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AMDIS and CHART Update (I)

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Abstract

A working group for updating atomic and molecular collision data in the NIFS database AMDIS (electron scattering) and CHART (ion scattering) has been organized. This group has searched and reviewed literatures for collecting relevant atomic data which are to be included into the database. This is a summary report of the activities of this working group.

Keywords: cross sections, rate coefficients, collisional ionization, collisional excitation, charge transfer, heavy particle collision, electron-ion collisions, database

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1 Introduction

The Data and Planning Center at The National Institute for Fusion Science, Japan (NIFS) has had a long history of effective collection of collision data and their critical evaluation and compilation, and of making these data available for general users. NIFS also has had a long history of productive collaborative effort of data compilation with other data centers around the world including IAEA data unit and ORNL fusion data center. The Atomic and Molecular Numerical Database System of the NIFS has developed and is opened publicly making it available for registered users. The current system can be readily used by connection through internet at URL=<http://dbshino.nifs.ac.jp/>.

Data compilation and evaluation of atomic and molecular data for fusion research was initiated by working groups organized by Professors K. Takayanagi, H. Suzuki et al. in the Institute of Plasma Physics, Nagoya Univ. (IPP), the predecessor of NIFS, in 1975 [1]. This work has continued in Research Information Center in IPP, Nagoya from 1979 to 1989 [2], has extended its activity for including plasma surface interaction data and then evolved into in the Data and Planning Center of NIFS since 1989 [3].

The retrieval and display systems were developed as a joint research program with Drs. Y. Kanada, K. Takasugi and R. Ogasawara et al., which have become available for users since 1981 until 1997 through a main frame computer (FACOM) [4, 5]. In 1997 the systems were moved into a unix computer and its retrieving system was changed to be accessed by using a browser for internet. In Appendix A we describe the current database system and how to use the database for retrieving.

As recent development of the database system, we organized a new subgroup of numerical database for recombination processes of ions in 1999 and will do so other subgroups for molecular processes starting in 2002.

In order to update the database and keep its quality and content more complete and comprehensive, we need the continued effort of the data compilation. For this purpose, we formed a working group as a joint research program for data update of cross sections of ionization and excitation by electron impact (AMDIS) and cross sections of charge transfer, excitation and ionization by heavy particle collision (CHART).

In this report we summarize the activities of the working group for data compilation. Compiled numerical data are included into the database.

References

- [1] Cross sections for Atomic Processes. Vol.1, IPPJ-DT-48 (1975), Vol.2, IPPJ-DT-50(1976), edited by K. Takayanagi, H. Suzuki.
- [2] IPPJ-AM series, IPP, Nagoya Univ., Japan.
- [3] NIFS-DATA series, National Institute for Fusion Science, Japan.
- [4] T. Kato, Y. Itikawa, Y. Kanada, and R. Watanabe, *Physica Scripta* 23 (1981) 198.
- [5] T. Kato et al. *J. Nucl. Mater.* 128 & 129 (1984) 1006.

2 Electron-impact excitation and ionization of atomic ions

One of the numerical databases maintained by the Data and Planning Center, NIFS, is AMDIS. It contains cross section data for the electron-impact excitation and ionization of atomic ions. Those cross sections are useful particularly for diagnostics and modeling of fusion plasmas. To update the content of AMDIS, a working group has been organized. The followings are a brief summary of the activity of the group.

Since a large amount of data are expected to be available for the present processes, the task of the update is divided according to the number of bound electrons (N) of the ions: (a) $N=1,2,3$ (D. Kato) (b) $N=4-9$ (A. Igarashi) (c) $N=10-28$ (K. Moribayashi) (d) $N \geq 29$ (Y. Itikawa). The name in the parentheses indicates the member of the group who is assigned to the respective isoelectronic sequence of ions. In addition, some data from Russian research groups have been recently reported for various targets, and these data are also newly included in this database (L. Pichl). For each isoelectronic sequence, the following procedure is taken:

- (i) prepare a list of relevant literature
- (ii) review the literature to assess the cross section reported
- (iii) select the cross section data to be input into the database
- (iv) write up a brief explanation of the data selected

Considering the cross section data already kept in the AMDIS, the literature published in 1990-2000 is surveyed this time. The lists of the literature have been prepared mainly by Y. Itikawa (refs 1 and 2, and the list for 2000 attached as Appendix B of this report). Some of the papers report rate coefficients as a function of electron temperature, instead of or in addition to cross sections. Though the present version of AMDIS can store only the cross section data, those rate coefficients are also compiled for future input into AMDIS.

The following subsections give a list of ion species for which cross section data are collected. When rate coefficients are available, a letter (r) is inserted after the reference number. Experimental (theoretical) data are indicated by a letter E (T).

- (1) Itikawa, Y., *Atom. Data Nucl. Data Tables*, **63**, 315 (1996):
Annotatated bibliography on electron collisions with atomic positive ions: Excitation and ionization, 1990-1994
- (2) Itikawa, Y., *Atom. Data Nucl. Data Tables*, **80**, 117 (2002):
Annotatated bibliography on electron collisions with atomic positive ions: Excitation and ionization, 1995-1999

2.1 $N=1,2,3$

Reviewed literatures for the hydrogenlike through the lithiumlike sequences are listed in Table 1. In the table, theoretical and experimental literatures are categorized by letters of T and E, respectively. The literatures which report rate coefficients or effective collision strengths are indicated by (r) in the last column.

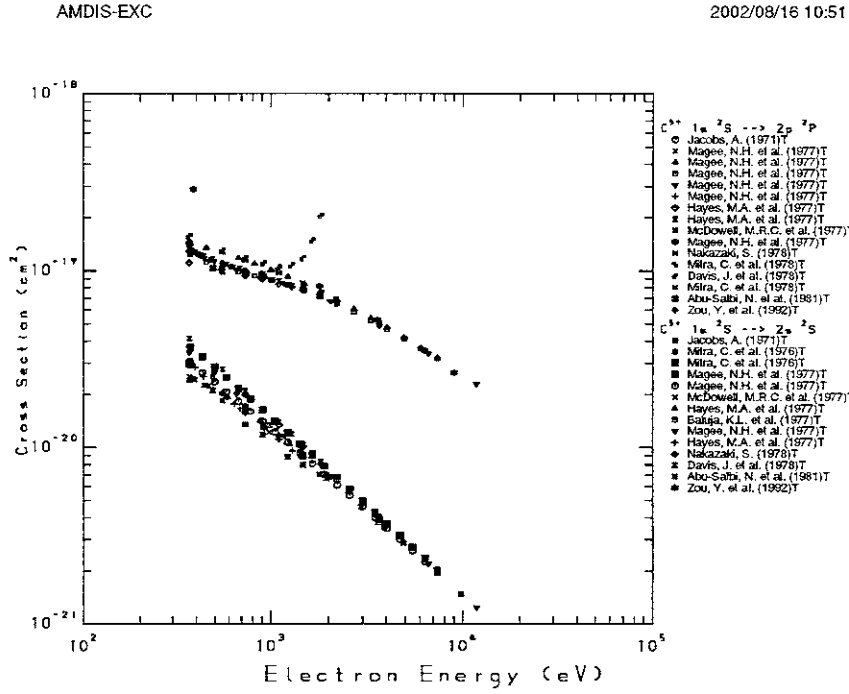
Only indirect measurements by X-ray spectroscopy of trapped ions are available for highly charged heavy ions, while direct and precise measurements are available for light ions of $Z \leq 10$ with the crossed or merged beam techniques. As the available experiments for the very highly charged ions increased in the last decade, detail examinations of the relativistic and quantum-electrodynamics theories became feasible.

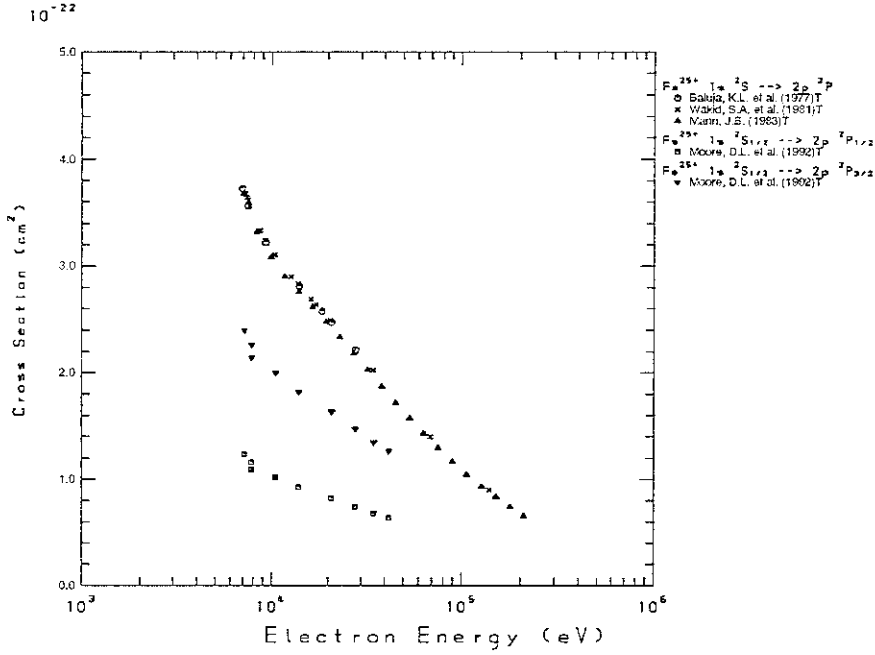
Table 1: reference table for N=1-3

Process	Nuclear charge	References
H-like		
Excitation	1-6	T [2]
	1,6,10,14,20,26	T [3] (r)
	2	T [37, 38] (r)
	2-5	T [4]
	2,6,10,13,18	T [5]
	2,26	T [15] (r)
	2,26,92	T [24] (r)
	6	T [36] (r)
	10	T [34] (r)
	14	T [39] (r)
	20	T [41] (r)
	26	T [43] (r)
	26,54,67,79,92	T [1]
Ionization	1-28	T [10] (r)
	2,6,8,9,12-14,16,17,26,29	T [28]
	42,66,79,83,92	E [11]
	42,66,79,83,92	T [26]
	92	E [46]
He-like		
Excitation	16	T [14, 42] (r)
	16,20,26	T [6] (r)
	18	T [23] (r)
	22-26	E [22]
	26,54	T [16]
	28	T [29] (r)
Ionization	2-28	T [10] (r)
	3,6,8,9,12-14,16,17,26,29	T [28]
	10	T [7]
	92	T [25]
	92	E [46]
Li-like		
Excitation	5	E [19]
	6	E [18, 20]
	6	E [21] (r)
	6	T [40] (r)
	6,8	T [8] (r)
	6-8,10,12-14,16,20,22,26,28,30,32,34,36,42	T [30, 31] (r)
	8	E [45]
	8-92	T [33]
	18	T [23] (r)
	22-26	E [22]
	26	T [13] (r)
Ionization	3,4,7	T [12]
	3-28	T [10] (r)
	5	E [19]
	6-29	T [27]
	7,8,10	E [32]
	8	E [9]

Table 1: (continued.)

Process	Nuclear charge	References
	22–26	E [44]
	56	E [35]
	92	E [17]
	92	T [25]

Figure 1: Excitation cross section of C^{5+} by electron impact.

Figure 2: Excitation cross section of Fe^{25+} by electron impact.

2.2 N=4-9

Tables 2-7 show references for ions with 4-9 electrons.

Table 2: reference table for N=4

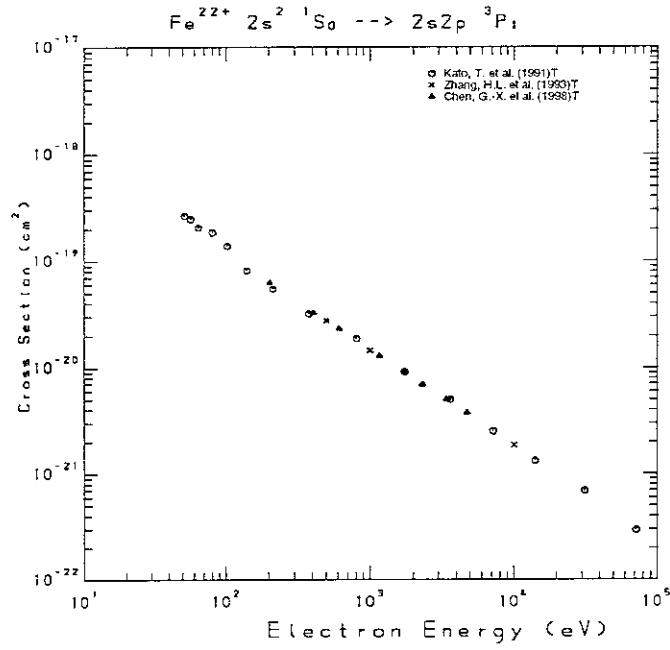
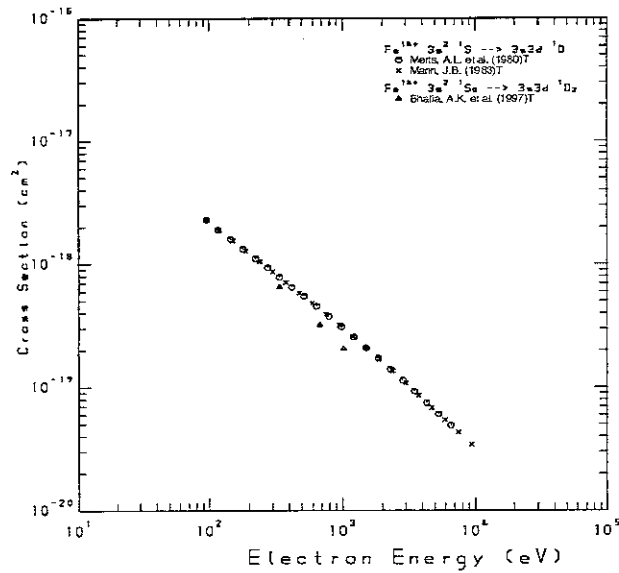
Process	Nuclear charge	References
Be-like		
Excitation	4-28	T [109]
	5	[153]
	6	T [86] (r)
	6-54	T [147] (r)
	6-92	T [185]
	21-30	T [123] (r)
	7	T [124] (r)
	8	T [49] (r) [69] [89] (r) [59] (r) [104] [175]
	10	T [104] [125] (r) [146] (r)
	14	T [59] (r) [69] [89] (r)
	18	T [137] (r)
	21-30	T [123] (r)
	26	T [59] (r) [69] [76] (r) [89] (r) [100] (r) [104] [173] [187] (r)
	42	T [59] (r) [69] [89] (r) [113]
	54	T [104]
Ionization	5	T [87] [163] [154]
	6	T [163] [171] (r)
	8	E [183]
	10	E [150] (r) [160]

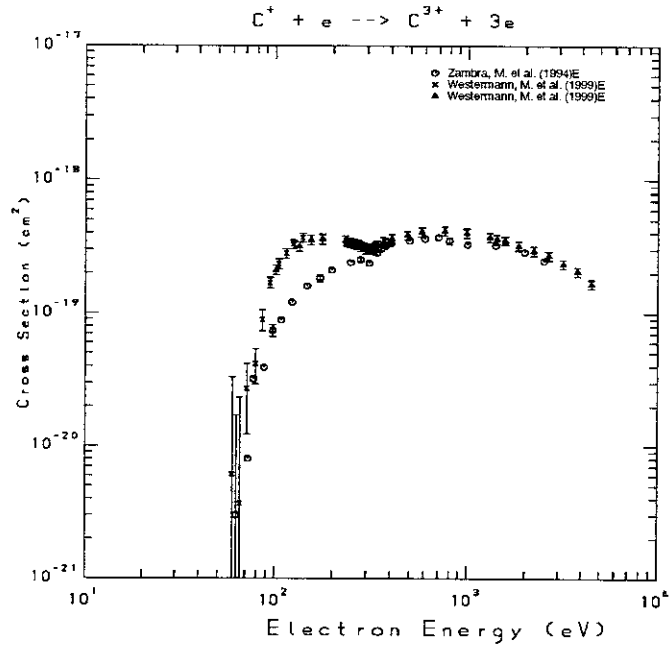
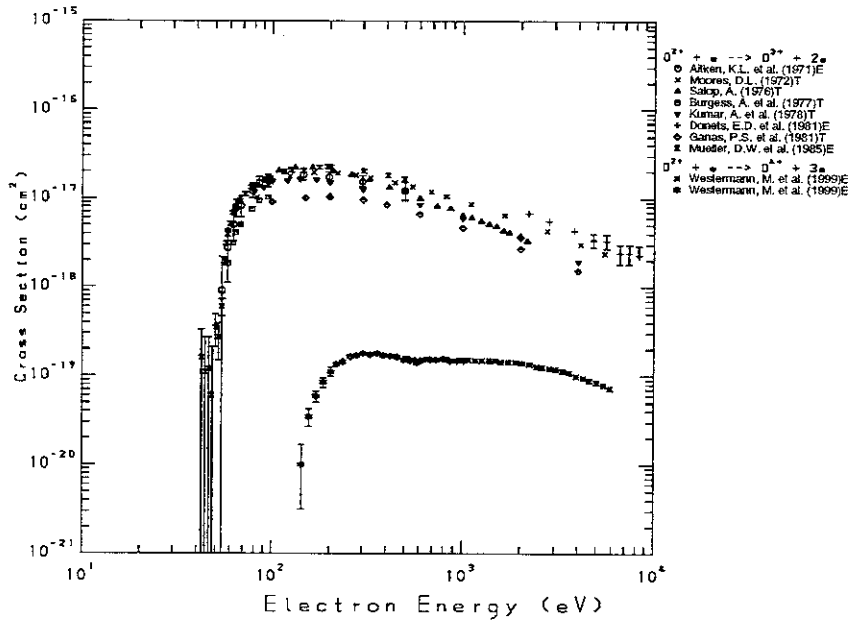
Table 2: (continued.)

