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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

2nd (Final) IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

September 25-26, 2000, IAEA Headquarters
Vienna, Austria

SUMMARY REPORT

Prepared by: R.E.H. Clark

November 2001

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

The proceedings and conclusions of the 2nd Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies", held on September 25 and 26, 2000 at the IAEA Headquarters in Vienna, are briefly described. This report includes a summary of the presentations made by the meeting participants and a review of the accomplishments of the Co-ordinated Research Project (CRP). In addition, short summaries from the participants are included indicating the specific research completed in support of this CRP.

Reproduced by the IAEA in Austria
November, 2001

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1. Introduction

The 2nd and final Research Co-ordination Meeting (RCM) of the participants of the IAEA Co-ordinated Research Project (CRP) on "Charge Exchange Cross Section Data for Fusion Plasma Studies" was held on September 25-26, 2000, at the IAEA Headquarters in Vienna, Austria. The objectives of the meeting were:

a) to review the results of the work done within the individual CRP projects in the period between the 1st and 2nd RCM;

b) to summarise the overall accomplishments of the CRP over its entire duration;

c) to agree on a method of submitting final reports of work accomplished and their publication;

d) to agree on a plan for assessing and submitting cross section data generated from this CRP for inclusion in the IAEA database.

The meeting was attended by the principal scientific investigators of the individual CRP projects except for W. Fritsch and N. Toshima who were not able to attend. L. Errea attended in the place of A. Riera. The list of meeting participants is attached as Appendix 1.

2. Brief Meeting Proceedings

The meeting began with a welcoming address by Mr. D.D. Sood, Director of the Division of Physics and Chemistry. The Meeting Agenda was adopted without change (see Appendix 2). The meeting then continued with five sessions, the first four devoted to reports of the latest work from each individual project, and the fifth session devoted to formulating conclusions for the CRP and discussion of publication of final results and assessment and transmittal of cross section data for inclusion in the IAEA database.

The first session of the meeting was chaired by M. Kimura and included results presented by H.P. Winter, B. Zygelman, and J.P. Hansen.

The first speaker of the session, **HP. Winter** from the Institut für Allgemeine Physik in Austria, began with a summary of the different plasma regions in a Tokamak reactor and the types of data needed for understanding the plasma in each region. He presented a complete survey of the state of currently available charge exchange data accumulated over the past ten years. He then summarised the results of his recent measurements using the Low Energy Ion Beam Unit for Scattering Studies and Applications (LIBUSSA). He emphasized the importance of needing to know the fraction of metastable states in the beam, as these states have a much different cross section and can cause significant deviations in measurements. He described the method of using an attenuation cell to filter out metastable states. He is hopeful that these measurements can be pushed down to energies as low as 100 electron volts.

The second talk of this session was presented by **B. Zygelman**. He described recent advances in the theoretical studies at the University of Nevada at Las Vegas. His work is based on ab initio calculations followed by use of quantum close coupling theory. He described his package of codes for work on molecular systems. The first step is the calculation of potential surfaces. Following this structure calculation, dynamic collision processes can be calculated. With the recent large advances in computational power, it is possible to include a large number of channels in these calculations. Currently the computer package for the molecular part is available for hydrogenic ions colliding with hydrogen. Work on non-adiabatic transition theory is in process.

The final talk of the first session was given by **J.P. Hansen**. Hansen mentioned that there is a Training Center at the University of Bergen with opportunities for students to do research for a period of three to six months. He then described current work on their theoretical approach to the solution of the time dependent Schödinger equation. His recent work seems to resolve discrepancies in cross sections for C^{+5} on hydrogen and he presented recommended cross sections. He has codes that are available for one and two electron systems.

The second session was held in the afternoon of the first day and was chaired by J.P. Hansen. Reports were presented by C.C. Havener, K. Okuna, R. Hoekstra, and H.B. Gilbody.

The first presentation of the second session was by **C.C. Havener** of the Oak Ridge National Laboratory, USA. He presented measurements of total electron capture cross sections for multiply charged ions on neutrals. He described the method of using electron impact ionisation measurements to detect the presence of metastable states in the beam. He found that the low energy measurements free from metastable states were an order of magnitude lower than previously recommended data. He investigated the scaling of cross sections in various systems. Some systems indicated that scaling with charge works well, while in other systems it does not.

The second talk of this session was presented by **K. Okuno** of Tokyo Metropolitan University of Japan. Okuna described his recent measurements of cross section data for krypton ions on CO and for carbon, nitrogen, and oxygen ions on helium and hydrogen. He found that at low energies general scaling laws do not seem to apply. The cross sections are very energy dependent and this dependence is determined by competition between the interaction range and the orbit radius.

R. Hoekstra of KVI Atomic Physics, the Netherlands, gave the third talk of the second session. He noted the importance of the use of charge exchange for temperature and density diagnostics. He described his experimental technique to measure state selective cross sections. His results for ions of carbon, nitrogen, helium, and oxygen on hydrogen were presented. He noted that there is a strongly changing triplet/singlet ratio in the measurements. His results indicated that some scaling seems possible.

H.B. Gilbody gave the fourth and final talk of the second session. Gilbody presented his method of translational energy spectroscopy (TES) for measurement of state selective electron capture. This method has been extended to double translational energy spectroscopy (DTES) which can be used to select either the ground or metastable part of an atomic beam. This allows the identification of features in a measurement as to their origin from the ground of metastable state. Absolute cross sections are not yet possible through the DTES method, but in some cases the ratio of the two can be measured. The method has been of great help in resolving some discrepancies in cross sections obtained at different sites.

The third session began on the morning of the second day of the meeting. It was chaired by M. Panov. L. Gulyas, R. McCarroll, R.K. Janev, and L. Errea gave presentations of their research.

The first presentation, by **L. Gulyas** of the Institute of Nuclear Research of the Hungarian Academy of Science, was on the continuum distorted wave method (CDW). Gulyas presented a comprehensive overview of the CDW method using model potentials. This method has been applied to a number of systems and the results compared to experiment. In all cases, the CDW theory agrees well with experiment at the higher energies where the theory is expected to be valid.

The next presentation was given by **R. McCarroll** of the Universite P. et M. Curie, Paris, France. McCarroll built on the presentation given at the first RCM, in comparisons of theory with experiment. In many cases there is good agreement, but some troubling cases give good reason to examine closely additional aspects of the theoretical methods. Dr. McCarroll gave a thorough summary of many aspects of the theory. He pointed out the defects of the PSS method and the ad hoc remedies. He summarised the electron translation factors and finally, the common translation factors. He emphasized that it would be desirable to have more experimental activity for larger molecules and close collaboration between chemical dynamics and electron scattering.

R.K. Janev of the Macedonian Academy of Sciences gave the third presentation of this session. The first part of his presentation focused on charge exchange cross sections for protons with helium, hydrogen and hydrocarbons. The method employed was a close coupling approach using atomic orbitals. Janev then went on to studies of H^+ on H_2 using the methods of classical trajectory surface hoping (CTSH) and infinite order sudden approximation (IOSA). Finally, collisions of H^+ with hydrocarbons were examined. Of particular interest was a construction of scaling laws to predict approximate cross sections for systems not yet studied.

The final talk of the third session was presented by **L. Errea**, who attended the meeting as the representative for A. Riera. Errea presented the results of work done on non-adiabatic processes in ion collisions with H_2. The methods employed were summarised results presented for a number of systems. Plans for extending calculations to lower velocities were discussed along with additional extensions to the theory employed.

The fourth session of the RCM began in the afternoon of the second day and was chaired by B. Zygelman. Presentations were made by M. Kimura and M. Panov.

The first talk of this session was presented by **M. Kimura** of Yamaguchi University, Japan. Kimura discussed his recent results using molecular orbital close coupling calculations for charge transfer cross sections with projectiles of H^+ and C^+ on targets of H_2, D_2, CO, CO_2, and a variety of hydrocarbons. Kimura presented a number of results of calculations, including differential cross sections. He compared some of his cross sections with experiment where available.

The final presentation of the session was by **M. Panov** of the Ioffe Phisical-Technical Institute of RAS, St-Petersburg, Russia. Panov described the work done at his institute on collisions of multiply charged ions with atomic hydrogen and of alpha particles with helium-like systems. Absolute values for total cross section for one electron capture were measured for a number of multiply charged ions colliding with hydrogen. The TES method was used to determine the particle excited state populated in the collision. Results were presented in tabular and graphical form. The collisions of alpha particles with helium-like ions were studied with the close coupling method using quasi-molecular orbitals. These results were compared with experiment where available and with other theory.

The final session, chaired by **R.E.H. Clark**, was devoted to a summary of the results of the CRP and a discussion of the final reports and the publication of the results. The conclusions reached in this session are summarised in the next section.

3. Meeting Conclusions and Recommendations

The assessment of the overall success of the CRP in achieving its objectives was done on the basis of brief reports of the meeting participants for the activities within each CRP project for the duration of the CRP. Their reports are attached in Appendix 3. Both these reports and the presentations at the RCM indicate that the CRP has achieved its basic goal: to generate, using both experimental and theoretical techniques, new charge exchange cross section data for collision systems of prime interest in fusion research in energy ranges where such data are fragmentary or non-existent. On average about ten publications have been published by each of the participating CRP groups within the scope of their CRP projects. The CRP effort had produced very important data contributions in the field of charge exchange cross sections.

