ISSN 0915-6364

NATIONAL INSTITUTE FOR FUSION SCIENCE

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(Received - June 29, 1995)

NIFS-DATA-27 July 1995

RESEARCH REPORT
NIFS-DATA Series

NAGOYA, JAPAN

Multiple-Ionization Cross Sections of Atoms and Positive Ions by Electron Impact

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Abstract

For the first time, semiempirical formulae for multiple-ionization (MI) cross sections σ_n of atoms and ions by electron impact are suggested for ejection of three or more electrons $n \geqslant 3$. The formulae have been deduced on the basis of available experimental data on σ_n and the assumption of the Born-Bethe dependence of σ_n on the incident electron energy E.

A comparison of the cross section described by the semiempirical formula suggested with experimental data available for neutral atomic targets from Ne up to U and ejection up to 13 electrons and with those for positive ions from Ar^+ up to W^{4+} with ejection up to four electrons shows that the formulae can be used for estimation of MI cross sections σ_n, $n \geqslant 3$, from threshold up to high electron energies $E \approx 10^5$ eV for an arbitrary atomic or ionic target.

[keywords: atomic collisions, ionization potential, multiple electron ionization, effective cross section]

Contents

1. Introduction

The problem of the multiple ionization (MI) arising in electron-atom and ion-atom collisions is of a high interest both for our understanding of many-electron processes (multi- electron transitions, electron correlation effects[1-2]) and for different physical applications such as plasma kinetics problems, charge-state evaluation of atoms exposed to an electron beam, contribution of Auger and shake-off processes and others[3-4].

In the case of MI of atoms and positive ions by electron impact the available experimental data on the cross sections σ_n are often not consistent and complete and large discrepancies exist among MI cross sections, in particular for large numbers n of the ejected electrons (see a compilation[5]). The quantum mechanical calculations of MI cross sections even for $n > 2$ are still unknown, therefore analytical semiempirical formulae constitute a special interest.

A semiempirical formalism to predict double- and triple-ionization cross sections in the vicinity of ionization threshold of some specific atomic targets is applied in ref.[6]. A scaling of multiple-ionization cross sections and semiempirical formulae for σ_n are considered in ref.[7].

Our aim in this work is to investigate the multiple-ionization process in electron-atom and electron-ion collisions

$$e + A^{z+} \rightarrow e + A^{(z+n)+} + ne, \quad n > 1 \qquad (1)$$

and to obtain a semiempirical formula for MI cross section σ_n which could describe its behavior on the average in a wide range of the incident electron energy.

2. Basic Formulae

The measured threshold energy E_{th} for MI cross sections σ_n corresponds to the minimal ionization energy I_n required to remove n outmost electrons (see, e.g.,[8-9]), i.e.

$$E_{th} = I_n = \sum_{i=0}^{n-1} I_{i,i+1}, \qquad (2)$$

where $I_{i,i+1}$ is the one-electron ionization energy from the charge i to i+1. For example, the minimal energy I_6 required for ionization of six electrons in Kr is estimated to be[24-25]: I_6 = $I(Kr) + I(Kr^{+}) + I(Kr^{2+}) + I(Kr^{3+}) + I(Kr^{4+}) + I(Kr^{5+})$ = 14.0 eV + 27.89 eV + 41.78 eV + 55.67 eV + 70.31 eV + 84.52 eV = 294.17 eV.

Each target atom or ion is characterized by its own set of the minimal ionization energies I_n, so it is natural to choose I_n as a scaling parameter for the incident electron energy E

$$u = E/I_n - 1 \qquad (3)$$

similar to a single ionization.

Our analysis of the experimental data available on MI cross sections σ_n for atoms and ions by electron impact showed that the majority of the cross sections has a similar shape for all targets and all cases with $n \geqslant 3$ and the electron- impact energy dependence is described with the universal Born- Bethe type formula[10]:

$$F(u) = \left(\frac{u}{u+1}\right)^c \frac{\ln(u+1)}{u+1}, \quad u = E/I_n - 1, \qquad (4)$$

where the constant c = 1 for neutral targets (z = 0) and c = 0.75 for positive ions (z > 1) (Fig. 1).

Unfortunately, the energy dependence of double-ionization cross sections σ_2 (n = 2) can not be described properly with Eq.(4) and will be considered separately.

We write an expression for σ_n in the form:

$$\sigma_n(u) = \frac{C(n, N)}{(I_n/Ry)^2} F(u) \; [10^{-18} cm^2], \quad n \geqslant 3, \tag{5}$$

where 1Ry = 13.6 eV. Then the coefficient C(n,N) should depend only on two parameters - the number of the ejected electrons n and the total number of the target electrons N. The analysis of the available experimental data with a fixed number of the ejected electrons n but different numbers of the target electrons N has shown that the constant C(n, N) can be written in the form:

$$C(n, N) = a(n) \; N^{b(n)} \tag{6}$$

where *a* and *b* are the approximation parameters. They were obtained by fitting Eqs.(5) and (6) to the experimental data at low as well as at high electron energies. As the references of experimental data for electron-atom collisions we used the results of[8-9,11-23]. Most of the electron-ion cross sections ions were measured using the crossed beam technique.

Finally, the expression of MI cross section σ_n for electron-atom and electron-ion collisions can be written in the form:

$$\sigma_n(u) = \frac{a(n) \; N^{b(n)}}{(I_n/Ry)^2} \left(\frac{u}{u+1}\right)^c \frac{\ln(u+1)}{u + 1} \; [10^{-18} cm^2], \quad n \geqslant 3, \tag{7}$$

where the constant *c* is given in eq.(4). The analysis has also shown that it is possible to describe MI cross sections of atoms and ions by the same set of fitting parameters a(n) and b(n). We note that the parameters a(n) and b(n) given in Table 1 are the smooth functions of n.

For ejection of $3 \leqslant n \leqslant 10$ electrons the values for a(n) and b(n) are listed in Table 1; for $n \geqslant 10$ one can use the asymptotic values:

$$a(n) \approx 1350/n^{-5.7}, \quad b(n) = const = 2, \quad n \geqslant 10. \tag{8}$$

Table 1. Fitting parameters a(n) and b(n) in Eq.(7) for removal of $3 \leqslant n \leqslant 10$ electrons from atoms or ions.

n	a(n)	b(n)
3	6.30	1.20
4	0.50	1.73
5	0.14	1.85
6	0.049	1.96
7	0.021	2.00
8	0.0096	2.00
9	0.0049	2.00
10	0.0027	2.00

According to Eq.(7) the cross section σ_n reaches its maximum at $u_{max} \approx 3.2$, $E_n^{max} \approx 4.2\ I_n$, i.e.,

$$\sigma_n^{max} \approx 0.27\ a(n)\ N^{b(n)} (I_n/Ry)^{-2} [10^{-18} cm^2]. \tag{9}$$

Eq.(9) gives quite good estimate for the cross section maximum σ_n^{max} and the corresponding electron energy E_n^{max}. For example, for experimental triple-ionization cross section of Bi atoms[15] we have:

$$\sigma_3^{max} = 2.7\text{x}10^{-17}\text{cm}^2, \quad E_3^{max} = 170 \text{ eV},$$

meanwhile Eq. (9) gives (I_3 = 51.3 eV):

$$\sigma_3^{max} = 0.27\text{x}6.3\text{x}(83)^{1.20}(51.3/13.6)^{-2}\ 10^{-18}\text{cm}^2 = 2.40\text{x}10^{-17}\text{cm}^2$$

and E_3^{max} = 4.2x51.3 = 215 eV, respectively.

4. Comparison with experimental data

A comparison of the present semiempirical formula (7) with typical experimental data on MI cross sections of neutral atoms and positive ions is given in Figs. 2 - 26 and 27 - 52, respectively. Figures of the MI cross sections are presented in the order of increasing of the target nuclear charge. The minimal ionization potentials I_n were calculated from Tables[24-25]. The values for I_n of some atoms and ions are given in Tables 2 and 3.

Table 2. The minimal ionization energies I_n, eV, for neutral atoms.

Atom	Number of the target electrons N	I_1	I_2	I_3	I_4	I_5	I_6
He	2	24.6	79.0				
Ne	10	21.6	62.7	126	223	349	
Mg	12	7.65	22.6	103	212	353	539
Ar	18	15.8	43.4	84.3	144	219	310
Fe	26	7.87	23.5	56.2	114	197	305
Cu	29	7.73	29.0	77.3	153	256	386
Ga	31	6.00	25.8	56.7	118	214	344
Ge	32	7.90	24.3	58.6	105	192	317
Se	34	9.75	32.1	66.3	112	183	269
Kr	36	14.0	41.9	83.7	139	209	294
Ag	47	7.58	29.1	70.1	131	211	310
In	49	5.79	23.9	51.9	106	184	284
Sn	50	7.34	22.4	53.1	94.8	169	267
Sb	51	8.64	26.0	52.8	98.0	155	250
Te	52	9.01	28.3	58.1	98.4	160	233
Xe	54	12.13	35.7	70.8	117	177	249
Pb	82	7.42	23.0	55.3	98.9	166	254
Bi	83	7.29	24.4	51.3	97.4	156	241
U	92	6.0	17.6	35.7	66.6	116	185

Table 2 (continued)

Atom	Number of the target electrons N	I_7	I_8	I_9	I_{10}	I_{11}	I_{12}	I_{13}
Kr	36	400	542	703				
Xe	54	347	459	630	832	1064	1328	1656

Table 3. The minimal ionization energies I_n, eV, for positive ions.

Ion	Number of the target electrons N	I_3	I_4	Ion	Number of the target electrons N	I_3	I_4
Ar^+	17	128	203	Mo^+	41	87	
Ar^{2+}	16	176		Mo^{2+}	40	130	
Fe^+	25	106		Mo^{3+}	39	173	
Fe^{2+}	24	173		Mo^{4+}	38	253	
Fe^{3+}	23	278		Xe^+	53	105	165
Fe^{4+}	22	324		Xe^{2+}	52	141	213
Fe^{5+}	21	400		Xe^{3+}	51	178	
Ni^+	27	117		Xe^{6+}	48	381	
Ni^{2+}	26	192		Cs^+	54	106	167
Ni^{3+}	25	276		La^{2+}	55	130	
Ni^{4+}	24	360		W^+	73	80	
Kr^+	35	125		W^{2+}	72	118	
Kr^{2+}	34	168		W^{3+}	71	160	
Rb^+	36	127	200	W^{4+}	70	240	

4. Conclusion

A comparison of the cross section described by the semiempirical formula (7) with experimental data available for neutral atomic targets from Ne up to U and ejection up to 13 electrons and with those for positive ions from Ar^{+} up to W^{4+} with ejection up to four electrons has shown that in the most cases considered the accuracy of the present formula is a factor of 2 or even better. Two cases are exceptional: quintuple ionization of Ne atoms (Fig. 4) and triple ionization of La^{2+} (Fig. 48) ions where the discrepancy between the semiempirical formula (7) and experimental data is more than one order of magnitude. To make more general conclusions it is necessary to perform further experimental investigations with better accuracies.

It was found semiempirically that σ_n depends mainly on three atomic parameters: the minimal ionization energy I_n, required to remove n electrons from the target, the total number of the target electrons N and the number of the ejected electrons n. For large n, one has the following asymptotic behavior:

$$\sigma_n \sim \frac{N^2}{n^{\sigma} I_n^2} F(u), \qquad u = E/I_n - 1, \qquad n \gg 1,$$

where F(u) is the universal function (Eq.(4)) for any $n \geqslant 3$ and arbitrary neutral target.

Therefore, as the number of the ejected electrons n increases the multiple-ionization cross section approximately decreases as $\sigma_n \sim n^{-\sigma}$.

Of course, the present empirical formula (7) based on the Born-Bethe approximation can not describe properly the energy dependence near cross section maximum where the indirect processes are known to play a significant role. However, the formula suggested is very simple and can be used for estimation of multiple-ionization cross for an arbitrary atomic or ionic target in a wide range of the incident electron energy.

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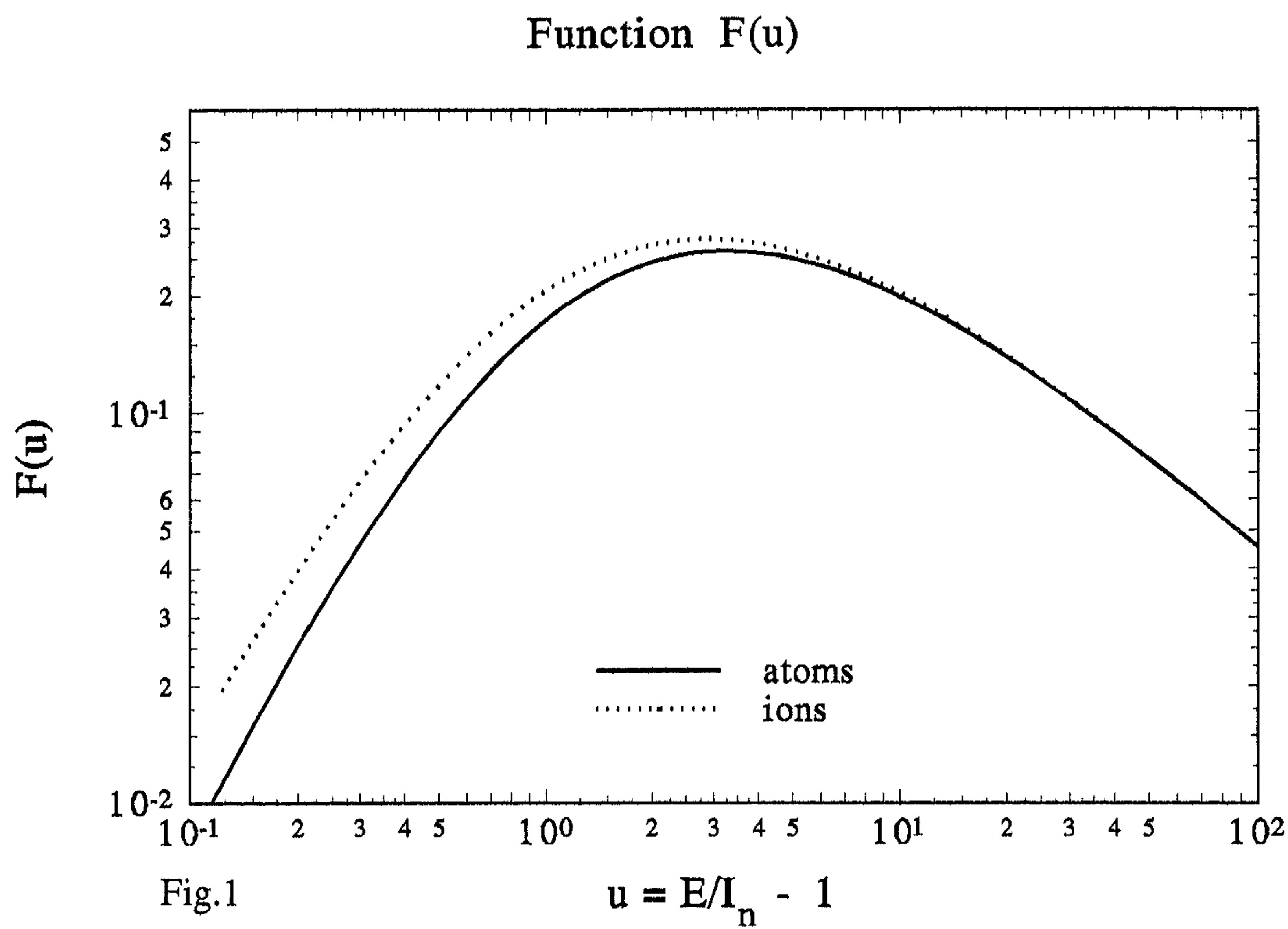

Function F(u)
F(u)
5
4
3
2
10-1
6
5
4
3
2
10-2
10-1
2
3
4
5
100
2
3
4
5
101
2
3
4
5
102
atoms
ions
u = E/In - 1
Fig.1