Process	Nuclear charge	References
		T [139] [172] (r) [188] [189]
	16	T [140] (r)
	18	T [139] [176] (r) [177] (r)
	20	T [140] (r)
	24	T [75] (r)
	26	T [80] (r) [94] [140] (r)
	28	T [58] (r)
	36	T [94]
	54	T [94]
	92	E [161]
		T [144]

Table 3: reference table for N=5

Process	Nuclear charge	References
		B-like
Excitation	5	T [133]
	5-28	T [126]
	6	E [135]
		T [50] [67] (r) [82] (r) [156]
	7	T [50] [82] (r) [91] (r) [128] (r)
	8	T [50] [131] (r) [134] (r)
	8-92	T [132]
	10	T [85] (r) [131] (r) [134] (r)
	12	T [134] (r) [168]
	12-14	T [131] (r)
	14	T [134] (r)
	18	T [131] (r)
	20	T [131] (r) [179] (r)
	26	T [131] (r) [134] (r) [148] [151] [164] (r) [165] (r) [170] (r)
Ionization	6	E [106] [183]
		T [171] (r)
	8	T [145] (r) [183]
	10	E [150] (r) [160]
		T [139] [172] (r) [188]
	18	T [139] [176] (r) [177] (r)
	24	T [75] (r)
	26	T [80] (r) [94]
	28	T [58] (r)
	36	T [94]
	92	E [161]

Figure 3: Excitation cross section of Fe^{22+} by electron impact.Figure 4: Excitation cross section of Fe^{22+} by electron impact.

Figure 5: Ionization cross section of C^+ by electron impact.Figure 6: Ionization cross section of O^{2+} by electron impact.

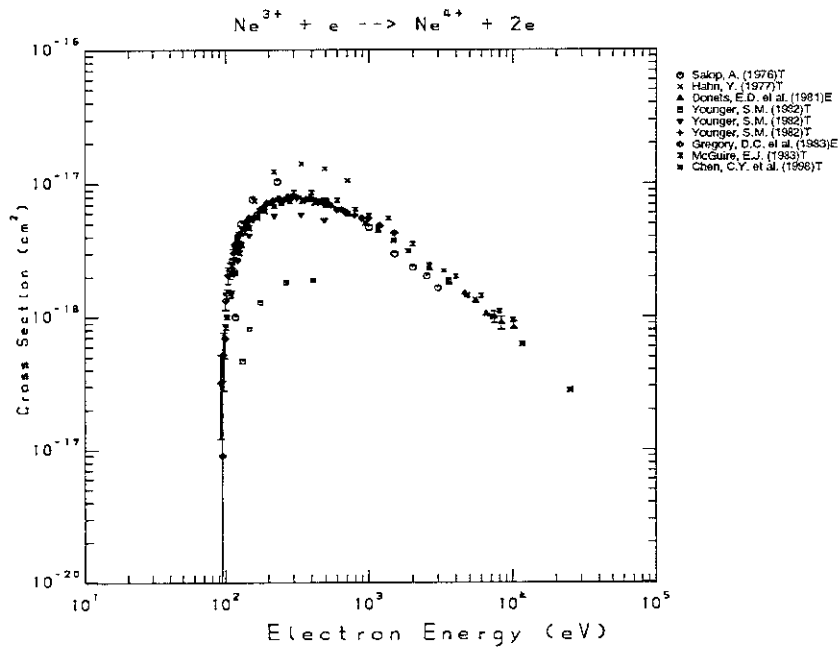
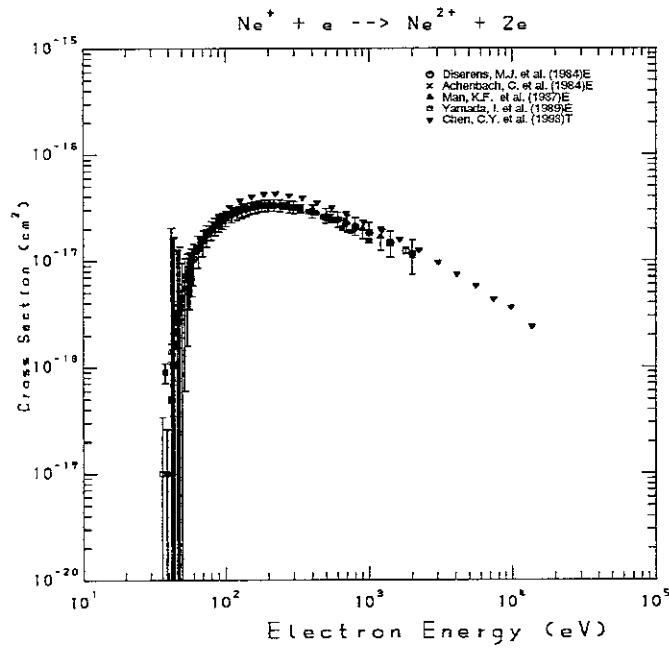
Figure 7: Ionization cross section of Ne^{3+} by electron impact.Figure 8: Ionization cross section of Ne^{+} by electron impact.

Table 4: reference table for N=6

Process	Nuclear charge	References
C-like		
Excitation	6	T [116]
	7	T [129] (r) [178] (r)
	7-16	T [119] (r)
	8	T [66] [93] (r) [95]
	9	T [83] (r)
	9-54	T [157] [166]
	10	T [70] (r)
	11	T [83] (r)
	12	T [68] [138]
	13	T [83] (r)
	14	T [96]
	15-19	T [83] (r)
	20	T [47] (r) [63] (r) [65] [79] (r) [97]
	21-28	T [130] (r)
	26	T [64] (r)
Ionization	7	E [106]
	8	E [183]
	10	E [150] (r) [160]
		T [139] [172] (r) [188]
	18	T [139] [176] (r) [177] (r)
	24	T [75] (r)
	26	T [80] (r)
	28	T [58] (r)
	92	E [92] [161]
		T [56] [90]

2.3 N=10-28

We found 20 papers in which the cross sections of electron impact processes of Ne-like to Ni-like ions are investigated. Among them 10 papers show the ionization cross sections. The excitation auto-ionization dominates in these ions. The experimental measurements are for $\text{Ti}^{+},^{2+},^{4-6+},^{11+}$, Cr^{13+} , Ar^{7+} , Cl^{+} , Si^{4-7+} , Al^{22+} , Ca^{+} and numerical calculations are for those of Fe^{15+} and Ar^{2+} . On the other hand, in the excitation processes, 10 papers are found for experimental measurement and numerical calculation. The cross sections for $\text{Si}^{2+,3+}$, Ar^{7+} are measured, while those of Co^{2+} , Fe^{14+} , Ni^{12+} are calculated.

Table 5: reference table for N=7

Process	Nuclear charge	References
N-like		
Excitation	7	T [117]
	8	E [136]
		T [101] (r) [102] (r) [103] (r) [120] (r) [121] (r) [149] [180] (r)
	10	T [181] (r) [182] (r)
	12	T [164] (r) [169]
	16	T [184] (r)
	12-92	T [191]
Ionization	8	E [106] [183]
	10	T [139] [172] (r) [188]
	12	T [164] (r)
	13	T [152]
	14	E [105]
		T [152] [164] (r)
	18	T [139] [176] (r) [177] (r)
	24	T [75] (r)
	26	T [80] (r)
	28	T [58] (r)
	92	E [161]
		T [56] [90]

Table 6: reference table for N=8

Process	Nuclear charge	References
O-like		
Excitation	8	T [118]
	9	T [73] [88]
	9-18	T [111] (r)
	20	T [108]
	36	T [78]
Ionization	10	E [150] (r)
		T [139] [172] (r) [188]
	14	E [105] [152]
	18	T [139] [176] (r) [177] (r)
	24	T [75] (r)
	26	T [80] (r)
	28	T [58] (r)
	92	E [161]

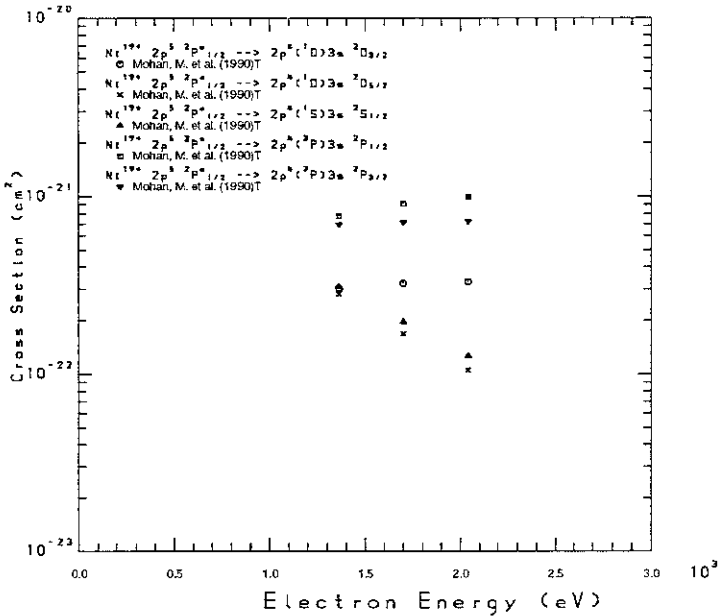


Figure 9: Excitation cross section of Ni^{17+} by electron impact.

Table 7: reference table for N=9		
Process	Nuclear charge	References
F-like		
Excitation	9	T [110]
	10-26	T [127] (r)
	18-23	T [167] (r)
	14	T [51] (r) [52] (r)
	17	T [72] (r)
	22-92	T [74]
	26	T [84] [98] (r) [112] (r)
	28	T [53] (r) [55] (r)
	34	T [112] (r) [162] [174] [186]
	42	T [112] (r)
	47	T [112] (r)
	54	T [112] (r)
	63	T [112] (r)
Ionization	10	E [106] T [139] [172] (r) [188]
	14	E [105] T [190]
	18	T [139] [141] [176] (r) [177] (r)
	24	T [75] (r)
	26	T [80] (r)
	28	T [58] (r)
	92	E [161]

Table 8: Reference table for N=10-28		
Process	Ion species	References
Excitation	Si ³⁺	E [197]
	Ar ⁷⁺	E [198]
	Ar ²⁺	T [201]
	Fe ¹⁵⁺	T [202]
	Ar ⁶⁺	E [206]
	Si ²⁺	E [207]
	Si ²⁺	E [208]
	Ni ¹²⁺	T [209] (CS)
	Fe ¹⁴⁺	T [210]
	Co ⁺	T [211]
Ionization	Cl ⁺	E [192]
	Ti ¹¹⁺	E [193]
	Cr ¹³⁺	E [193]
	Ar ⁷⁺	E [194]
	Mg ⁺	E [195]
	Ti ⁵⁺	E [196]
	Si ^{6+,7+}	E [199]
	Si ^{4+,5+}	E [200]
	Ti ^{1-,2-,4+,6+}	E [203]
	Al ²⁺	E [204]
	Ca ⁺	E [205]

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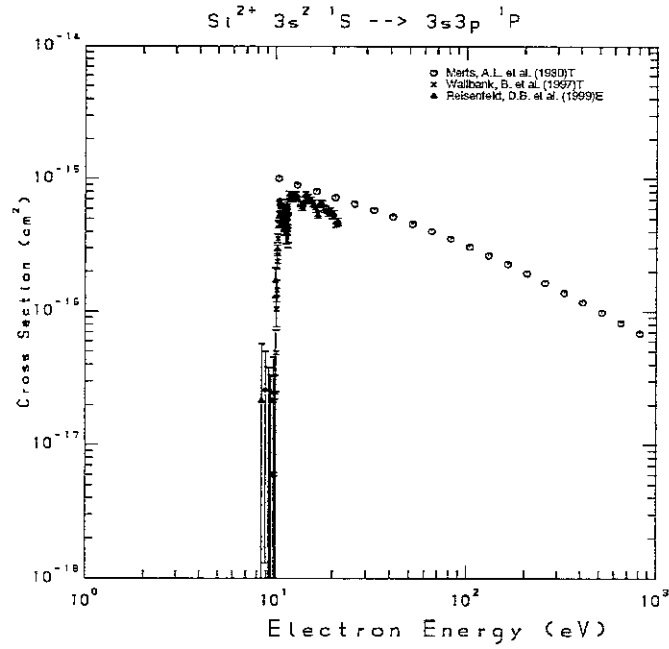


Figure 10: Excitation cross section of Si²⁺ by electron impact.

2.4 $N \geq 29$

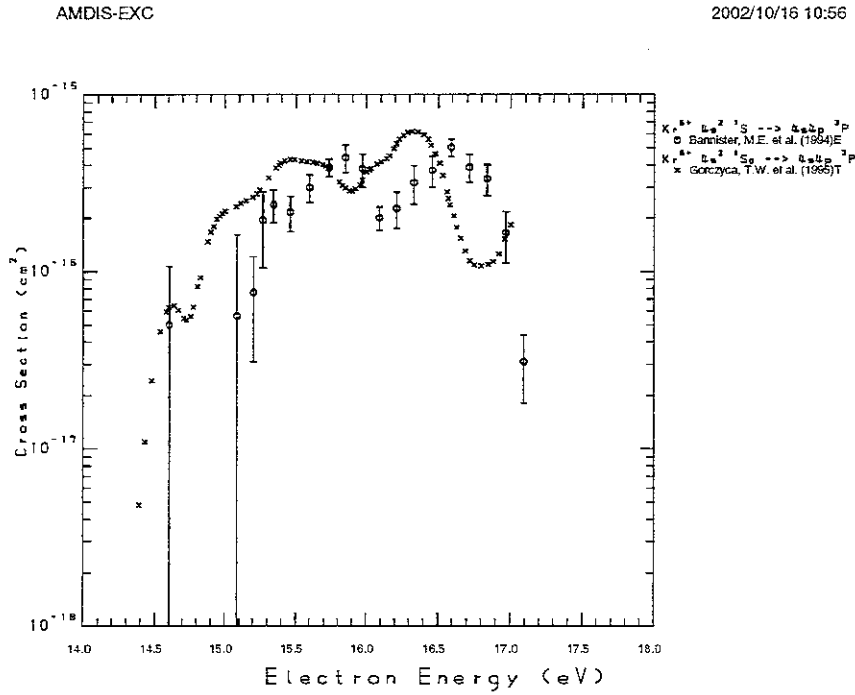
Cross section data have been collected for the ions listed in the following tables. In the tables, the ions are listed in ascending order of atomic number (Z). For excitation, experimental data are available only for Zn^+ , Kr^+ , Kr^{6+} , Sr^+ and Ba^+ , while most of the data available for ionization are experimental.

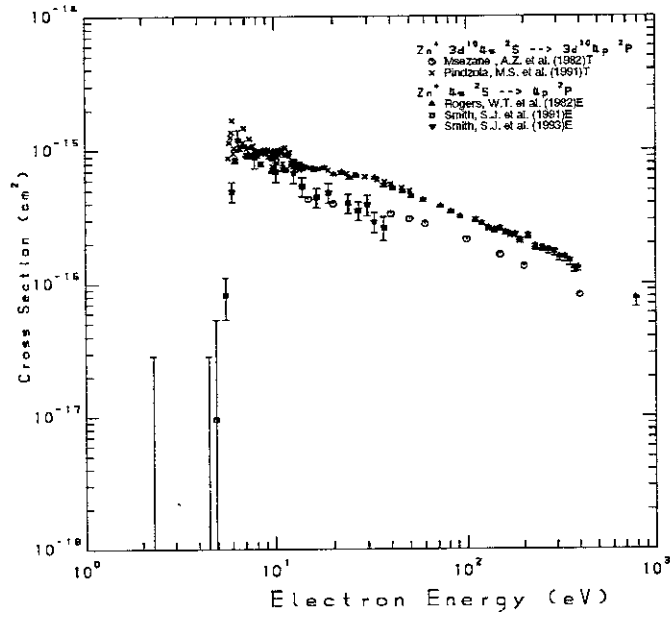
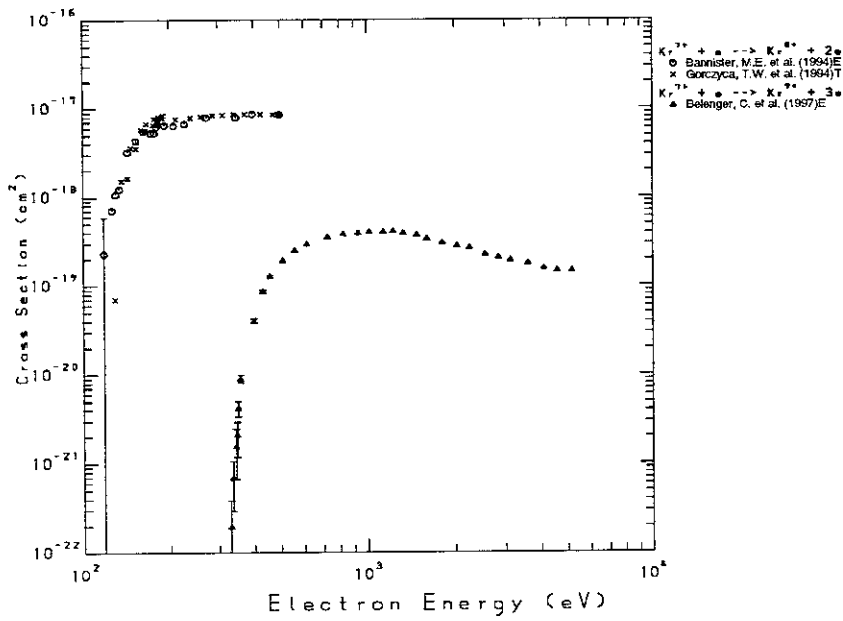
Table 9: Reference table for $N \geq 29$