These new charge exchange cross sections are expected to be of immediate use in the area of charge exchange spectroscopy in connection with beam diagnostics. There is a new CRP on the general topic of plasma diagnostics for fusion. It is expected that results from this just completed CRP will be of value in the new CRP. Furthermore, it is probable that the new CRP will identify new processes for which further work on charge exchange will be needed. It is expected that some of the researchers from the charge exchange CRP will be able to give some support to the new CRP on plasma diagnostics.

Based on the above assessments and discussions at the final session of the RCM, the meeting participants have arrived at the following conclusions:

1) The extension of measurements by R. Hoekstra to very low energies is very significant;

2) A significant improvement in matching theory with experiment on ion-molecule collisions has been achieved;

3) Significant new data on collision of hydrogenic ions with hydrocarbons is now available;

4) The new subroutines available through the work of J.P. Hansen is a significant advance;

5) The molecular orbital close coupling method represents a significant new direction in calculations of cross sections;

6) There are new experimental data with higher accuracy then ever before now available;

7) The role of metastable states is confirmed as significant and the DTES method is an important development in distinguishing ground state and metastable contributions;

8) Scaling remains a difficult task with significant deviations at low energies;

9) A strong need for complementary theoretical approaches was recognized.

The meeting participants agreed that it would be of value to submit review papers on the work performed on the individual projects of the CRP for publication in the *Atomic and Plasma-material Interaction Data for Fusion* (APID) series. The format will be the same as published in the summary report INDC(NDS)-402 and was distributed at the RCM.

A final recommendation reached at the meeting was on the topic of support for computer codes developed for atomic and molecular calculations in general. Some concern was expressed that if institutional support for such computer codes is not maintained, a significant loss of calculational capability would be lost, especially when a very small number, often just one, researcher at the institution has primary responsibility of such a code. It was recommended that the Atomic and Molecular Data Unit of the IAEA look into forming a network for support of such code work, with the goal being to encourage the home institutions continued support by, for example, writing letters of reference in support of proposals for support and perhaps sponsoring meetings of code developers.

Appendix 1

2^{nd} (Final) IAEA Research Co-ordination Meeting of the Agency's Co-ordinated Research Programme on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

25-26 September 2000, IAEA Headquarters, Vienna, Austria

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Appendix 2

2nd (Final) IAEA Research Co-ordination Meeting of the Agency's Co-ordinated Research Programme on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

25-26 September 2000, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, 25 September **Meeting Room: B0545**

09:30 - 10:00 Opening: Adoption of Agenda

Session 1: Latest Results

Chairman: M. Kimura

10:00 - 10:30	HP. Winter:	Charge exchange between slow doubly charged ions and simple molecules - survey on existing data and recent measurements
10:30 - 11:00	B. Zygelman:	Theoretical studies of charge transfer, involving multiply charged ions, at low collision velocities
11:00 - 11:30	***Coffee Break***	
11:30 - 12:00	J.P. Hansen:	Charge transfer at low energies in C^{6+} - H collisions
12:00 - 13:30	***Lunch***	

Session 2: Latest Results II

Chairman: J.P. Hansen

13:30 - 14:00	C. Havener:	Recent measurements of low energy charge-exchange cross sections for collisions of multicharged ions on neutral atoms and molecules
14:00 - 14:30	K. Okuno:	Charge changing cross sections of multiply charged C, N and O ions colliding with He and H_2 at low energies below 1 keV/amu
14:30 - 15:00	***Coffee Break***	
15:30 - 16:00	R. Hoekstra:	Photon Emission Spectroscopy of Low-Energy Charge Transfer Reactions

16:00 - 16:30 H.B. Gilbody: Measurements of state-selective electron capture by slow multiply charged ions in specified ground metastable states

17:30 - 19:00 ***Reception***

Tuesday, 26 September

Session 3: Latest Results III

Chairman: M. Panov

09:30 - 10:00 L. Gulyas: CDW theory of electron capture by ion impact with model potential description of the target

10:00 - 10:30 R. McCarroll: Low energy charge exchange involving systems with two active electrons

10:30 - 11:00 ***Coffee Break***

11:00 - 11:30 R. Janev: Charge exchange cross section database for proton collisions with hydrocarbon molecules

11:30 - 12:00 L. Errea: Charge exchange and vibrational distribution in ion-H_2 collissions

12:00 - 13:30 ***Lunch***

Session 4: Latest Results IV

Chairman: B. Zygelman

13:30 - 14:00 M. Kimura: Charge transfer from hydrocarbons by H+ impact at low-to-intermediate energies

14:00 - 14:30 M. Panov: The electron capture by multiply charged ions to state selected electron states from atomic hydrogen (experiment) and by alpha-particles from helium-like atomic systems (theory)

14:30 - 15:00 ***Coffee Break***

Session 5: Formulation of Final CRP Outcome and Form of Publication

Chairman: R.E.H. Clark

15:00 - 17:00 Discussion of form of publication of final reports Method of transmitting final outcomes to A+M Data Unit Meeting Conclusions

17:00 - ***Adjournment of Meeting***

Summary Reports from CRP Participants

Recommended Partial Cross Sections for Electron Capture in $C^{6+}+H(1s)$ Collisions

J. Caillat[1,2], A. Dubois[1] and J. P. Hansen[2]

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Abstract

We report $n\ell$-selective capture cross sections for the $C^{6+}-H(1s)$ collision system at low and intermediate impact energies. The present converged results take into account important trajectory effects for $C^{5+}(n = 5)$ capture channels and allow for the extension of the analytical fits proposed by Janev *et al* in *At. Data Nucl. Data Tables* **55** 201 in the 0.1 – 60 keV amu^{-1}energy range.

An important limitation to the heating of fusion plasmas arises from the presence of non-negligible impurity ions in the medium [1, 2]. Among others, plasma modeling and diagnostics require the knowledge of accurate cross sections of electron transfer from atomic hydrogen to fully stripped carbon and oxygen ions. For both systems Janev *et al* [2] proposed analytical fits of capture cross sections based on reliable theoretical and experimental data, when available in the $0.1 - 1000$ keV amu^{-1} impact energy range.

Since the seventies, the C^{6+}– H(1*s*) collision system has been widely studied which makes it a benchmark system for atomic collisions involving highly charged ions [3]. The two main capture channels are the C^{5+} ($n = 4$) and C^{5+} ($n = 5$) manifolds,

$$C^{6+} + H(1s) \rightarrow C^{5+}(4\ell) + H^{+}$$
$$C^{6+} + H(1s) \rightarrow C^{5+}(5\ell) + H^{+}$$

For the dominant C^{5+} ($n = 4$) capture cross sections, experimental data and theoretical predictions were found to be in good agreement and the fits covered the entire energy domain of interest, cf. figure 1. However, severe discrepancies were reported for electron capture to the $C^{5+}(n = 5)$ shell at low impact energies ($0.1 - 10$ keV amu^{-1}). These disagreements, as well as the lack of data for minor channels, prevented Janev*et al* to extend their fits to the low energy range [2].

We have recently reported new results for that system [4, 5] with special emphasize in the low energy range where the above mentioned discrepancies were observed. By a detailed analysis of the mechanisms responsible for the capture processes and of the inter nuclear trajectory effects [4], we have proposed a set of cross sections reliable in this range. These data are reported in the present paper.

We use a non-perturbative semi-classical approach, within the straight-line inter nuclear trajectory approximation. The electron wave function is expanded on a set of target- and projectile-centered atomic orbitals. The projectile orbitals are furthermore modified with Electron Translational Factors in order to take into account the relative motion of the two atomic centers. Inserting this expansion in the time-dependent Schrödinger equation leads to a set of coupled differential equations for the coefficients *c*. These coupled equations are solved numerically for given impact energies E_{coll} and a well chosen set of trajectories, characterized by the impact parameter *b*. From the expansion coefficients after collision the probabilities and cross sections for transition from initial atomic state *i* to final atomic states *f* can be evaluated, respectively

$$P_{i\rightarrow f}\left(E_{coll}, b\right) = \left|c_f\left(t \rightarrow \infty, E_{coll}, b\right)\right|^2 \qquad (1)$$

$$\sigma_{i\rightarrow f}\left(E_{coll}\right) = 2\pi \int_0^\infty b\, db\, P_{i\rightarrow f}\left(E_{coll}, b\right) \qquad (2)$$

However, for $C^{5+}(n = 5)$ capture, the small impact parameter range (b $\leq$ 4 a.u.) is very dominant in the integration of eq. 2, and trajectory effects due to the strong repulsive interaction between the collision partners in the final

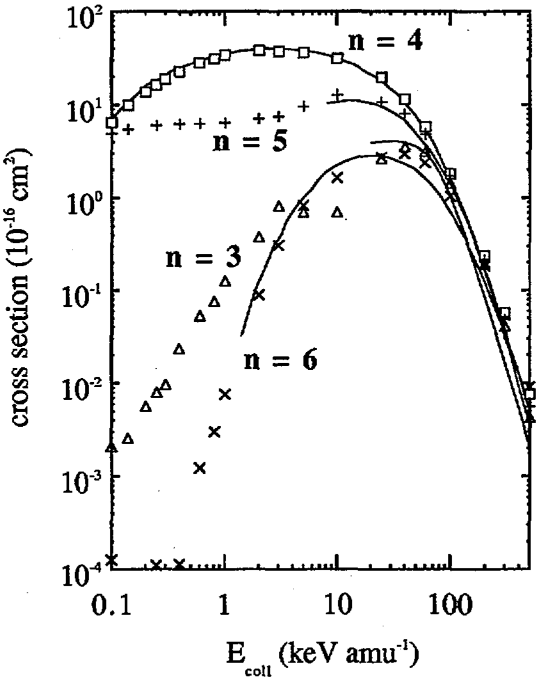

Figure 1: Electron capture cross sections from H(1s) to C^{5+}(n=3–6). Our results: △, n=3; □, n=4; +, n=5; ×, n=6. Recommended data [2]: ——, n=3–6.

channel were found very important [4]. To take into account the departure from straight-line trajectory, we have performed Classical Trajectory Monte Carlo (CTMC) [9] calculations to obtain realistic deflection functions. The trajectory effects were then introduced in the semi-classical results by replacing the impact parameter b in $P_{i\to f}$ (E_{coll}, b) (eq. 2) by an averaged closest approach distance evaluated from the CTMC results [4].