$e + Ne^{0+} \rightarrow e + Ne^{3+} + 3e$

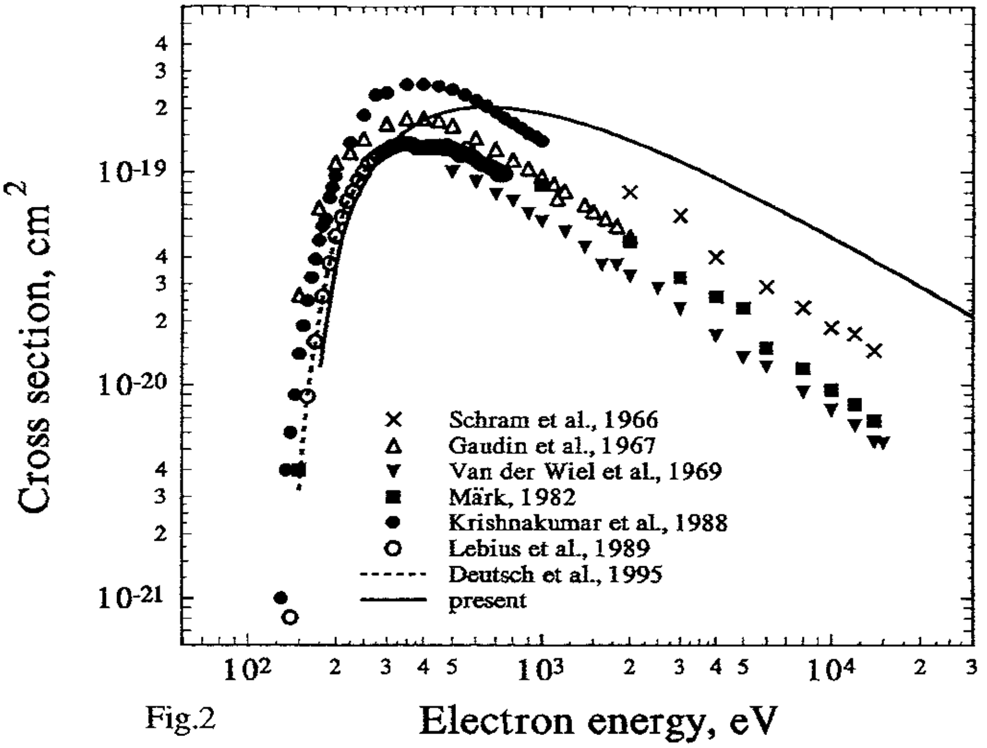


Fig.2

$e + Ne^{0+} \rightarrow e + Ne^{4+} + 4e$

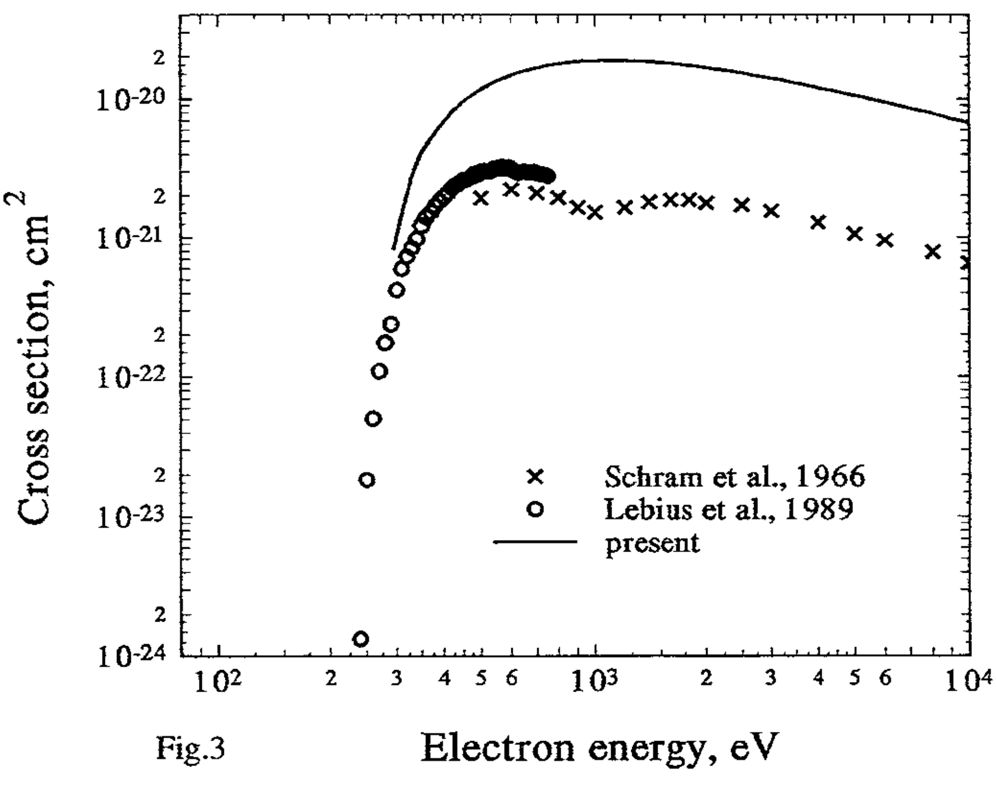


Fig.3

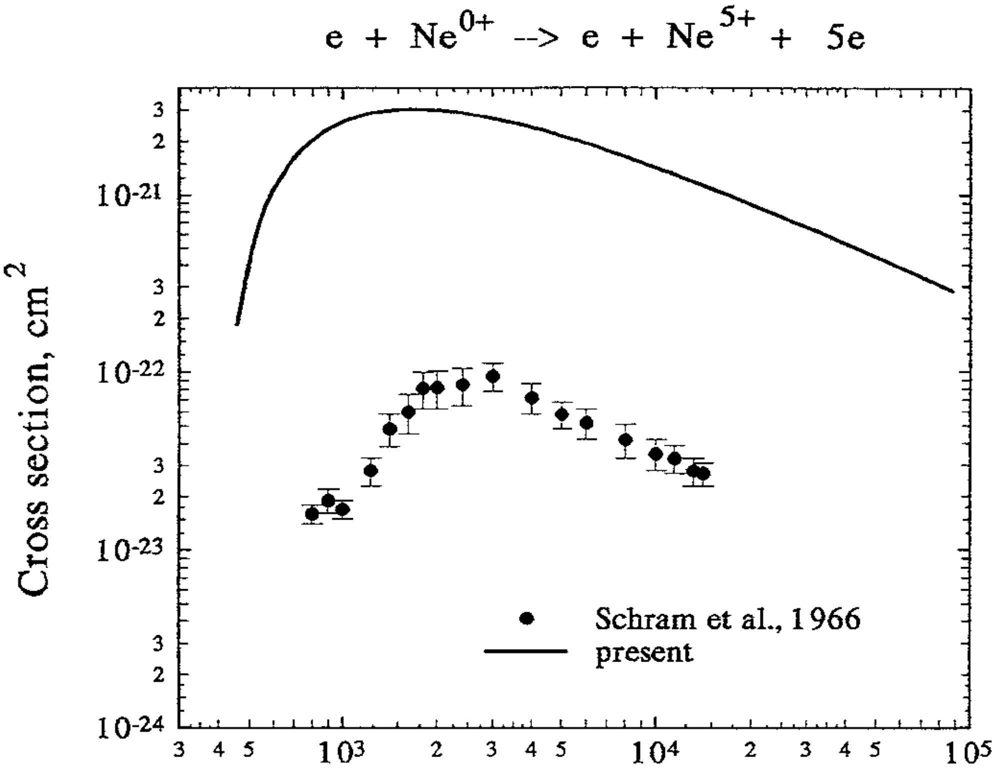

e + Ne^{0+} --> e + Ne^{5+} + 5e
Cross section, cm^2
Electron energy, eV
Schram et al., 1966
present

Fig.4

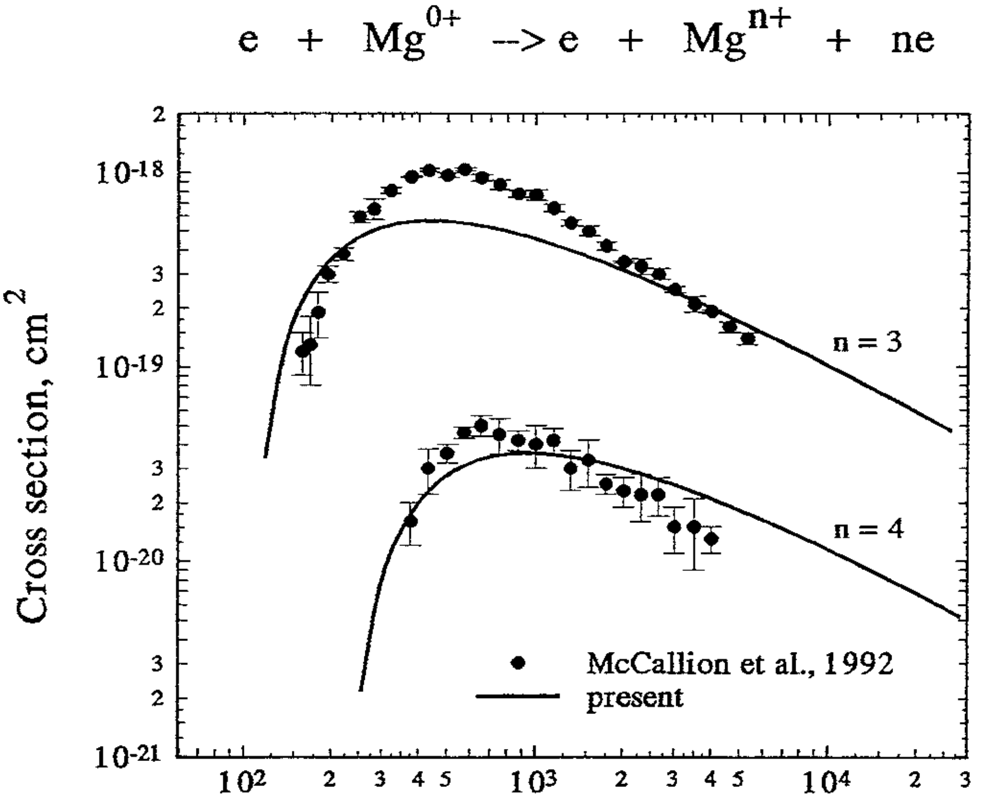

e + Mg^{0+} --> e + Mg^{n+} + ne
Cross section, cm^2
Electron energy, eV
n = 3
n = 4
McCallion et al., 1992
present

Fig.5

$e + Ar^{0+} \rightarrow e + Ar^{n+} + ne$

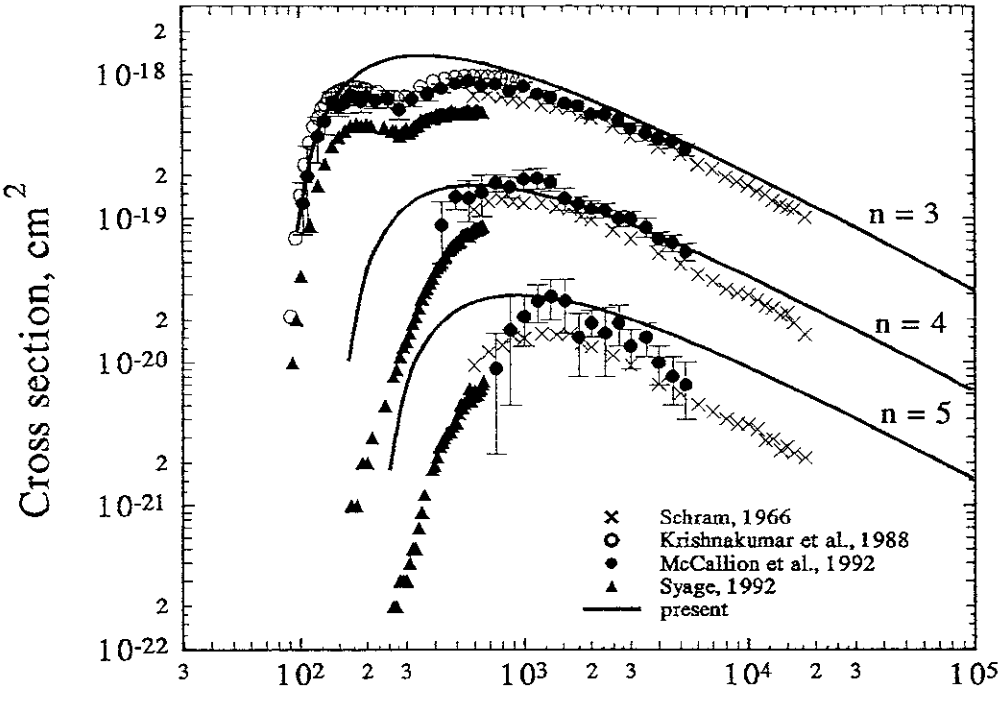


Fig.6

$e + Fe^{0+} \rightarrow e + Fe^{n+} + ne$

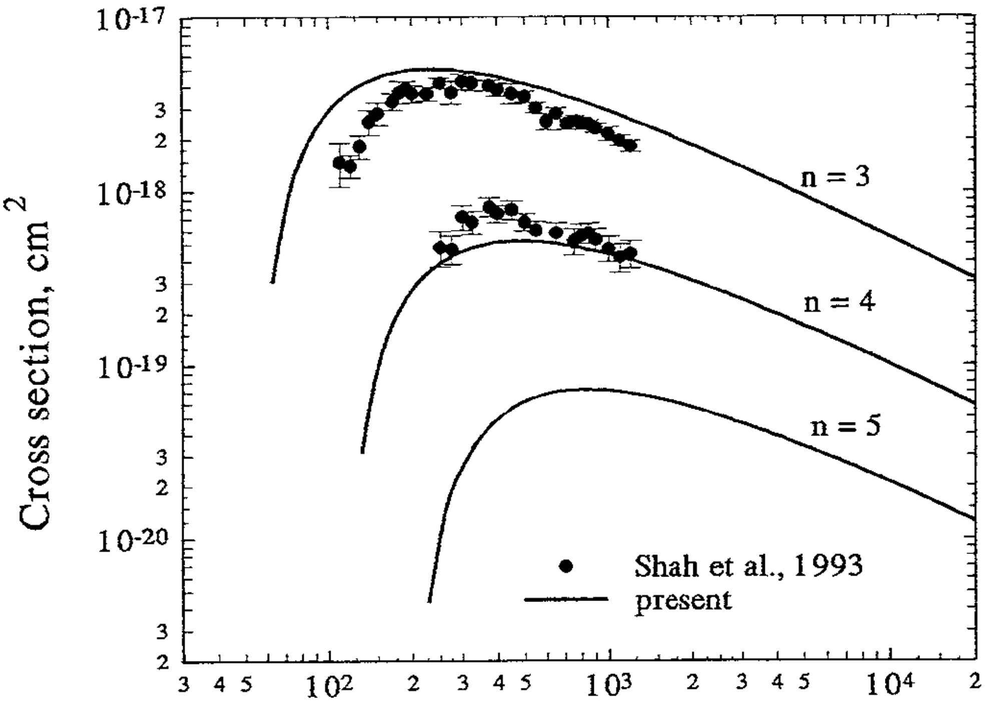
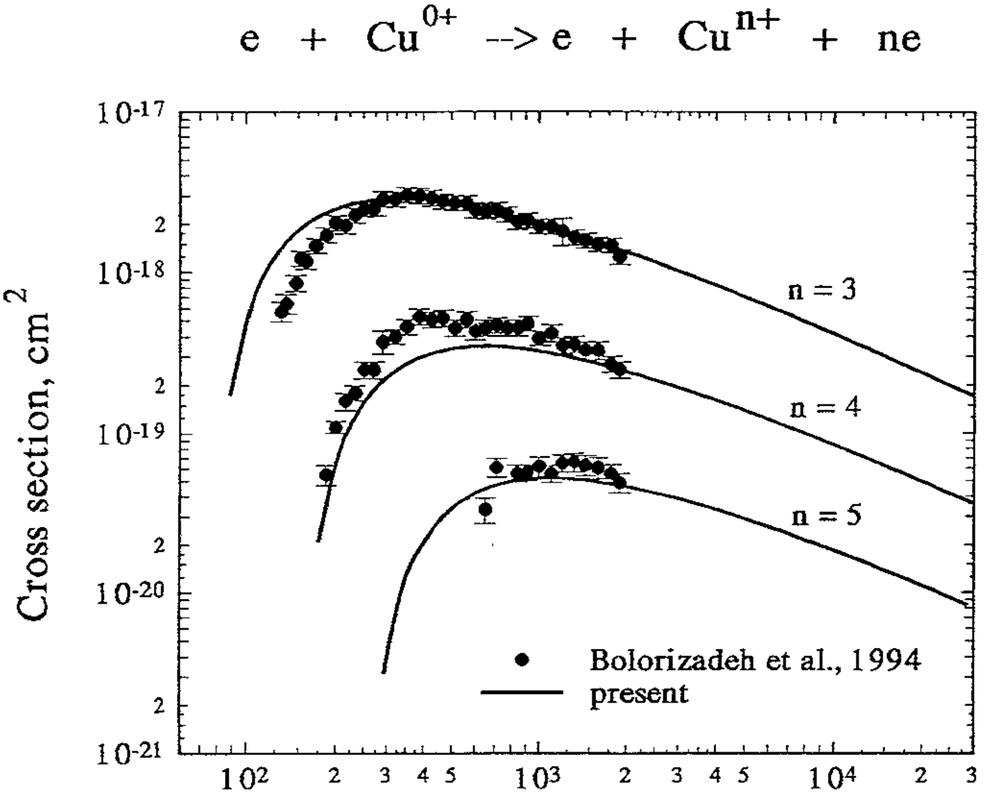
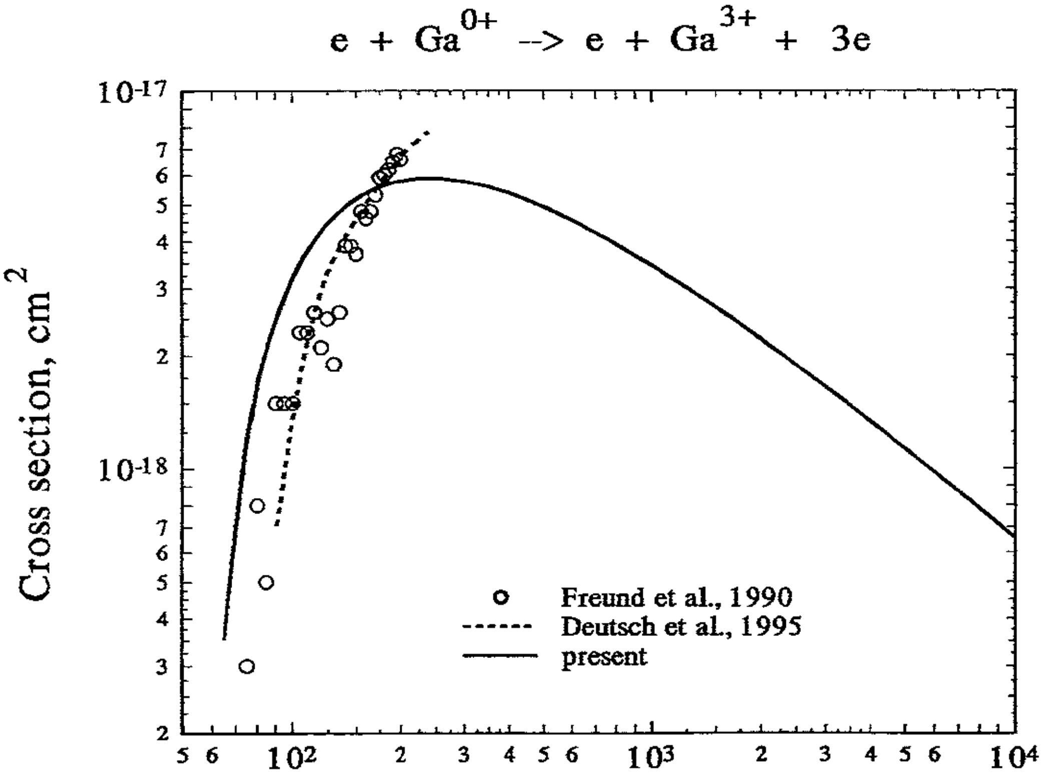


Fig.7



e + Cu^{0+} --> e + Cu^{n+} + ne
Cross section, cm^2
n = 3
n = 4
n = 5
Bolorizadeh et al., 1994
present
Electron energy, eV

Fig.8



e + Ga^{0+} --> e + Ga^{3+} + 3e
Cross section, cm^2
Freund et al., 1990
Deutsch et al., 1995
present
Electron energy, eV

Fig.9

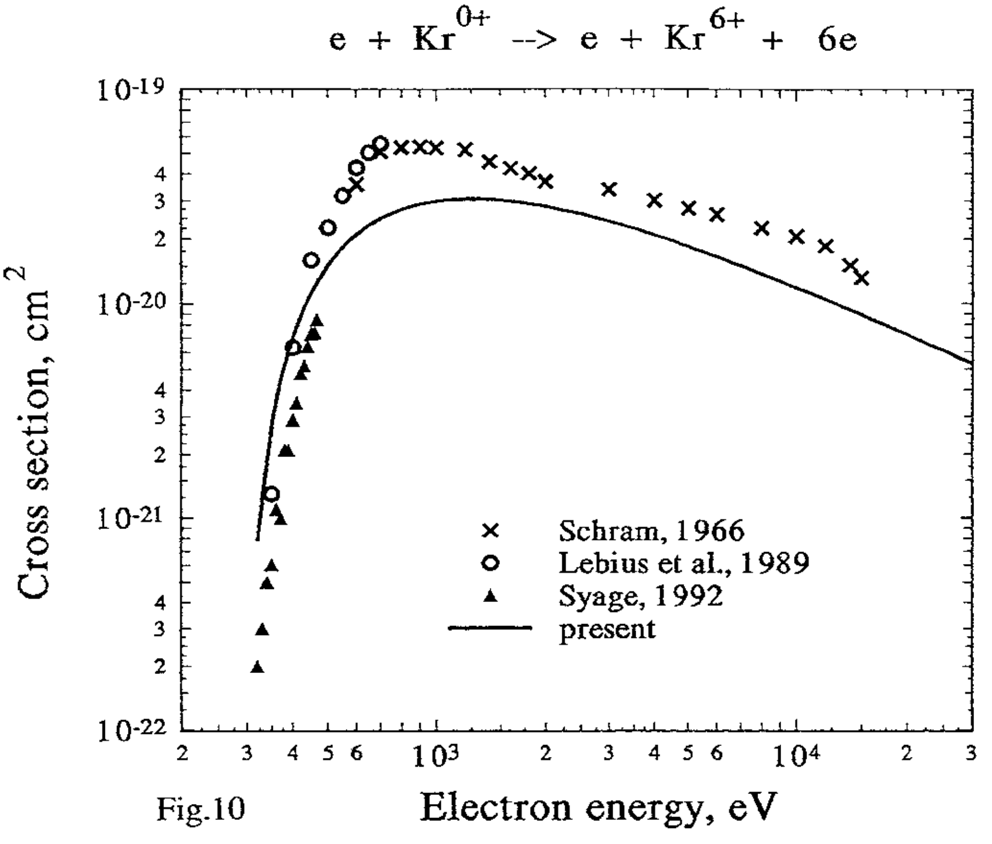

e + Kr^{0+} --> e + Kr^{6+} + 6e
Cross section, cm^2
Electron energy, eV
Schram, 1966
Lebius et al., 1989
Syage, 1992
present