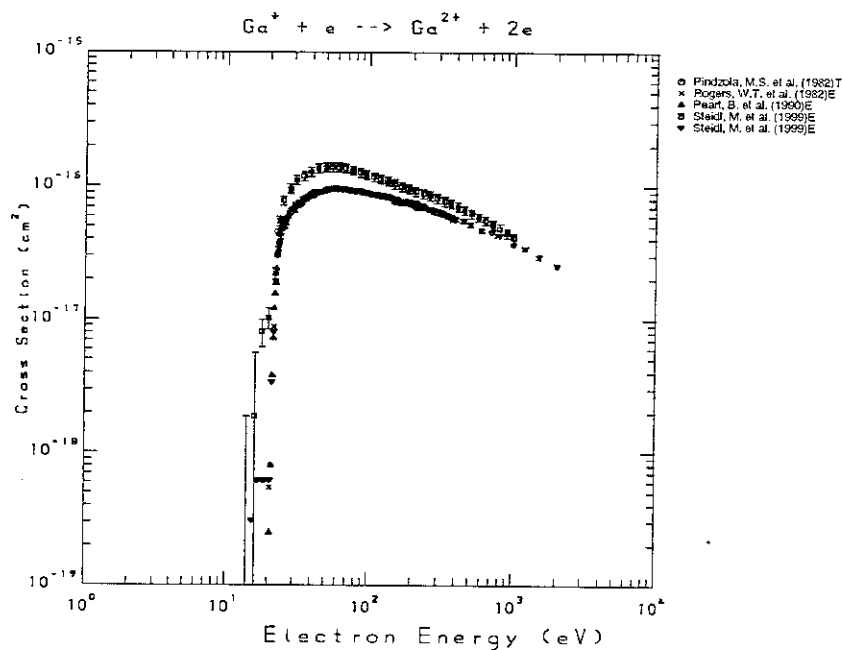
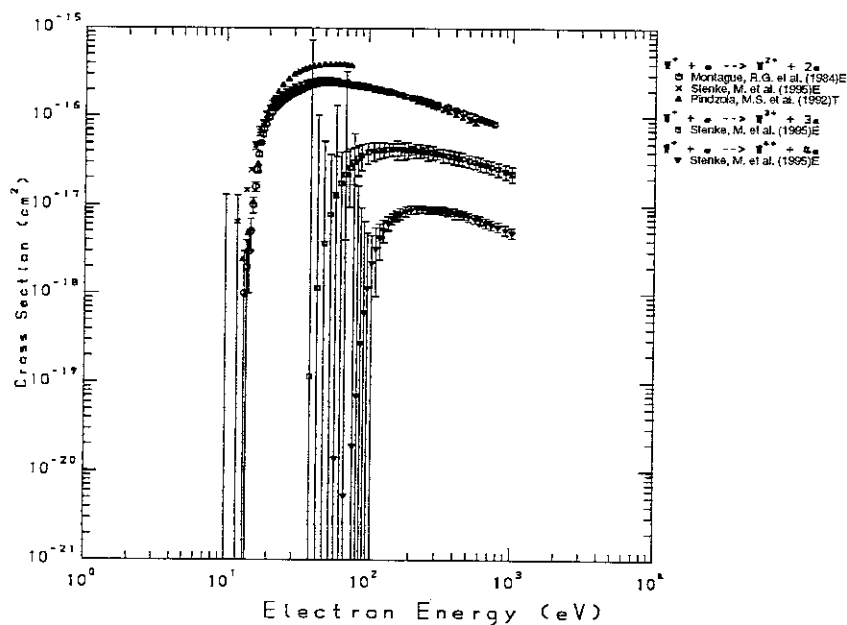
Process	Ion species	References
Excitation	Zn^+	E [238] [243] T [241]
	Kr^+	E [239]
	Kr^{2+}	T [248] (r)
	Kr^{3+}	T [247] (r) [248] (r)
	Kr^{4+}	T [248] (r)
	Kr^{6+}	E [244] T [245]
	Sr^+	E [240] T [242]
	Xe^{2+}	T [249] (r)
	Xe^{3+}	T [246] (r) [249] (r)
	Xe^{5+}	T [249] (r)
	Ba^+	E [240] T [249] (r)
	Ba^{3+}	T [249] (r)
	Cu-like ($Z=60-92$)	T [237]
Ionization	Zn^+	E [215]
	Ga^+	E [214] [236]
	Ge^+	E [230]
	Se^+	E [222] (r)
	Kr^+	E [230]
	Kr^{2+}	E [213] [219]
	Kr^{4+}	E [221] [223] T [225]
	Kr^{5+}	E [221] T [225]
	Kr^{6+}	T [225] [233]
	Kr^{7+}	E [221] [223] T [225] [232]
	Sr^+	E [231]
	Mo^+	E [229] [235]
	Mo^{2+}	E [229] [235]
	Mo^{3+}	E [229] [235]
	Mo^{4+}	E [226] (r) [229] [235]
	Mo^{5+}	E [226] (r) [229] [235]
	Mo^{6+}	E [229] [235]
	Mo^{7+}	E [229]
	Mo^{8+}	E [229]
	Mo^{11+}	T [251] (r)
	Mo^{12+}	T [233]
	Ag^{16+}	T [251] (r)
	Cd^+	E [224]
	In^+	E [218] (r) [230]
	Te^+	E [222] (r)
	Xe^+	E [218] (r)
	Xe^{2+}	E [213] [219]
	Xe^{6+}	E [223]
	Xe^{8+}	E [223] [252]
	Xe^{23+}	T [251] (r)
	Xe^{24+}	T [233]
	Cs^+	E [231]

Table 9: (continued.)

Process	Ion species	References
	Ba ⁺	E [220]
	Ba ²⁺	E [216] [252]
	Ba ³⁺	E [216]
	Pr ²⁸⁺	T [250] (r) [251] (r)
	Pr ²⁹⁺	T [233]
	Eu ³²⁺	T [251] (r)
	Dy ³⁵⁺	T [250] (r) [251] (r)
	Dy ³⁶⁺	T [233]
	Ta ⁸⁺	E [223]
	W ⁺	E [227] [228] T [217]
	W ²⁺	E [227] [228]
	W ³⁺	E [227] [228]
	W ⁴⁺	E [227] [228] T [234]
	W ⁵⁺	E [227] [228] T [234]
	W ⁶⁺	E [227] [228] T [234]
	W ⁷⁺	E [227]
	W ⁸⁺	E [227]
	W ⁹⁺	E [227]
	W ¹⁰⁺	E [227]
	U ¹⁰⁺ , U ¹³⁺ , U ¹⁶⁺	E [212] [223]

Figure 11: Excitation cross section of Kr^{6+} by electron impact.

Figure 12: Excitation cross section of Zn^+ by electron impact.Figure 13: Ionization cross section of Kr^{7+} by electron impact.

Figure 14: Ionization cross section of Ga^+ by electron impact.Figure 15: Ionization cross section of W^+ by electron impact.

2.5 H, He, N, O, Ar, Xe, Au, Pb, Ti, Kr, Sn, Ta, U

New electron impact data by theoretical group in the Joint Institute for Nuclear Research in Dubna are to be added into the NIFS databases. The processes presently covered are

$$X^{q+} + e^- \rightarrow X^{(q+1)+} + 2e^-,$$

for the electron energy range from ionization threshold up to 200 keV. Here X stands for the atomic targets and their respective positive ions,

$$X = H, He, N, O, Ar, Xe, Au, Pb, Ti, Kr, Sn, Ta, U.$$

The data is a compilation of experimental results [255, 256] and "Atom" code simulations (Coulomb-Born approximation with exchange term in the partial wave representation, including at least three target outer-most shells) [257]. Numerical results are fitted, and also tabulated including the fitting error. All parameters for the fitting formulas are given. The authors claim the accuracy within a factor of two as compared to the experimental results, which is demonstrated by several examples in the introduction of the Dubna report [253].

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3 Charge transfer and ionization by ion impact on atoms and molecules

Among many databases stored in NIFS, CHART is primarily concerned with excitation, charge transfer and ionization in ion impacts on atoms and molecules in a wide range of impact energies for a variety of collision pairs. Since the last effort of the data compilation and publication in late 80th, more new experimental and theoretical investigations have been reported, and corresponding new cross section data have become available for revision as well as new addition to the database. Accordingly, we undertake the present effort to update the current database and reexamine the contents. It has been known that H_2 , CO_2 , and O_2 molecules are present in the reactor as impurities, and various hydrocarbons were recently found to be produced near the divertor edge where the plasma temperature is low. Hence, the information of their spectroscopic data and the dynamical behavior of these molecules is important for the modeling and other applications. But reliable data concerning these molecules were still quite limited. Recently, more systematic studies on molecular targets have been carried out for charge transfer and ionization including the classification of fragmented species, and certainly these data should be included in the database. Hence, a particular effort was placed on molecular targets in the current project, although new data for atomic targets were also critically evaluated and included. In this report, we divide this section into two sub-sections, (i) atomic targets (Morishita) and (ii) molecular targets and their fragmented species (Kusakabe, Imai, Kimura, Motohashi).

3.1 Atomic targets

For atomic targets, we are concerned with primarily H^+ , He^+ , C^{q+} , and O^{q+} ions since these ions are most important plasma species not only in fusion, but also other applied fields such as astrophysics, aerospace science, and technological applications. Furthermore, these ions are repeatedly studied at different energy regions for various inelastic processes for better precision. As for targets, we selected neutral species of these ionic species because these neutrals are abundantly present as impurities in the fusion reactor. Recent measurements for these species below 100 keV/u are believed to be more reliable because of better experimental and theoretical tools and techniques used. Hence, the present revision for these collision pairs may significantly improve over old data particularly for charge transfer.

Table 10: Reference table for atomic targets

Projectile ionic species:	H^+ , He^{q+} ($q = 1, 2$), C^{q+} ($q = 1 - 6$), O^{q+} ($q = 1 - 8$)
Target atomic species:	C, N, O
Energy region:	a few eV- a few MeV
References:	[1] - [15]

(a) Carbon ions on H atom

Table 11: Reference for Carbon ions on H atom

System	References	Experiment/Theory	Energy (keV/u)
$C^{2+} + H$	[1]	T	0.1-150
$C^{3+} + H$	[2]	T	0.05-9
$C^{3+} + H$	[3]	T	0.05-10000
$C^{4+} + H$	[4]	E	0.006-1
$C^{4+} + H$	[5]	T	0.01-2
$C^{4+} + H$	[6]	T	0.01-10
$C^{5+} + H$	[7]	T	0.0001-10
$C^{6+} + H$	[8]	T	1-400
$C^{6+} + H$	[9]	T	0.1-500

(b) Heavy-atom targets

Table 12: Reference for heavy atoms

System	References	Experiment/Theory	Energy (keV/u)
H^+ + Mg	[10]	E	90-2000
He^{2+} + Mg	[10]	E	43-500
Al^{3+} + H	[11]	T	0.5-10
H^+ + Fe	[12]	E	70-500
He^{2+} + Fe	[12]	E	37.5-360
H^+ + Cu	[13]	E	70-720
He^{2+} + Cu	[13]	E	35-360
H^+ + Ga	[14]	E	38-1440
He^{2+} + Ga	[14]	E	38-1440
H^+ + Pb	[15]	E	50-600
He^{2+} + Pb	[15]	E	50-600

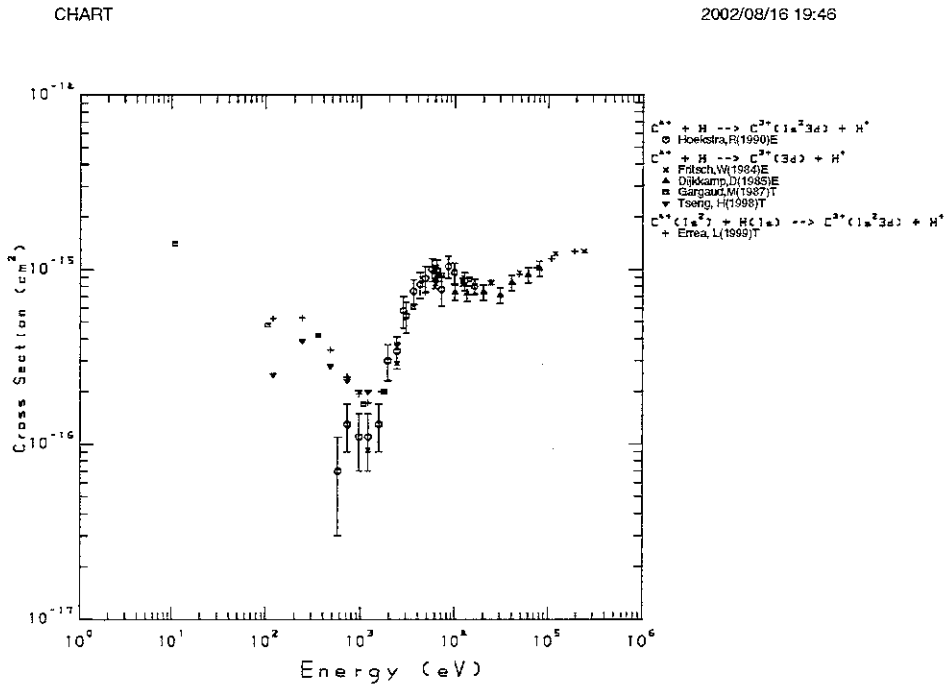
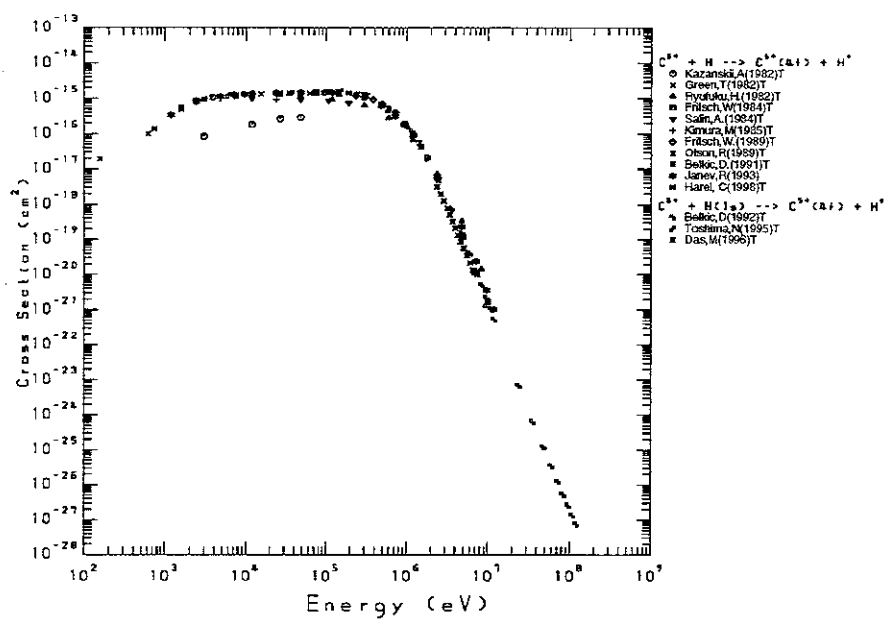
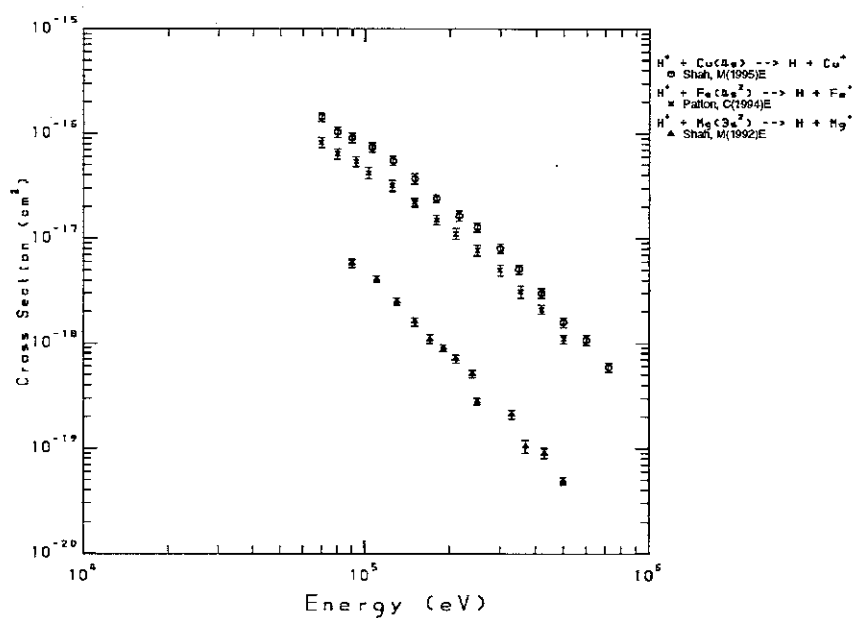


Figure 16: Charge transfer cross section of $C^{4+} + H$ collision.

3.2 Molecular targets

Most of gaseous as well as condensed species around us are present apparently in a form of molecules. Therefore, collision processes between ions and molecules are of basic importance for understanding

Figure 17: Charge transfer cross section of $C^{6+} + H$ collision.Figure 18: Charge transfer cross section of $H^+ + Cu$ collision.

a variety of phenomena and applications. Yet, the present knowledge of collision processes involving molecular targets is very limited and the amount of collision data is scarce. Charge transfer from molecular targets is among those whose data are urgently required in many applied fields because charge transfer makes a dominant contribution to the total cross section below 100 keV/u, or so over ionization. Here we attempt to review cases of some selective molecular species as shown in Table 13.

As described, H_2 , CO, CO_2 , and O_2 molecules are known to be abundantly present, and various types of hydrocarbons (C_nH_m , where $n=1-4$ and $m=2, 4, 6, 8, 10$) have been observed near the divertor edge. Hence, various inelastic collision processes for these large hydrocarbons are also important which provide essential ingredients for the modeling of plasma and carbon behavior.

Except for research journals, we consulted some data books, and these include:

- (1) International Bulletin on Atomic and Molecular Data for Fusion: IAEA, No.42 (1991)-58 (2000).
- (2) CIAMDA 98 (An Index to the Literature on Atomic and Molecular Collision Data Relevant to Fusion Research): IAEA (1998).
- (3) Bibliography on Electron Transfer Processes in Ion-Ion/Atom/Molecule Collisions-Updated 1997-: H. Tawara, NIFS-DATA-42, (1997).
- (4) Cross Sections for Charge Transfer of Hydrogen Atoms and Ions Colliding with Gaseous Atoms and Molecules: Y. Nakai, T. Shirai, T. Tabata and R. Ito, At. Data and Nucl. Data Tables 37, 69 (1987).
- (5) Data on Collisions of Hydrogen Atoms and Ions with Atoms and Molecules (1) (Cross Sections for Charge Transfer of H, H^+ with H_2 , N_2 , O_2 , C and Carbon Containing Molecules): Y. Nakai, A. Kikuchi, T. Shirai and M. Sakata, JAERI-M 83-013 (unpublished).

For hydrocarbons, very few investigations have been carried out to date. Therefore, we undertook the effort to carry out a joint experimental and theoretical study of charge transfer from these hydrocarbons by H^+ , C^+ , O^+ ion impacts below 100 keV. We have also carried out a careful study of the effect of vibrational states of the target.

Furthermore, some ionic projectiles in the second row of the periodic table ($Li^{q+} - Ne^{q+}$) in collisions with H_2 and D_2 targets were studied relatively frequently, and hence, charge transfer and ionization cross section data for these projectiles are newly included in this report.

Molecular ions after charge transfer are often unstable and undergo dissociation or Coulomb explosion to smaller neutral and ionic species. These dissociation processes are important, but very few studies has been carried out as described in the next section. Charge transfer study from molecules other than H_2 and D_2 is very rare as exemplified in this report, and in future, we need to direct our effort toward this direction.