The basis set used in the calculations consists of the H(1s) initial state and of all the states spanning the $C^{5+}(n = 1-6)$ shells. This basis set does not include hydrogen excitation and ionisation channels so that it is not expected to give very accurate cross sections above 60 keV amu^{-1}[7]. Indeed Figure 1 shows that the capture cross sections are slightly overestimated (typically 50% at 200 keV amu^{-1}) in our model compared to the recommended data [2]. However in the low energy range the basis set is adequate and describes correctly the $(CH)^{6+}$ molecular curves and the important avoided crossings [4]. Our results are in excellent agreement with recent molecular-orbital calculations of Harel *et* *al* [6]: for example at 0.3 keV amu^{-1}, differences between the two data sets are less than 5% for the important channels and below 50% for the minor C^{5+}($n = 3$) and C^{5+}($n = 6$) channels.

E_{coll}	0.05	0.0625	0.1	0.14	0.2*	0.25	0.3*	0.4	0.6	0.81*
$3s$	1.88^{-6}	2.32^{-6}	1.46^{-5}	5.06^{-5}	2.30^{-5}	2.13^{-5}	1.85^{-5}	1.37^{-5}	4.12^{-4}	7.28^{-4}
$3p$	3.00^{-6}	7.83^{-6}	2.91^{-5}	2.13^{-5}	2.99^{-5}	4.49^{-5}	4.74^{-5}	3.92^{-5}	2.67^{-4}	1.21^{-3}
$3d$	5.93^{-6}	5.08^{-6}	8.23^{-5}	1.24^{-5}	3.58^{-5}	4.41^{-5}	6.30^{-6}	6.00^{-5}	5.61^{-4}	1.09^{-3}
n=3	1.08^{-5}	1.52^{-5}	1.26^{-4}	8.42^{-5}	8.88^{-5}	1.10^{-4}	7.22^{-5}	1.13^{-4}	1.24^{-3}	3.02^{-3}
$4s$	3.70^{-1}	3.72^{-1}	4.90^{-1}	6.48^{-1}	8.94^{-1}	1.05^{+0}	1.34^{+0}	1.61^{+0}	2.12^{+0}	2.07^{+0}
$4p$	8.38^{-1}	9.51^{-1}	1.46^{+0}	1.97^{+0}	2.79^{+0}	3.30^{+0}	4.01^{+0}	4.69^{+0}	6.42^{+0}	7.23^{+0}
$4d$	9.95^{-1}	1.15^{+0}	1.87^{+0}	2.22^{+0}	3.01^{+0}	3.93^{+0}	4.91^{+0}	7.06^{+0}	9.49^{+0}	1.12^{+1}
$4f$	1.13^{+0}	1.43^{+0}	2.67^{+0}	5.06^{+0}	7.07^{+0}	7.93^{+0}	8.42^{+0}	9.29^{+0}	1.00^{+1}	1.07^{+1}
n=4	3.34^{+0}	3.90^{+0}	6.49^{+0}	9.90^{+0}	1.38^{+1}	1.62^{+1}	1.87^{+1}	2.26^{+1}	2.80^{+1}	3.13^{+1}
$5s$ →	1.83^{-1}	1.87^{-1}	5.46^{-1}	5.79^{-1}	5.59^{-1}	3.15^{-1}	2.55^{-1}	3.34^{-1}	6.58^{-1}	7.51^{-1}
	5.44^{-1}	4.39^{-1}	8.53^{-1}	7.83^{-1}	6.81^{-1}	3.66^{-1}	2.88^{-1}	3.64^{-1}	6.89^{-1}	7.71^{-1}
$5p$ →	1.98^{-1}	3.75^{-1}	5.16^{-1}	8.76^{-1}	1.12^{+0}	1.09^{+0}	8.36^{-1}	6.78^{-1}	1.29^{+0}	1.59^{+0}
	5.89^{-1}	8.78^{-1}	8.06^{-1}	1.19^{+0}	1.37^{+0}	1.26^{+0}	9.45^{-1}	7.39^{-1}	1.35^{+0}	1.63^{+0}
$5d$ →	3.26^{-1}	5.68^{-1}	5.05^{-1}	6.72^{-1}	1.17^{+0}	1.12^{+0}	1.12^{+0}	1.45^{+0}	1.77^{+0}	1.83^{+0}
	9.71^{-1}	1.33^{+0}	7.89^{-1}	9.10^{-1}	1.43^{+0}	1.30^{+0}	1.27^{+0}	1.59^{+0}	1.85^{+0}	1.88^{+0}
$5f$ →	8.67^{-1}	1.12^{+0}	1.68^{+0}	1.26^{+0}	1.32^{+0}	1.69^{+0}	2.09^{+0}	2.28^{+0}	1.74^{+0}	1.51^{+0}
	2.58^{+0}	2.62^{+0}	2.63^{+0}	1.70^{+0}	1.61^{+0}	1.97^{+0}	2.36^{+0}	2.49^{+0}	1.82^{+0}	1.55^{+0}
$5g$ →	9.65^{-1}	1.10^{+0}	1.69^{+0}	2.08^{+0}	1.64^{+0}	1.78^{+0}	1.79^{+0}	1.45^{+0}	8.77^{-1}	6.96^{-1}
	2.87^{+0}	2.57^{+0}	2.64^{+0}	2.81^{+0}	2.00^{+0}	2.07^{+0}	2.02^{+0}	1.59^{+0}	9.17^{-1}	7.15^{-1}
n=5 →	2.54^{+0}	3.35^{+0}	4.94^{+0}	5.46^{+0}	5.82^{+0}	6.00^{+0}	6.09^{+0}	6.21^{+0}	6.34^{+0}	6.37^{+0}
	7.55^{+0}	7.84^{+0}	7.72^{+0}	7.39^{+0}	7.10^{+0}	6.97^{+0}	6.89^{+0}	6.77^{+0}	6.64^{+0}	6.54^{+0}
$6s$	6.03^{-5}	1.13^{-5}	4.91^{-5}	1.22^{-4}	5.71^{-4}	1.04^{-3}	8.54^{-4}	1.32^{-3}	3.14^{-3}	4.74^{-3}
$6p$	7.77^{-5}	1.71^{-5}	9.23^{-5}	3.51^{-4}	1.07^{-3}	1.03^{-3}	2.65^{-3}	3.06^{-3}	8.01^{-3}	1.21^{-2}
$6d$	2.03^{-4}	3.81^{-5}	1.79^{-4}	2.77^{-4}	6.03^{-4}	2.16^{-3}	2.01^{-3}	4.32^{-3}	1.31^{-2}	1.20^{-2}
$6f$	2.33^{-4}	1.13^{-4}	3.50^{-4}	3.99^{-4}	8.52^{-4}	1.31^{-3}	1.43^{-3}	5.91^{-3}	1.48^{-2}	2.16^{-2}
$6g$	4.26^{-4}	1.93^{-4}	5.41^{-4}	5.08^{-4}	1.01^{-3}	1.23^{-3}	1.58^{-3}	5.56^{-3}	9.62^{-3}	1.65^{-2}
$6h$	6.58^{-4}	2.52^{-4}	8.93^{-4}	9.33^{-4}	1.60^{-3}	1.22^{-3}	1.18^{-3}	3.61^{-3}	4.73^{-3}	9.19^{-3}
n=6	1.66^{-3}	6.24^{-4}	2.10^{-3}	2.59^{-3}	5.70^{-3}	8.00^{-3}	9.70^{-3}	2.38^{-2}	5.34^{-2}	7.62^{-2}

Table 1: Electron transfer cross sections (in 10^{-16} cm^2) from H(1s) to C^{5+}($n\ell$), n = 3–6 at low collision energies E_{coll} (in keV amu^{-1}). For transfer to C^{5+}(5ℓ) the trajectory modified cross sections are shown by "→" and pure straight-line results are reported underneath in smaller font.

The $n\ell$-partial and n-partial ($n = 1-6$) capture cross sections are reported in table 1 for 10 impact energies from .05 keV amu^{-1} to .81 keV amu^{-1} and in table 2 for 10 impact energies from 1 keV amu^{-1} to 200 keV amu^{-1}. As concluded in [4] for electron capture to C^{5+}($n\ell$) we recommend the use of the trajectory modified cross sections, in good agreement with the data of Green *et al* [8] (for information pure impact-parameter results are also reported in smaller font).

