%) with the experimental data for most species. For Ar^{++} , the agreement is rather poor but not very bad (within about 40%). There are two exceptional cases (C^{3+} , Mg^+) for which the formula gives very poor results. (For some species, an apparent disagreement is found near threshold, but it may be due to a contamination of incident ion beams with metastable species.)

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This satisfactory nature of the formula is attributed to the following reasons. The functional form of X_j is properly chosen and flexible enough to reproduce the sensitive cross section in the region near threshold. Based on the detailed comparison with a fairly large number of experimental data, the parameters are adjusted deliberately depending not only on the subshell of the ejected electron but also on the ionic species. Moreover the way of the variation of the parameters is at least qualitatively

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reasonable, though Lotz said nothing about that explicitly. With q increased and N fixed, for instance, the parameter a_j increases and b_j decreases. This accounts for the effect of the increase in the Coulomb attraction between the incident electron and the ion.

Finally we should mention several disadvantages of this formula. First, the parameters in the formula were determined purely empirically, so that it is almost impossible to improve them or to extend the applicability of the formula. Second, this formula cannot give the correct asymptotic value at $X_j \longrightarrow \infty$. Third, the determination of the parameters is solely based on the experimental data. Thus the experimental error, if any, directly affects the values of the parameters. Moreover, if an autoionization contributes to the experimental data Lotz used, the parameters thereby determined do not represent those for direct ionization. In other words, this formula may include, at least partly, the effect of autoionization.

(2) Lotz (II)

A graphical comparison shows that this formula gives ionization cross sections in agreement with the experimental data within 20-40% of error, except for C^{3+} , Ne^+ , Na^+ , Mg^+ , and Ar^{5+} . As shown in the graphs, this formula is better, on the whole, than that of Golden and Sampson (GS3). The basic principle of derivation is the same for both the formulas. The GS3 is even more elaborate than the Lotz(II).

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The former (GS3) takes into account the dependence on the subshell of the ejected electron in a more detailed manner than the latter. That is, the numerical coefficients in GS3 depend on the subshell j. The functional form of GS3 is more realistic than that of Lotz (II). In the case of Lotz (II), therefore, these defects seem to be cancelled by the error inherent in the model of hydrogenic ion.

Two disadvantages should be mentioned here about this formula. First, due to the simple functional form of X_j, this formula often cannot reproduce detailed structure of the cross section (e.g., that near threshold), though it gives a fairly good overall feature. Second, this formula is not assured to become correct with increasing Z/N, as the GS formula does.

(3) Golden and Sampson

An extensive comparison shows that the scaling factor, GS3, is better than GS1 or GS2 in most cases. Some examples are shown in Figs. 2 - 5. There are two exceptional cases. For many of singly charged ions, none of the factors can give a satisfactory result. In such cases, the experimental dependence on X_j is much different from the formula. (Mg⁺⁺ is included in this class.) It is evident that the experimental cross sections for lithium-like ions (C³⁺, N⁴⁺, O⁵⁺) have an autoionization contribution. If we subtract the contribution, the resulting values are more likely to be fit by GS1 than GS3. Aside from these two

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exceptional cases, the GS3 gives ionization cross sections in agreement with the experimetal data within about 20 % for most species and within about 40 % for some poor cases $(N^{3+}, 0^{4+}, Ar^{5+})$. The numerical values of the parameters in the formula have been revised several times to improve the formula. The most recent ones are used to produce the cross sections shown in the present report.

The advantages of this formula are: (i) The way of derivation of the formula is quite clear, so that it is relatively easy to improve that or to extend its applicability. An effect of autoionization, for example, is not included in this formula. The effect, if necessary, can be simply added to the result of this formula. (ii) In principle, this formula converges to the correct one as the ratio Z/N increases. (This tendency is not clearly shown, however, in the present comparison, probably because the value of Z/N is at most 3.5 here.) (iii) In particular the parameters in the formula GS3 are dependent only on the subshell of the ejected electron. This simplifies very much the cross section calculation.

From the graphs it is shown that the formula GS3 systematically provides smaller cross sections at higher energies than the experimental ones. This may be related to the fact that the formula is forced to go to the Bethe asymptote of hydrogenic ions, not of real ones, at $X_i \longrightarrow \infty$.

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5. Conclusions

First of all, we propose a new type of scaling factor, GS3, for the formula of Golden and Sampson. This factor has been found better than the two factors, GS1 and GS3, proposed originally by Golden and Sampson.

From the detailed comparisons of Lotz (I), Lotz (II), and GS3, the following conclusions are reached.

- For the cases of q = 1 3, the formula of Lotz (I) is the best.
- (2) An overal! feature of the cross section, especially for the case with q > 1, is reasonably well given by Lotz (II).
- (3) The formula GS3 is not better than Lotz (I) or Lotz(II), but usable for q > 1. This formula should give, in principle, more accurate results for ions with larger Z/N.
- (4) In the case where a significant contribution of autoionization is expected, the contribution should be estimated separately and added to the direct-ionization cross section obtained by Lotz (II) or GS3. It is rather unclear whether the cross section given by Lotz

(I) includes no contribution of autoionization.

When any of those empirical formulas is used, one should take into account the cautions mentioned in the previous sections.

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Appendix: Other empirical formulas

There are many other empirical formulas^{2,3,4,7,8,9)} proposed for ionization cross sections. Comparative studies have also been made for them. As a conclusion, we have found no better formulas than those proposed by Lotz or Golden and Sampson. Furthermore, all those formulas have problems either in the derivation or in its applicability. Two of them are shown below as an example.