Table 13: Reference for molecular targets

Projectile ionic species:	H^+ , D^+ , He^{q+} ($q = 1, 2$), Li^{q+} ($q = 1-3$), Be^{q+} ($q = 1-4$), B^{q+} ($q = 1-5$), C^{q+} ($q = 1-6$), N^{q+} ($q = 1-7$), O^{q+} ($q = 1-8$), F^{q+} ($q = 1-9$), Ne^{q+} ($q = 1-10$)
Target atomic species:	CO, CO_2 , H_2O , C_nH_m (hydrocarbons)
Energy region:	1 eV - a few hundred keV
Search of papers published:	Primarily since 1990, but we also include a few prior to 1990.
References:	[16] - [76]
Projectile ionic species:	H^+ , H_2^+ , D_2^+
Target molecular species:	H_2 , D_2
References:	[102], [107], [108], [122], [125], [136], [144], [160], [169], [171], [173], [177], [182], [184], [188], [196], [220], [245], [256], [298]

Table 13: (continued.)

Projectile ionic species:	$\text{He}^{q+}(q=1,2)$
Target molecular species:	H_2, D_2
References:	[79], [83], [84], [90], [96], [98], [108], [121], [122], [125], [135], [155], [163], [164], [194], [205], [213], [218], [220], [228], [231], [234], [236], [244], [249], [257], [261], [262], [273], [275], [278], [279], [284], [285]
Projectile ionic species:	$\text{Li}^{q+}(q=1-3)$
Target molecular species:	H_2
References:	[99], [117], [246], [252]
Projectile ionic species:	$\text{Be}^{q+}(q=1-4)$
Target molecular species:	H_2
References:	[139], [237], [267], [294]
Projectile ionic species:	$\text{B}^{q+}(q=1-5)$
Target molecular species:	H_2
References:	[100], [101], [103], [139], [267]
Projectile ionic species:	$\text{C}^{q+}(q=1-6)$
Target molecular species:	H_2, D_2
References:	[89], [93], [94], [95], [97], [100], [101], [105], [108], [109], [110], [113], [114], [115], [116], [118], [122], [124], [126], [128], [129], [135], [137], [138], [140], [143], [154], [157], [158], [161], [162], [175], [176], [178], [179], [180], [190], [211], [212], [215], [216], [221], [229], [230], [232], [238], [246], [250], [253], [254], [255], [259], [260], [263], [264], [265], [277], [286], [297], [299], [300], [301]
Projectile ionic species:	$\text{N}^{q+}(q=1-7), \text{N}_2^{q+}(q=1,2)$
Target molecular species:	H_2, D_2
References:	[89], [94], [97], [100], [105], [108], [109], [111], [113], [124], [130], [141], [142], [145], [151], [152], [156], [157], [158], [161], [162], [166], [172], [176], [178], [179], [183], [186], [191], [193], [198], [199], [201], [206], [232], [235], [253], [277], [287], [289], [290], [291], [292], [299], [301]
Projectile ionic species:	$\text{O}^{q+}(q=1-8)$
Target molecular species:	H_2, D_2
References:	[85], [86], [89], [92], [94], [97], [100], [104], [105], [108], [109], [110], [113], [124], [126], [127], [130], [135], [138], [149], [150], [157], [158], [159], [161], [162], [176], [178], [179], [180], [183], [192], [197], [204], [208], [209], [211], [212], [216], [221], [225], [226], [232], [233], [235], [239], [243], [246], [247], [251], [260], [266], [268], [276], [277], [282], [283], [288], [295], [299], [301], [302]
Projectile ionic species:	$\text{F}^{q+}(q=1,6-9)$
Target molecular species:	H_2
References:	[82], [87], [161], [162], [200], [204], [219], [222], [223], [227], [240], [241], [248], [251]
Projectile ionic species:	$\text{Ne}^{q+}(q=1-10)$
Target molecular species:	H_2, D_2
References:	[91], [106], [108], [111], [113], [120], [132], [134], [135], [147], [149], [153], [161], [162], [165], [168], [170], [178], [179], [183], [203], [210], [242], [301]

Table 13: (continued.)

Projectile ionic species:	$H^+, H_2^+, D_2^+, H_3^+, D_3^+$
Target molecular species:	N_2, O_2
References:	[80], [88], [107], [136], [148], [174], [185], [202], [228], [274], [280], [287]
Projectile ionic species:	$He^{q+}(q=1,2)$
Target molecular species:	N_2, O_2
References:	[77], [78], [81], [83], [84], [119], [131], [133], [135], [146], [163], [164], [167], [187], [189], [207], [228], [234], [236], [249], [258], [269], [275], [296]
Projectile ionic species:	Li^+
Target molecular species:	N_2
References:	[80]
Projectile ionic species:	$B^{q+}(q=1-4)$
Target molecular species:	N_2, O_2
References:	[133], [272], [294]
Projectile ionic species:	$C^{q+}(q=1-6)$
Target molecular species:	N_2, O_2
References:	[93], [94], [109], [124], [135], [143], [190], [264], [265]
Projectile ionic species:	$N^{q+}(q=1-4,6), N_2^{q+}(q=1,2)$
Target molecular species:	N_2, O_2
References:	[94], [109], [123], [124], [145], [181], [186], [195], [270], [271], [290], [291]
Projectile ionic species:	$O^{q+}(q=1-3,8), O_2^+$
Target molecular species:	N_2, O_2
References:	[85], [86], [92], [94], [109], [112], [124], [135], [159], [197], [214], [224], [281], [283], [293]
Projectile ionic species:	F^+
Target molecular species:	N_2
References:	[82]
Projectile ionic species:	$Ne^{q+}(q=1-10)$
Target molecular species:	N_2, O_2
References:	[81], [120], [133], [135], [147], [217], [303]

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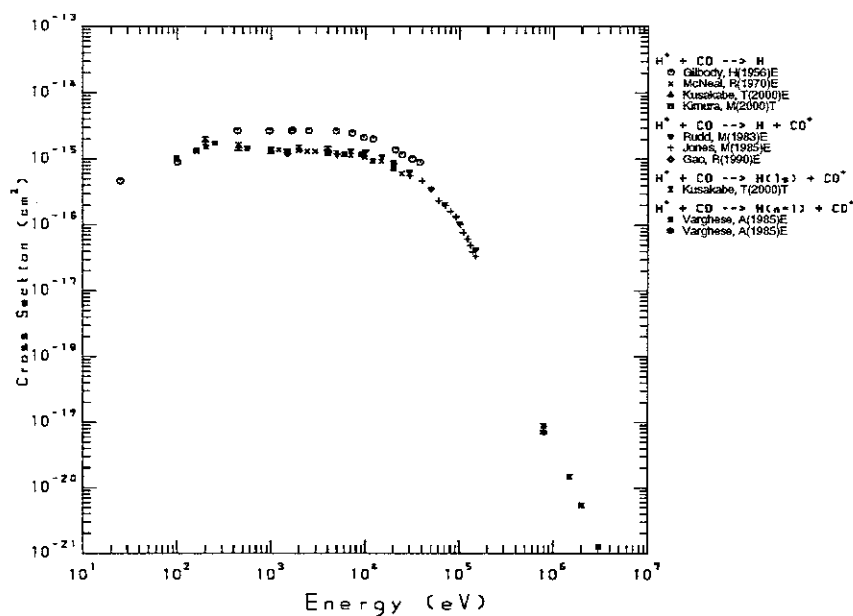


Figure 19: Charge transfer cross section of $\text{H}^+ + \text{CO}$ collision.

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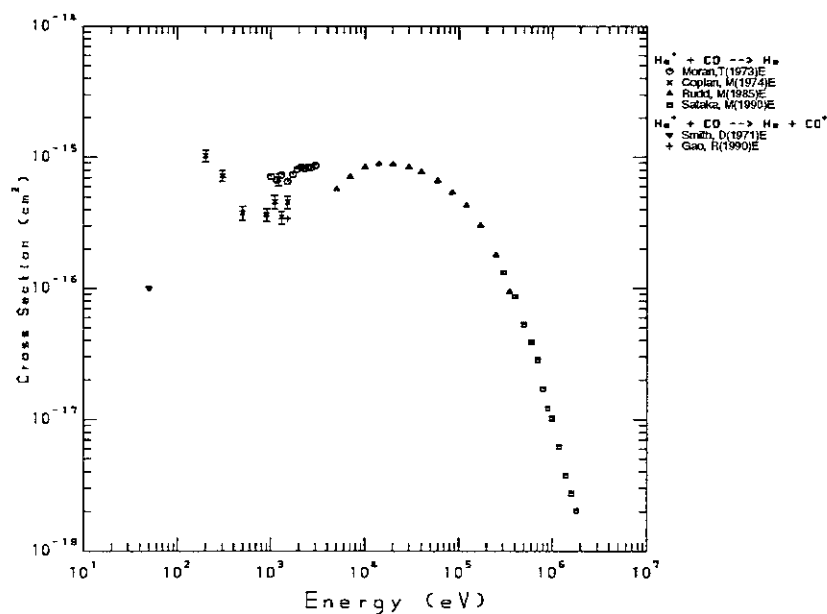
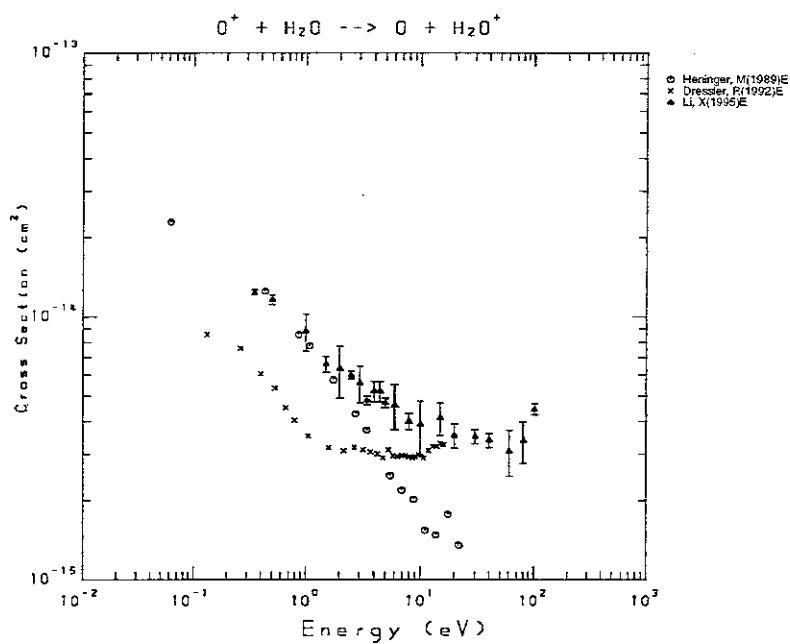


Figure 20: Charge transfer cross section of $\text{He}^+ + \text{CO}$ collision.

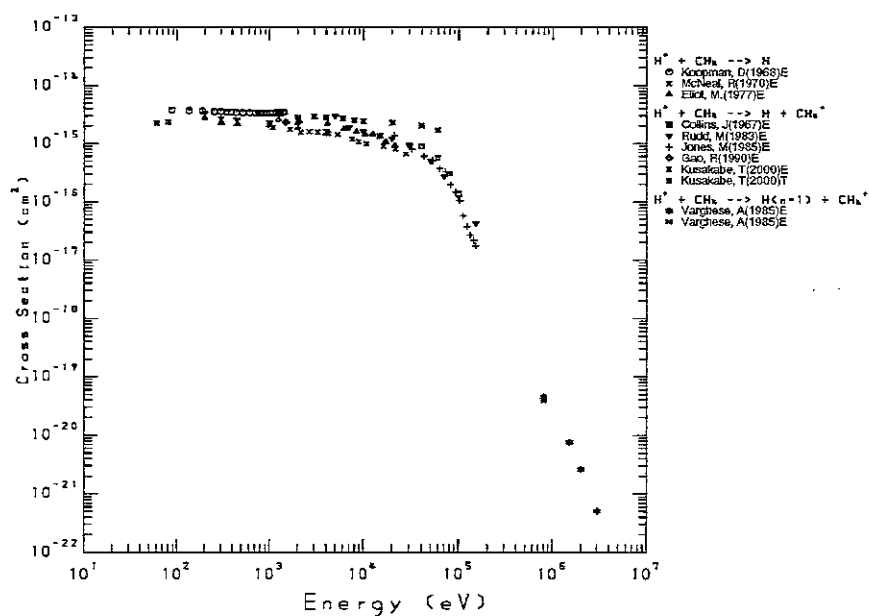
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Figure 21: Charge transfer cross section of $O^+ + H_2O$ collision.

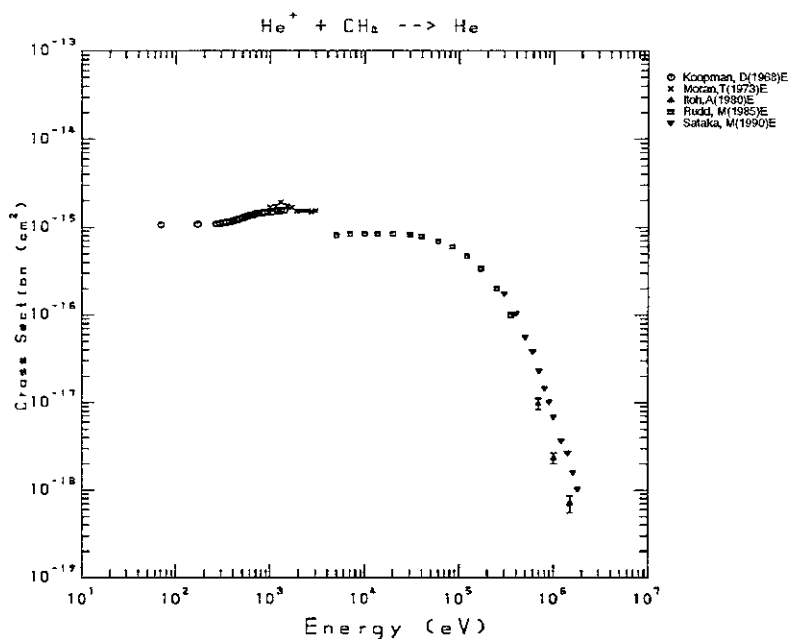
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Figure 22: Charge transfer cross section of $H^+ + CH_4$ collision.

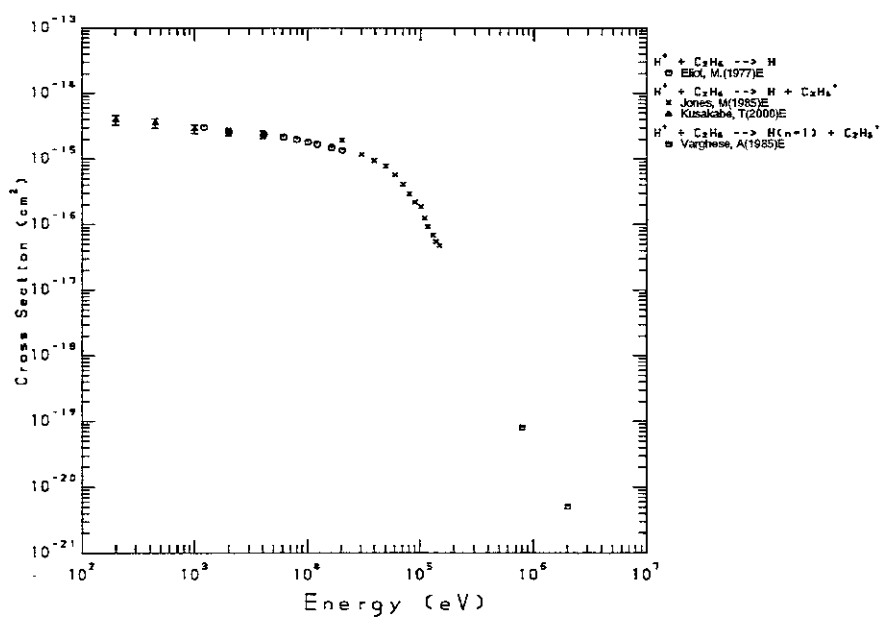
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Figure 23: Charge transfer cross section of $\text{He}^+ + \text{CH}_4$ collision.

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Figure 24: Charge transfer cross section of $\text{H}^+ + \text{C}_2\text{H}_6$ collision.

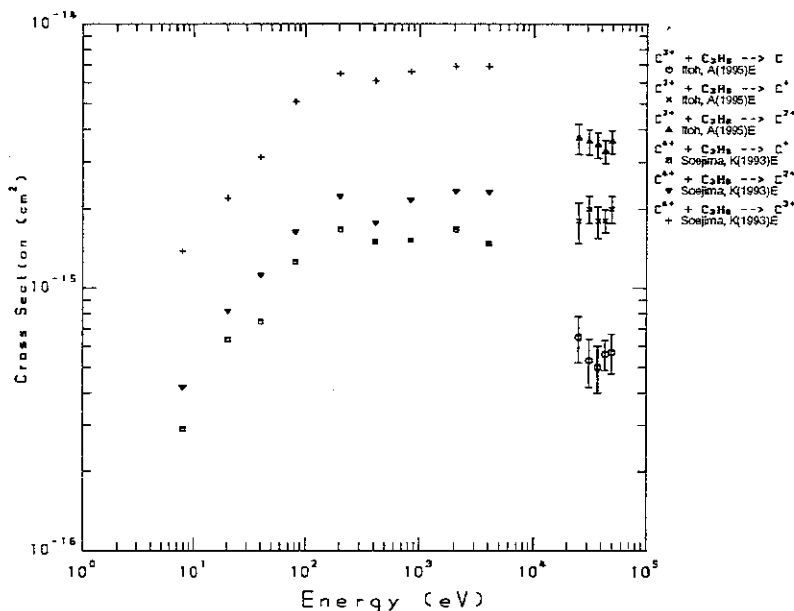


Figure 25: Charge transfer cross section of $C^{q+} + C_3H_8$ collision.

3.3 Fragmented Species from Molecular Targets

Fragmentation or dissociation of molecule is one of the most fundamental processes among chemical reactions. Most of molecular ions (positively, or negatively charged) are often unstable, and after the short life-time, they are likely to dissociate. Hence, dissociation processes via charge transfer of ion-molecule collisions are especially important in the plasma of ionosphere and nuclear fusion, because the corresponding cross sections are very large (in size). There has been very scarce, however, of quantitative studies on dissociative ion-molecule collisions in intermediate energy from 1 eV to 100 keV. In this subsection, cross sections, branching ratios of ion production, and the kinetic energy distributions (KERD) of fragment ions released are compiled and analyzed.