Trajectory effects were interpolated from figure 4 in [4] for 3 impact energies (.2, .3 and .81 keV amu^{-1}) marked by "*" in table 1 (CTMC predictions not

E_{coll}	1.0	2.0	3.0	5.0	10.0	25.0	40.0	60.0	100.	200.
$3s$	1.07^{-3}	1.40^{-2}	7.23^{-2}	2.34^{-1}	3.32^{-1}	3.58^{-1}	3.52^{-1}	1.06^{-1}	5.09^{-2}	1.29^{-2}
$3p$	4.05^{-3}	4.66^{-2}	1.45^{-1}	3.94^{-1}	7.54^{-1}	1.07^{+0}	1.16^{+0}	8.98^{-1}	1.99^{-1}	1.82^{-2}
$3d$	2.47^{-3}	2.88^{-2}	9.07^{-2}	2.03^{-1}	5.56^{-1}	1.31^{+0}	1.48^{+0}	1.37^{+0}	7.97^{-1}	1.56^{-1}
n=3	7.60^{-3}	8.94^{-2}	3.08^{-1}	8.31^{-1}	1.64^{+0}	2.74^{+0}	2.99^{+0}	2.38^{+0}	1.05^{+0}	1.87^{-1}
$4s$	3.13^{+0}	2.40^{+0}	2.52^{+0}	1.80^{+0}	1.04^{+0}	3.99^{-1}	1.56^{-1}	9.54^{-2}	6.88^{-2}	1.15^{-2}
$4p$	8.21^{+0}	9.03^{+0}	8.54^{+0}	7.31^{+0}	4.22^{+0}	1.66^{+0}	1.04^{+0}	5.96^{-1}	1.27^{-1}	1.69^{-2}
$4d$	1.15^{+1}	1.37^{+1}	1.36^{+1}	1.39^{+1}	1.06^{+1}	5.44^{+0}	2.16^{+0}	8.62^{-1}	4.43^{-1}	1.10^{-1}
$4f$	1.11^{+1}	1.29^{+1}	1.28^{+1}	1.31^{+1}	1.55^{+1}	1.20^{+1}	8.15^{+0}	4.26^{+0}	1.18^{+0}	9.91^{-2}
n=4	3.40^{+1}	3.80^{+1}	3.74^{+1}	3.61^{+1}	3.13^{+1}	1.95^{+1}	1.15^{+1}	5.82^{+0}	1.81^{+0}	2.37^{-1}
$5s$	6.98^{-1}	2.60^{-1}	2.26^{-1}	1.81^{-1}	1.54^{-1}	1.30^{-1}	8.05^{-2}	1.02^{-1}	6.51^{-2}	9.80^{-3}
$5p$	1.55^{+0}	7.21^{-1}	6.26^{-1}	6.16^{-1}	6.58^{-1}	5.51^{-1}	5.53^{-1}	3.31^{-1}	9.17^{-2}	1.42^{-2}
$5d$	1.79^{+0}	1.20^{+0}	1.04^{+0}	1.29^{+0}	1.53^{+0}	1.36^{+0}	7.75^{-1}	5.64^{-1}	3.36^{-1}	8.08^{-2}
$5f$	1.60^{+0}	2.46^{+0}	2.17^{+0}	2.72^{+0}	3.17^{+0}	2.61^{+0}	2.36^{+0}	1.76^{+0}	7.26^{-1}	8.50^{-2}
$5g$	7.89^{-1}	2.39^{+0}	3.41^{+0}	4.79^{+0}	7.27^{+0}	5.98^{+0}	4.26^{+0}	2.10^{+0}	4.93^{-1}	2.69^{-2}
n=5	6.42^{+0}	7.03^{+0}	7.47^{+0}	9.61^{+0}	1.28^{+1}	1.06^{+1}	8.04^{+0}	4.86^{+0}	1.71^{+0}	2.17^{-1}
$6s$	4.46^{-3}	1.60^{-2}	3.20^{-2}	1.65^{-2}	2.21^{-2}	4.22^{-2}	5.64^{-2}	8.76^{-2}	6.09^{-2}	9.19^{-3}
$6p$	2.16^{-2}	4.60^{-2}	9.25^{-2}	5.30^{-2}	5.15^{-2}	1.88^{-1}	2.51^{-1}	2.16^{-1}	8.89^{-2}	1.25^{-2}
$6d$	3.41^{-2}	9.44^{-2}	1.28^{-1}	8.64^{-2}	1.11^{-1}	3.33^{-1}	3.40^{-1}	3.81^{-1}	2.65^{-1}	6.34^{-2}
$6f$	2.66^{-2}	4.72^{-2}	2.19^{-1}	8.65^{-2}	1.42^{-1}	5.52^{-1}	8.67^{-1}	9.16^{-1}	5.04^{-1}	7.15^{-2}
$6g$	2.31^{-2}	5.29^{-2}	2.24^{-1}	2.67^{-1}	1.44^{-1}	7.46^{-1}	1.18^{+0}	1.01^{+0}	3.89^{-1}	3.10^{-2}
$6h$	1.56^{-2}	1.23^{-1}	1.23^{-1}	2.00^{-1}	2.35^{-1}	7.94^{-1}	8.84^{-1}	5.20^{-1}	1.24^{-1}	5.15^{-3}
n=6	1.25^{-1}	3.80^{-1}	8.19^{-1}	7.09^{-1}	7.06^{-1}	2.66^{+0}	3.58^{+0}	3.13^{+0}	1.43^{+0}	1.93^{-1}

Table 2: Electron transfer cross sections (in 10^{-16} cm^2) from H($1s$) to C^{5+}($n\ell$), $n = 3$–6 at medium collision energies E_{coll} (in keV amu^{-1}).

available). These effects were considered identical for the different ℓ states in the C^{5+}($n = 5$) shell. Note finally that trajectory effects are not significant for all other channels (C^{5+}($n = 3, 4, 6$)) compared to the uncertainty of the data. Thus trajectory-modified cross sections are not reported in these cases.

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Recent Measurements of Low Energy Charge Exchange Cross Sections for Collisions of Multicharged Ions on Neutral Atoms and Molecules

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At the ORNL Multicharged Ion Research Facility (MIRF), charge exchange (CX) cross sections have been measured for multicharged ions (MCI) on neutral atoms and molecules. The ORNL ion-atom merged-beams apparatus was used to measure single electron capture by MCI from H at eV/amu energies. A gas cell was used to measure single and double electron capture by MCI from a variety of molecular targets at (q x keV) collision energies.

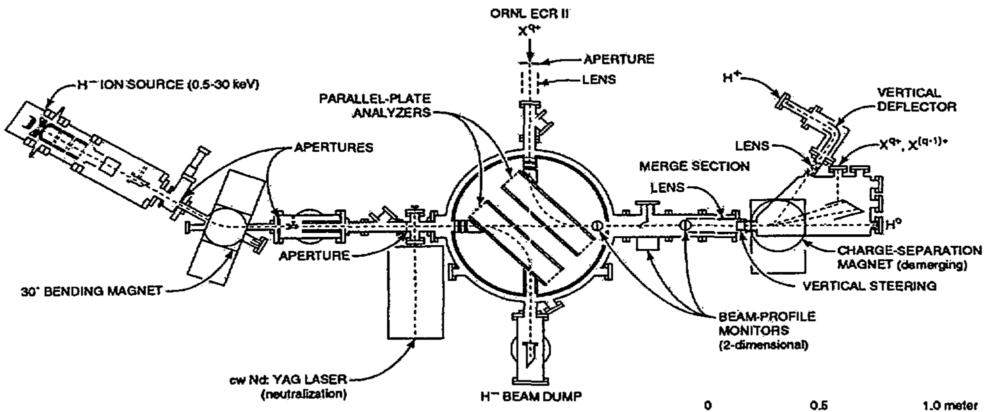

Figure 1. Schematic of the ORNL ion-atom merged-beams apparatus.

Figure 1 shows a schematic of the ORNL ion-atom merged-beams apparatus. A 6-8 keV ground state neutral atomic hydrogen or deuterium beam is produced via photo-detachment of a $H^-(D^-)$ beam as it passes through the inner cavity of a YAG laser. The neutral beam is electrostatically merged with an intense multicharged q x (8-25) keV ion beam from the ECR ion source. Measurements of the horizontal and vertical profiles of the two beams at three positions along the merge-path are used to calculate the form factor or beam-beam overlap. At the end of the merge path the signal H^+ is demerged from the primary beams and detected in a channel electron multiplier. The absolute cross section is determined directly from experimental parameters that include the primary beam intensities, form factor, beam-beam signal rate, merge path length, and velocities of the beams. Beam-beam signals are inherently low (Hz) and must be separated from large backgrounds (kHz) by a two-beam modulation technique.

The merged-beams experiment has been successful in providing benchmark total electron capture measurements for several collision systems with a variety of multicharged ions (see Table 1) on H or D. References for most measurements can be found at the web site www-cfadc. phy.ornl.gov/mirfhome or in the merged-beams reviews (Havener 97, Phaneuf 1999). The Cl^{7+} + H(D) measurements can be found in (Thompson 01) and the Mo^{q+} + H(D) in (Havener 01). The feasibility of using the merged-beams technique to measure state-selective cross sections was investigated for Si^{4+} + D (Wu & Havener 1998).