Fig.10

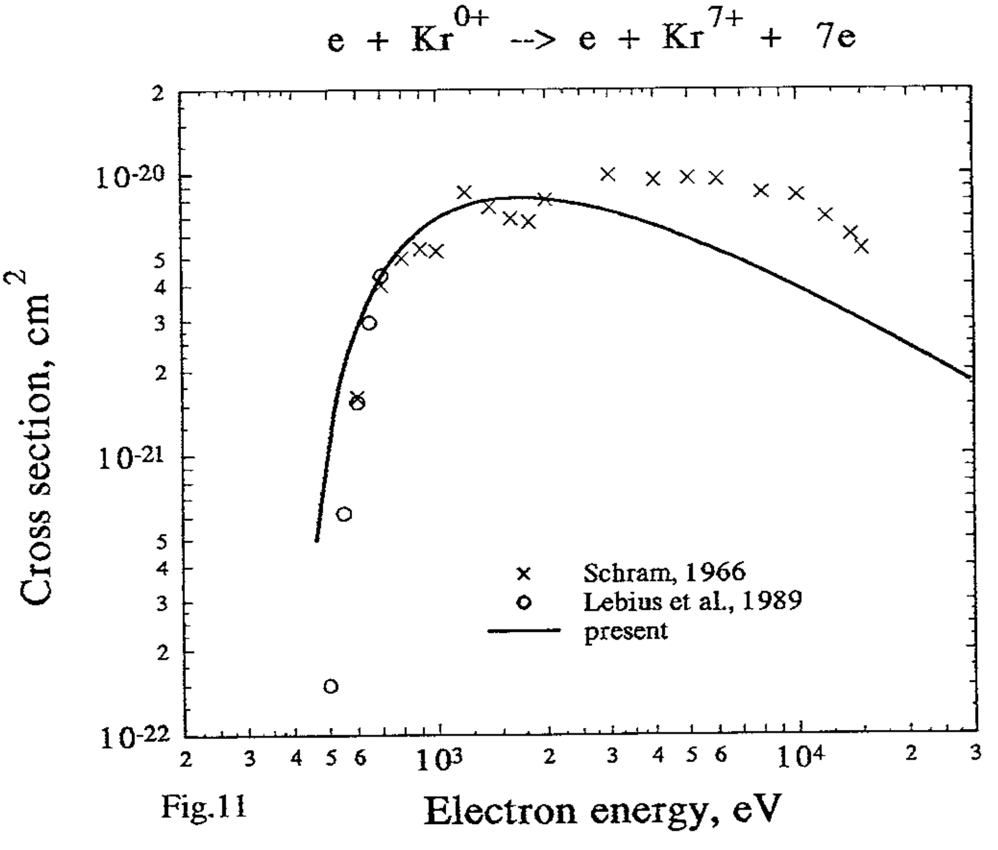
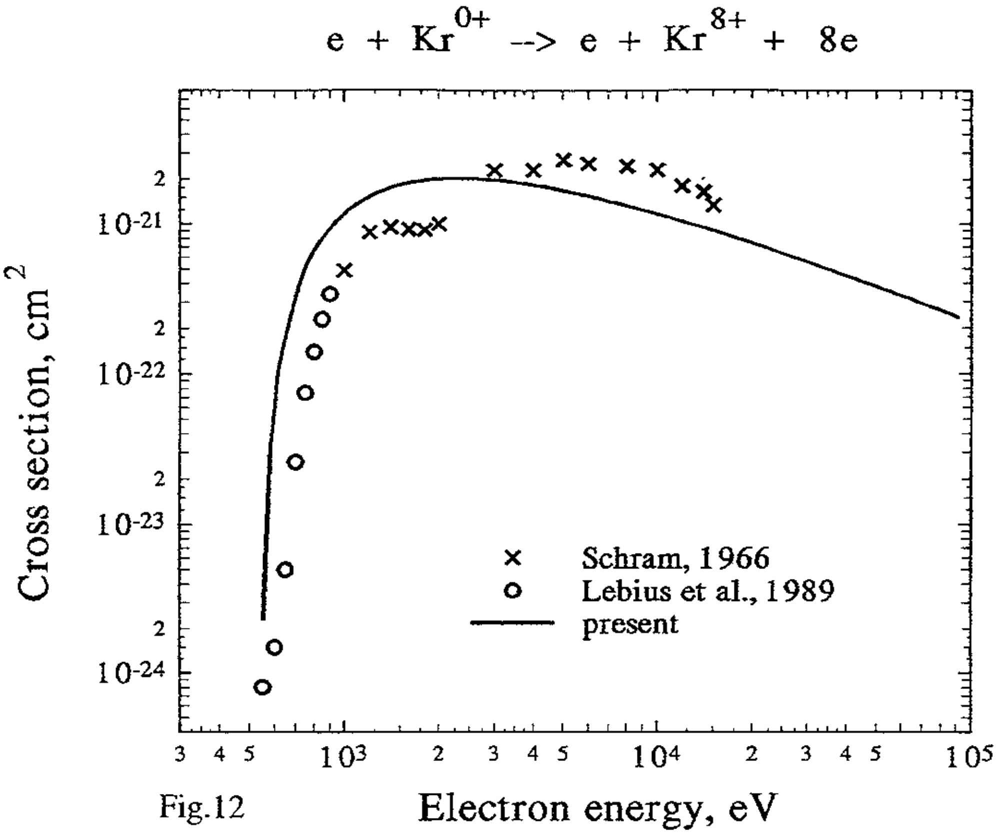
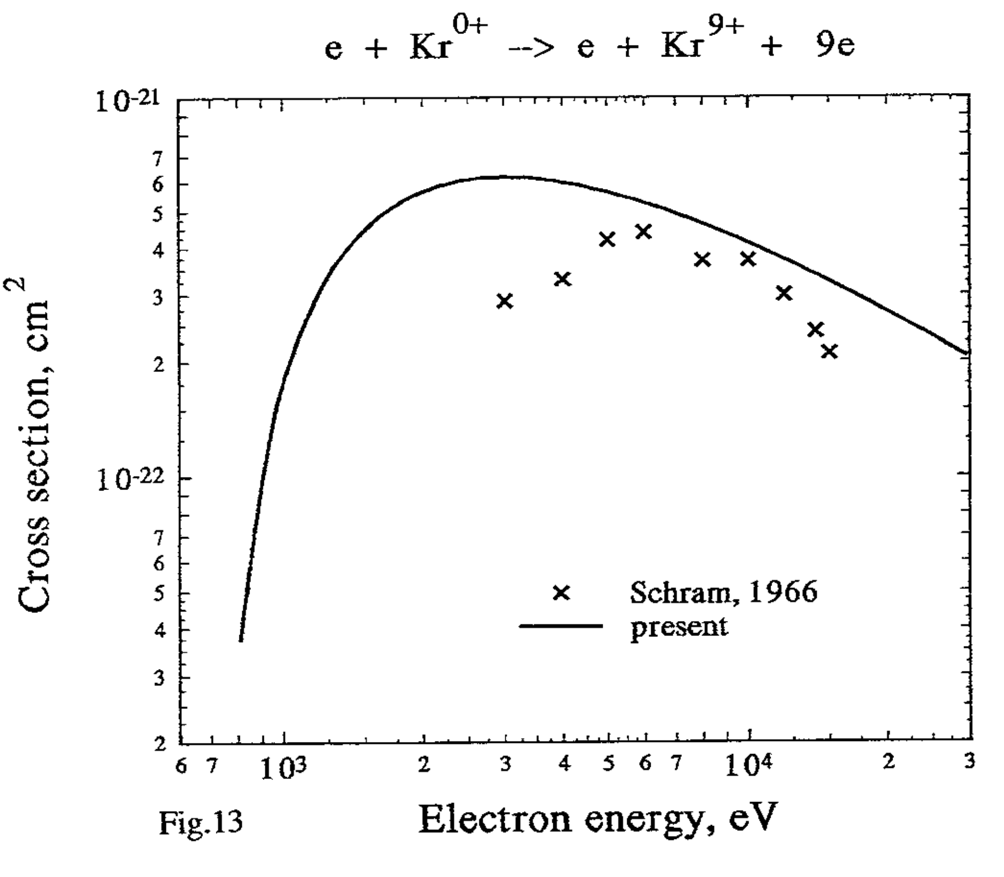

e + Kr^{0+} --> e + Kr^{7+} + 7e
Cross section, cm^2
Electron energy, eV
Schram, 1966
Lebius et al., 1989
present

Fig.11



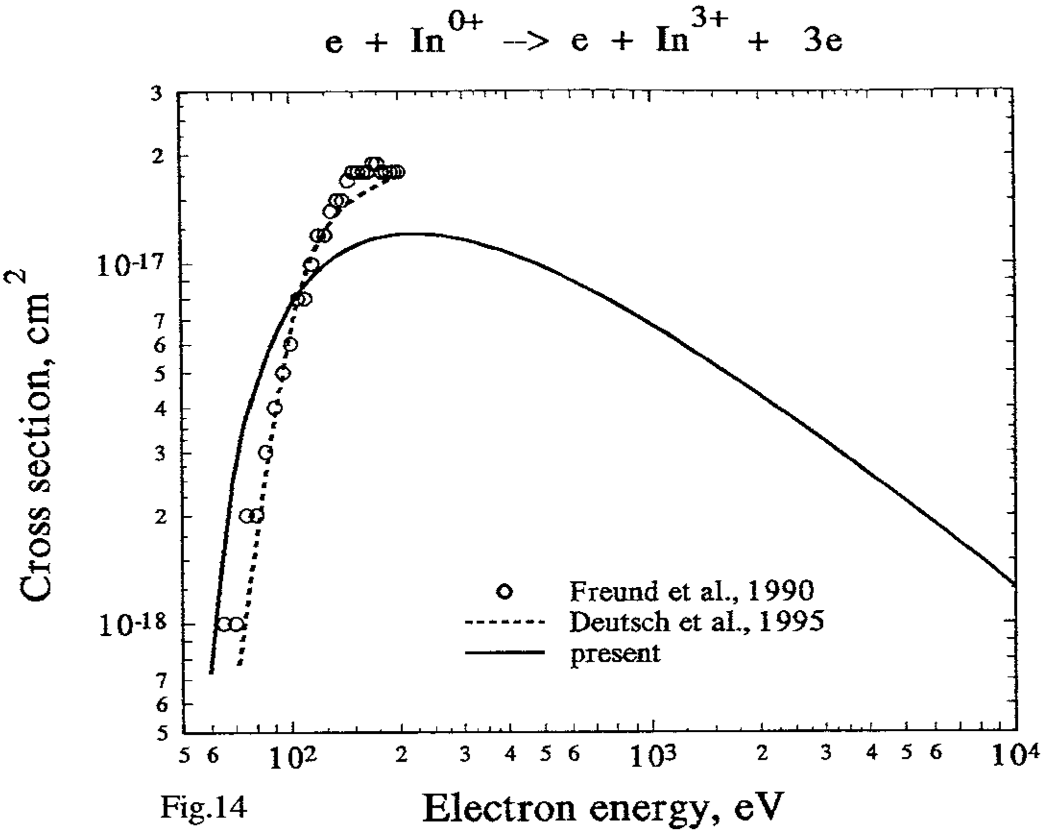
e + Kr^{0+} --> e + Kr^{8+} + 8e
Cross section, cm^2
Electron energy, eV
× Schram, 1966
o Lebius et al., 1989
present

Fig.12



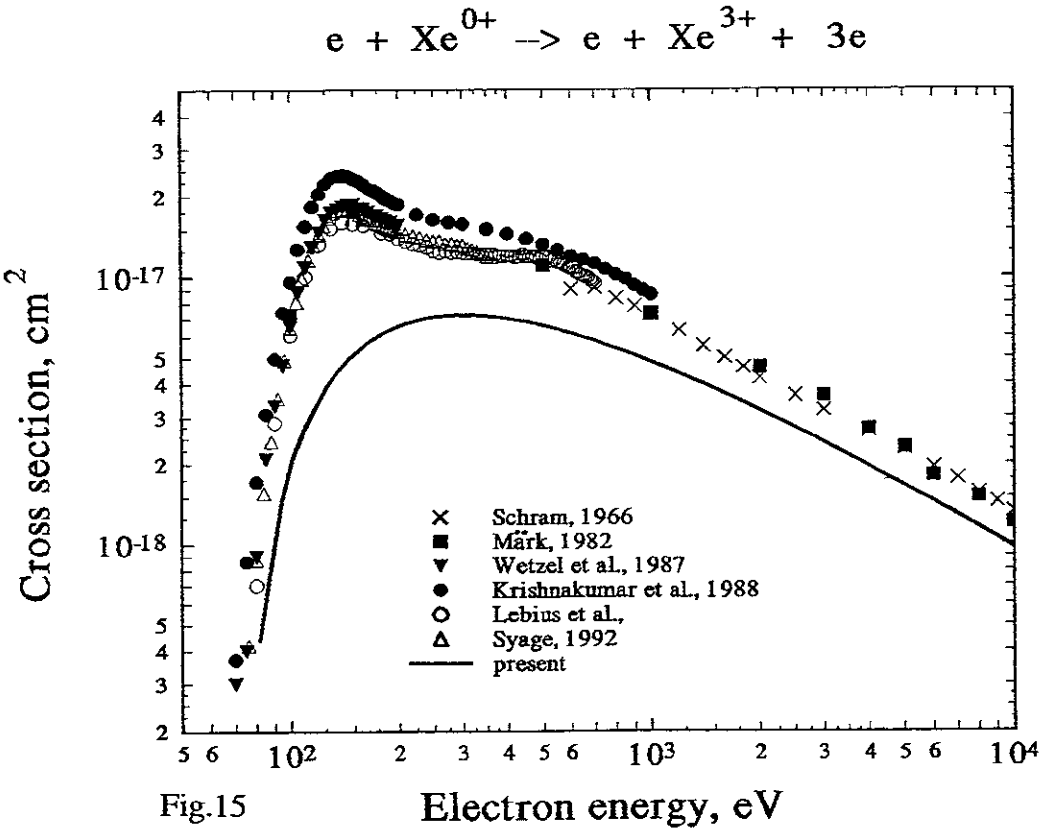
e + Kr^{0+} --> e + Kr^{9+} + 9e
Cross section, cm^2
Electron energy, eV
× Schram, 1966
present

Fig.13



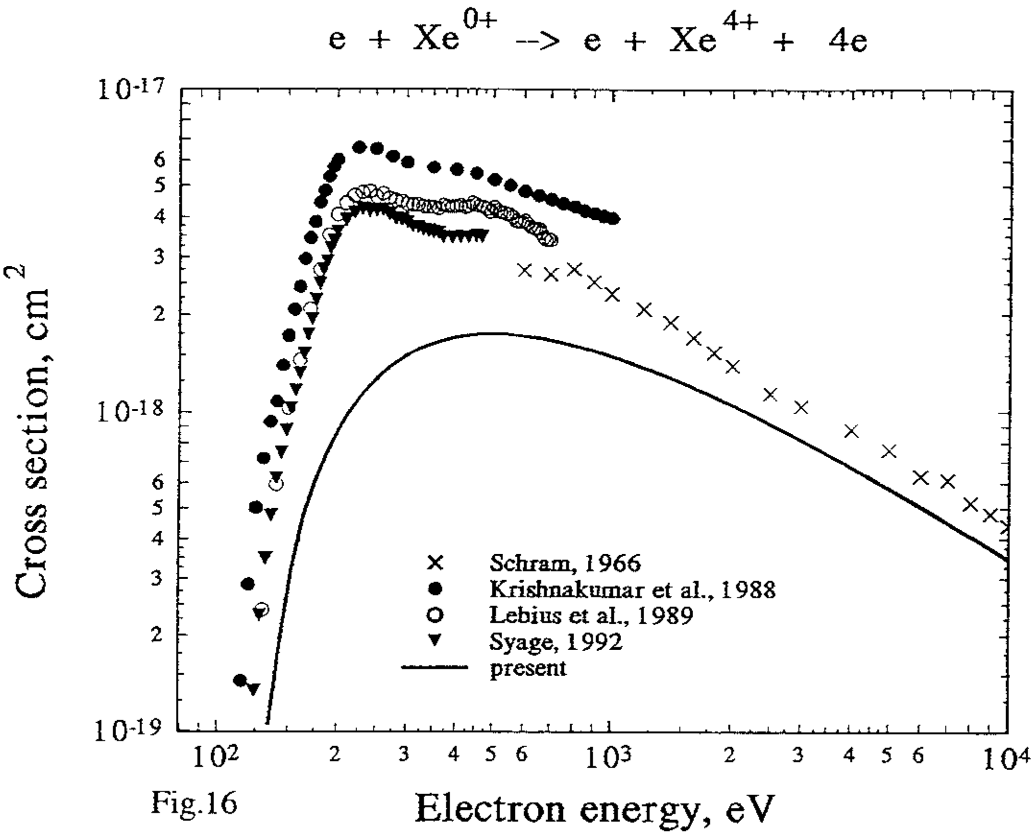
e + In^0+ --> e + In^3+ + 3e
Cross section, cm^2
Electron energy, eV
Freund et al., 1990
Deutsch et al., 1995
present

Fig.14



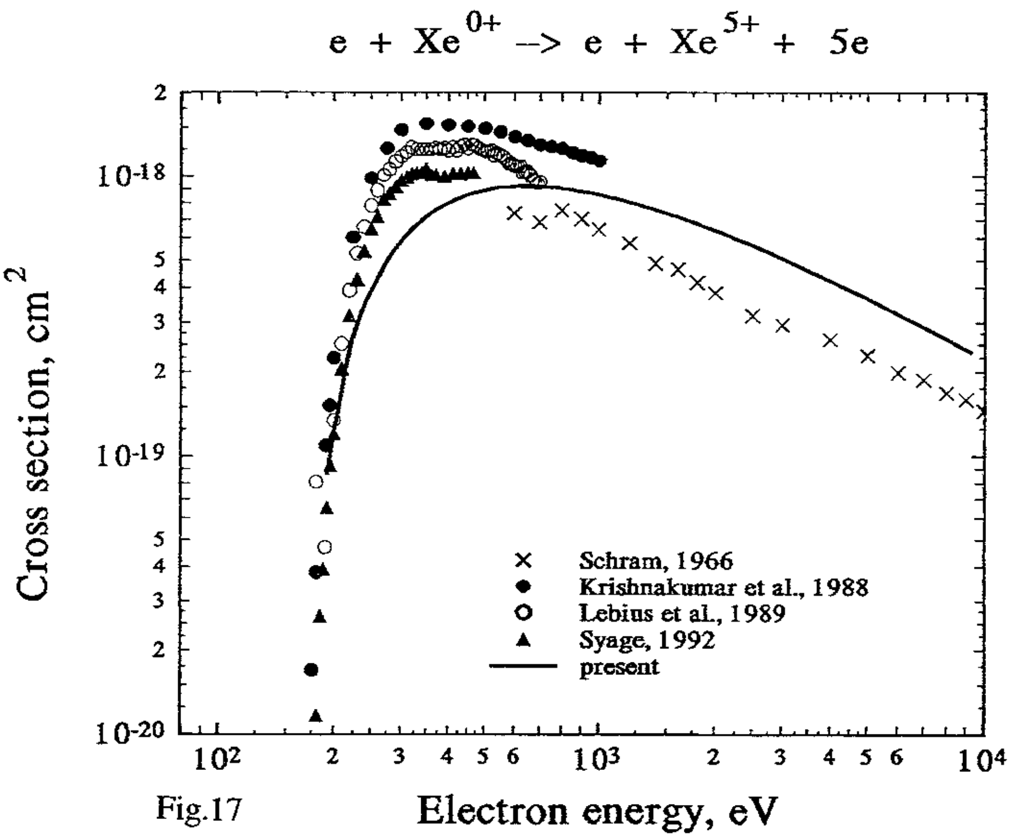
e + Xe^0+ --> e + Xe^3+ + 3e
Cross section, cm^2
Electron energy, eV
Schram, 1966
Märk, 1982
Wetzel et al., 1987
Krishnakumar et al., 1988
Lebius et al.,
Syage, 1992
present