Papers on the dissociative charge transfer of ion-molecule collisions that were published in the period from 1990 to 2000 were researched. Twelve papers on the studies of cross sections and six papers on the studies of branching ratios of ion production, and KERDs of fragment ions were found in four journals (Physical Review A, Physical Review Letters, The Journal of Chemical Physics, and Journal of Physics B). Incident ions in the present research were limited to H^+ , C^{q+} , N^{q+} , O^{q+} , and rare gas ions. Target molecules were H_2 , N_2 , O_2 , CO , CO_2 , H_2O , and the simple hydrocarbon molecules. Collision energy is in the range from 1 eV to 100 keV. Charge transfer processes are believed to be dominant in this energy range over ionization and elastic channels. Cross section measurements were very scarce because most studies on dissociative ion-molecule collisions were carried out by using the mass spectrometry or analyses of fragmentation dynamics. Therefore physical quantities, for example the branching ratios for dissociation and the KERD of fragment ions, were studied through the cross section data. Many studies on reaction rate coefficients in the collision energy less than 1 eV are excluded. Dissociation processes via direct ionization by fast ion impact in the energy range larger than 100 keV are also excluded though many studies in collisions between highly charged ions (HCIs) and molecules conform to this case. Cross section measurements of dissociative charge exchange in collisions between highly charged ions and molecules are very few because total charge exchange cross sections are measured by the beam attenuation method in many cases. Rare gas ions are frequently used in the cross section measurements due in part to that these rare gases are easy to handle. The number of optical emission cross-section measurements is less than

that of ion production cross section measurements because of their weak signals. There are no theoretical investigations, to the author's knowledge, on the dissociative charge transfer between ion and molecules except for H₂, D₂, and HD. Each cross section data is necessary to be checked by other experimental and theoretical studies.

The KERDs of fragment ions were investigated in HCl-molecule collisions in many cases to verify the Coulomb explosion mechanism. It is difficult to convert the branching ratio into the cross-section because the intensity ratio among fragment ions was not measured in many cases.

Table 14: Reference for molecular fragmentation via charge transfer

Projectile ionic species:	H ⁺ , D ⁺ , He ^{q+} (q = 1, 2) , C ^{q+} (q = 1-6), N ^{q+} (q = 1-7), O ^{q+} (q = 1-8), Ne ^{q+} (q = 1-10)
Target atomic species:	H ₂ , CO, CO ₂ , O ₂ , NO, NO ₂ , H ₂ O, C _n H _m (hydrocarbons)
Energy region:	1 eV - a few hundred keV
References:	[304] - [326]

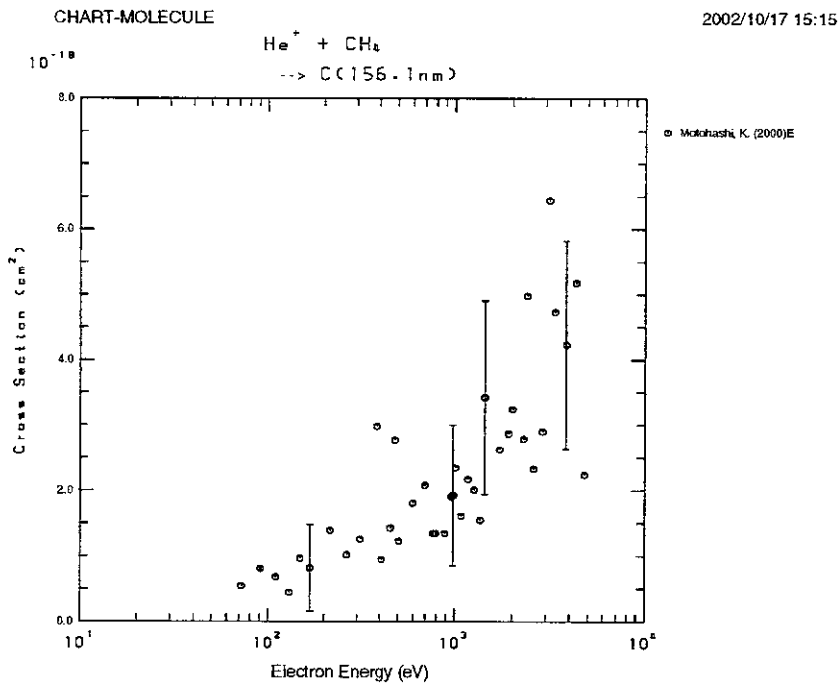


Figure 26: Emission cross section of carbon λ 156.1nm spectral line produced in He⁺ + CH₄ collision. This graph is from new database for molecules (CMOL, i.e. Chart-MOLecule) which is now in preparation.

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A Manual for the AMDIS and CHART databases at NIFS

A.1 Introduction

The National Institute for Fusion Science (NIFS) continuously develops an Atomic and Molecular Numerical Database System in the following 4 categories:

AMDIS¹: a database of cross sections for ionization, excitation, recombination, and dissociation of atoms, ions, and molecules by electron impact. Rate coefficients for recombination are also included;

CHART²: a database of cross sections for charge transfer and ionization of atoms, ions, and molecules by ion collisions;

SPUTY³: a database of sputtering yields for monatomic solids by ions; and

BACKS⁴: a database of light ions particle- and energy-backscattering coefficients from solids as functions of energy and angle.

These databases include numerical data along with the bibliographic information. Numerical data can be displayed in two modes, either as a numerical table or a graph. Users can specify the plot regions of the graph. The output figures can be downloaded as a PDF file or a Postscript file for printing.

Furthermore, we have recently been building two new databases for molecular collisions, “**AMOL**” (for electron collisions with AMDIS-type-molecules) and “**CMOL**” (for heavy particle collisions with CHART-type-molecules). The AMOL and CMOL databases will include all collisional processes for molecules, such as dissociative attachment and dissociative ionization. The numerical data covered will be the cross sections and rate coefficients, and also some additional information, such as the branching ratios of dissociation. We will start collecting data for hydrogen molecule, hydrocarbons and other molecules important for plasma physics.

These databases are available on the internet at URL=<http://dbshino.nifs.ac.jp/>. They are free of charge for the research purpose of registered users. The registration form can be found at the same URL address.

Bibliographic databases are also available via <http://dbshino.nifs.ac.jp/>. They can be used independently or in a connection with the numerical database, both being cross-linked. We have 3 bibliographic databases: two of them are built on the data extracted from INSPEC for fusion sciences and plasma physics, “**FUSION**” and for atomic and molecular physics “**AM**”, and one contains the bibliography for atomic collisions compiled by Oak Ridge National Laboratory, USA, “**ORNL**”.

In the following, we briefly describe how to use the numerical databases AMDIS and CHART.

A.2 AMDIS

The AMDIS database consists of 4 groups: “**IONIZATION**” for ionization cross sections by electron impact, “**EXCITATION**” for excitation cross sections by electron impact, “**DISSOCIATION**” for dissociation cross sections of molecules by electron impact, and “**RECOMBINATION**” for recombination cross sections and rate coefficients by electron impact. Here we describe how to retrieve data from this database.

A.2.1 IONIZATION

(a) Retrieving data

In order to retrieve the data, users need to specify at least one item in the input fields. Filling out all the input fields is not required. Figure A1 shows the data retrieval page.

The main input fields and examples of input values are shown in Table A1.

To specify an author including the initial of the first name, you need to use brackets { } such as “{Einstein, A}”. If you want to search for two author names using the logical ‘AND’, input “A & B”, and if you want to search for two authors names with logical ‘OR’, input “A | B”. These rules of using { }, &, | are valid for

¹originally Atomic and Molecular Data Interactive System

²CHARGE Transfer

³SPUTtering Yields

⁴BACK Scattering

AMDIS IONIZATION
[Help]

Element*

Initial ionic state:

Number of electrons (if you want to search for isoelectronic sequence.)

Final ionic state:

☐ Theoretical
 ☐ Experimental
 ☐ Evaluated

Author* :

Year of Publication : From : To : (YYYY)

Additional conditions for search:

[Type Table] [Journal Table]

↓	↓		↓	↓	↓
↓	↓	Record number	↓	↓	↓
↓	↓	Author(s)*	↓	↓	↓
↓	↓	First Author*	↓	↓	↓
↓	↓	Element*	↓	↓	↓
↓	↓	Journal Name	↓	↓	↓
↓	↓	Journal Name Abbreviated	↓	↓	↓
↓	↓	Title*	↓	↓	↓
↓	↓	Reference number	↓	↓	↓
↓	↓	Type of theory or experiment	↓	↓	↓
↓	↓	Initial configuration	↓	↓	↓
↓	↓	Final configuration	↓	↓	↓
↓	↓	Type of TOF, abbreviated	↓	↓	↓

Transition energy (eV) From : To :

Minimum incident energy From : To :

Maximum incident energy From : To :

SORT KEY

For items marked with *, put a word as an input string without using %, which is faster for getting results. Please do not bracket string with "%" character. For more details, see the help page.

Figure A1: Data retrieval in AMDIS-IONIZATION (page snapshot).

the input fields marked with ‘*’. Also, the items marked with “*” (Element, Author etc.) do not distinguish between the lower case and upper case letters, but all the other items do.

You can select theoretical, experimental, or evaluated data. If no selection is specified, all kinds of data are retrieved.

As mentioned above, when one input field is filled at least, the database can retrieve data. For example, if you fill only “C” in the Element field, the database retrieves cross section data for all ionic stages of carbon. If two or more fields are filled, all are combined using “AND” as the retrieving condition.

There are other additional items summarized in Table A2 which can be specified. These items can be combined using “AND” or “OR”, as you set.

After filling in the desired input field, please click “**Search Data**” button to start the data retrieval. If the number of data hits exceeds 300 records, the output is truncated, and only the first 300 records are shown.

Table A1: Main input fields and examples of input values for retrieving data in AMDIS-IONIZATION

Field name	Example of input values	Comments
Element*	“H” or “He”	Chemical Symbol.
Initial ionic state	“1” or “10” or “-1”	Number.
Number of electrons	“2”	For isoelectronic sequences. Number.
Final ionic state	“1” or “-1”	Number
Author*	“Bohr” ”{Einstein, A}” “Bohr & Einstein” “Bohr Einstein”	Use brackets when including the first name initial. For Bohr AND Einstein. For Bohr OR Einstein.
Year of publication	“From 1990 To 2000” “From 1992 To 1992”	For one year only.

Table A2: Additional input fields and examples of input values for retrieving data in AMDIS-IONIZATION

Field name	Example of input values	Comments
Record number	“003221”	Number of the record in the database.
Author(s)*	“Spitzer”	The same rules as described above.
First author*	“Zhang”	
Element*	“Fe”	Chemical symbol.
Journal name	“{Phys. Rev. A}”	Use brackets when using the period.
Journal name abbreviated	“PRA”	Refer to Table A3 for journal name abbreviations.
Title*	“Ionization%” “%ionization%”	You need to input the exact full title, or specify the first word as “Ionization%”. To specify a word included in the title. Use % at both ends.
Reference number	“1972T010”	Reference record number in the database.
Type in theory or experiment	“Born”	Confer Table A4 for the list of methods.
Initial configuration	“1s2” “1s 2s”	= 1s ² = 1s2s
Final configuration	“2s 2p 3P1”	= 2s2p ³ P ₁
Type of T. or E., abbreviated	“B” for Bron	Confer Table A4 for the list of methods.
Transition energy	“From 5 to 15”	In the units of eV.
Minimum incident energy	“From 1 To 10”	Select the region of minimum energy (eV).
Maximum incident energy	“From 10 To 20”	Select the region of maximum energy (eV).

Retrieved data can be sorted in the ascending order for the specified sorting keys, which are Element (EL), First author (AU1), Publication year(DP), Initial ionic state (IST, INS), and Final ionic state (FIS).

Table A3: Journal names and abbreviations in AMDIS

Abbreviated Journal name	Journal Name
AA	Astron. & Astrophys.
AAS	Astron. Astrophys. Suppl. Ser.
ACP	Atomic Collision Processes, Proceedings of 3rd ICPEAC.
ACS	Atomic Col. Solids, Brighton
ADN	Atomic Data and Nuclear Tables
AFP	Arkiv For Physik
AIP111	AIP Conf. Proc. No.111
AJP	Aust. J. Phys.
AJR	Aust. J. Sci. Res. A
APJ	Astrophys. J.
APJS	Astrophys. J. Suppl.
APP	Appl. Phys.
APPA	Appl. Phys.
APPL	Appl. Phys. Lett.
APSS	Appl. Surf. Sci.
AM	Adv. Atom. Mol. Phys.
ANA	Ann. d'Astrophys.
ANP	Ann. de Phys.
AZA	A. Z. Angew. Phys.
BA	Bull. Am. Astr. Soc.
BAU	Bull. Acad. USSR. Phys. Ser.
BC	Bull. Astron. Inst. Czech
BN	Bull. Astr. Inst. Netherlands
BSCF	Bull. Soc. Chim. Fr.
BT	Butsuri
CEN	C. E. N. Report
CFADC	CFADC Data Collections and Codes (http://www-cfadc.phy.ornl.gov/data_and_codes/)
CJP	Can. J. Phys.
CMP	Comments At. Mol. Phys.
CP	Chem. Phys.
CPL	Chem. Phys. Lett.
CRAS	Compt. Rend. Acad. Sci.
CSAC	Case Studies in Atomic Collision Physics 2nd. E. W. McDaniel and M.R.C.McDowell (North-Holland) Chap.4
DAR	Douglas Adv. Res. Lab. Res. Communic.
EPJD	Eur. Phys. J. D
FPU	Fiz. Plazmy (USSR)
GMR	General Mills. Report
GRL	Geophys. Res. Lett.
HPAA	Helv. Phys. Acta. A
HT	High Temp.
IB	Ionic Bombardment
IBSLA	Ion Beam Surf. Layer Analysis, Karlsruhe
ICP10	10th ICPEAC, Abstracts of papers
ICP11	11th ICPEAC, Abstracts of papers
ICP4	4th ICPEAC, Abstracts of papers
ICP5	5th ICPEAC, Abstracts of papers

Table A3: (continued.)

Abbreviated Journal name	Journal Name
ICP6	6th ICPEAC, Abstracts of papers
ICP7	7th ICPEAC, Abstracts of papers
ICP8	8th ICPEAC, Abstracts of papers
ICP9	9th ICPEAC, Abstracts of papers
ICPIG9	IX Proc. Int. Conf. Phenom. Ioniz. Gases, Bucharest
IET	Instr. Exp. Tech.
IJP	Indian J. Phys.
INDC	INDC(NDS)
IPC28	Inst. Phys. Conf. Ser. No.28
IPG5	Ioniz. Phenom. in Gases, Munch, ed. by H. Maecker
IPG6	Ioniz. Phenom. Gases, Paris
IPJ	Max-Planck-Institut fuer Plasmaphysik Report IPP-JET
IPP	IPP
IPM	IPPJ-AM
IQ	Information quarterly No.6
ISIAT4	Proc. 4th Symposium Ion Sources and Ion Application Technology, Tokyo
JAERIM	JAERI-M
JACS	J. Amer. Chem. Soc.
JAP	J. Appl. Phys.
JCI	J. Chim. Phys.
JCP	J. Chem. Phys.
JEC	J. Electron. Control
JES	J. Electr. Spectros. and Rel. Pheno.
JETP	JETP USSR (Russian)
JGR	J. Geophys. Res.
JILA	JILA Report
JJPA	Jpn. J. Appl. Phys.
JNM	J. Nucl. Mater.
JMT	J. Appl. Mechan. Tech. Phys.
JNB	J. of Res. of the National Bureau of Standards
JO	J. Opt. So. Am.
JPB	J. Phys. B
JPD	J. Phys. D.
JPE	J. Phys. E
JPS	J. Phys. Soc. Jpn.
JQ	J. Quant. Spectrosc. & Radiat. Transfer
JS	J. Sci. Res. A
JVSJ	J. Vac. Soc. Japan
LAS	Los Alamos Scientific Laboratory Report
LJP	Le J. de Physique
MC	Mem. Coll. Sci. Kyoto Imperial Univ. A
MNR	Mon. Not. R. Astron. Soc.
MR	Mem. R. Astron. Soc.
MSR	Mem. Soc. R. Sci. Liege
MT	Measuring Technique
NASATR	NASA Tech. Report
NC	Nuovo Cimento
NCA	Nuovo Cimento A
NCB	Nuovo Cimento B
NF	Nucl. Fusion
NFS	Nucl. Fusion Suppl.

Table A3: (continued.)

Abbreviated Journal name	Journal Name
NIFS	NIFS-DATA
NIM	Nucl. Instrum. & Methods
NMIA	Nucl. Instrum. Methods Phys. Res. Sect. A
NMIB	Nucl. Instrum. Methods Phys. Res. Sect. B
NPIG	Nonequilib. Proc. in Part. Ioniz. Gases
NRL	NRL Memo. Rept.
NT	Nucl. Technol.
OIS	Opt. & Spectrosc.
OMS	Org. Mas. Sp.
OR	ORNL/TM
ORNL	ORNL
ORO	Oakridge Operation Office
OS	Opt. Spectry.
PA	Publ. Astron. Soc. Pac.
PASJ	Publ. Astron. Soc. Jpn.
PACPP	Pro. Symposium on Atomic Collision. Processes in Plasma (Culham Laboratory, Sept. 14-16, 1994)
PC	Private Communication
PCA	Physica B&C
PCS	Physica Scripta.
PF	Phys. Fluids
PHC	Physica
PI	Proc. Indian Natl. Sci. Acad. A
PL	Phys. Lett.
PLA	Phys. Lett. A
PMA	Philos. Mag. A
PPS	Proc. Phys. Soc.
PPSA	Proc. Phys. Soc. A
PR	Phys. Rev.
PRA	Phys. Rev. A
PRA	Phys. Rev. B
PREP	Physics Reports
PRL	Phys. Rev. Lett.
PRRS	Philips Res. Rep. Suppl.
PRSA	Proc. R. Soc. London A
PS	Planet. & Space Sci.
PSP	Proc. Symp. on Sputtering (Inst. fuer Allg. Phy., Techn. Univ. Vienna)
PSSA	Phys. Status Solidi A
PTP	Prog. Theor. Phys.
PTRS	Philos. Trans. R. Soc. London A
PWIJ	Proc. Int. Symp. Plasma Wall Interaction, Jülich (Pergamon, Oxford, 1977)
RE	Rad. Effects
REEP	Radio Eng. Electron Physics (USSR)
REL	Radiat. Eff. Lett.
RPA	Rev. Phys. Appl.
RMP	Rev. Mod. Phys.
RSI	Rev. Sci. Instrum.
SAA	Sov. Astron.-AJ
SFB	SFB 82-05-104
SFT	Symp. Fusion Tech.
SFT9	Proc. 9th Symp. Fusion Technology, Pergamon

Table A3: (continued.)