Table 1. A list of the multicharged ions used in ORNL ion-atom merged-beams measurements. Total electron capture cross sections have been measured for the above ions with H or D.

Ion q =	1	2	3	4	5	6	7	8	9	10	11
B				X							
C	X		X	X							
N		X	X	X	X						
O			X	X	X						
Ne			X	X							
Si				X							
Cl							X				
Mo				X	X		X		X		X

The following is a short discussion of some of the results pertinent to this report. Theoretical predictions of charge exchange cross sections can be very sensitive to the quasi-molecular potentials used in the calculations. This was demonstrated by merged-beams measurements (Pieksma et al. 1998) for B^{4+} + H(D) when compared to recent theory. Merged-beams measurements (Bliek et al. 1997) for C^{4+} were performed with sufficient resolution that structure was observed near the peak in the cross section where several dominant capture channels compete. The observation of this structure has led to a reevaluation (Tseng and Lin 1998) of theory, but as yet no calculation of C^{4+} has been able to reproduce the structure. More dramatic structure has been observed in merged-beams measurements (Pieksma et al. 1997) for N^{2+} + H.

There is a considerable amount of previous experimental work in ion-atom collisions at 100 eV/amu and above. While there have been recent experiments which select ions in either ground or metastable states, a significant fraction of the previous measurements did not fully characterize the metastable content of their ion beam. Merged-beams measurements [Stancil 98] for C^{+} + D show that the recommended data for fusion (Janev et al. 1988) are too high at low energies and are based on previous measurements using a thermal-dissociation atomic hydrogen target (Nutt et al. 1979). These measurements used a C^{+} beam, which was probably contaminated with metastables. The merged-beams measured cross section is over an order of magnitude lower at eV/amu energies and was taken with a C^{+} beam essentially free of metastables. The metastable content of ion beams at ORNL can be estimated by observing electron-impact ionization below threshold. The ionization measurements were performed using the ORNL electron-ion crossed-beams apparatus (Bannister 1996). It is important to note that the electron capture process by ground state C^{+} ion from H is endothermic by 2.33 eV (Stancil et al. 1998). For endothermic reactions, the cross section decreases with decreasing energy, becoming exponentially small at the lowest energies near threshold. ORNL molecular-orbital coupled-channel calculations (Stancil et al. 1998) verify this lower cross section for the C^{+} ground state.

Recent measurements with the merged-beams apparatus involve heavier and higher charge state ions. Measurements with Mo^{q+}, q=4,5,7,9,11 which were limited to higher collision energies due to the 25 kV maximum acceleration voltage of the present ECR ion source, were found to generally follow the q scaling experimentally found by Phaneuf (1983) for Fe^{q+} + H, q=3-14. Our recent cross section measurements (Thompson et al. 2001) with Cl^{7+} exhibit a strong energy dependence with a decrease in the cross section toward eV/amu energies, in contrast to the slightly increasing cross section previously observed for other 7+ ions. To investigate this energy dependence MOCC calculations were performed for N^{7+} + D (calculations for Cl^{7+} are tedious due to the number of states involved). The calculated cross section for N^{7+} decreases toward lower energies and agrees with the Cl^{7+} measurements, suggesting that the Ne-like core of Cl^{7+} plays no significant role in the electron capture process for this collision system. The fact that the cross section does not remain flat toward decreasing energies shows that the actual quasi-molecular structure and associated dynamics remain important even for high charge states ions with multielecton cores.

Presently, the negative ion source on the ion-atom merged-beams apparatus is being upgraded to a new Cs negative ion sputter source which will allow measurements with a wide variety of neutral atom and molecular beams. Any negative ion whose extra electron is bound by less that 1 eV can be photodetached with the current YAG laser and used to produce a neutral beam. Such neutral beams include Li, B, Na, Al, P, K, Ca, Cr, Fe,... and molecular beams such as O_2, CH_2,....The merged-beams technique is the only technique available to explore collisions at eV/amu energies and below for these atomic targets. For vapor targets like Fe that can only be produced at high temperatures, the electron capture process is virtually unexplored. For symmetric collisions like Fe^{q+} + Fe it will be important to access the relative contribution of the single to the multiple electron capture resonant processes.

Measurements of single and double electron capture by MCI from a variety of molecular targets were performed using a gas cell for collision energies from 100 eV/amu to 3000 eV/amu. A highly collimated MCI beam was directed through a gas cell and the electron capture products, $X^{(q-1)+}$ and $X^{(q-2)+}$ were subsequently separated from the primary beam with a parallel-plate electrostatic analyzer. Measurements were performed with As^{2+} + O_2, N_2, H_2; P^{2+} + O_2, N_2, H_2; B^+ + CH_4, CO_2, CO, H_2, N_2; B^{3+} + H_2; and $S^{5+,7+}$ + CO_2, CO, H_2, H_2O. In general the ion-molecule CX measurements show the same trends with the ionization potential as the classical over barrier model, especially for larger q. For B^{3+} + H_2, single and double CX measurements show fair agreement with existing molecular-orbital close-coupling calculations (Bacchus-Montabonel 1999).

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Cross Sections for Ion-molecular Reactions in Hydrogen Systems and for Charge Transfer Reactions of Slow Multiply Charged Ions

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Cross sections of ion-molecular reactions in hydrogen systems of H^+-H_2, H_2^+-H_2 and H_3^+-H_2 and charge transfer cross sections of multiply charged ions in atomic and molecular targets are presented in graphs and tables of the part A, B and C. All data presented for 99 collision systems have been measured systematically using an octo-pole ion beam guide (OPIG) technique till now since 1985. The part A is for ion-molecular reactions in hydrogen systems. In the lower energy region below few eV in center-of-mass systems, it is seen obviously at a glance that the ion-molecular reaction in hydrogen systems is dominated by H_3^+ formation process. In the energy region from few eV to few hundred eV in center-of-mass systems, many reaction channels of decay processes from intermediate molecular states seem to be opened resonantly. Some of cross section data in the part B for charge transfer reactions of low-charged ions produced by a conventional electron impact type (Nier type) ion source should be noted to strongly depend on the electron impact energy due to contamination of low lying metastable states in projectile ions. The part C is for charge transfer reactions of multiply charged ions extracted from a small type of electron beam ion source (Mini-EBIS). In measurements using the mini-EBIS, no evidence of metastable ions existing in the primary ion beam has been found except for doubly charged ion beam. The higher energy end of the present cross sections are connected with previous data in fairly good.

CONTENTS

Table 1. List of reaction systems in the Part A.

No.	projectile	targets	No.	projectile	targets
A1	$^{1}H^{+}$	H_2, D_2	A4	$^{2}D_2^{+}$	H_2, D_2
A2	$^{2}D^{+}$	H_2	A5	$^{1}H_3^{+}$	H
A3	$^{1}H_2^{+}$	H_2, D_2	A6	$^{2}D_3^{+}$	H_2, D_2

Table 2. List of collision systems in the Part B.

No.	projectile	targets	No.	projectile	targets
B1	$^{20}Ne^{2+}$	He, H_2, N_2	B4	$^{84}Kr^{2+}$	He, Ne, Kr
B2	$^{40}Ar^{2+}$	He, Ne, Ar,Kr	B5	$^{86}Kr^{3+}$	Kr
B3	$^{40}Ar^{3+}$	He, Ne, Ar,Kr			

Table 3. List of collision systems in the Part B.

No.	projectile	targets	No.	projectile	targets
C1	$^{3}He^{2+}$	He, H_2, N_2, O_2, CO	C17	$^{40}Ar^{4+}$	Ne
C2	$^{13}C^{2+}$	He, H_2	C18	$^{38}Ar^{5+}$	Ne
C3	$^{13}C^{3+}$	He, H_2	C19	$^{40}Ar^{6+}$	He, Ne, H_2
C4	$^{12}C^{4+}$	He, Ne, Ar, Kr, H_2, N_2, O_2, CH_4, C_2H_6, C_3H_8, n-C_4H_{10}	C20	$^{40}Ar^{7+}$	He, Ne, H_2
			C21	$^{40}Ar^{8+}$	He, Ne, H_2
C5	$^{12}C^{5+}$	He, H_2	C22	$^{40}Ar^{9+}$	He, Ne, H_2
C6	$^{13}C^{6+}$	He, H_2	C23	$^{40}Ar^{11+}$	He, H_2
C7	$^{14}N^{2+}$	He, H_2	C24	$^{86}Kr^{3+}$	CO
C8	$^{14}N^{3+}$	He, H_2	C25	$^{84}Kr^{4+}$	CO
C9	$^{14}N^{4+}$	He, H_2	C26	$^{84}Kr^{5+}$	CO
C10	$^{14}N^{5+}$	He, H_2	C27	$^{84}Kr^{6+}$	CO
C11	$^{14}N^{6+}$	He, H_2	C28	$^{84}Kr^{7+}$	Ne, CO
C12	$^{16}O^{2+}$	He, H_2	C29	$^{84}Kr^{8+}$	Ne, N_2, O_2, CO
C13	$^{16}O^{3+}$	He, H_2	C30	$^{84}Kr^{9+}$	Ne, CO
C14	$^{18}O^{4+}$	He	C31	$^{127}I^{24+}$	He
C15	$^{16}O^{5+}$	He, H_2	C32	$^{127}I^{25+}$	He
C16	$^{16}O^{6+}$	He, H_2	C33	$^{127}I^{26+}$	He