Fig.15



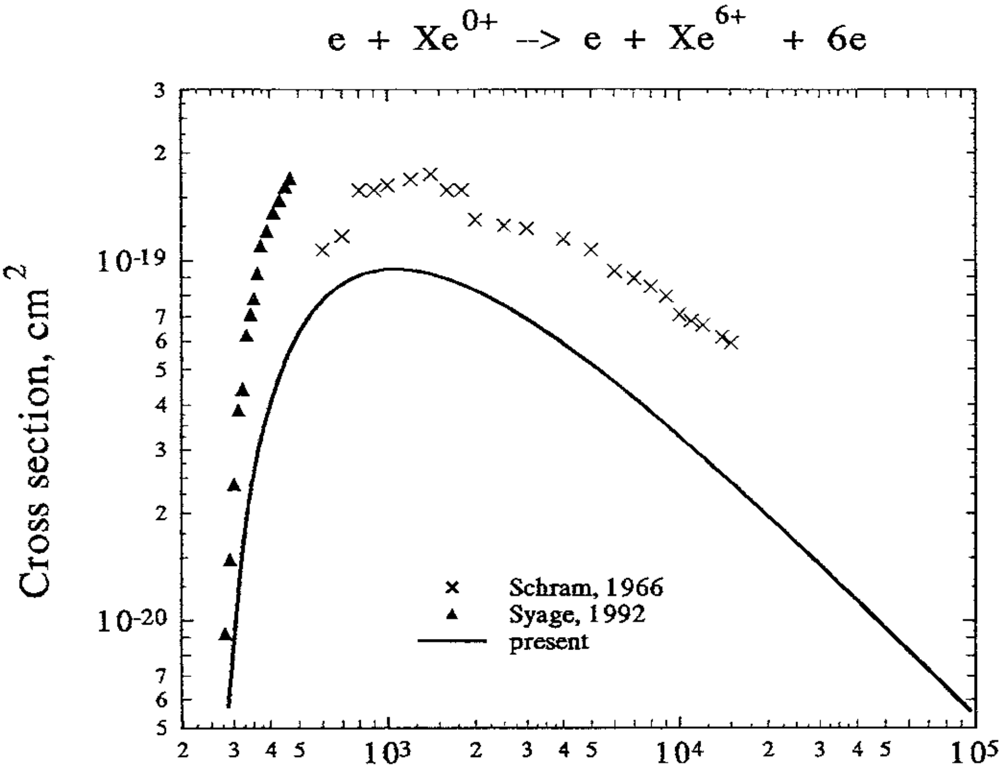
e + Xe^0+ --> e + Xe^4+ + 4e
Cross section, cm^2
Electron energy, eV
Schram, 1966
Krishnakumar et al., 1988
Lebius et al., 1989
Syage, 1992
present

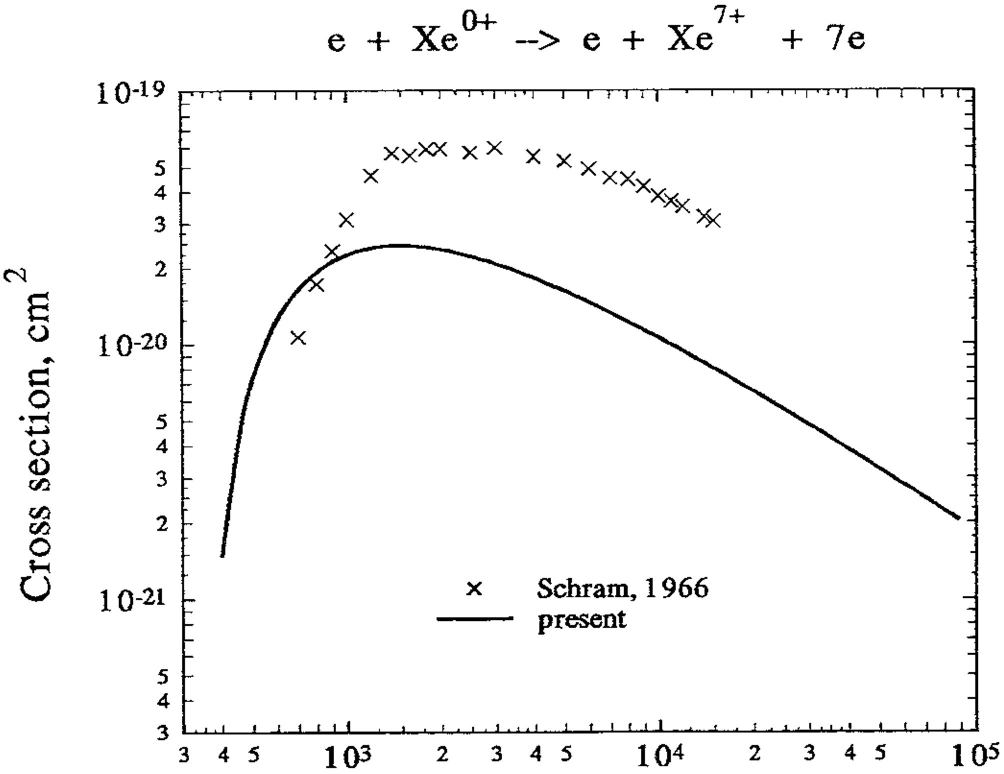
Fig.16

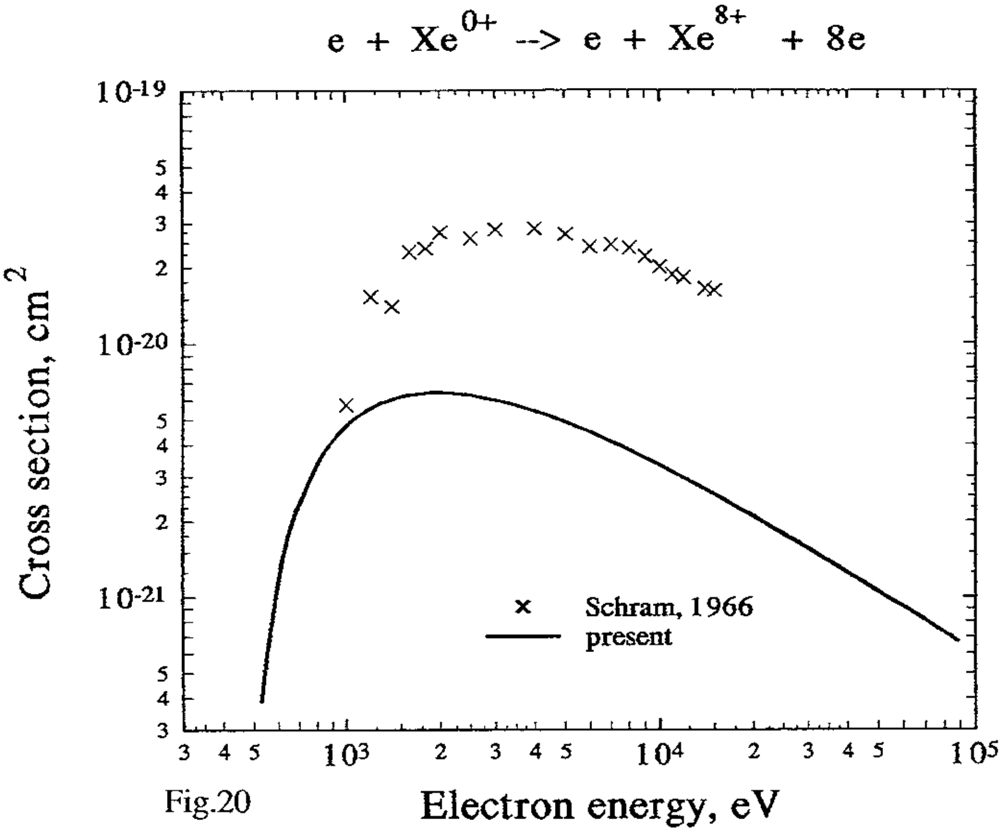


e + Xe^0+ --> e + Xe^5+ + 5e
Cross section, cm^2
Electron energy, eV
Schram, 1966
Krishnakumar et al., 1988
Lebius et al., 1989
Syage, 1992
present

Fig.17

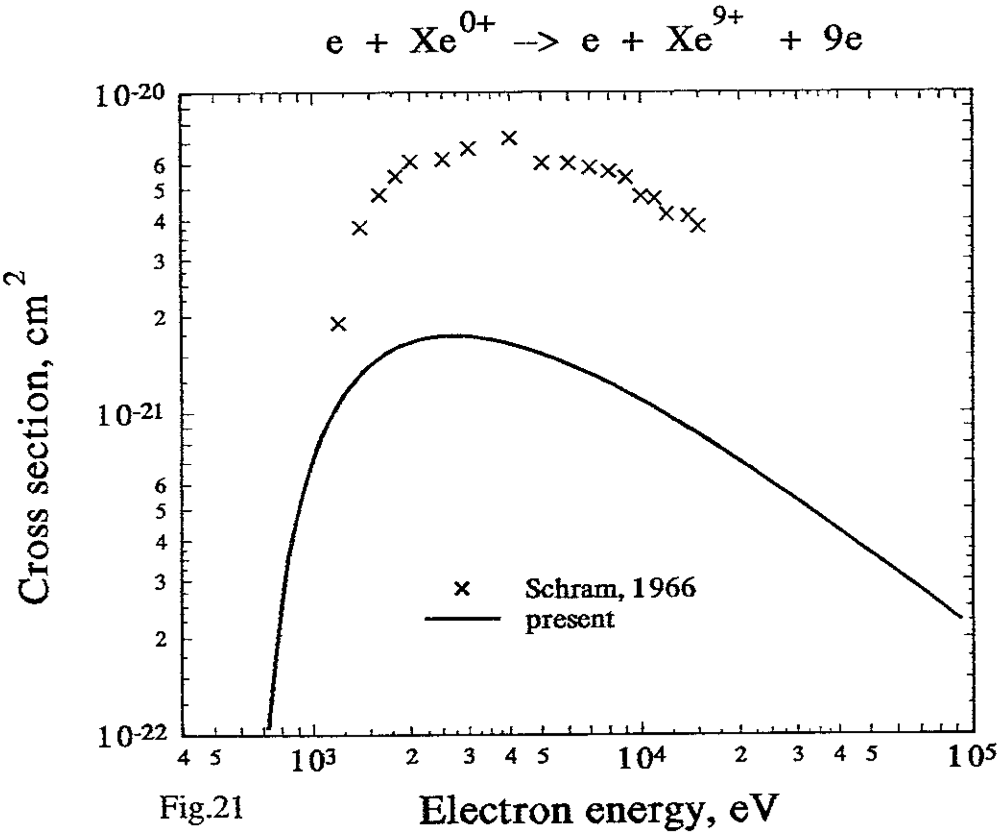

e + Xe^0+ --> e + Xe^6+ + 6e
Cross section, cm 2
Electron energy, eV
Schram, 1966
Syage, 1992
present
Fig.18


e + Xe^0+ --> e + Xe^7+ + 7e
Cross section, cm 2
Electron energy, eV
Schram, 1966
present
Fig.19



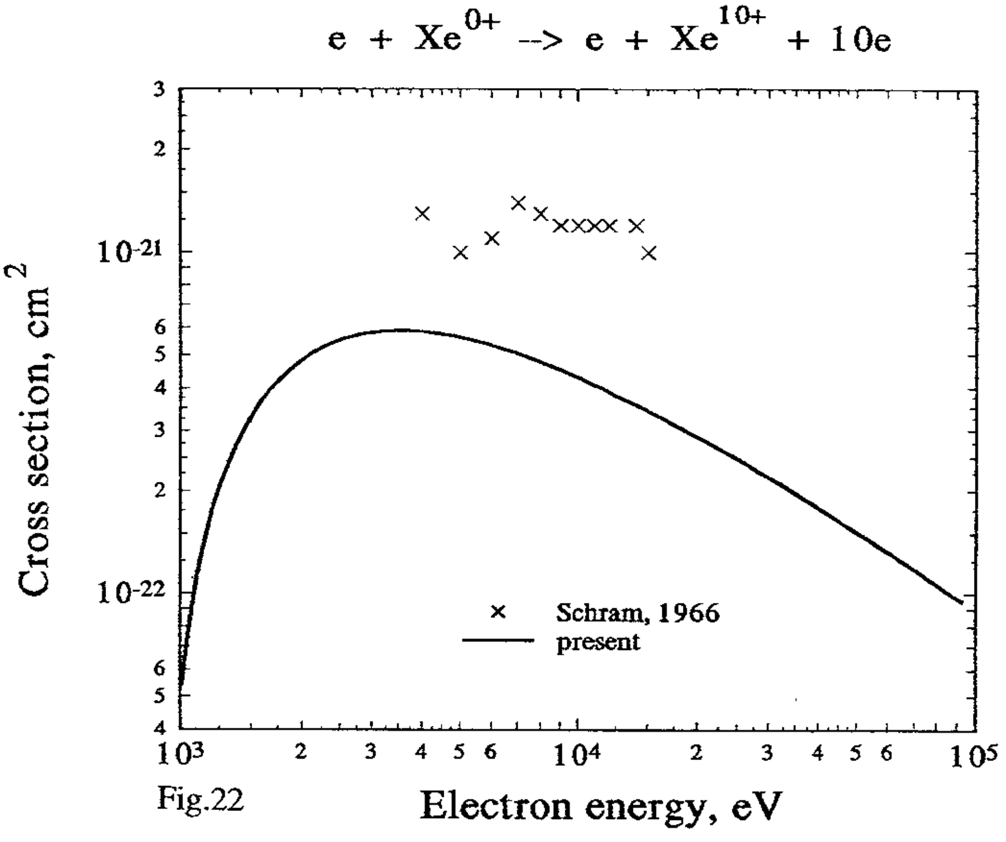
e + Xe^{0+} --> e + Xe^{8+} + 8e
Cross section, cm^2
Electron energy, eV
Schram, 1966
present

Fig.20



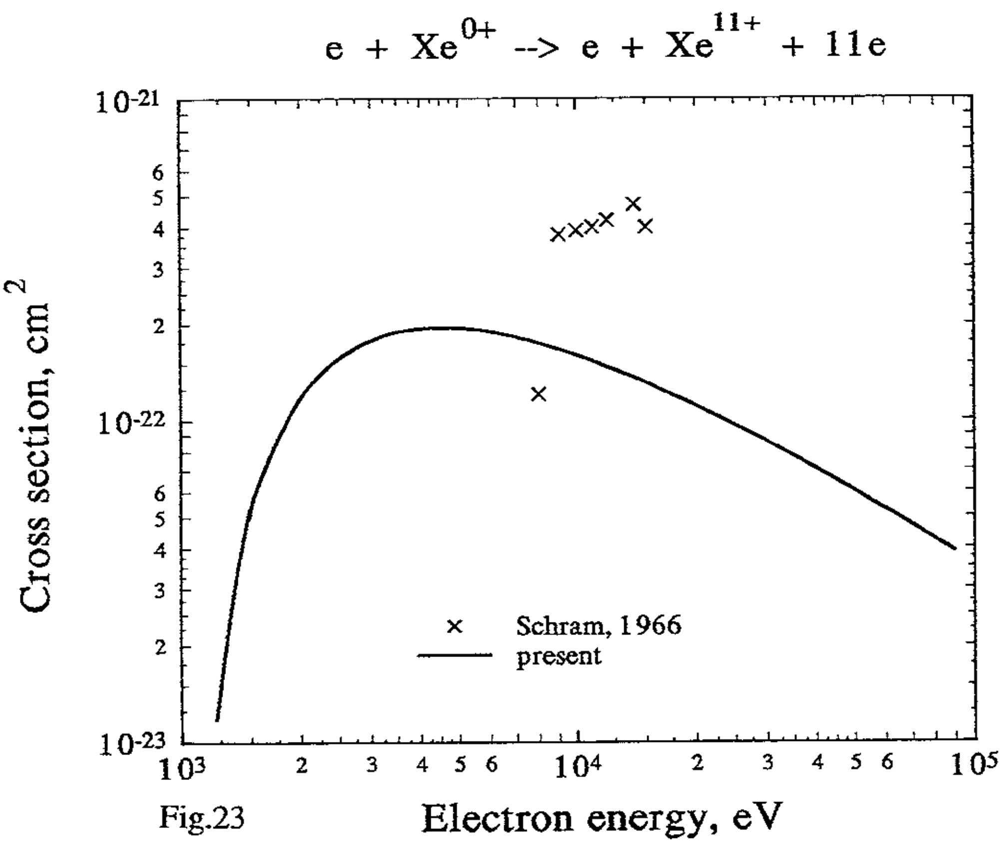
e + Xe^{0+} --> e + Xe^{9+} + 9e
Cross section, cm^2
Electron energy, eV
Schram, 1966
present

Fig.21



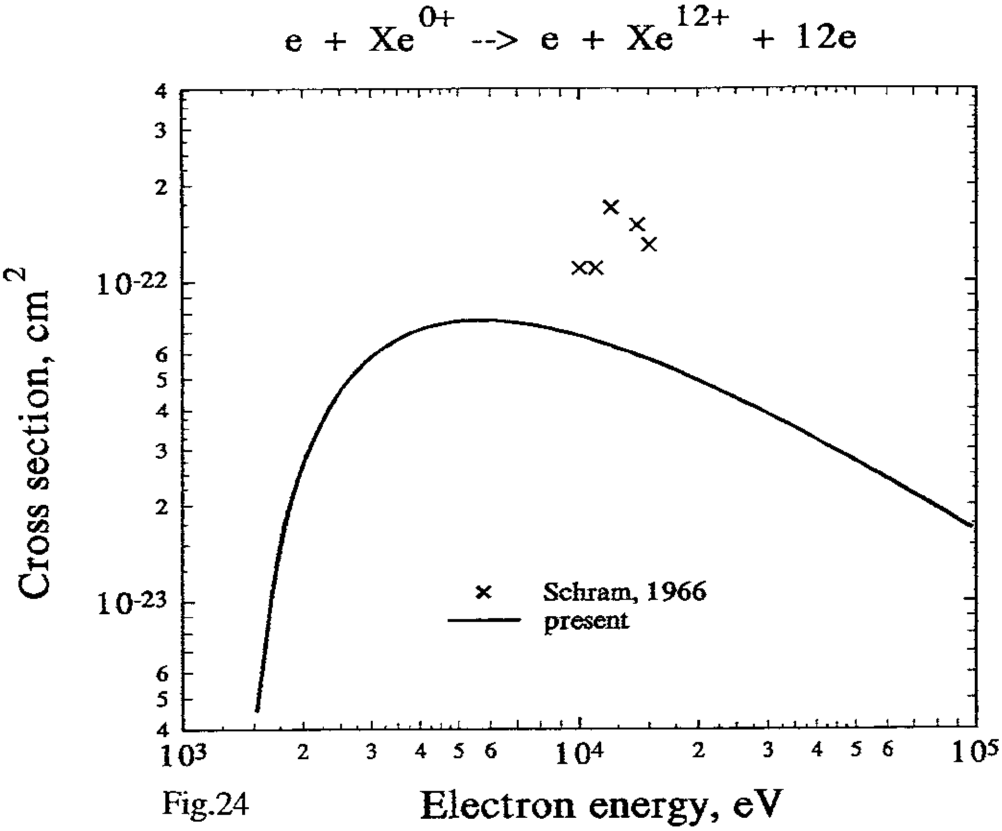
e + Xe0+ --> e + Xe10+ + 10e
Cross section, cm2
10-21
10-22
Electron energy, eV
103
104
105
Schram, 1966
present