Abbreviated Journal name	Journal Name
SIA	Surface and Interface Analysis
SIP	Int. J. Mass Spectrometry and Ion Phys.
SIP2	Int. J. Mass Spectrom. Ion Processes
SNF	Supplement to the journal Nuclear Fusion
SP	Sol. Phys.
SPD	Sov. Phys.-Dokl.
SPJ	Sov. Phys.-JETP
SPJL	Sov. Phys.-JETP Lett.
SPTP	Sov. Phys.-Tech. Phys.
SPS	Sov. Phys.-Solid State
SS	Surface Sci.
TA	Tr. Inst. Fiz. Akad. Nauk Latv. SSR
TAA	The Airglow and the Aurorae, ed. By Armstrong and Dalgarno
TANS	Trans. AM. Nucl. Soc.
THS	Thesis
TSF	Thin Sol. Fi.
TVS7	Trans. 7th Natl. Vacuum Symposium, Pergamon
TVSW	Trans. Vac. Symp., Washington D.C.
UCRL	UCRL-14214
UF	Ukr. Fiz. Zh. (Russian)
VCSS	Vacc. Congr. & Solid Surf., Vienna
ZN	Z. Naturforsch. a
ZP	Z. Physik
ZPA	Z. Phys. A
ZPB	Z. Phys. B
ZPD	Z. Phys. D

Table A4: Method names and their abbreviations in AMDIS

Abbreviation for the method	Name (type) of the theoretical or experimental method
B	Born
BC	Crossed beam method
BEA	Binary encounter approximation
BM	Beam method
BO	Born Oppenheimer
BOH	Born-Ochkur
BT	Bethe
BU	Born uniform
BX	Born with exchange
CB I	Coulomb Born I
CB I X	Coulomb Born I with exchange
CB II	Coulomb Born II
CB X CI	Coulomb Born with exchange, conf. int.
CBB	Coulomb Born Bely
CBO I	Coulomb Born Oppenheimer I
CBO II	Coulomb Born Oppenheimer II
CBT I	Coulomb Bethe I
CBT II	Coulomb Bethe II
CC	Close coupling

Table A4: (continued.)

Abbreviation for the method	Name (type) of the theoretical or experimental method
CC NX	Close coupling without exchange
CC NX 2	Close coupling without exchange 2-levels
CC NX 5	Close coupling without exchange 5-levels
CC X	Close coupling with exchange
CC X 10	Close coupling with exchange 10-levels
CC X 14	Close coupling with exchange 14-levels
CC X 2	Close coupling with exchange 2-levels
CC X 3	Close coupling with exchange 3-levels
CC X 5	Close coupling with exchange 5-levels
CC X 6	Close coupling with exchange 6-levels
CC X 9	Close coupling with exchange 9-levels
CCC	Convergent close-coupling
CCO	Coupled channels with optical potential
CDW	Coulomb distorted wave
CDW I	Coulomb distorted wave I
CDW II	Coulomb distorted wave II
CG	Coulomb Glauber
CGOH	Coulomb Glauber Ochkur
CL	Classical
CM	Configuration mixing
CPCO	Coulomb projected Coulomb Oppenheimer
DRPD	Double Retarding Potential Difference
DW	Distorted wave
DW NX	Distorted wave without exchange
DW X	Distorted wave with exchange
DW X CI	Distorted wave with exchange, conf. int.
DW,CC	Distorted wave or Close coupling
DWB	Distorted wave Born
DWB X	Distorted wave Born with exchange
DWBO	Distorted wave Born Oppenheimer
DWCB	Distorted wave Coulomb Born
DWPO I	Distorted wave polarized orbital I
DWPO II	Distorted wave polarized orbital II
DWPO III	Distorted wave polarized orbital III
DWU	Distorted wave uniform
EBIT	Electron beam ion trap
ECIP	Exchange classical impact parameter
EM	Empirical
ER	Exact resonance
ER+DW	Exact resonance and distorted wave
ERM	Eleven-state R matrix
EV	Evaluation
FBA	First Born approximation
FOEC	First-order exchange Coulomb
FOMBT	First Order Many Body Theory
FRM	Five-state R matrix
G	Glauber
GCPB	Generalized Coulomb projected Born
GCPBO	Generalized Coulomb projected Born Oppenheimer
GM	Growth method
GREEN.F	Green function
IP	Impact parameter

Table A4: (continued.)

Abbreviation for the method	Name (type) of the theoretical or experimental method
LGT	Laser-generated target
MB	Merged beam
MBT	Many-Body theory
MCDF	Multiconfiguration Dira Fock
MCE	Multichannel Eikonal approximation
MCHF	Multiconfiguration Hartree Fock
MCHF DW	Hartree Fock and Distorted wave
MCDF	Multiconfiguration Dirac Fock
MCQDT	Multichannel quantum-defect theory
MG	Modified Glauber
MO	Modified Oppenheimer approximation
MOT	Magneto-optical trap
MVC	Matrix variational calculation
O	Others
OF	Orthogonalized function
OF X	Orthogonalized function with exchange
OH	Ochkur
P	Plasma
RCB	Relativistic Coulomb Born
RCBO	Relativistic Coulomb Born Oppenheimer
RDW	Relativistic distrtd-wave
RER-MAT	Relativistic R matrix
RM	R matrix
SC	Semi classical
SCB	Simplified Coulomb Born
SCB I	Simplified Coulomb Born I
SCB II	Simplified Coulomb Born II
SCON	Smoothly connected method
SE	Semi empirical
SG	Static gas
SOP	Second order potential
TE	Trapped electron
TI	Trapped ion
TOF	Time of flight
UDWPO II	Unitarized distorted wave polarized orbital II
VAR	Variational
VPS	Vainshtein, Presnyakov and Sobelman

(b) Displaying the data

Figure A2 shows an example of the data retrieval result. A list of processes for the retrieved data is shown first, such as $C + e \rightarrow C^+ + 2e$, from which you can select some processes to see the related numerical data and bibliographic information. The default is all data records.

The retrieved data on the bibliographic information can be seen when either “**Standard**” or “**Custom**” is selected. The available information includes the theoretical or experimental method and further details, as well as the journal name, volume and page numbers, paper title, and year of publication. Figure A3 shows an example of the “Standard” list. Users can select items to be shown in the “Custom” mode.

For the numerical data to be displayed, select the “**Numerical Data Tables or Graphs**” option. After selecting one of these three options, click the “display” button and proceed to the data displaying page.

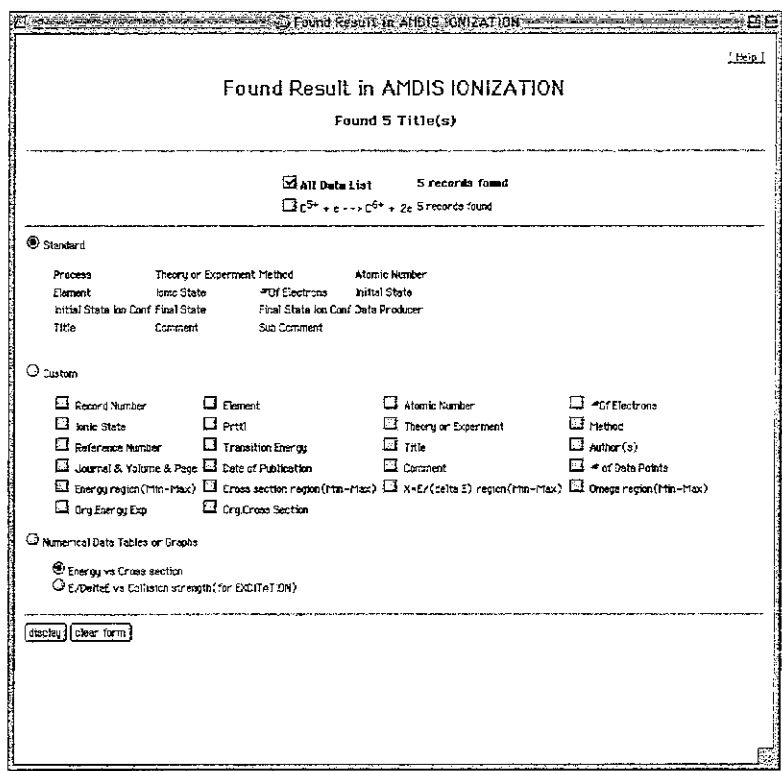


Figure A2: Example of data retrieval result in AMDIS-IONIZATION.

When selecting the “Numerical Data Tables and Graphs”, a list of all data (for each publication) is shown and you can select some of them to be displayed, as shown in Fig. A4. In the list the first author, journal name, volume number, year of publication, page number, and incident energy region (eV) are shown in a row. If you check the “Line Option” for a record, the data points in the output graph will be connected with a line.

The link at the “Reference” for each data record brings you to search the bibliographic databases. A new window is popped up after clicking at this link and the record numbers in AM and ORNL databases are shown. By clicking the particular record number you can view the data from the bibliographic databases.

For displaying the numerical data table, select “Data Display” and click the “display” button. The numerical data consist of the incident energy X (eV), cross section Y (cm^2), and the cross section errors ΔY (cm^2) in plus and minus directions. These are shown horizontally or vertically, as selected. When outputting the data vertically, as seen in Fig. A5, the cross section error ΔY is shown to be 0, even when no data for cross section errors are included in the database. When outputting the data horizontally, ΔY are shown only when the error data are included in the database. Information on the publication and number of data points (NDP) are listed as well.

For drawing the graphs, select “Graph Display” and click the “display” button. You may change the plotting conditions, see Table A5 for details. A graph (gif file) is displayed in your browser, and a PDF file and a Postscript file are also available for download, as shown in Fig. A6.

A.2.2 EXCITATION

(a) Retrieving data

In order to retrieve the data, users need to specify at least one item in input fields, similarly to IONIZATION. Figure A7 shows the retrieving page. The main input fields as listed in Table A6 are different from IONIZATION. For specifying the initial and final states, only the LS term expressions are currently accepted. See section A.2.1(a) for more details on the input fields. Also, the additional conditions to be specified for the data retrieval are almost identical as in IONIZATION (Table A2).

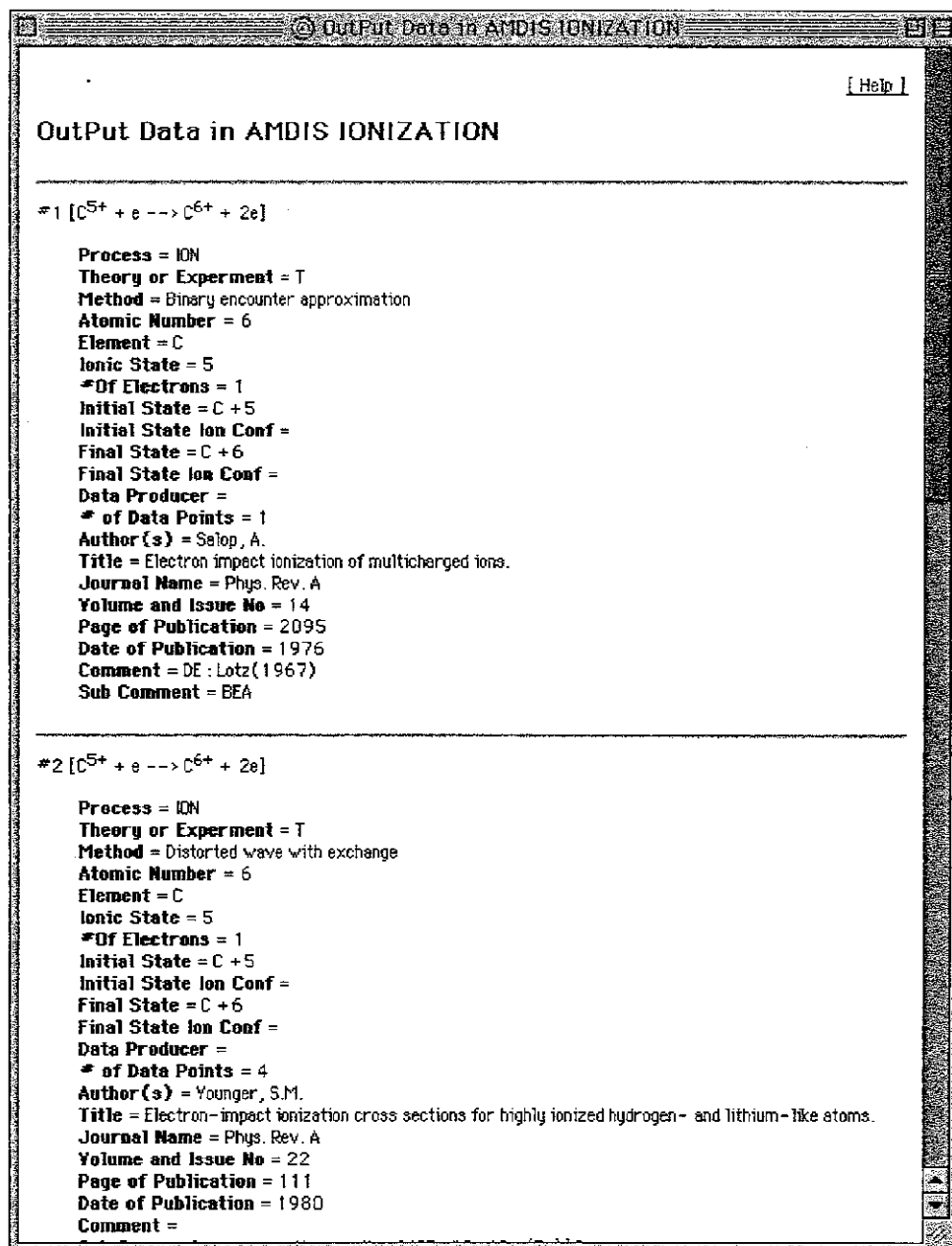


Figure A3: Example of the data retrieval output in the "Standard" mode in AMDIS-IONIZATION.

Table A5: Drawing conditions for graphs

Items	Choices	Comment
MODE		To set the plotting mode.
	AUTO	Automatic plot (default).
	FIX	Specify the plotting scale and the region.
	FREE	Specify the plotting scale, the region is automatically defined.
	FLEX	Specify the plotting scale and the region, but the plotting region might be altered automatically.
LOG		To set the plot scale.
	LIN	For a linear scale plot.
	LOG	For a logarithmic scale plot.
MESH		To set the ticks and their numerical labels.
	NONE	Only ticks.
	SCALE	Ticks and numbers (default).
	MESH	Ticks, numbers, and horizontal or vertical lines to draw the "mesh".
MAX		Specify the maximum value for the plotting region. Should be a real number, such as 1e-12, not like -12 even for logarithmic scale.
MIN		Specify the minimum value for the plotting region. Same as above.
AUTHOR		To select the position where all the symbols and references (author name and publication year, T (theoretical data) or E(experimental data)) are shown.
	frame-out	On the right, outside of the plotting box (default).
	upper-right	The upper-right corner in the box.
	upper-left	The upper-left corner in the box.
	lower-left	The lower-left corner in the box.
	lower-right	The lower-right corner in the box.
CURVE		To draw an empirical formula.
	0	No empirical curve (default).
	1	Draw Lotz's empirical formula for $Z < 31$ for ionization. No empirical curve is available for excitation, recombination, and dissociation. The charge transfer database (CHART) has empirical formulas.
FITTING CURVE		To draw the fitting curve.
	0	No fitting curve (default).
	1	Draw a polynomial fitting curve.
Y-ERROR PLOT		To plot the error bars for the cross section.
	On	Draw the error bars (default).
	Off	No error bars are displayed.

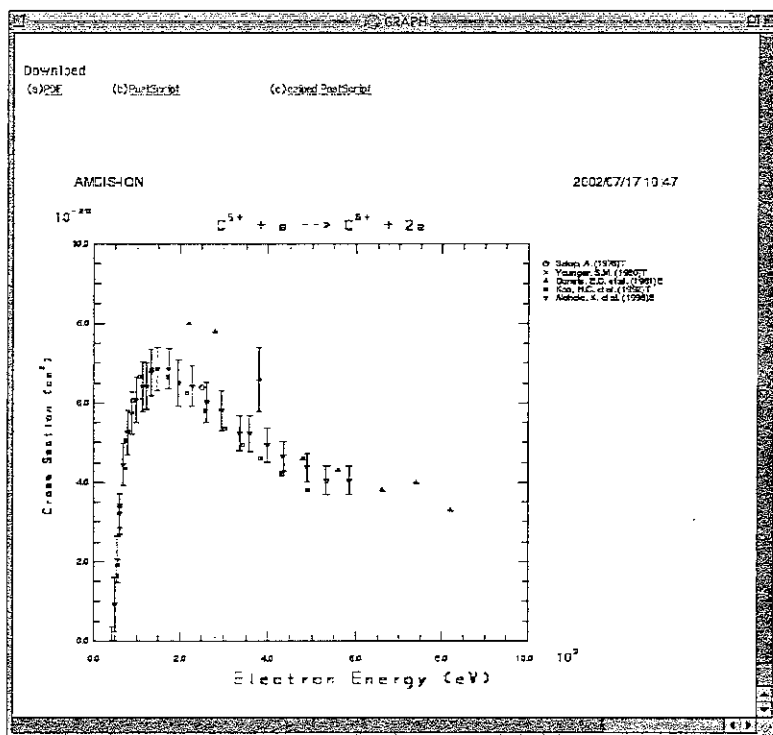


Figure A6: Example of the graphic output for the numerical data in AMDIS-IONIZATION.

(b) Displaying data

A list of processes for all data retrieved is shown at first, such as “ $\text{Li}^+\{1s2p\ ^3P \rightarrow 1s2p\ ^1P\}$ ”, from which you can select some in order to check the related numerical data. The default is all data. See section A.2.1(b) for the details on displaying the data.

In case of EXCITATION, users can select the unit for numerical data. The default is energy (eV) vs. cross section (cm^2). Another selection is $E/\Delta E$ vs. collision strength (which is often symbolized as Ω).

A.2.3 DISSOCIATION

(a) Retrieving data

Similarly to the previous databases, users need to specify at least one item in the input fields for the data retrieval. Figure A8 shows the data retrieval page. Main input fields and examples of input values are shown in Table A7.

Please be careful when inputting the molecular name in the ‘Element’ field. Without “%”, you do not obtain any results. We do not have much data in this sub-database. Data on the following molecules are included (as of July 16, 2002): CD, CD₂, CD₃, CD₄, CH, CH₂, CH₃, CH₃OH, CH₄, CO, CO₂, C₂, C₂H, C₂H₂, C₂H₄, C₂H₆, C₃H₈, H₂, H₂O, NO, N₂, O₂, SiH₄, and Si₂H₆ (202 records).

The new databases for molecule collision processes should also include dissociation. Therefore, the data from the present AMDIS-DISSOCIATION database will be used for the new database “AMOL” in the future.