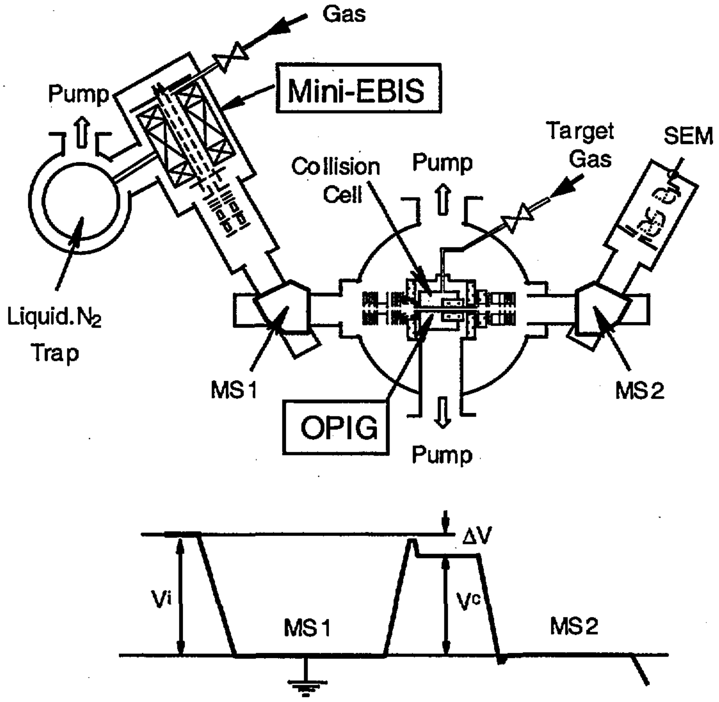
1. Introduction

In the last two decades after development of ion source which can produce highly charged ions, a great deal of information concerning on charge transfer reactions of multiply charged ions in collisions with neutrals has been accumulated. Cross section data for such reactions are not only considerable fundamentals on atomic physics but also quite important for fusion and astrophysical plasma research. However the low energy data below 1 keV/u which is most necessary for plasma diagnosis of fusion plasma still has been lacking even now.

In the low energy cross section measurements, there are some technical difficulties, especially in preparation of a stable beam of highly charged ions with a narrow energy spread and in detection of large angle scattered ions. In 1985, we had succeeded in overcoming these difficulties in development of an octo-pole ion beam guide (OPIG) technique in which a high frequency oscillating RF field prevents ion beam from diverging. The OPIG is just a powerful tool for low energy ion-collision experiments. Because the lower limit of beam energy has been gone down with great strides without intensity loss and cross section measurements has been possible with an almost constant beam intensity in the energy range of $E_{lab} = q\times(0.5\sim2000)$ eV in the laboratory systems where there is no data [1-2]. At first, this technique also displayed it's great power in detection of product ions in ion-molecular reactions of hydrogen systems. And then, in 1987, we had also developed a small size electron beam ion source (mini-EBIS) for the low energy atomic collision research [3]. The new idea of cooling the magnetic solenoid with liquid nitrogen was very effective not only in miniaturizing the solenoid coil and its power supply but also in creating a good vacuum required for production of highly charged ions. The mini-EBIS can supply a moderate intensity beam of highly charged ions with a narrow energy spread in the DC mode operation. By using a combination technique of the OPIG and the mini-EBIS [4], charge changing cross sections of multiply charged ions in collisions with atoms and molecules have been systematically measured at energies below 1 keV/amu since 1988 and are still continuing. Here, all of cross sections measured for 99 collision systems will be presented.

2. Experimental setup and experimental procedure

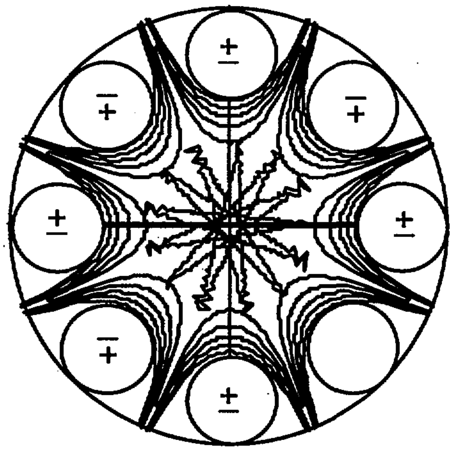
The apparatus used in presented cross section measurements is fundamentally like a tandem mass spectrometer which is consisted of an ion source, a mass selector, a collision cell, a mass analyzer and an ion detector in cascade as shown schematically in Fig.1. The arrangement of electric potentials in general operation is also shown at the lower side in Fig.1. In the original setup, a Nier type ion source which is of a conventional electron impact type was used as an ion source and it was displaced by the mini-EBIS which can produce highly charged ions in 1987. Fig.1 shows of the present setup used since 1987. As details have been reported previously [1,

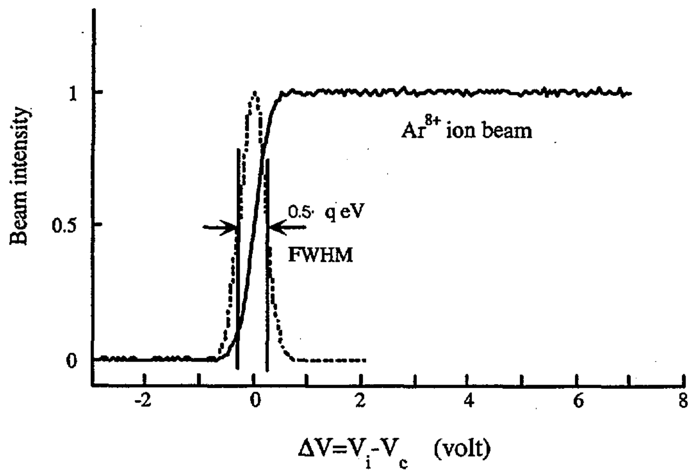


4], only a brief description is given here.

The ions extracted from the ion source are accelerated and the desired m/q is selected by MS1, then, the ion beam is decelerated to the desired energy before injection into the collision ce).5mmφ and an outlet pipe of 7 mmφ inner diameter and of 70 m the OPIG which consists of eight poles with a diameter of 1.5 m nbled as it penetrates through inscribing the outlet pipe. High fr to the poles equally spaced around an axis alternatively in op lectric field created in the OPIG modulates and confines only th ticles and never affects the drift motion along the axis. The co ential and the simulated trajectory of ionic motion in the OPIG

Fig.1. Schematic diagram of the experimental setup used since 1987.
The arrangement of electric potentials is shown in the lower side; vacuum envelop is grounded , and V_i and V_c are potentials at the ion source and the collision cell, respectively.





are shown in Fig.2. The injected ions are guided through the OPIG upon the next stage of an ion lens system without intensity loss and they are accelerated again. Primary and product ions ar netic m/q analyzer, MS2, and detected by a secondary el ssure was determined using an MKS baratron pressure ga ned by the charge q times the potential difference ΔV be the collision cell potential V_c, $E_{lab}= q×ΔV = q×(V_i-V_c)$. U tial V_c was changed. As the careful tuning of the beam in OPIG is achieved, the beam intensity is almost constant until it falls off rapidly near the zero energy as seen in Fig.3. This is a great merit of using the OPIG for the low energy cross section measurements. Cross sections were measured by the initial growth method with a continuous change of target gas pressure which was at all times low enough to ensure single collision conditions. Energy spreads of the projectile ion beam extracted from a Nier type ion source and from the mini-EBIS were typically of q×0.3 eV and of q×(0.4~0.7) eV, respectively.

Fig.3. Intensity curve of Ar^{8+} beam extracted from the mini-EBIS as a function of the difference ($ΔV = V_i-V_c$) between potentials at the ion source (V_i) and the collision cell (V_c).

3. Explanation of graphs and tables

All measured cross sections are presented in graphs as a function of collision energy of E_{cm} in the center-of-mass systems but E_{lab} in the laboratory systems and E_{amu} because of comparison among results using different isotope species. Their numerical data are summarized in tables as a function of E_{lab}/q, E_{cm} $(=E_{lab}×m_2/(m_1+m_2))$ and $E_{amu}(=E_{lab}/m_1)$, where q is the charge state of projectile ion and m_1 and m_2 are masses of the projectile and the target, respectively.

Statistical uncertainties of presented cross sections were less than ±10% and systematic errors for each parameter measurements were commonly estimated to be in ±10% for the collision length, in ±5% for target pressure and less than ±5% for signal counting, respectively.

The gross uncertainties of measured cross sections can be estimated to be ±20% at the most if the collecting efficiency by using the OPIG is perfect for product ions.