Fig.22



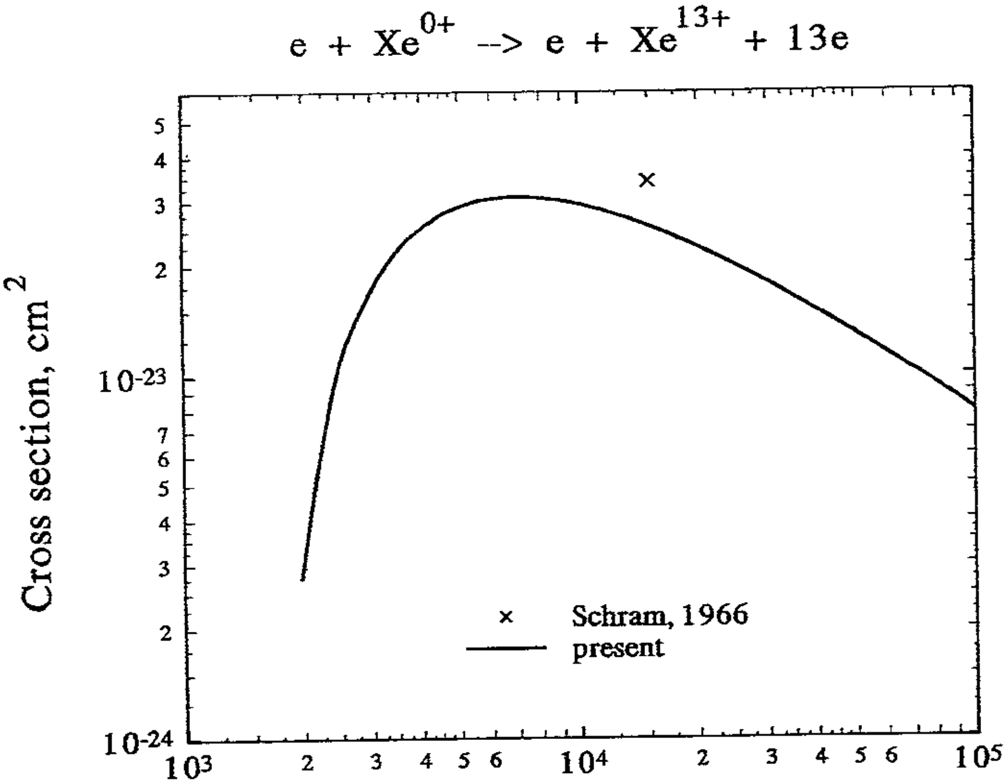
e + Xe0+ --> e + Xe11+ + 11e
Cross section, cm2
10-21
10-22
10-23
Electron energy, eV
103
104
105
Schram, 1966
present

Fig.23



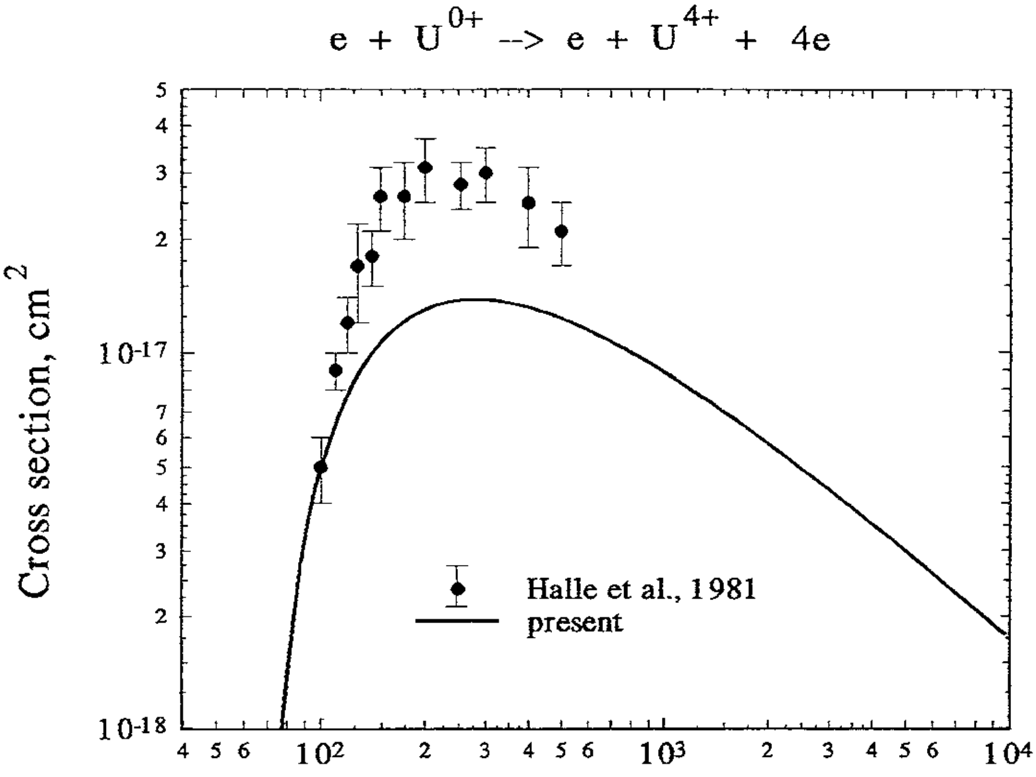
e + Xe0+ --> e + Xe12+ + 12e
Cross section, cm2
Electron energy, eV
Schram, 1966
present
10-22
10-23
103
104
105

Fig.24



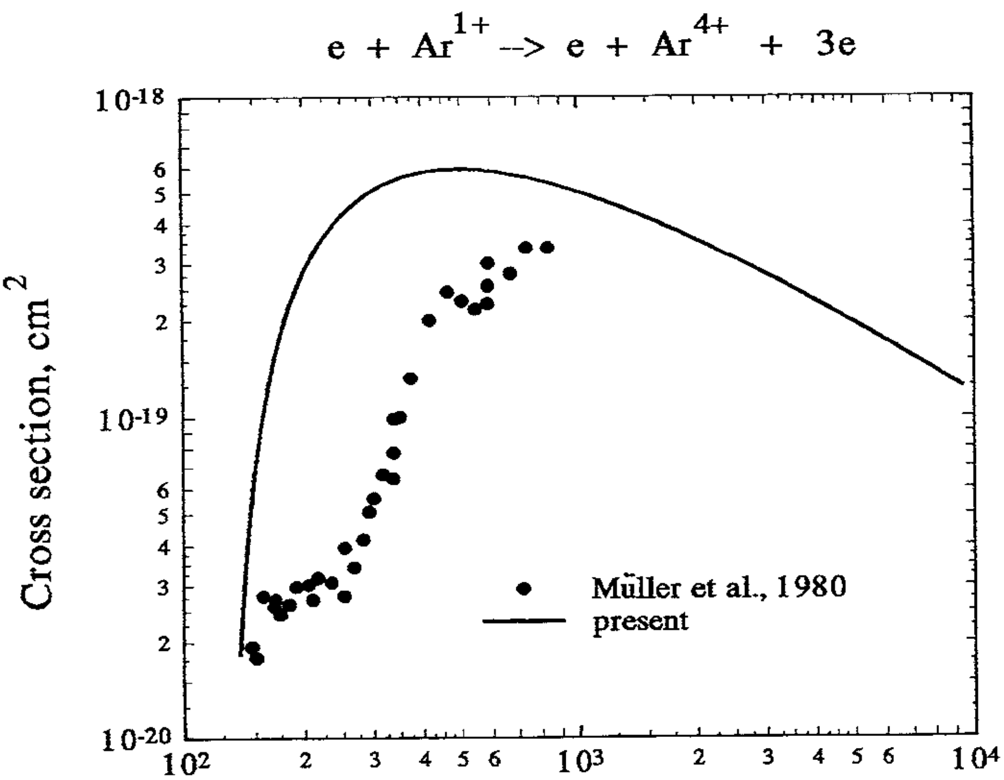
e + Xe0+ --> e + Xe13+ + 13e
Cross section, cm2
Electron energy, eV
Schram, 1966
present
10-23
10-24
103
104
105

Fig.25



e + U^{0+} --> e + U^{4+} + 4e
Cross section, cm^2
10-17
10-18
10^2
10^3
10^4
Halle et al., 1981
present
Electron energy, eV

Fig.26



e + Ar^{1+} --> e + Ar^{4+} + 3e
Cross section, cm^2
10-18
10-19
10-20
10^2
10^3
10^4
Müller et al., 1980
present
Electron energy, eV

Fig.27

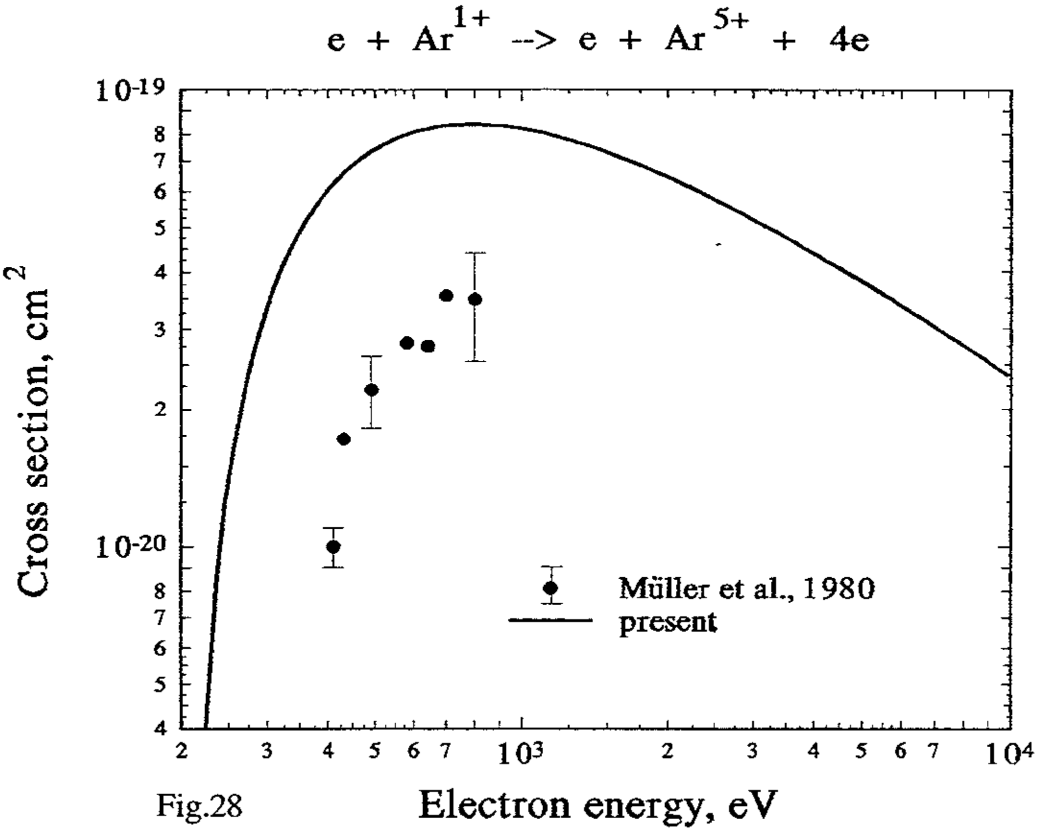

e + Ar^{1+} --> e + Ar^{5+} + 4e
Cross section, cm^2
10^{-19}
8
7
6
5
4
3
2
10^{-20}
8
7
6
5
4
2 3 4 5 6 7 10^3 2 3 4 5 6 7 10^4
Müller et al., 1980
present
Electron energy, eV

Fig.28

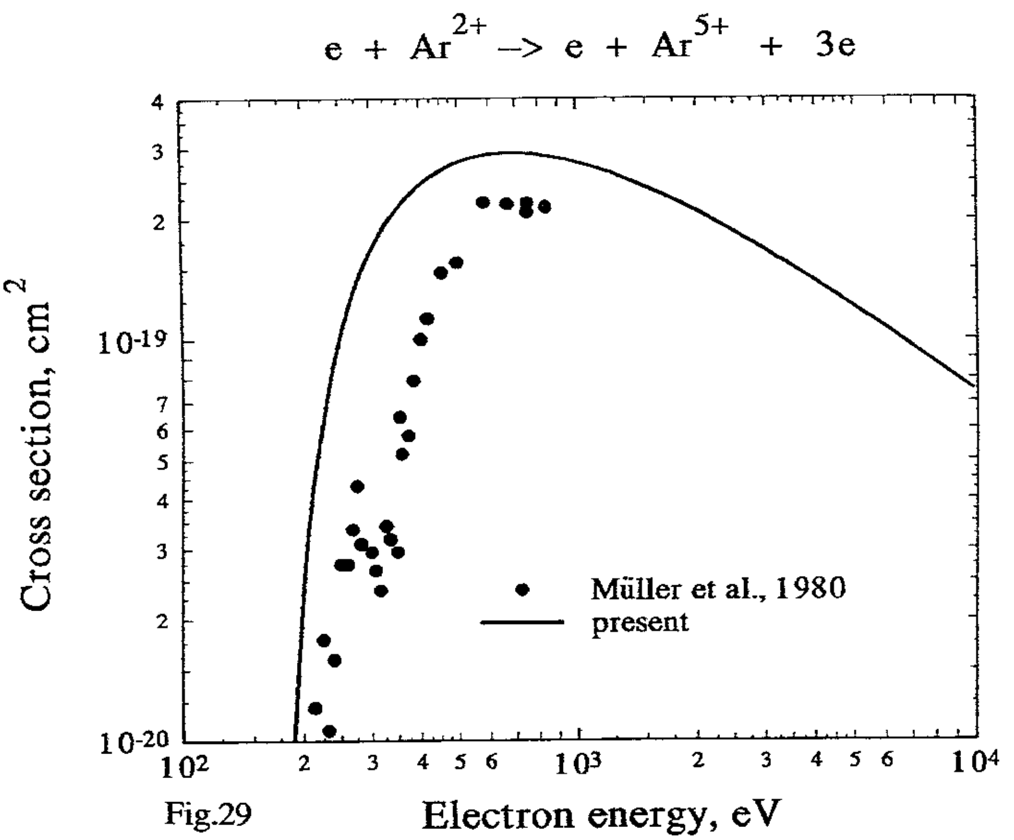

e + Ar^{2+} --> e + Ar^{5+} + 3e
Cross section, cm^2
4
3
2
10^{-19}
7
6
5
4
3
2
10^{-20}
10^2 2 3 4 5 6 10^3 2 3 4 5 6 10^4
Müller et al., 1980
present
Electron energy, eV