See section A.2.1(a) for more details on the input fields for data retrieval. The additional conditions to be specified are almost the same as in IONIZATION (Table A2).

(b) Displaying data

A list of all processes for the retrieved data is shown at first, such as “ $\text{C}_2\text{H}_6 + e \rightarrow \text{CH}_2^+$ ”, from which you

AMDIS EXCITATION
[Help]

Search Data Form Clear

Atomic Number
 Element*
 Ionic State
 Number of electrons (if you want to search for isoelectronic sequence.)

Initial state: Configuration or or
 Multiplicity(2S+1)
 Orbital Ang Momentum(L) or or
 Statistical Weight(2J+1)
 Final state: Configuration or or
 Multiplicity(2S+1)
 Orbital Ang Momentum(L) or or
 Statistical Weight(2J+1)

☐ Theoretical ☐ Experimental ☐ Evaluated

Author* :
 Year of Publication : From : To : (YYYY)

Additional conditions for search:

[Type Table] [Journal Table]

		Author(s)*		
		First Author*		
		Journal Name		
		Journal Name abbreviated		
		Title*		
		Record number		
		Reference number		
		Type of theory or experiment		
		Element*		
		Type of T or f, abbreviated		

Transition energy (eV) From : To :
 Minimum incident energy From : To :
 Maximum incident energy From : To :

SORT KEY

For items marked with *, put a word as an input string without using %, which is faster for getting results. Please do not bracket string with "%" character. For more details, see the help page.

Figure A7: Data retrieval in AMDIS-EXCITATION (page snapshot)

Table A6: Main input fields and examples of input values for the data retrieval in AMDIS-EXCITATION

Field name	Example of input values	Comments
Atomic Number	"1" or "2"	Number.
Element*	"H" or "He"	Chemical symbol.
Ionic state	"1" or "10" or "-1"	Number.
Number of electrons	"2"	For isoelectronic sequences.
Initial state/Final state		
Configuration	"1s2"	= 1s ²
	"1s 2s"	= 1s2s (put space between orbitals).
	"2s2 2p"	= 2s ² 2p
Multiplicity (2S+1)	"1" or "2"	
Orbital Ang. Momentum (L)	"S" or "P"	
Statistical Weight (2J+1)	"1" or "2"	
Author*	"Bohr"	
	"{Einstein, A}"	Use brackets when including the first name initial.
	"Bohr & Einstein"	For Bohr AND Einstein.
	"Bohr Einstein"	For Bohr OR Einstein.
Year of publication	"From 1990 To 2000"	
	"From 1992 To 1992"	For one year only.

The screenshot shows the AMDIS DISSOCIATION web interface. At the top, there's a title bar and a navigation bar with a "Help" link. Below the title, there are buttons for "Search Data" and "Form Clear". The main form contains several input fields: "Initial State Element*", "Ionic:", "Final State Element*", and "Ionic:". There are also checkboxes for "Theoretical", "Experimental", and "Evaluated". Below these, there are fields for "Author*" and "Year of Publication: From: To: (YYYY)". A section titled "Additional conditions for search:" contains a list of criteria with dropdown menus and radio buttons. The criteria include: "Author(s)*", "First Author*", "Journal Name", "Journal Name abbreviated", "Title", "Issue Number", "Reference number", "Type of theory or experiment", "Element*", and "Type of transition, abbreviated". At the bottom, there are fields for "Transition energy (eV) From: To:", "Minimum incident energy From: To:", and "Maximum incident energy From: To:". A "SORT KEY" section has three dropdown menus. A footer note states: "For items marked with *, put a word as an input string without using %, which is faster for getting results. Please do not bracket string with '*' character. For more details, see the help page."

Figure A8: Data retrieval in AMDIS-DISSOCIATION (page snapshot)

Table A7: Main input fields and examples of input values for the data retrieval in AMDIS-DISSOCIATION

Field name	Example of input values	Comments
Initial State/Final State		
Element*	"H2%" or "C2H6%"	Put "%" after the molecular name (or chemical symbol) every time, because this field has values such as "H2 +1" for H_2^{+1} inside the database. You may instead specify a molecule with its ionic state by using the 'ionic' field.
ionic	"1"	Number. Note that in case of "0" nothing goes in this field.
Author*	"Bohr" "{Einstein, A}" "Bohr & Einstein" "Bohr Einstein"	Use brackets when including the first name initial. For Bohr AND Einstein. For Bohr OR Einstein.
Year of publication	"From 1990 To 2000" "From 1992 To 1992"	For one year only.

can select some in order to check the related numerical data. The default is all data. See section A.2.1(b) for the details on displaying data.

A.2.4 RECOMBINATION

(a) Retrieving data

In case of RECOMBINATION, this database contains numerical data of recombination cross sections and rate coefficients, for which the electron distribution is either Maxwellian or non Maxwellian. Users need to choose the data type from the selection list: 'Cross section', 'Rate coefficients (all)', 'Rate coefficients (Maxwellian)', or 'Rate coefficients (Non-Maxwellian)'. Most of the data in the database now are rate coefficients.

There are three processes for recombination: radiative recombination (RR), dielectronic recombination (DR), and three body recombination (TBR). You may select some of them. If there is no selection, all kinds of the recombination processes are searched for. Some data include a combination of these processes; such data are stored as "RR+DR", for example, in the database. These are the main points of difference from other AMDIS databases. Other issues are similar to IONIZATION. Also, the additional conditions to be specified for the data retrieval are almost the same as in IONIZATION.

Table A8: Main input fields and examples of input values for the data retrieval in AMDIS-RECOMBINATION

Field name	Example of input values	Comments
Element*	"H" or "He"	Chemical symbol.
Initial ionic state	"1" or "10" or "-1"	Number.
Number of electron	"2"	For isoelectronic sequences. Number.
Final ionic state	"0" or "1"	Number.
Author*	"Bohr" "{Einstein, A}" "Bohr & Einstein" "Bohr Einstein"	Use brackets when including the first name initial. For Bohr AND Einstein. For Bohr OR Einstein.
Year of publication	"From 1990 To 2000" "From 1992 To 1992"	For one year only.

(b) Displaying data

A list of processes for the data retrieved is shown at first, such as " $C^+(2s2p^2\ ^4P) \rightarrow C(2s^22p3d\ ^3E)$ (DR: RC-M)", or " $O^{5+}(1s^22s\ ^2P) \rightarrow O^{4+}$ (DR: RC-NM)" or " $O^{5+} \rightarrow O^{4+}$ (RR+DR: RC-M)". DR, RR, TBR or RR+DR on the right-hand-side indicate the various kinds of recombination processes, RC or RC-M means the rate coefficients in Maxwellian electron distribution, while RC-NM means the rate coefficients in a non Maxwellian electron distribution. CS means the cross section.

Users can select some processes for looking up the bibliographic information and numerical data. The default is all data. See section A.2.1(b) for details on displaying the data, since almost all items are the same as in IONIZATION. Some data have fitting formulas and fitting coefficients as bibliographic information.

Found Result in AMDIS RECOMBINATION

Found 10 Title(s)

☒ **All Data List** **10 records found**

- ☐ $O^{5+}(1s^22s\ ^2S) \rightarrow O^{4+}$ (DR: RC-NM) 2 records found
- ☐ $O^{5+}(2p\ ^2P_{1/2}) \rightarrow O^{4+}$ (DR: RC) 1 records found
- ☐ $O^{5+}(2p\ ^2P_{3/2}) \rightarrow O^{4+}$ (DR: RC) 1 records found
- ☐ $O^{5+}(2s\ ^2S_{1/2}) \rightarrow O^{4+}$ (DR: RC) 2 records found
- ☐ $O^{5+} \rightarrow O^{4+}$ (DR: RC-M) 1 records found
- ☐ $O^{5+} \rightarrow O^{4+}$ (RR+DR: RC-M) 3 records found

☒ **Standard**

Record Number	Process	Theory or Experiment Method
Atomic Number	Element	Ionic State # of Electrons
Y Axis Unit Type	Initial Ionic State	Initial Configuration Final Ionic State
Final Configuration	Fitting Equation	Fitting Parameters Data Producer
# of Data Points	Reference Number	Author(s) Title
Journal Name	Volume and Issue No	Page of Publication Date of Publication
Comment	Sub Comment	Graph No. AM Record No.
DRNL Record No.		

☐ **Custom**

☐ Record Number	☐ Prt1	☐ Process	☐ Element
☐ Atomic Number	☐ # of Electrons	☐ Y Axis Unit Type	☐ X Axis Original Unit
☐ Ionic State	☐ Initial Ionic State	☐ Initial Configuration	☐ Final Ionic State
☐ Final Configuration	☐ Theory or Experiment	☐ Method	☐ Fitting Equation
☐ Fitting Parameters	☐ Data Producer	☐ # of Data Points	☐ Reference Number
☐ Transition Energy	☐ Energy Region(Min-Max)	☐ Title	☐ Author(s)
☐ Journal & Volume & Page	☐ Date of Publication	☐ Comment	☐ Sub Comment
☐ DRNL Record No.	☐ AM Record No.	☐ Graph No.	

☒ **Numerical Data Tables or Graphs**

X Axis Data Type: ☒ eV ☐ K

Figure A10: Data retrieval in AMDIS-RECOMBINATION (page snapshot)

A.3 CHART

(a) Retrieving data

CHART is the database for ion - atom/molecule collision cross sections. Charge transfer (CT) and ionization (ION) processes are included. Figure A11 shows the page image of data retrieval. In most cases 'Element A' is a projectile ion and 'Element B' is a target element which also includes some molecules such as H₂, D₂, CO, CO₂, H₂O, CH₄, C₂H₄, C₂H₆, C₃H₈, n - C₄H₁₀, C₃F₈, c - C₄F₁₀, NO, N₂, NH₃, etc.

Figure A11: Data retrieval in CHART (page snapshot)

Sign should be attached for the charge state such as "+1" and the rule for writing the excited states is different from AMDIS. Subscripts and superscripts are shown with (). As for the molecular chemical symbols, write "H₂O" for H₂O, similarly to the DISSOCIATION.

For additional conditions, some items are similar to AMDIS (cf. Table A2). The different items are listed in Table A10. These items can be combined with the logical "AND" or "OR", as you set.

(b) Displaying data

Table A9: Main input fields and examples of input values for the data retrieval in CHART

Field name	Example of input values	Comments
A / B		
Element (A / B)*	"H" or "He"	Chemical symbol.
Atomic number	"1" or "2"	Number.
Atomic mass	"1" or "4"	Number (integer).
Initial charge number	"+1" or "+10" or "-1"	Sign and number.
Final charge number	"+0" or "+9"	Sign and number.
Initial/Final excited state	"1s(2)"	= 1s ²
	"(2)P"	= ² P
	"1s(2)2s2p"	= 1s ² 2s2p
Author*	"Bohr"	
	"{Einstein, A}"	Use brackets when including the first name initial.
	"Bohr & Einstein"	For Bohr AND Einstein.
	"Bohr Einstein"	For Bohr OR Einstein.
Year of publication	"From 1990 To 2000"	
	"From 1992 To 1992"	For one year only.

Table A10: Additional input items and examples for the data retrieval in CHART (items common with AMDIS are excluded)

Field name	Example of input values	Comments
Element	"Ar / CH4"	Both A and B elements must be input.
A Element	"Ar" or "H"	Same as that one in the main field.
B Element	"CH4" or "Ne"	Same as that one in the main field.
Method	"BA"	= "Beam attenuation". Abbreviated name of methods listed in Table A11
Reference ID	"1972C010"	Reference record number in the database.
Reference ID(H)	"20"	Reference record number for the hydrogen target case in the database.
Reference ID(H2)	"20"	Reference record number for the hydrogen molecule target case in the database.
Process	"CT" or "ION"	Select charge transfer or ionization processes.

Table A11: Theoretical and experimental methods listed in CHART

Abbreviation	The method (theoretical or experimental)
CE	Charge equilibrium
BA	Beam attenuation
CD	Condensor
BC	Crossed beam
DT	Drift tube
GR	Group rate of fast beam
MO	Molecular orbital method
PS	Perturbed stationary state method
MOE	Molecular orbital expansion method
UDW	Unitarized distorted-wave method
CTMC	Classical trajectory Monte Carlo method
ODM	One-electron diatomic molecular method
AO	Atomic orbital method
SP	Super promotion model
PS	Photon spectroscopy method
GM	Growth method
PIS	Photoionization ion source
COIN	Coincidence
O	Others

Figure A12 shows an example of the data retrieval result. A list of processes for the retrieved data is shown first, such as $\text{C}^{6+} + \text{H} \rightarrow \text{C}^{5+}(2\text{p}) + \text{H}^+$, from which you can select some processes to see the related numerical data and bibliographic information. The default is all data records.

The retrieved data on the bibliographic information can be seen when either “**Standard**” or “**Custom**” is selected. The available information includes the theoretical or experimental method and further details, as well as the journal name, volume and page numbers, paper title, and year of publication. Figure A13 shows an example of the “Standard” list. Users can select items to be shown in the “Custom” mode.

For the numerical data to be displayed, select the “**Numerical Tables or Graphs**” option, and “**Data Display**” for data tables or “**Graph Display**” for drawing the graphs, and then click the “display” button. Figure A14 shows an example of “vertically written” numerical data. The incident energy X (eV) and cross section Y (cm^2) are shown. Numerical data for the cross section errors can be seen only when selecting “Y_Error_Data” in “Custom” mode. For drawing the graphs, you may change the plotting conditions, see Table A5 for details. A graph (gif file) is displayed in your browser, and a PDF file and a PostScript file are also available for download, as shown in Fig.A15.

Found Result in CHART

Found 5 Title(s)

☒ All Data List
5 records found

☐ $C^{6+} + H \rightarrow C^{5+} (2p) + H^+$
3 records found

☐ $C^{5+} + H(1s) \rightarrow C^{5+} (2p) + H^+$
2 records found

Standard

Id_Number	Record Number	Process	Elements_A
Atomic_No_A	Atomic_Mass_A	Initial_Charge_No_A	Initial_Excited_A
Final_Charge_No_A	Final_Excited_A	Elements_B	Atomic_No_B
Atomic_Mass_B	Initial_Charge_No_B	Initial_Excited_B	Final_Charge_No_B
Final_Excited_B	Theory_or_Experiment	Method	Title
Fig_No	Comment	Prttlf	Prttlr

Select Output Data

☐ Id_Number	☐ Record Number	☐ Process	☐ Elements
☐ Elements_A	☐ Atomic_No_A	☐ Atomic_Mass_A	☐ Initial_Charge_No_A
☐ Initial_Excited_A	☐ Final_Charge_No_A	☐ Final_Excited_A	☐ Elements_B
☐ Atomic_No_B	☐ Atomic_Mass_B	☐ Initial_Charge_No_B	☐ Initial_Excited_B
☐ Final_Charge_No_B	☐ Final_Excited_B	☐ Theory_or_Experiment	☐ Method
☐ No_Data_Points	☐ X_Axis_Data	☐ Y_Axis_Data	☐ Y_Error_Data
☐ Reference_Id	☐ Reference_Id_H	☐ Reference_Id_H2	☐ Author(s)
☐ Title	☐ Journal Name	☐ Volume	☐ Page
☐ Year	☐ Fig_No	☐ Figure_Title	☐ Comment
☐ Prtllf	☐ Prtllr	☐ Prtll	

Numerical Data Tables or Graphs

Data Display

☒ write horizontally
☐ write vertically

Graph Display

☒ Energy(eV) vs Cross section(cm^2)
☐ Energy(eV/bmu) vs Cross section(cm^2)

MODE	LOG	MESH	MAX	MIN
X-AXIS 0: AUTO	2: NONE	1: SCALE	0	0
Y-AXIS 0: AUTO	2: NONE	1: SCALE	0	0
AUTHOR: 0 frame-out	CURVE: 0			

There are theoretical/empirical curves available only for the target H, H₂, and He.

display
clear form

Figure A12: Example of data retrieval result in CHART.

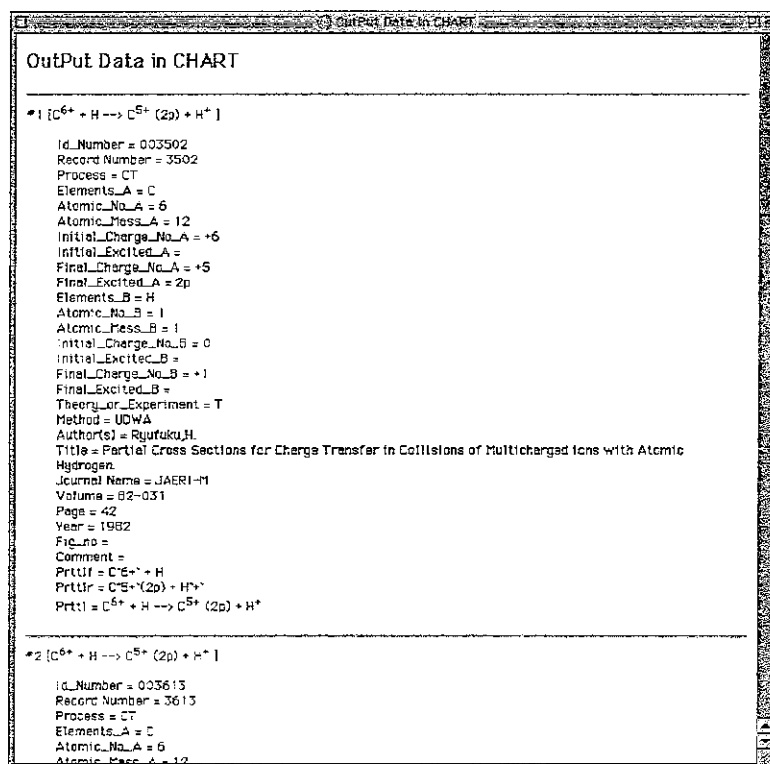


Figure A13: Example of data retrieval output in the “Standard” mode in CHART.