3.1 Part A: Ion-molecule reactions in hydrogen systems

Ion-molecule reactions in hydrogen systems were investigated by the experimental setup with a Nier type ion source. In graphs and tables of the part A, formation cross sections of product ions observed in collision systems listed in table 1 are presented together with attenuation cross sections of σ(att) and contributions of secondary processes are denoted by δ( ). These cross sections are unpublished data measured during 1985-1986. Especially in cross section measurements for every hydrogen systems, there is much difference between the attenuation cross section and sum of reaction cross sections measured. This reason is concluded to be that attenuation cross section includes those for target excitation processes followed with energy loss and/or large angle scattering, and also reaction cross sections measured for very slow product ions is underestimated due to the ion trapping effects of the OPIG. The latter effects are confirmed by experimental evidence of secondary processes occurring even in very thin targets.

From comparison of presented data, following cross sections and related processes are resolved for each hydrogen systems of A^+/B_2, A_2^+/B_2 and A_3^+/B_2 as shown in Fig.4-6, where A and B are

Fig.4. Resolved cross sections related following processes for the A^+/B_2 system.

$A^+ + B_2 \rightarrow AB + B^+ + 0$ eV $\sigma(B^+)$ (1)
$\rightarrow AB^+ + B - 1.83$ eV $\sigma(AB^+)$ (2)
$\rightarrow A + B_2^+ - 1.83$ eV $\sigma(B_2^+)$ (3)
$\rightarrow A + B + B^+ - 4.48$ eV $\sigma(B^+)$ (4)
$\rightarrow A^+ + B_2^+ + e - 15.43$ eV $\sigma(B_2^+)$ (5)

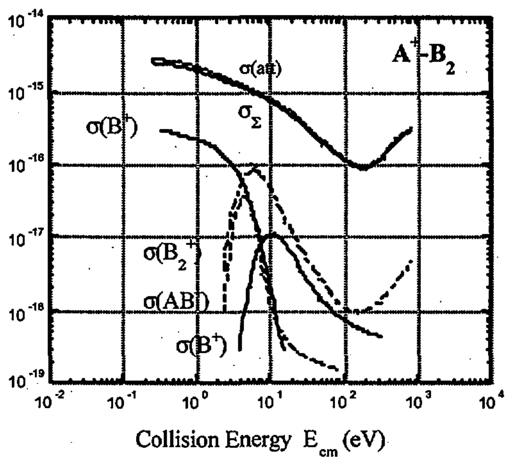
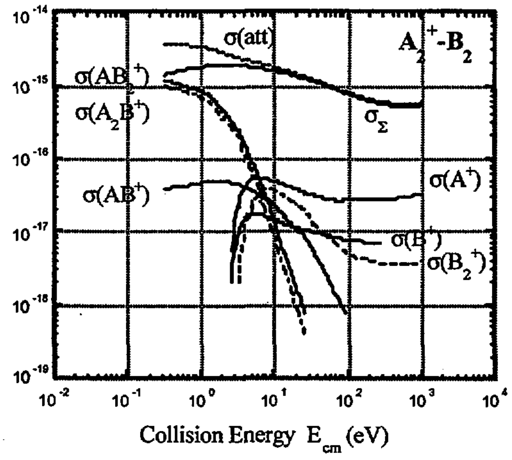


Fig.5. Resolved cross sections related following processes for the A_2^+/B_2 system.

$A_2^+ + B_2 \rightarrow A_2B^+ + B + 2.06$ eV $\sigma(A_2B^+)$ (6)
$\rightarrow AB_2^+ + A + 2.06$ eV $\sigma(AB_2^+)$ (7)
$\rightarrow AB^+ + AB + 0$ eV $\sigma(AB^+)$ (8)
$\rightarrow A + A + B_2^+ - 4.47$ eV $\sigma(B_2^+)$ (9)
$\rightarrow A^+ + A + B_2 - 2.75$ eV $\sigma(A^+)$ (10)
$\rightarrow A_2 + B_2^+ + 0$ eV $\sigma_C(B_2^+)$ (11)



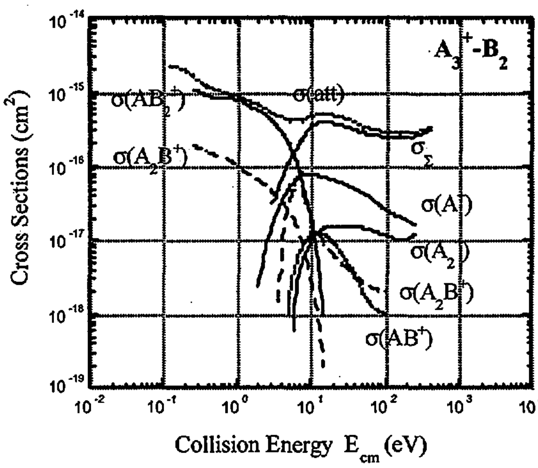


Fig.6. Resolved cross sections related following processes for the A_3^+/B_2 system.

$A_3^+ + B_2 \rightarrow A_2B^+ + AB + 0$ eV $\quad \sigma(A_2B^+)$ (12)
$\rightarrow A_2B^+ + A + B - 4.47$ eV $\quad \sigma(A_2B^+)$ (13)
$\rightarrow AB_2^+ + A_2 + 0$ eV $\quad \sigma(AB_2^+)$ (14)
$\rightarrow AB_2^+ + A + A - 4.47$ eV $\quad \sigma(AB_2^+)$ (15)
$\rightarrow AB^+ + A_2 + B - 6.52$ eV $\quad \sigma(AB^+)$ (16)
$\rightarrow AB^+ + AB + A - 6.52$ eV $\quad \sigma(AB^+)$ (16')
$\rightarrow A^+ + A_2 + B_2 - 4.81$ eV $\quad \sigma(A^+)$ (17)
$\rightarrow A_2^+ + A + B_2 - 6.52$ eV $\quad \sigma(A_2^+)$ (18)
$\rightarrow A_2^+ + AB + B - 6.52$ eV $\quad \sigma(A_2^+)$ (18')
$\rightarrow A_2 + AB + B^+ - 4.81$ eV $\quad \sigma(B^+)$ (19)
$\rightarrow A_2 + A + B_2^+ - 6.52$ eV $\quad \sigma(B_2^+)$ (20)

element of H or D. The σ_Σ indicates the difference between $\sigma(\mathrm{att})$ and sum of measured reaction cross sections.

3.2. Part B: Charge transfer of low-charged rare gas ions from a Nier type ion source

In the part B, single-, double- and triple-electron capture cross sections of low-charged rare-gas ions extracted from the Nier type ion source are presented in graphs and tables as a function of collision energy of E_{cm} in the center-of-mass systems. Cross section data for symmetric collision systems of Ar^{2+}/Ar, Ar^{3+}/Ar, Kr^{2+}/Kr and Kr^{3+}/Kr were reported in details [1] [2]. In these symmetric collision systems, it was known that low energy collisions were dominated by an attractive potential due to induced dipole, symmetric resonant charge transfer cross sections σ_{q0} of $A^{q+} + A \rightarrow A + A^{q+}$ for q=2 and 3 increased with the decrease of collision energy at the end energy measured and their cross section values almost agreed with a half of the classical orbiting cross section (Langevin cross section), $\sigma_L = 2\pi q(\alpha/2E_{cm})^{1/2}$, where α is the polarizability of the target atom [5].

Generally, the doubly charged rare gas ions of Ne^{2+}, Ar^{2+} and Kr^{2+} produced by a conventional electron impact type ion source include low-lying metastable states of $^1D_2$ and $^1S_0$ added to the ground state of $^3P_{1/2,3/2}$. Practically, σ_{21} and σ_{20} measured in collision systems of Ar^{2+}/He and Kr^{2+}/He except for Ne^{2+}/He strongly depended on electron impact energies. So, the electron impact energy of E_e for production of the projectile ions used is shown in each graph. From the pressure dependence of product ions, partial cross sections were determined of $\sigma_{21}(^1D_2)$ and $\sigma_{21}(^3P)$ in Ar^{2+}/He system and of $\sigma_{21}(^1S_0)$ and $\sigma_{21}(^1D_2)$ in Kr^{2+}/He. That a very steep threshold structure of σ_{21} in Ne^{2+}/He appears at $E_{cm} \approx 16$ eV is quite different from others and very interesting.

3.3. Part C: Charge transfer of multiply charged ions from the mini-EBIS

In the part C, charge changing cross sections of multiply charged ions extracted from the mini-EBIS are presented in graphs and tables. The metastable state ions very frequently include in the primary beam from a plasma based ECR-type ion source and such contaminants can have significant and dramatic effects on the observed cross sections. However it should be noted that the source used in the present experiment is of a different type and the pressure in the mini-EBIS under operating collisions was lower than 10^{-9} Torr. At such low densities, metastable ions even if they are produced will be quenched during long confinement times in the DC operation and there is little probability of metastable production via electron capture collisions. We have found no evidence of metastable ions in beams from the mini-EBIS except for C^{2+} and O^{2+} beams. Some of presented data already were detailed in [6] for He^{2+}/He and He^{2+}/H_2, in [7] for He^{2+}/CO, N_2 and O_2, and Kr^{q+}/Ne, N_2, O_2 and CO (q=7-9), in [4] for C^{4+}, N^{4+} and O^{4+}/He, in [8] for C^{4+}/Ar and $C_nH_{2(n+1)}$ (n=1~4), in [9] for C^{4+}/H_2, N_2 and O_2, in [10] for Ar^{q+}/H_2 (q=6-9,11), in [11] for Ar^{q+}/He (q=6-9,11) and I^{q+}/He (q=24-26), in [12] for Ar^{q+}/Ne, and in [13] for C^{q+}/He and H_2 (q=2-5). In these measurements, the product ions are identified by q'/m for the final charge states of q' and measured cross sections include contributions from the transfer ionization processes in addition to the pure electron capture cross section.