Fig.29

$e + Ni^{1+} \rightarrow e + Ni^{4+} + 3e$

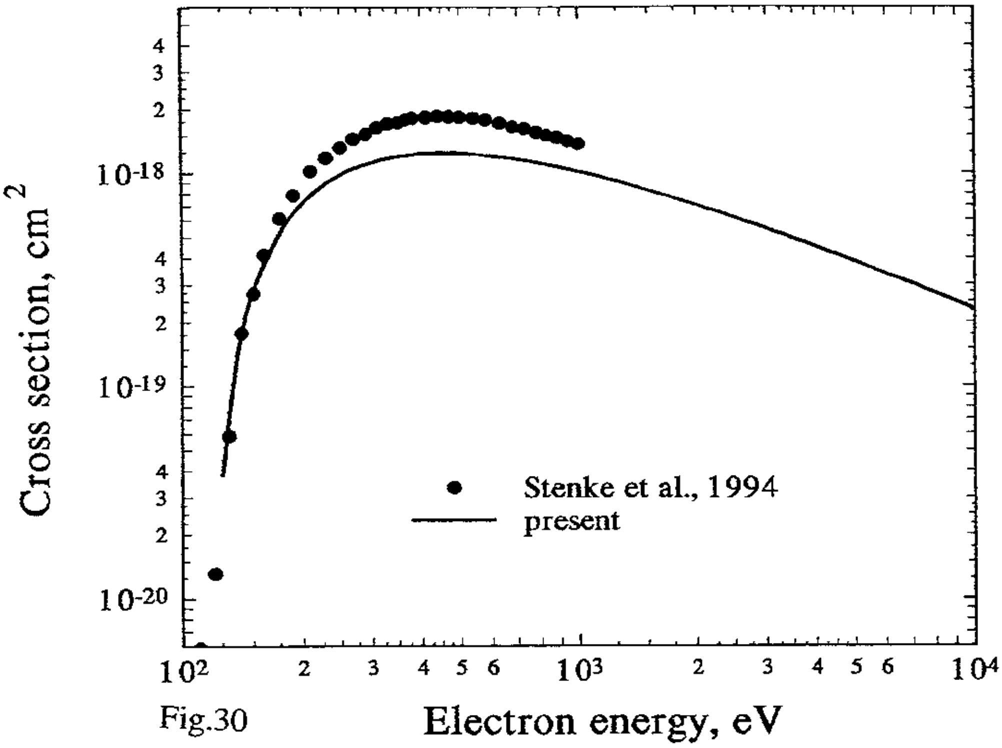


Fig.30

$e + Ni^{2+} \rightarrow e + Ni^{5+} + 3e$

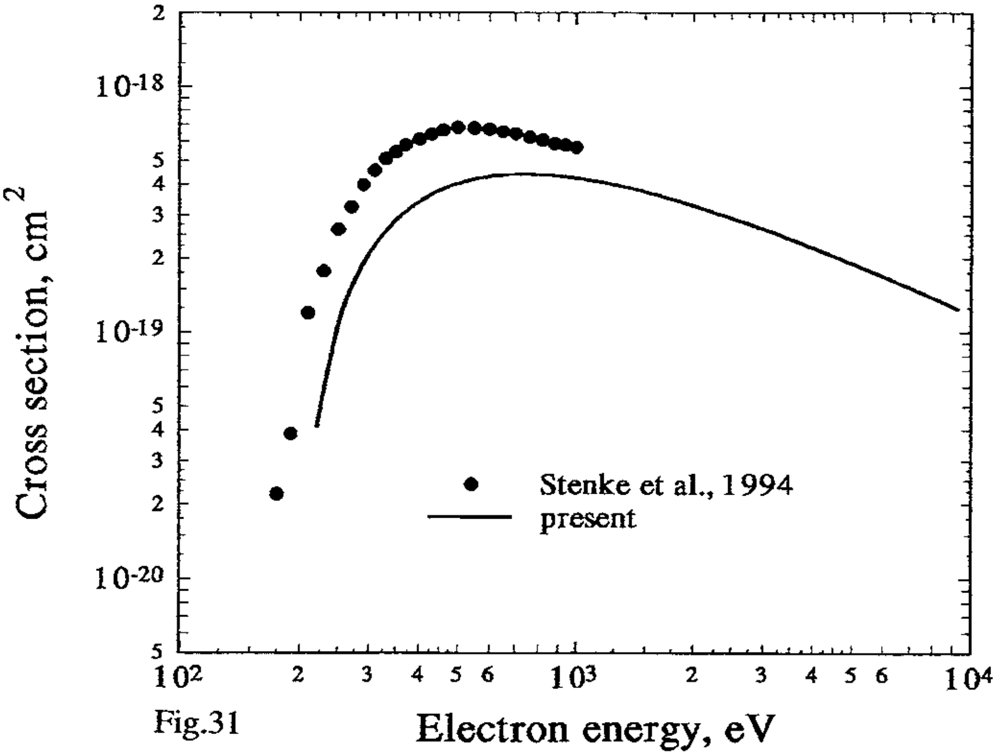


Fig.31

$e + Ni^{3+} \rightarrow e + Ni^{6+} + 3e$

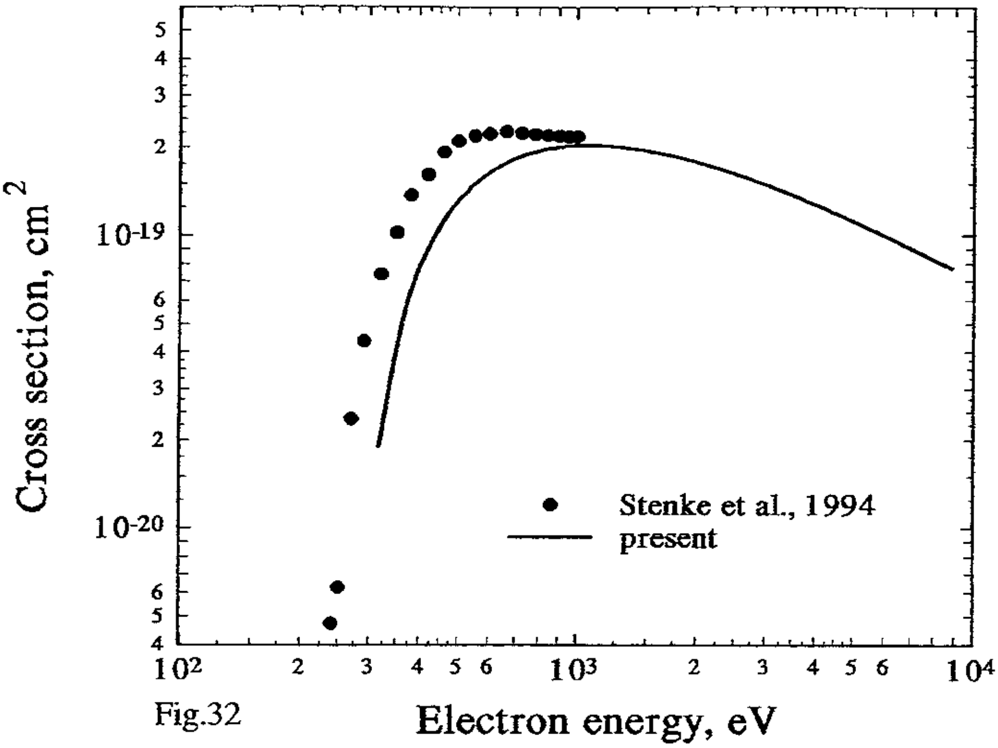


Fig.32

$e + Ni^{4+} \rightarrow e + Ni^{7+} + 3e$

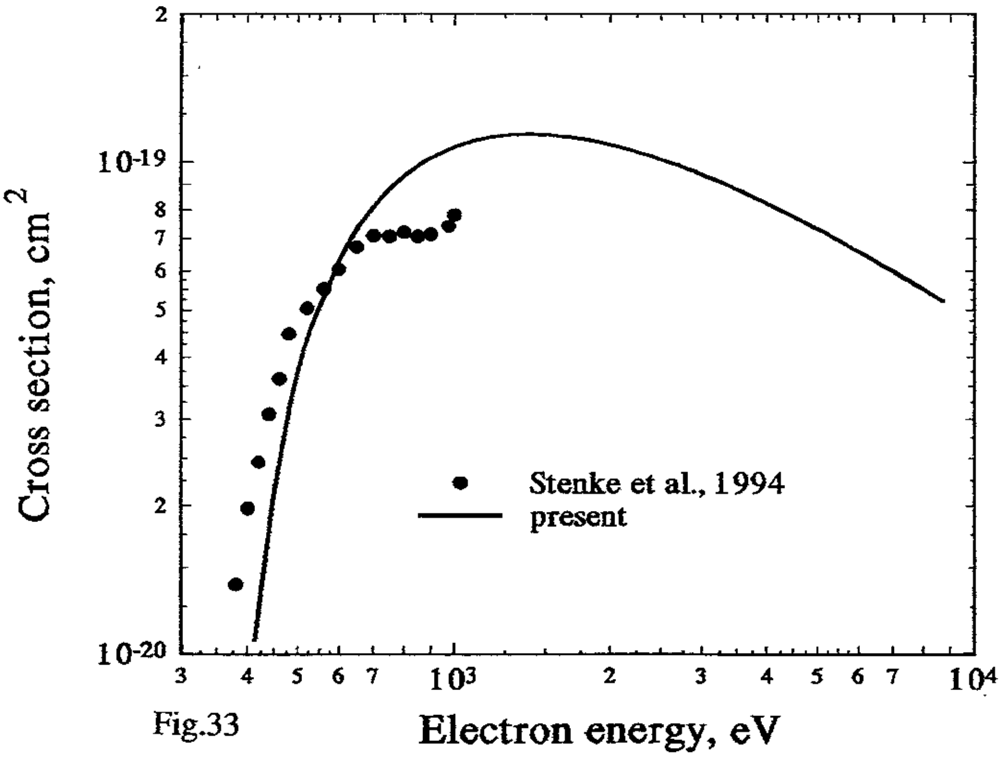
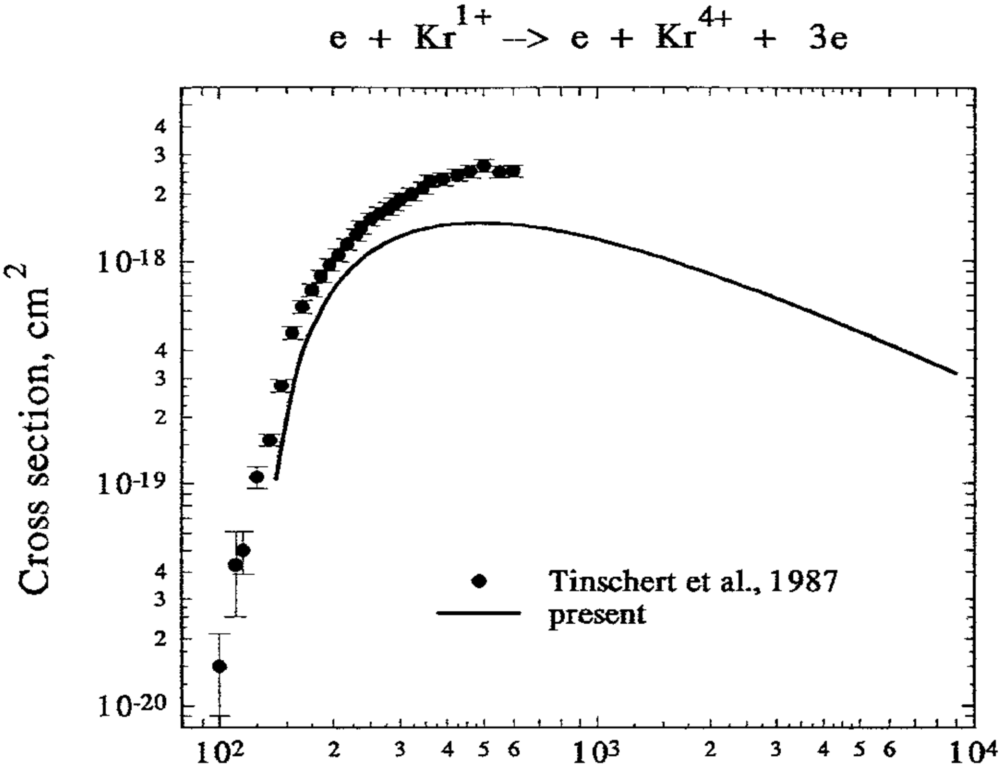
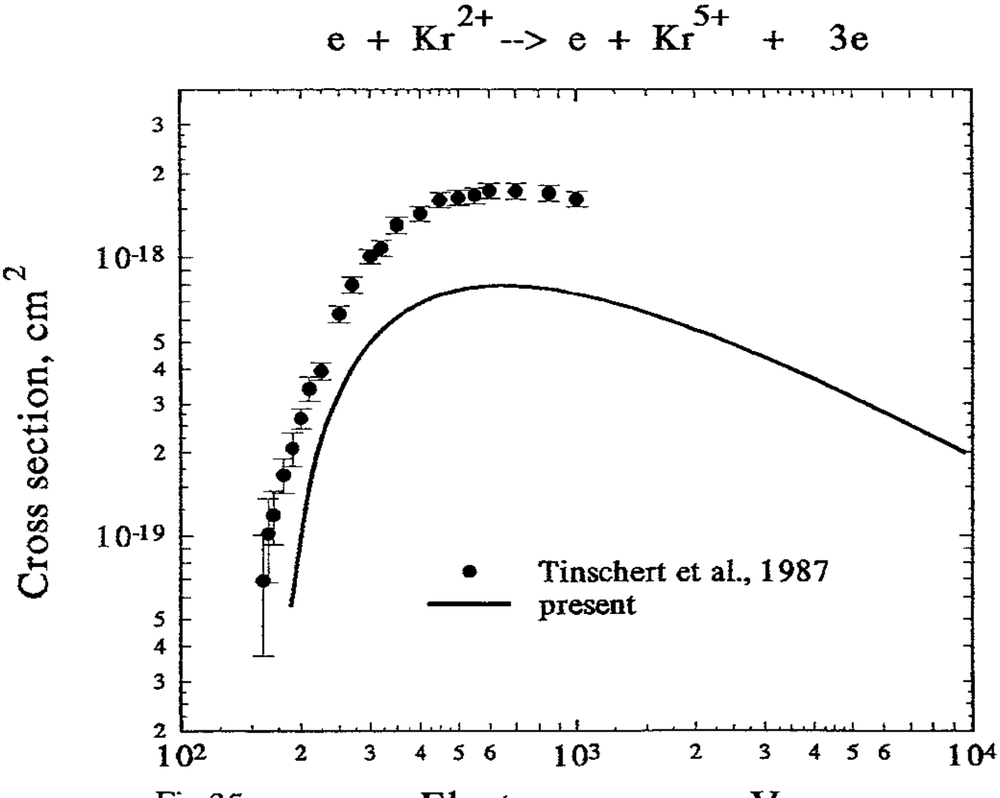
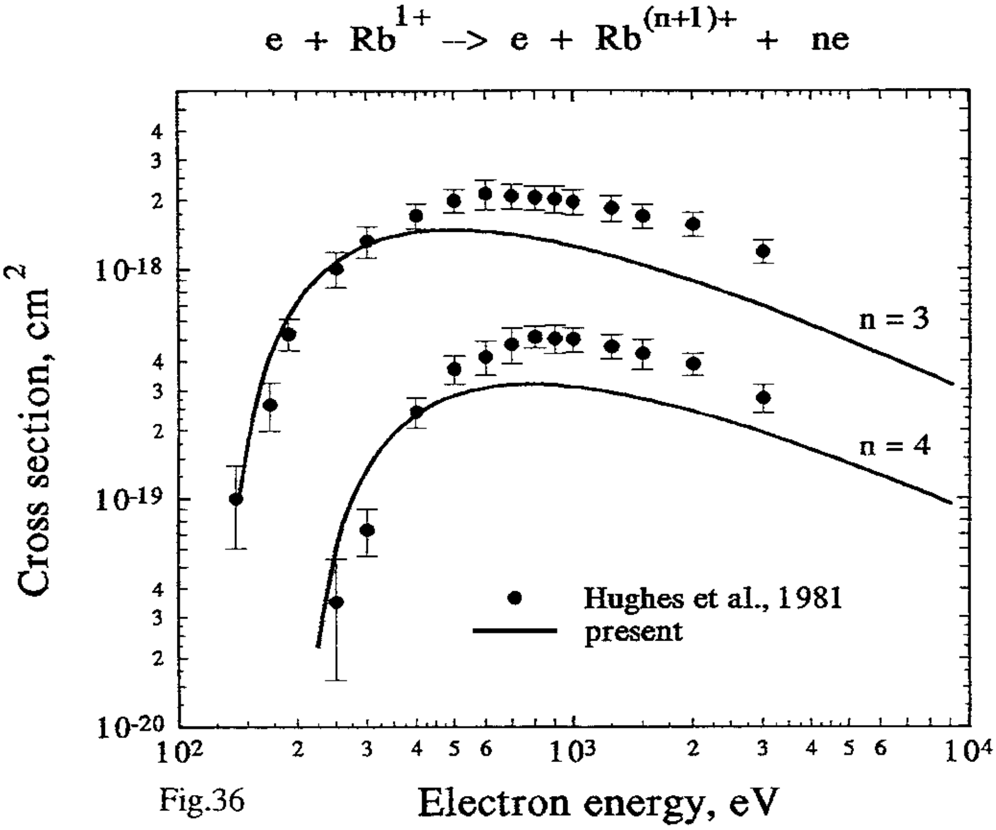


Fig.33

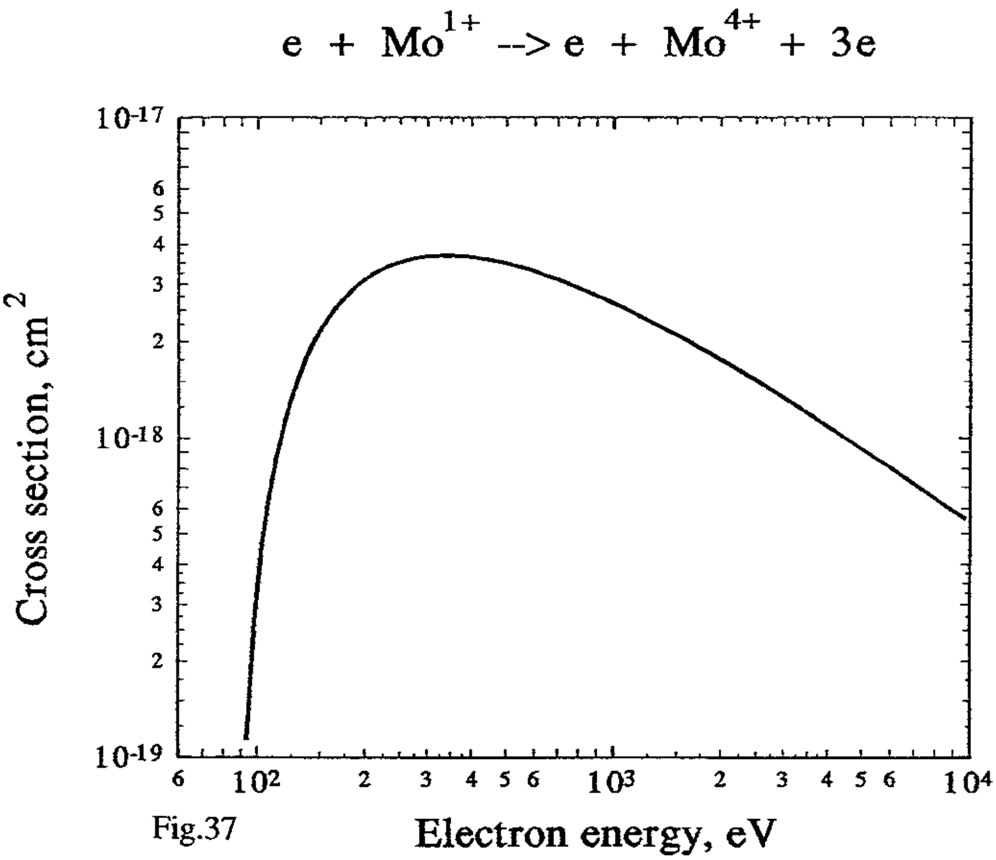

e + Kr1+ --> e + Kr4+ + 3e
Cross section, cm2
Electron energy, eV
Tinschert et al., 1987
present
10-18
10-19
10-20
102
103
104
Fig.34


e + Kr2+ --> e + Kr5+ + 3e
Cross section, cm2
Electron energy, eV
Tinschert et al., 1987
present
10-18
10-19
102
103
104
Fig.35



e + Rb^{1+} --> e + Rb$^{(n+1)+}$ + ne
Cross section, cm^2
10^{-18}
10^{-19}
10^{-20}
n = 3
n = 4
Hughes et al., 1981
present
10^2
10^3
10^4
Electron energy, eV

Fig.36



e + Mo^{1+} --> e + Mo^{4+} + 3e
Cross section, cm^2
10^{-17}
10^{-18}
10^{-19}
10^2
10^3
10^4
Electron energy, eV