(a) Drawin²⁾

$$Q_j = 2.34 \times 10^{-16} (\frac{I^H}{I_j})^2 \xi'_j \frac{X_j - 1}{X_j} \ln(1.25bX_j), (A.1)$$

where b = 2(q+1)/(q+2). The value of the parameter ξ'_j is given by Drawin²³⁾ for He, Li, C, N, O, Ne, Na, Mg, Al, Si, Ar, K. Drawin considers the ionization only from the outermost subshell. To take account of the contribution of inner shells, he modifies the number of the electrons. The derivation of (A.1) is essentially the same as that of Lotz (I), i.e., based purely empirically on experimetal data. The rule of the determination of the parameter is unclear, so that this formula can be applied only to the ions listed above.

(b) Seaton⁴⁾

$$Q_{j} = 1.9 \times 10^{-16} \left(\frac{I^{H}}{I_{j}}\right)^{2} \xi_{j} \left(1 - \frac{1}{X_{j}}\right).$$
 (A.2)

This has been obtained so as to fit the experimental data

for $X_j \leq 2$. Many astrophysicists employ this formula in their, studies, but its application should be limited in the threshold energy region.

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Table 1. Nomenclature of the symbols

<u>^</u>	$\mathbf{P}_{\mathbf{r}}$
^v j	Partial Ionization cross section (in cm) from
	the subshell j
Q o ^H	$= \sum_{j} Q_{j}$
Qj	ionization cross section (cm) of a hydrogenic ion
	with its electron in the subshell j
^E 0	Energy (in eV) of the incident electron
I _j	Ionization energy (eV) for the subshell j (For a
	hydrogenic ion, I_j^H is used.)
× _j	$= E_0 / I_j$
$\mathtt{I}^{\mathtt{H}}$	Ionization energy of atomic hydrogen (= 13.6 eV)
ξ _j	Number of equivalent electrons in the subshell j
nj	Principal quantum number of the subshell j
Z	Atomic number
N	Number of bound electrons
đ	Ionic charge (=Z - N)

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- Fig. 1. Reduced cross section for a hydrogenic ion with its electron in 1s state. Circles are the values calculated for $Z = \infty$ with the use of the Coulomb-Born-Exchange approximation. The solid line indicates the relation $X_{1s}Z^4Q_{1s}^H = 2.4 \times 10^{-16} \ln X_{1s}$.
- Fig. 2-5. Comparisons of the Golden-Sampson formula with three scaling factors: solid line for GS3; short-dashed line for GS2; long-dashed line for GS1.



Fig. 1

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Fig. 2



Fig. 3





Fig. 4

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II. Graphs of Experimental Data with the Results of

Processes

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Empirical Formulas

1. Index to graphs

Fig.no.

References

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1.	He^+ + e \longrightarrow He^{2+} + 2e	1, 19
2.	Li^+ + e \longrightarrow Li^{2+} + 2e	7, 10, 13, 19
3.	$B^{3+} + e \longrightarrow B^{4+} + 2e$	35
4.	c^+ + e $\longrightarrow c^{2+}$ + 2e	21
5.	c^{2+} + e $\longrightarrow c^{3+}$ + 2e	30
6.	c^{3+} + e $\longrightarrow c^{4+}$ + 2e	32, 33
7.	c^{4+} + e $\longrightarrow c^{5+}$ + 2e	35
8.	N^+ + e $\longrightarrow N^{2+}$ + 2e	4
9.	N^{2+} + e $\longrightarrow N^{3+}$ + 2e	21
10.	N^{3+} + e $\longrightarrow N^{4+}$ + 2e	35
11.	N^{4+} + e $\longrightarrow N^{5+}$ + 2e	32, 33
12.	N^{5+} + e $\longrightarrow N^{6+}$ + 2e	35
13.	0^+ + e $\longrightarrow 0^{2+}$ + 2e	21, 34
14.	o^{2+} + e $\longrightarrow o^{3+}$ + 2e	20
15.	o^{3+} + e $\longrightarrow o^{4+}$ + 2e	35
16.	o^{4+} + e $\longrightarrow o^{5+}$ + 2e	35
17.	0^{5+} + e $\longrightarrow 0^{6+}$ + 2e	33
18.	$Ne^+ + e \longrightarrow Ne^{2+} + 2e$	3, 34
19.	$Na^+ + e \longrightarrow Na^{2+} + 2e$	8, 12
20.	$Mg^+ + e \longrightarrow Mg^{2+} + 2e$	11
21.	$Mg^{2+} + e \longrightarrow Mg^{3+} + 2e$	18
22.	$Ar^+ + e \longrightarrow Ar^{2+} + 2e$	29, 34
23.	Ar^{2+} + e \longrightarrow Ar^{3+} + 2e	34

24.
$$Ar^{3+} + e \longrightarrow Ar^{4+} + 2e$$
 34
25. $Ar^{4+} + e \longrightarrow Ar^{5+} + 2e$ 34, 35
26. $Ar^{5+} + e \longrightarrow Ar^{6+} + 2e$ 34
27. $K^{+} + e \longrightarrow K^{2+} + 2e$ 8, 12

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2. Graphs (Experimental data with the results of the empirical formulas)

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All the symbols denote the experimental data obtained by beam method.

The results of the empirical formulas are indicated by

----- for $q \leq 3$, Lotz(I) and for q > 3, Lotz (II) ----- Lotz (II)

--- GS3



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Fig. 1





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Fig. 3



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Fig. 13





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Electron energy



Fig. 17





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Fig. 19















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Fig. 22



Fig. 23















ι, L ---> Ar



Fig. 25











Fig. 27

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