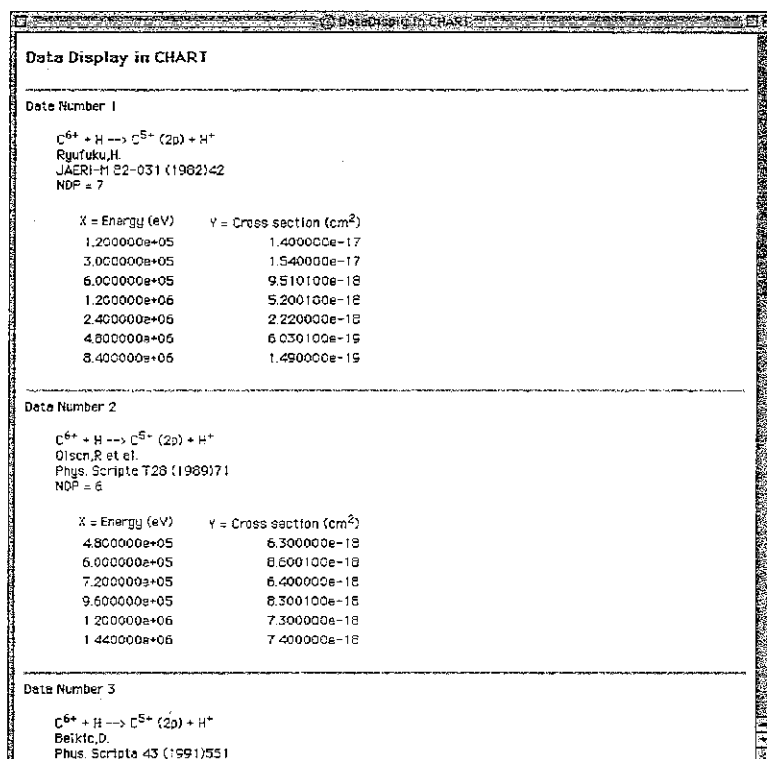


Figure A14: Example of a “vertically written” numerical table in CHART.

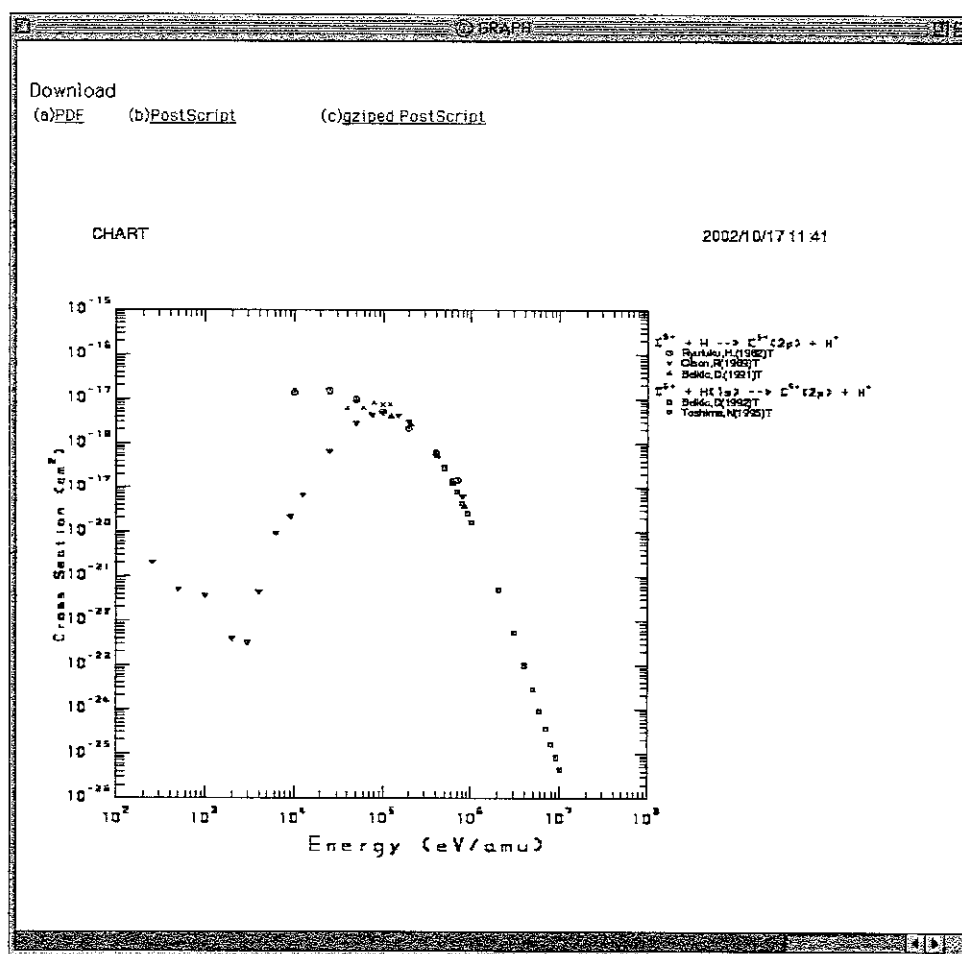


Figure A15: Example of the graphic output for the numerical data in CHART.

B. Bibliography on electron-impact excitation and ionization of atomic ions published in 2000

B.1 Experimental papers on electron-impact excitation and ionization of atomic ions published in 2000

00E1. A. Muller, H. Teng, G. Hofmann, R.A. Phaneuf and E. Salzborn
Phys. Rev. A **62**,062720 (2000)

Autoionizing resonances in electron-impact ionization of O^{5+} ions
[beam, Th-1000 eV, particularly near the threshold of K-shell ionization]
Ion $O\ VI$

00E2. S.J. Smith, J.B. Greenwood, A. Chutjian and S.S. Tayal
Astrophys. J. **541**,501 (2000)

Electron excitation cross sections for the $3s^2 3p^2\ ^3P - 3s 3p^3\ ^5S^o$ transition in S^{2+}
[merged beam, $3s^2 3p^2\ ^3P - 3s 3p^3\ ^5S^o$ 7-12 eV]
Exc $S\ III$

B.2 Theoretical papers on electron-impact excitation and ionization of atomic ions published in 2000

- 00T1. K.M. Aggarwal, N.C. Deb, F.P. Keenan and A.Z. Msezane
 J. Phys. B: At. Mol. Opt. Phys. **33**,L391 (2000)
 Collision strengths for transitions among the $3s^2$, $3s3p$ and $3p^2$ configurations of Fe XV
 [RM, transitions among $3s^2$, $3s3p$, $3p^2$, Th-160 Ryd]
 Exc Fe XV
- 00T2. N.R. Badnell and D.C. Griffin
 J. Phys. B: At. Mol. Opt. Phys. **33**,2955 (2000)
 Direct ionization of low-charge Li-like ions using a small pseudo-state basis
 [RM with pseudo-basis, Th-150 eV for Be, Th-300 eV for B, Th-450 eV for C]
 Ion Be II, B III, C IV
- 00T3. M.A. Bautista
 J. Phys. B: At. Mol. Opt. Phys. **33**,71 (2000)
 Electron-impact inner-shell excitation of Fe XVI
 [RM, $2p^63s - 2p^53\ell$ $3\ell'$ rate: 5×10^4 , 10^5 , 10^6 K]
 Exc Fe XVI
- 00T4. K.L. Bell and C.A. Ramsbottom
 Atomic Data Nucl. Data Tables **76**,176 (2000)
 Effective collision strengths for electron-impact excitation of S X
 [RM, FS transitions among $2s^22p^3$, $2s2p^4$, $2p^5$, $2s^22p^23s$, rate: $10^{4.6} - 10^{6.7}$ K]
 Exc S X
- 00T5. V.A. Bernshtam, Y.V. Ralchenko and Y. Maron
 J. Phys. B: At. Mol. Opt. Phys. **32**,5025 (2000)
 Empirical formula for cross section of direct electron-impact ionization of ions
 [empirical formula proposed and tested]
 Ion Ar III-VIII, Fe III, VI, VII, X, XII, XIV
- 00T6. K.A. Berrington, S. Nakazaki and P.H. Norrington
 Astron. Astrophys. Supp. **142**,313 (2000)
 Atomic data from the IRON Project XLI. Electron excitation rates among the $3d^2$ fine-structure levels of Ca-like Fe VII
 [RM, transitions among FS levels of $3d^2$, rate: $10^{4.3-6.0}$ K]
 Exc Fe VII
- 00T7. A.K. Bhatia and W. Eissner
 Atomic Data Nucl. Data Tables **76**,270 (2000)
 Atomic data and spectral line intensities for Fe VIII
 [DW, transitions among $3p^63d$, $3p^53d^2$, $3p^64s$, $3p^64p$, $3p^53d4s$ 10-70 Ryd]
 Exc Fe VIII
- 00T8. K. Butler and C.J. Zeippen
 Astron. Astrophys. Supp. **143**,483 (2000)
 Atomic data from the IRON Project XLII. Electron impact excitation of Fe XXI
 [RM, transitions among $2s^22p^2$, $2s2p^3$, $2p^4$, $2p3\ell$, rate]
 Exc Fe XXI
- 00T9. Z. Felfli, K.A. Berrington and A.Z. Msezane
 J. Phys. B: At. Mol. Opt. Phys. **33**,1263 (2000)
 Electron-impact ionization of Mg^+ near the 2p inner-shell edge
 [RM, 45-65 eV]

Ion Mg II

- 00T10. M.F. Gadi, A. Makhoute and M.H. Cherkani
Phys. Scr. **61**,437 (2000)
Electron-impact ionisation of Ne^{8+}
[1200-7100 eV]
Ion Ne IX
- 00T11. D.C. Griffin and N.R. Badnell
J. Phys. B: At. Mol. Opt. Phys. **33**,4389 (2000)
Electron-impact excitation of Ne^{4+}
[RM, transitions among $2s^2 2p^2$, $2s 2p^3$, $2p^4$, and $2s^2 2p^2 - 2s^2 2p^3$ ℓ , rate: $1 \times 10^4 - 1 \times 10^6$ K]
Exc Ne V
- 00T12. D.C. Griffin, N.R. Badnell and M.S. Pindzola
J. Phys. B: At. Mol. Opt. Phys. **33**,1013 (2000)
Electron-impact excitation of C^{3+} and O^{5+} : the effects of coupling to the target continuum states
[RM, transitions among $1s^2 \ell$, $3 \ell'$, $4 \ell''$ rate: $2.25 \times 10^4 - 3.6 \times 10^5$ K for C, $5 \times 10^4 - 8 \times 10^5$ K for O]
Exc C IV, O VI
- 00T13. D.C. Griffin, M.S. Pindzola and N.R. Badnell
Astron. Astrophys. Supp. **142**,317 (2000)
Electron-impact excitation of Fe^{7+}
[RM, $3p^6 3d - 3p^5 3d^2$, $3p^6 4f$ rate: $6.4 \times 10^4 - 3.2 \times 10^6$ K]
Exc Fe VIII
- 00T14. G.P. Gupta, N.C. Deb and A.Z. Msezane
Atomic Data Nucl. Data Tables **74**,257 (2000)
R-matrix calculation of electron impact excitation of fine-structure levels of Ne-like iron
[RM, $2p^6 - 2p^5 3 \ell$, 70-200 Ryd, rate: 250, 600, 1000 eV]
Exc Fe XVII
- 00T15. G.P. Gupta, N.C. Deb and A.Z. Msezane
Phys. Scr. **61**,175 (2000)
Electron impact excitation of fine-structure levels in neon-like Krypton (Kr XXVII) using R-matrix method
[RM, $2p^6 1S - 2p^5 3 \ell$ 150, 300, 500 Ryd, rate: 600, 1100, 2200 eV]
Exc Kr XXVII
- 00T16. E. Kimura, S. Nakazaki, K.A. Berrington and P.H. Norrington
J. Phys. B: At. Mol. Opt. Phys. **33**,3449 (2000)
Rate coefficients for electron impact excitation of helium-like ions within the Dirac R-matrix approach
[RM, $1s^2 - 1s 2 \ell$, $1s 3 \ell$ rate: $10^{6.0} - 10^{8.4}$ K]
Exc S XV, Ca XIX, Fe XXV
- 00T17. B.M. McLaughlin and K.L. Bell
J. Phys. B: At. Mol. Opt. Phys. **33**,597 (2000)
Electron collisional excitation of Ne III: ($1s^2 2s^2 2p^4$ $^3D_{2,1,0}$, 1D_2 , 1S_0) fine-structure transitions
[RM, FS transitions among $2s^2 2p^4 < 30$ Ryd, rate: $10^3 - 10^6$ K]
Exc Ne III
- 00T18. D.M. Mitnik, M.S. Pindzola and D.C. Griffin
Phys. Rev. A **62**,062711 (2000)
Influence of atomic radiative and collisional processes on the plasma modeling of Mg^{10+} at low

- electron densities
[RM, FS transitions among $1sn\ell$ $n=1-4$]
Exc Mg XI
- 00T19. M. Mohan, A. Hibbert, F. Keenan and P.G. Burke
Phys. Scr. **61**,71 (2000)
Collision strengths from ground levels of Ti XIII using relativistic-Breit-Pauli approximation
[RM, $2p^6\ 1S^e - 2p^53\ell$ 40-120 Ryd]
Exc Ti XIII
- 00T20. B. Nath and C. Sinha
Phys. Rev. A **62**,052713 (2000)
Triple differential cross sections for ionization of some heliumlike ions by electron impact
[TDCS, scaled]
Ion He-like
- 00T21. M.S. Pindzola, D.M. Mitnik, J. Colgan and D.C. Griffin
Phys. Rev. A **61**,052712 (2000)
Electron-impact ionization of Li^+
[RM, Th-500 eV]
Ion Li II
- 00T22. D. Porquet and J. Dubau
Astron. Astrophys. Supp. **143**,495 (2000)
X-ray photoionized plasma diagnostics with helium-like ions. Application to warm absorber-emitter in active galactic nuclei
[based on the calculation of Sampson et al., rate for $1s^2-1s2\ell$ for $Z=6,8,10,12,14$, $1s2\ell-1s2\ell'$ for $Z=8,10,12,14$]
Exc He-like
- 00T23. R. Rejoub and R.A. Phaneuf
Phys. Rev. A **61**,032706 (2000)
Electron-impact single ionization of multiply charged manganese ions
[beam, Th-4 keV]
Ion Mn VI-IX
- 00T24. M.P. Scott, H. Teng and P.G. Burke
J. Phys. B: At. Mol. Opt. Phys. **33**,L63 (2000)
Autoionizing states in electron-impact ionization of C^{3+}
[RM, AI 290-350 eV]
Ion C IV
- 00T25. S.J. Smith, J.B. Greenwood, A. Chutjian and S.S. Tayal
Astrophys. J. **541**,501 (2000)
Electron excitation cross sections for the $3s^23p^2\ 3P - 3s3p^3\ 5S^o$ transition in S^{2+}
[RM, $3s^23p^2\ 3P - 3s3p^3\ 5S^o$ 7-12 eV]
Exc S III
- 00T26. C.R. Stia, O.A. Fojon and R.D. Rivarola
J. Phys. B: At. Mol. Opt. Phys. **33**,1211 (2000)
Ionization of hydrogenic targets by electron impact
[TDCS, scaling law derived]
Ion H-like
- 00T27. P.J. Storey, H.E. Mason and P.R. Young
Astron. Astrophys. Supp. **141**,285 (2000)

Atomic data from the IRON Project XL. Electron impact excitation of the Fe XIV EUV transitions
 [RM, $3s^2 3p - 3s 3p^2, 3s^2 3d$ 10, 30 Ryd, rate: $10^{5.5-7.2}$ K]
 Exc Fe XIV

00T28. S.S. Tayal

Astrophys. J. **530**,1091 (2000)

Electron collision excitation of fine-structure levels in S IV

[RM, transitions among $3p, 3s 3p^2, 3d, 4s, 4p, 3p^4$ 0, 4, 6 Ryd, rate: $(1-40) \times 10^4$ K]

Exc S IV

00T29. S.S. Tayal

Astrophys. J. **544**,575 (2000)

Effective collision strengths of fine-structure transitions in Fe X, Fe XI, and Fe XIII

[RM, transitions among $3p^5 2p_{3/2}, 2p_{1/2}, 3s 3p^6 2s_{1/2}$ for Fe X; $3p^4 3p_{2,1,0} 1D_2, 1S_0$ for Fe XI;

$3p^2 3p_{2,1,0} 1D_2, 1S_0$ for Fe XIII rate: $(1-600) \times 10^4$ K]

Exc Fe X,XI,XIII

00T30. S.S. Tayal and L.M. Richardson

J. Phys. B: At. Mol. Opt. Phys. **33**,443 (2000)

Oscillator strengths and inelastic scattering of electrons from O II

[RM, $2s^2 2p^3 4S^o - 2D^o, 4P$ Th-40 eV, rate: $10^{3.6} - 10^{5.8}$ K]

Exc O II

00T31. H. Teng

J. Phys. B: At. Mol. Opt. Phys. **33**,L227 (2000)

Indirect processes in electron-impact ionization of Li^+

[RM for Al, 132-168 eV]

Ion Li II

00T32. H. Teng

J. Phys. B: At. Mol. Opt. Phys. **33**,L553 (2000)

Electron-impact ionization of Al^{2+} ions: a unified R-matrix calculation

[RM, 60-100 eV]

Ion Al III

00T33. H. Teng, P. Defrance, C. Chen and Y. Wang

J. Phys. B: At. Mol. Opt. Phys. **33**,463 (2000)

Electron-impact single ionization of Kr^{10+} and Kr^{11+} ions

[DW, < 3000 eV]

Ion Kr XI,XII

00T34. H.L. Zhang and D.H. Sampson

Phys. Rev. A **61**,022708 (2000)

Effective collision strengths for hyperfine-structure transitions with inclusion of resonance effects

[hyperfine transitions, rate: $(1-100) \times 10^6$ K]

Exc N VII, Fe XXIV

H-like (N=1)		
Exc	N VII	T34
Ion	T26	
He-like (N=2)		
Exc	T22	
	Mg XI	T18
	S XV	T16
	Ca XIX	T16
	Fe XXV	T16
Ion	T20	
	Li II	T21, T31
	Ne IX	T10
Li-like (N=3)		
Exc		
	C IV	T12
	O VI	T12
	Fe XXIV	T34
Ion		
	Be II	T2
	B III	T2
	C IV	T2, T24
	O VI	E1
C-like (N=6)		
Exc		
	Ne V	T11
	Fe XXI	T8
N-like (N=7)		
Exc		
	O II	T30
	S X	T4
O-like (N=8)		
Exc		
	Ne III	T17
Ne-like (N=10)		
Exc		
	Ti XIII	T19
	Fe XVII	T14
	Kr XXVII	T15
Na-like (N=11)		
Exc		
	Fe XVI	T3
Ion		
	Mg II	T9

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Ion	Mn VII	T23
Ca-like (N=20)		
Exc	Fe VII	T6
Ion	Mn VI	T23
	Fe VII	T5
Sc-like (N=21)		
Ion	Fe VI	T5
Cr-like (N=24)		
Ion	Fe III	T5
Mn-like (N=25)		
Ion	Kr XII	T33
Fe-like (N=26)		
Ion	Kr XI	T33

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A New Formula of the Energy Spectrum of Sputtered Atoms from a Target Material Bombarded with Light Ions at Normal Incidence; May 2001
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