Fig.37

$e + Mo^{2+} \rightarrow e + Mo^{5+} + 3e$

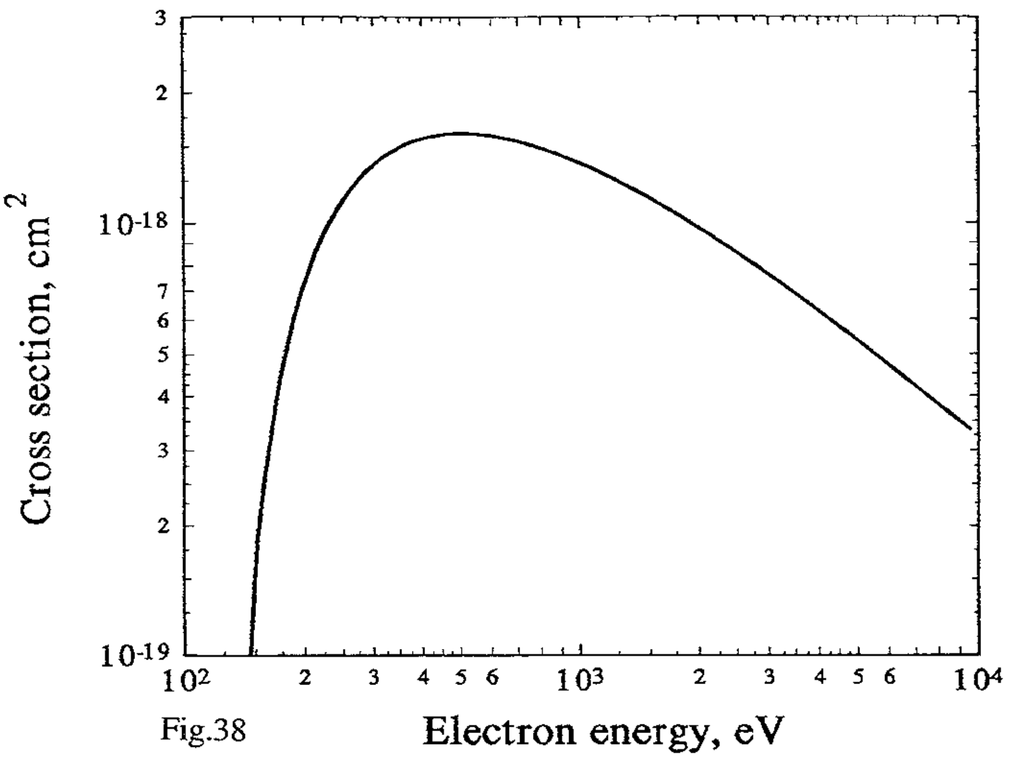


Fig.38

$e + Mo^{3+} \rightarrow e + Mo^{6+} + 3e$

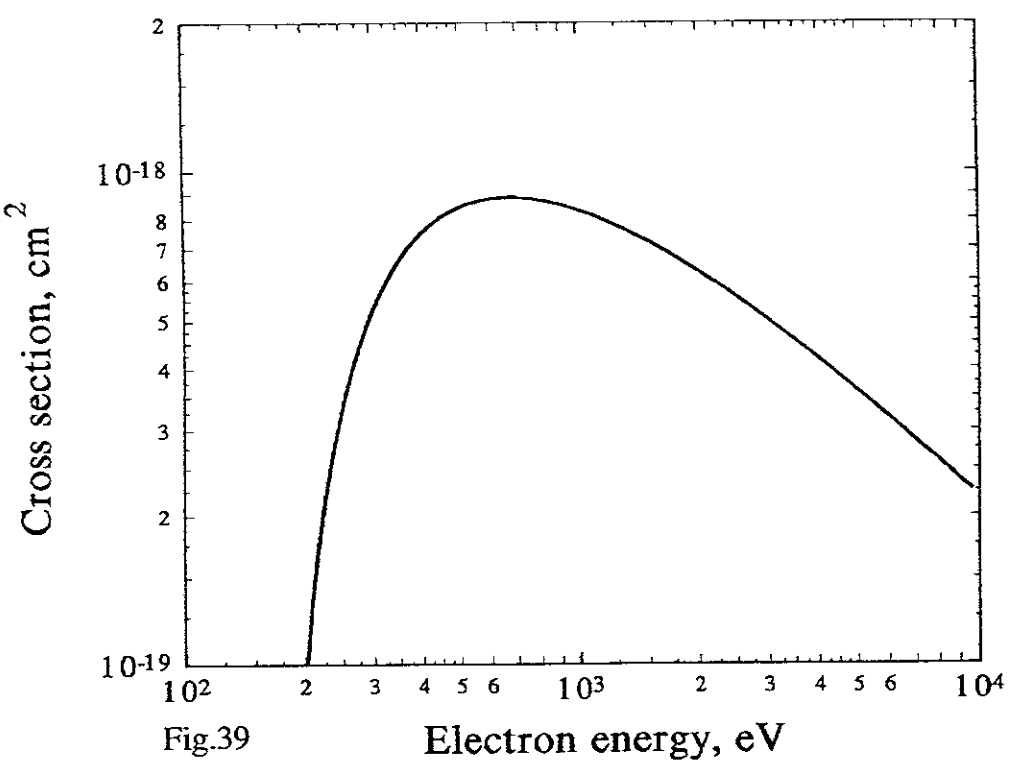
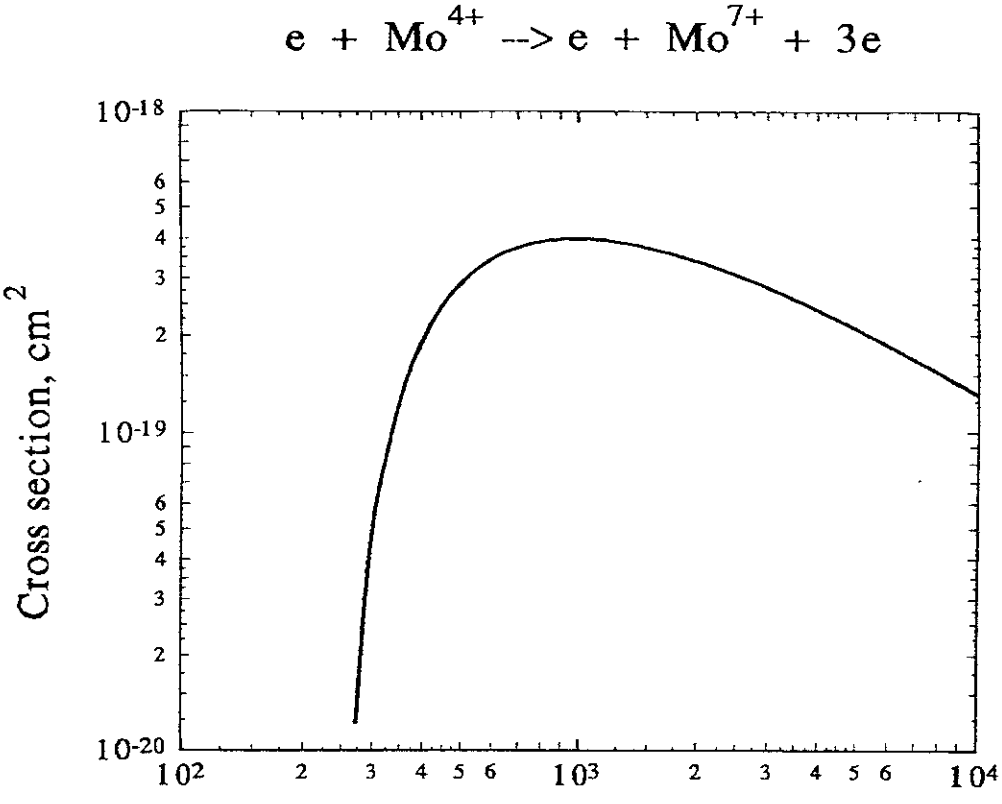
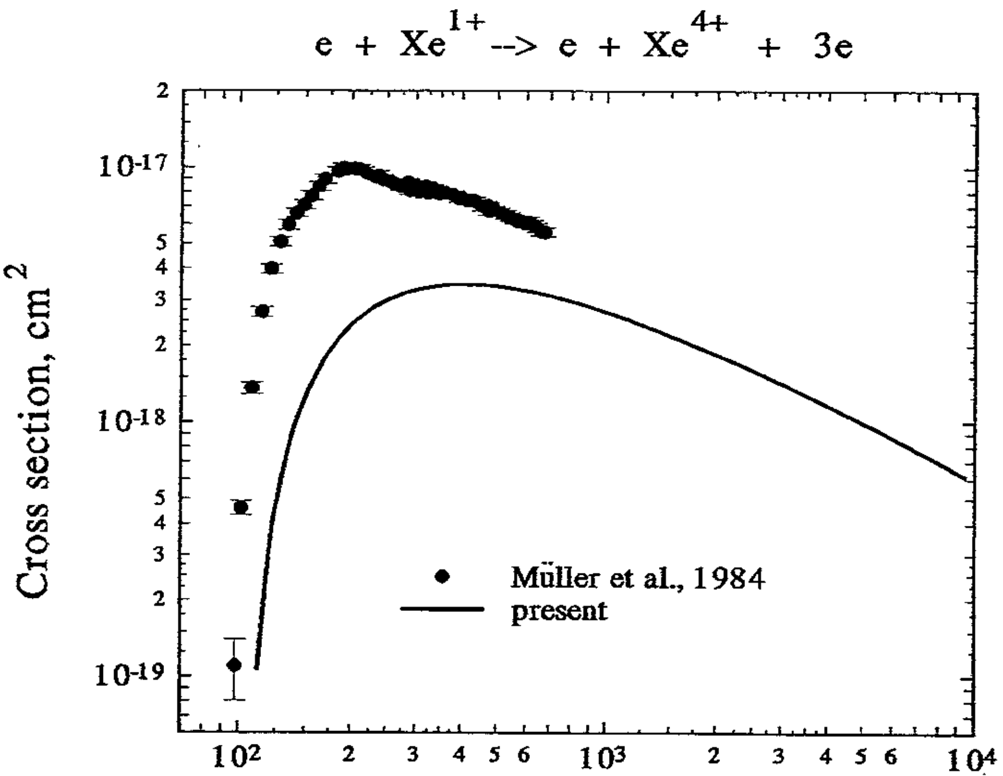


Fig.39



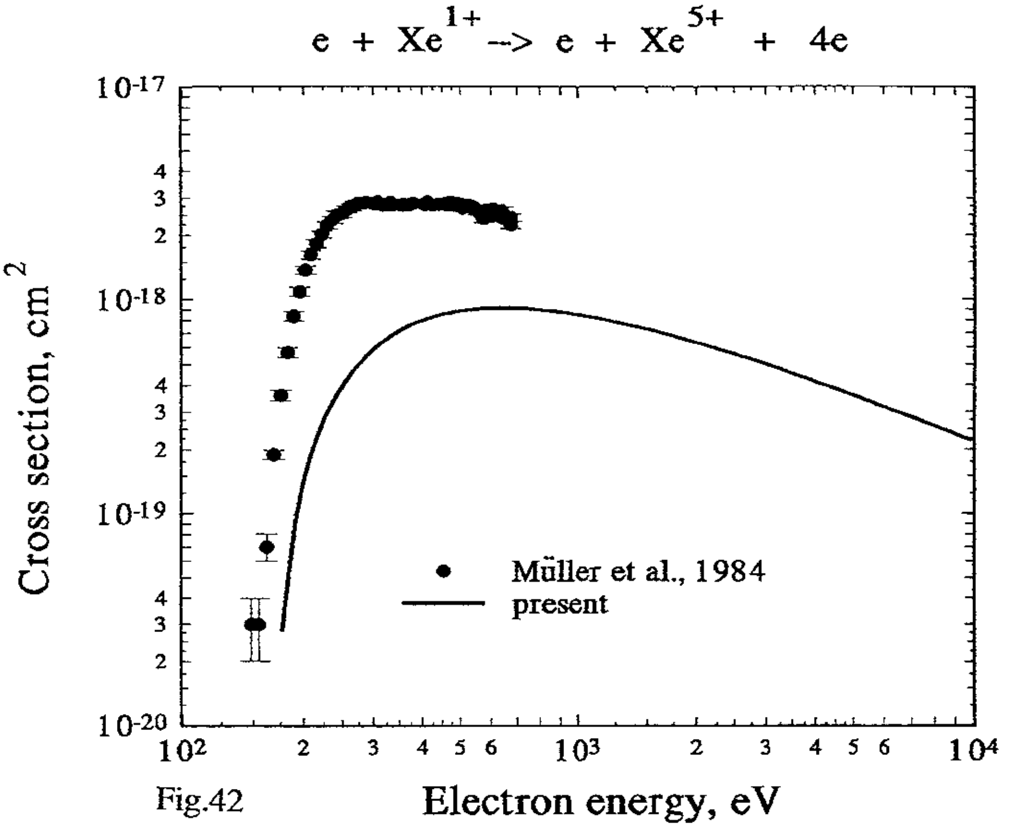
e + Mo^{4+} --> e + Mo^{7+} + 3e
Cross section, cm^2
Electron energy, eV

Fig.40



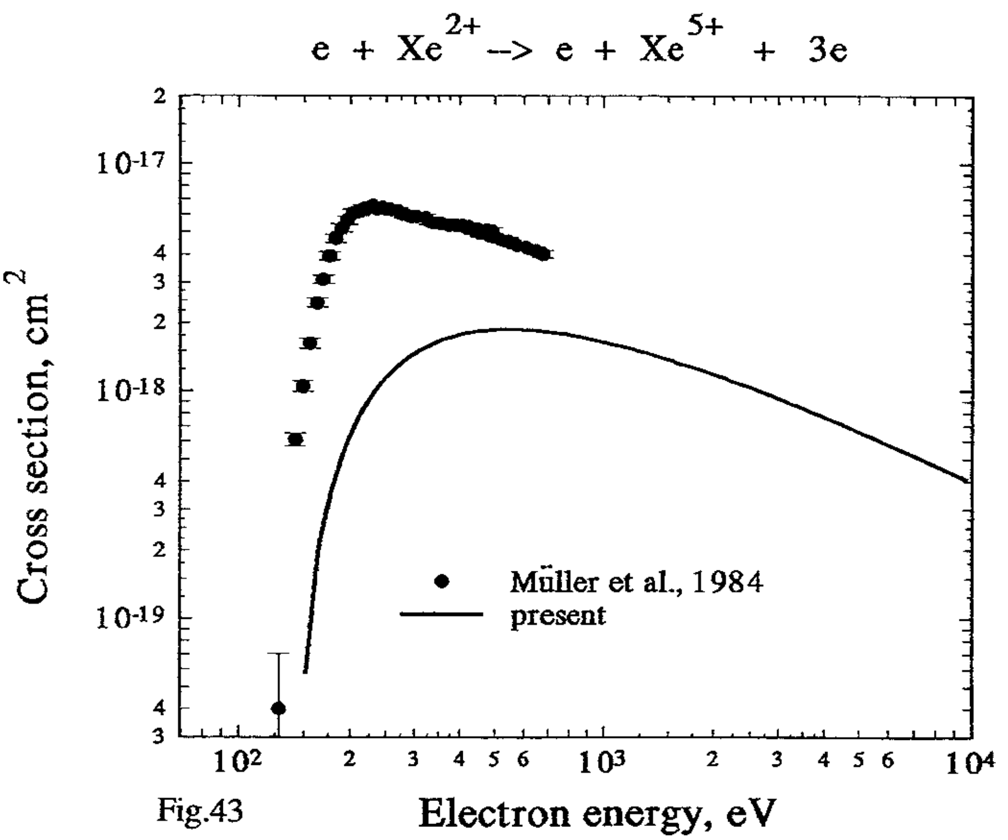
e + Xe^{1+} --> e + Xe^{4+} + 3e
Cross section, cm^2
Electron energy, eV
Müller et al., 1984
present

Fig.41



e + Xe^1+ --> e + Xe^5+ + 4e
Cross section, cm^2
10-17
4
3
2
10-18
4
3
2
10-19
4
3
2
10-20
Müller et al., 1984
present
10^2
2
3
4
5
6
10^3
2
3
4
5
6
10^4
Electron energy, eV

Fig.42



e + Xe^2+ --> e + Xe^5+ + 3e
Cross section, cm^2
2
10-17
4
3
2
10-18
4
3
2
10-19
4
3
Müller et al., 1984
present
10^2
2
3
4
5
6
10^3
2
3
4
5
6
10^4
Electron energy, eV

Fig.43

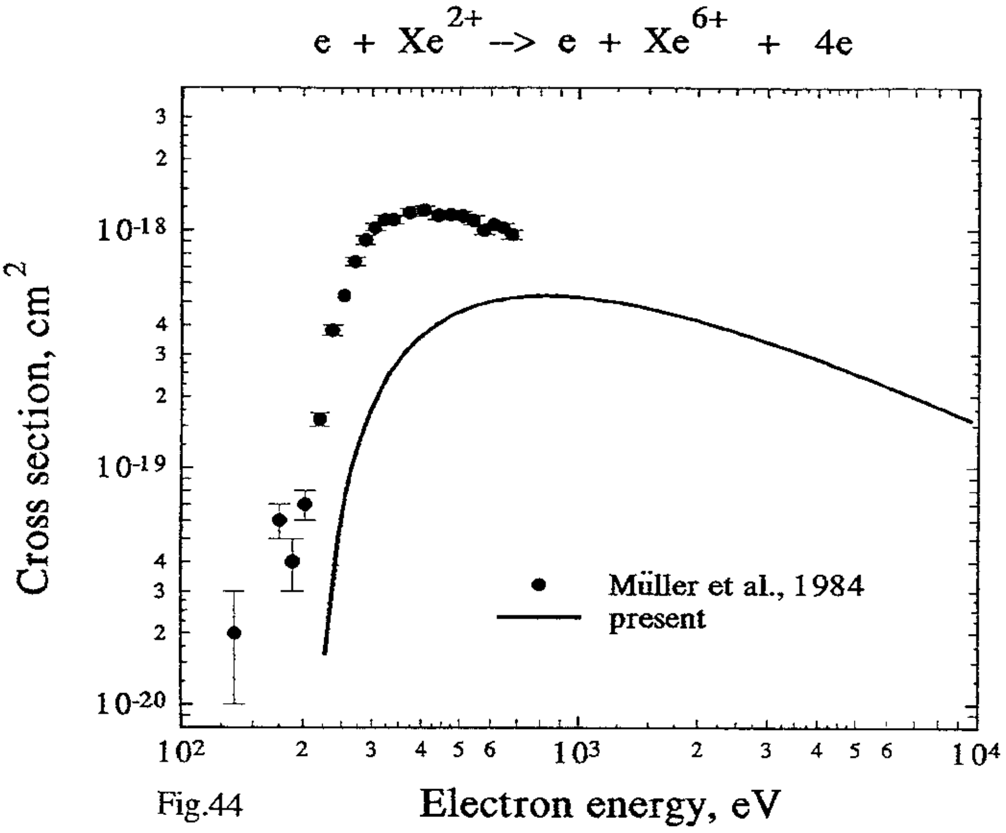

e + Xe 2+ --> e + Xe 6+ + 4e
Cross section, cm 2
Electron energy, eV
Müller et al., 1984
present

Fig.44

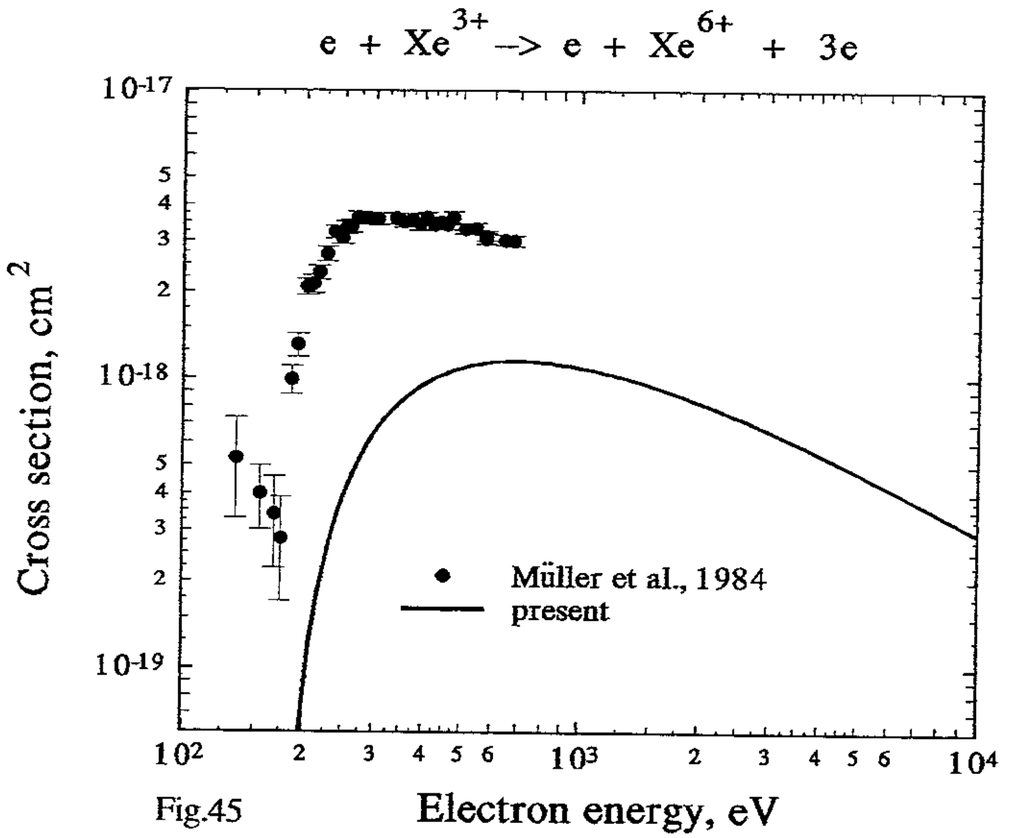
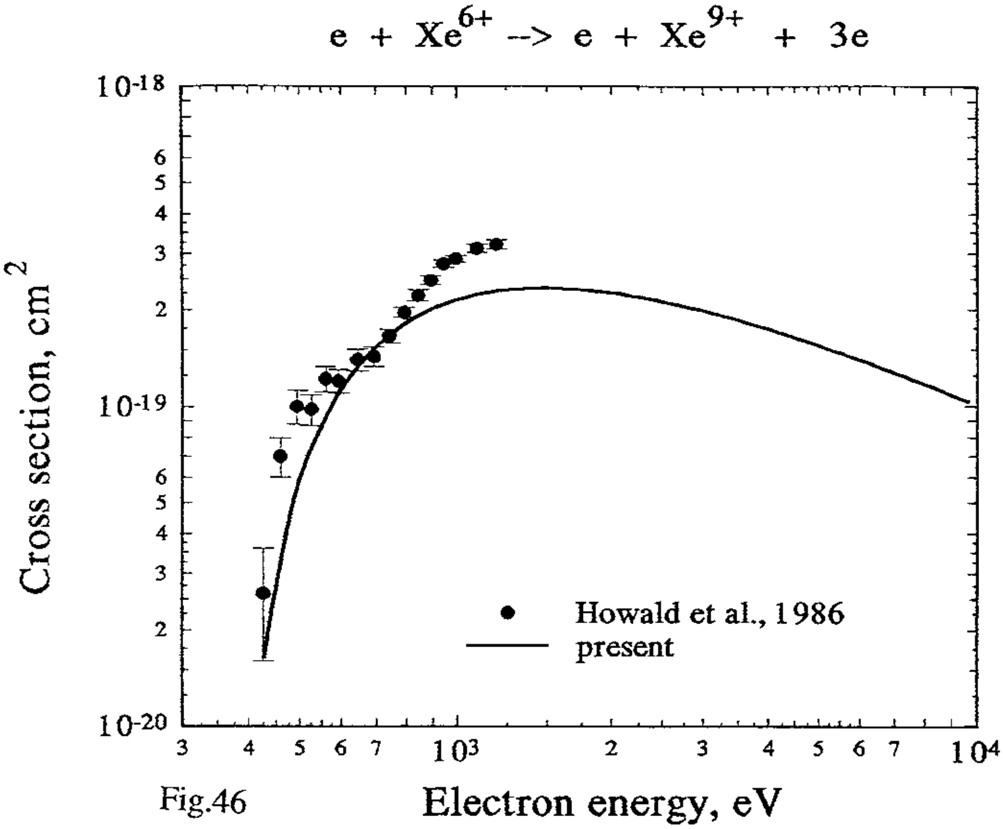
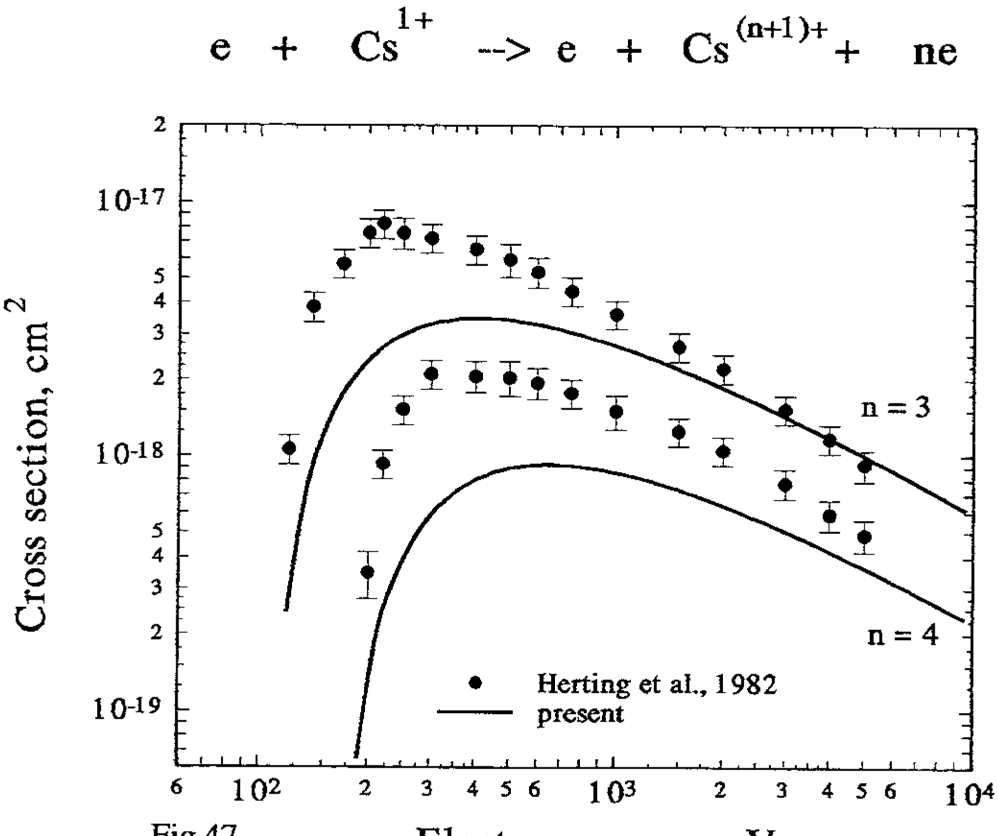

e + Xe 3+ --> e + Xe 6+ + 3e
Cross section, cm 2
Electron energy, eV
Müller et al., 1984
present

Fig.45



e + Xe6+ --> e + Xe9+ + 3e
Cross section, cm2
Electron energy, eV
Howald et al., 1986
present

Fig.46



e + Cs1+ --> e + Cs(n+1)+ + ne
Cross section, cm2
Electron energy, eV
n = 3
n = 4
Herting et al., 1982
present

Fig.47

$e + La^{2+} \rightarrow e + La^{5+} + 3e$

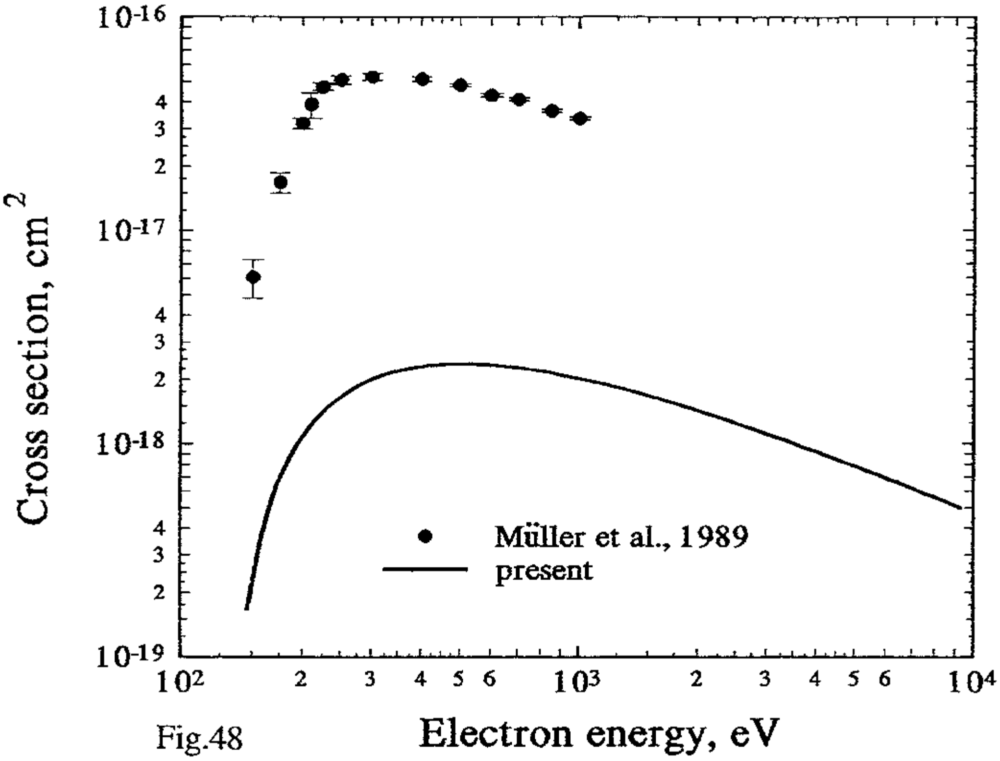


Fig.48

$e + W^{1+} \rightarrow e + W^{4+} + 3e$

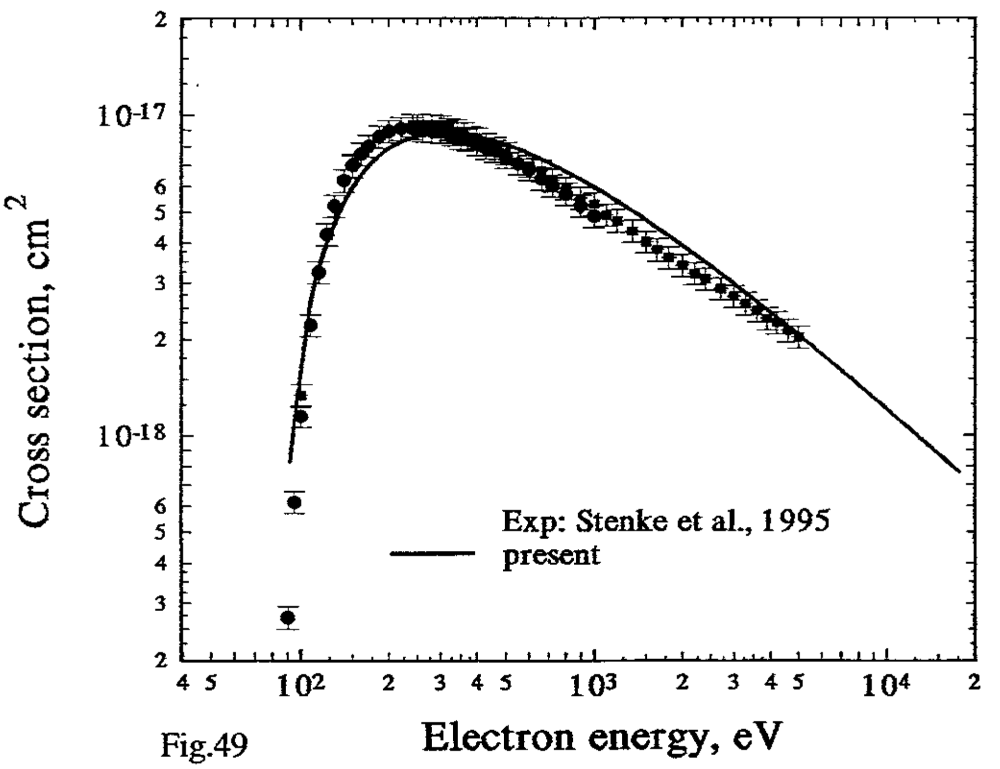


Fig.49

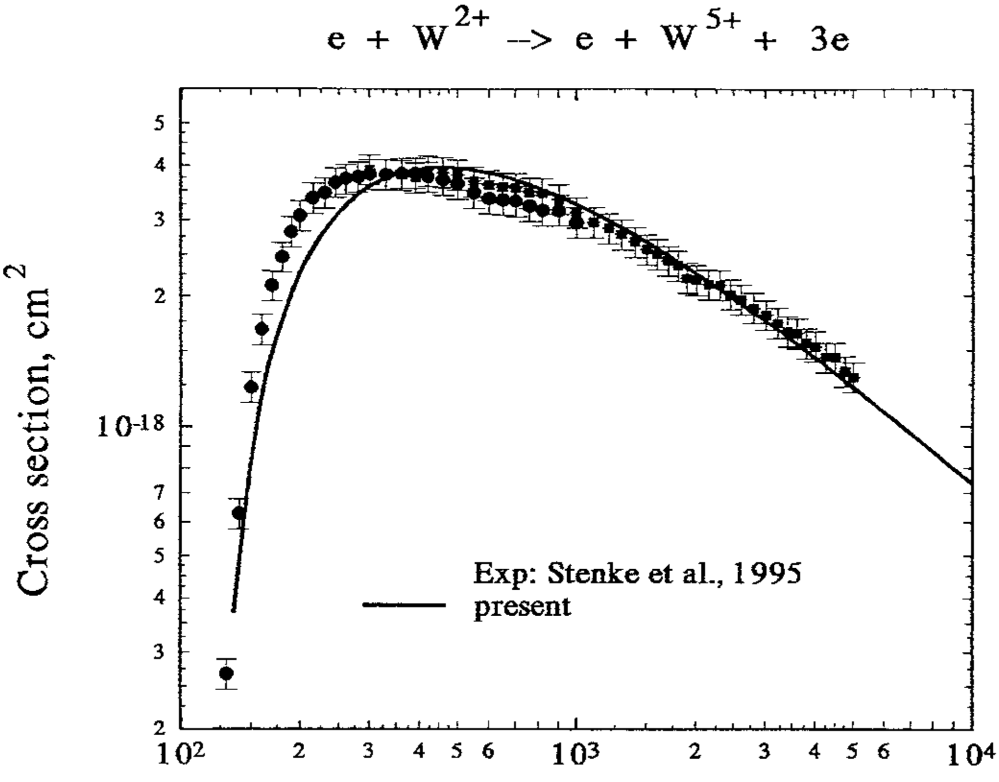

e + W^2+ --> e + W^5+ + 3e
Cross section, cm^2
10-18
Electron energy, eV
Exp: Stenke et al., 1995
present

Fig.50

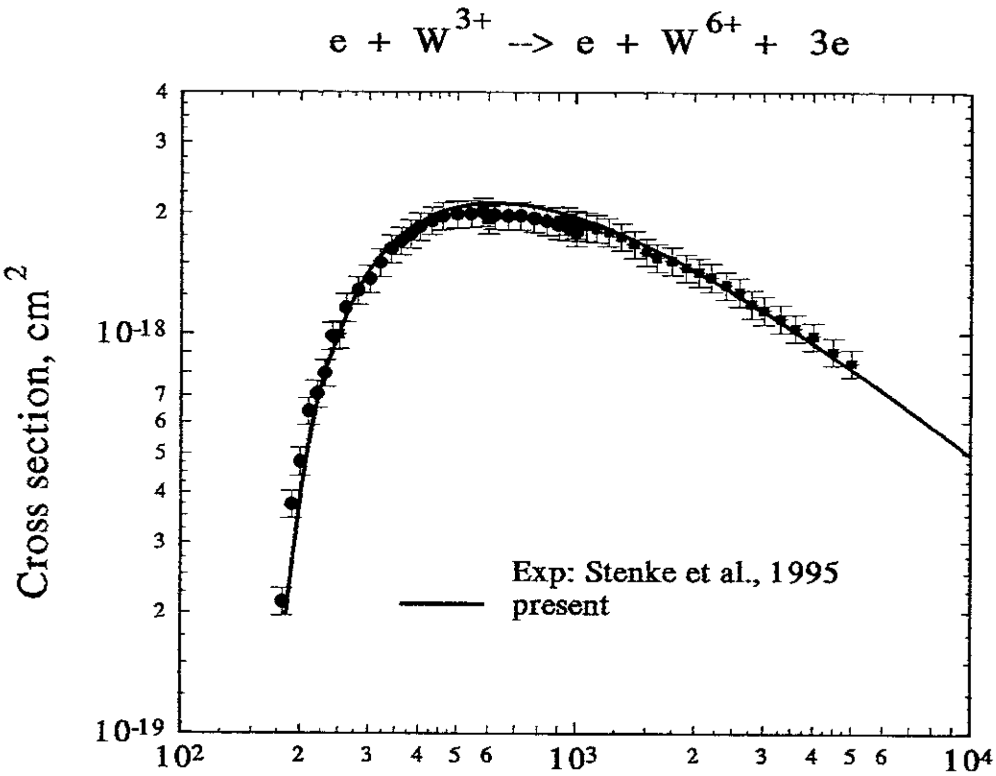

e + W^3+ --> e + W^6+ + 3e
Cross section, cm^2
10-18
10-19
Electron energy, eV
Exp: Stenke et al., 1995
present

Fig.51

$e + W^{4+} \rightarrow e + W^{7+} + 3e$

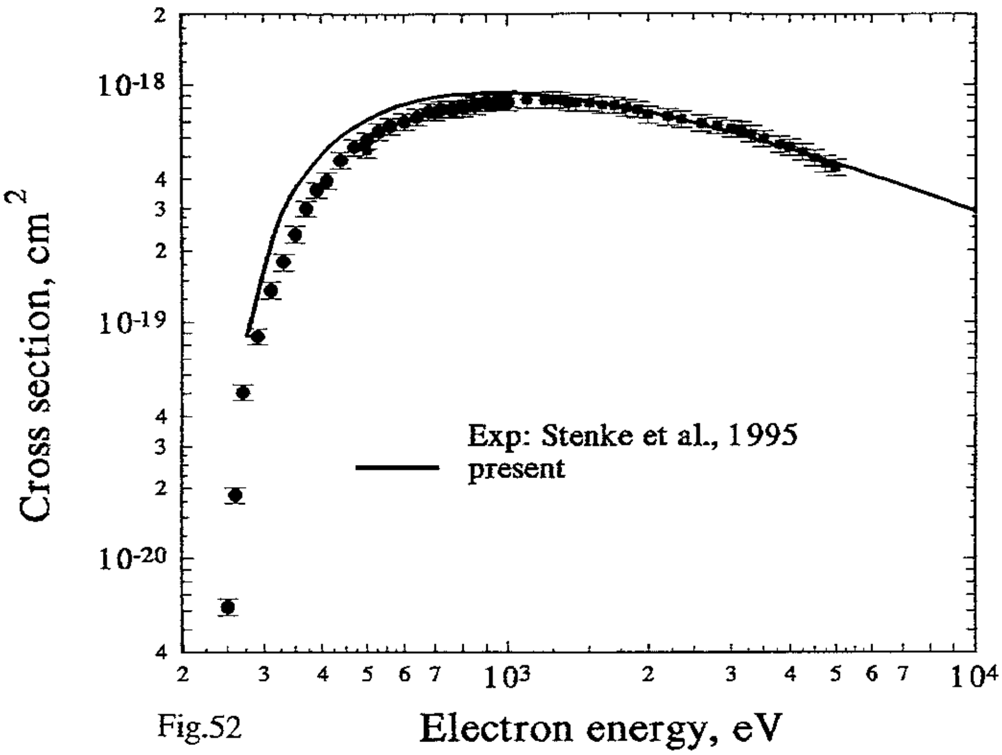


Fig.52

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Comparison of Ionization Rate Coefficients of Ions from Hydrogen through Nickel ; Sep. 1991

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Energy Dependence of Ion-Induced Sputtering Yields from Monoatomic Solids at Normal Incidence; Mar. 1995

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NIFS-DATA-26 N. Toshima and H. Tawara
Excitation, Ionization, and Electron Capture Cross Sections of Atomic Hydrogen in Collisions with Multiply Charged Ions; July 1995

ERRATA to the preprint NIFS-DATA-27 (1995):

1) The correct form of Eq. (8) is :

$$a(n) \approx 1350 / n^{5.7}, \; b(n) = const = 2.00, \quad n > 10, \tag{8}$$

2) The ref. [23] should be:

M.Stenke, K.Aichele, D.Hathiramani, G.Hofmann, M.Steidl, R.Völpel, E.Salzborn, Nucl. Instrum. Meth. Phys. Res. **B 98** (1995) 138