At low collision energies, the collision dynamics changes drastically giving rise to various new effects on the charge transfer reactions. The Coulomb electric field created by the ionic charge polarizes the neutral target and an ion-induced dipole leads to a mutual attraction between the collision partners. The induced dipole interaction can capture the ion in a spiraling trajectory closing to the target at sufficiently small impact parameters and the trajectory takes a circular orbit around the target at an appropriate impact parameter [5]. At sufficiently low collision energies where the collision is dominated by the ion-induced dipole, the orbiting cross section is enhanced in inverse proportion to the collision velocity. In various thermal reactions of singly charged ions, almost all reaction rates are constant. This signature is well known as the orbiting effects due to the ion-induced dipole interaction.

As the ionic charge-state becomes large, the enhancement of cross section due to the orbiting effects should be observed even at energies far much higher than thermal energy. This expectation was my initial motivation to start cross section measurements with multiply charged ions at low energies. It has been successfully confirmed that almost all measured charge transfer cross sections tend to increases at the low energy end studied [10],[11]. Only for Ar^{6+}-H_2 collisions there is Penning trap data at near thermal energy [14]. The thermal energy data places just on an extrapolation line of our single charge transfer cross sections converging to the Langevin cross section σ_L at the low energy end studied [5]. This agreement newly gives us rise to a fundamental interest how far the cross section goes up with decreasing collision energy. Furthermore, quantum mechanically orbiting resonance has been predicted that leads to sharp structures in the electron capture probability caused by the drastically increasing of the interaction time between the collision partners [15][16]. The experimental verification of the orbiting resonance is still one of future experiments with highly charged ions at low energies.

In slow collisions of He^{2+} and Kr^{8+} highly charged ions with H_2, N_2, O_2 and CO, charge transfer processes followed by fragmentation have been perfectly resolved by a new triple coincidence technique for three particle detection using twin OPIG systems [17]. Some new phenomena relevant to collision dynamics and oriented fragmentation have been found at low energies. The OPIG technique is very useful to trap and transport slow charge particles. Recently, Groningen's group also has applied the OPIG in state-selective electron capture experiments with slow highly charged ions [18][19].

3. References

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Summary Report on Research Project 10237/R0: State selective charge transfer at low energies

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Participants: G. Lubinski, Z. Juhasz, J.W. Turkstra, D. Meyer, R. Morgenstern.

Within the Co-ordinated Research Project on "Charge exchange cross section data for fusion plasma studies" the main objective of the KVI Atomic Physics group has been the production, assessment and recommendation of fundamental atomic physics data for fusion plasma research. The emphasis has been on charge transfer reactions between multicharged ions (A^{q+}) and neutrals (B), at energies of divertor and scrape-off-layer relevance. The electron transfer processes are schematically given by:

$$A^{q+} + B \rightarrow A^{(q-1)+}(nl) + B^{+}$$

with *nl* the principal and angular momentum quantum numbers of the state into which the donor electron is captured. Subsequentely to this reaction the $A^{(q-1)+}(nl)$ ion decays under photon emission, the process on which both passive and active charge exchange recombination spectroscopy (CXR) diagnostics is based.

For the diagnostics and modelling of divertor and edge-plasma regions, cross sections for collision energies well below 1 keV/amu are needed. We redesigned, reconstructed and took into operation a set-up to perform experiments in this yet unexplored low-energy regime. Ion beams were successfully decelerated down to energies as low as a few eV/amu.
First experiments were performed with He^{2+} and and He-like C^{4+}, N^{5+} and O^{6+} ions colliding on molecular hydrogen. These systems were chosen because, except for O^{6+}, there exist recent, elaborate quantum mechanical calculations for comparison. For He^{2+}, in accordance with theory we find that at low energies two-electron capture dominates fully over one-electron capture. But, the absolute values differ by a factor of 3 and in addition the final state distribution which determines the photon emission is distinctly different from theory. For N^{5+}, the experimental cross sections are much larger, more than an order of magnitude, than predicted by theory. Below 20 eV/amu, the dominant capture channel $N^{4+}(3s)$ is a factor of 1000 more efficient than predicted by theory. For C^{4+} ions the differences between theories and experiment are smaller but still considerable.

Altogether, all this seems to imply that low-energy charge-transfer calculations need to be considerably improved before they can be considered as a reliable basis for modelling and diagnostics of the scrape-off-layer and divertor regions in fusion plasma reactors.

On the database and modelling side work has been done in collaboration with the group of Summers (University of Strathclyde and JET Joint Undertaking) and the group of HP. Winter (Vienna) and J. Schweinzer (Garching). For Li beam based diagnostics, we have given support to the final data sets for diagnostics as prepared by the Vienna-Garching collaboration. The new assessments (Summers and coworkers, including the KVI group) of neutral beam stopping and excitation data led for the first time to agreement on an absolute scale of observed and calculated neutral beam densities and beam emission intensities.

Output (partly) related to the CRP on: "Charge exchange cross section data for fusion plasma studies"

Electron and neutral interactions with impurities in divertor plasmas
H.P. Summers, H. Anderson, N.R. Badnell, F.W. Bliek, M. Brix, F.J. de Heer, R. Hoekstra, D.C. Griffin, L.D. Horton, C.F. Maggi, M.G. O'Mullane and M.S. Pindzola
Plasma Phys. Rep. **25** (1999) 15

Lithium excitation by slow H^+ and He^{2+} ions
J.W. Turkstra, D. Meyer, R. Hoekstra, R. Morgenstern and J. Schweinzer
Phys. Rev. A. **60** (1999) 4627

Database for inelastic collisions of lithium atoms with electrons, protons and multiply charged ions

J. Schweinzer, R. Brandenburg, I. Bray, R. Hoekstra, F. Aumayr, R.K. Janev and HP. Winter
At. Nucl. Data. Tabl. **72** (1999) 239

Electron capture by slow multicharged ions from atoms, molecules and surfaces
R. Hoekstra and R. Morgenstern
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H. Anderson, M. von Hellermann, R. Hoekstra, L.D. Horton, A.C. Howman, R.W.T. Konig, R. Martin, R.E. Olson and H.P. Summers
Plasma Phys. Controll. Fusion. **42,** 781 (2000)

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EuroPhys. Lett. **49,** 41 (2000)

State selective electron-capture cross section measurements for low-energy collisions of He-like ions on H_2
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J. Phys. B: At. Mol. Opt. Phys. **33,** 5275 (2000)

Low-energy state-selective charge transfer by multiply charged ions
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Phys. Rev. Lett. **86,** 616 (2001)

Cross sections for electron capture from atomic helium by fully stripped ions

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Abstract

We give tables of theoretical cross sections for single electron capture from helium by fully stripped projectile ions with nuclear charge (Z) from 1 to 20, in the energy range 80–10000 keV/amu.

1 Introduction

The data produced in the present compilation has been obtained using the Continuum Distorted Wave (CDW) theory where the interaction between the active electron and the target is represented by model potential. We summarize the main concepts of the theory and refer to the literature for full details.

The energy range we are interested in corresponds to the intermediate and high impact energy range for which the first order of perturbative theories (eg. first-Born) is inadequate. At intermediate impact energies the response of the target atom to the projectile field is highly non linear while at high projectile velocities the contribution of double scattering can not be neglected. The usefulness of the CDW theory for describing the electron capture process in the energy range considered has been demonstrated by the comparison with experimental results in a number of previous studies [1, 2].

2 Theory

It is well known that perturbative methods such as a the Born series can not be applied in the case of long range potentials like the Coulomb interaction. The CDW approximation was proposed by Cheshire [3, 4] as a solution to this problem in the case of electron capture. It can be shown that it is a first order of a distorted-wave series and that this series is free of divergences arising from the incorrect treatment of the Coulomb potential [1, 2]. This model belongs to a family of multiple scattering approaches based on the Distorted-Wave Theory and includes contributions from higher order scattering terms in the conventional Born series [2]. Despite a few deficiencies discussed in [5] the CDW model has major advantages: (i) it accounts for the long-range behavior of the Coulomb potential and includes distortions in the entrance and exit channels on equal footing, (ii) the scattering amplitude is given analytically in the case of Coulomb potentials, (iii) the model gives reasonable agreement with experiments for a number of collision systems.

The extension of the CDW model to the case of multi-electronic targets has been done within the framework of the one active electron picture [1]. In this model there is only one active electron which is captured by the impinging projectile while the others remain frozen. Up to now this extension of the model has been limited by the use of Coulomb wave functions with an effective charge to describe the distortion by the residual target. This means that the potential created by the passive electrons is approximated by a Coulomb field. The major problems with this representation is that the target potential is chosen differently in the entrance and exit channels and that in many cases the Coulomb field is not accurate enough, specially at small distances, to represent the field produced by the passive electrons.

In a recent extension of CDW model these problems were solved by the use of spherically symmetric model potentials to represent the potential due to the projectile and target nuclei and the passive electrons bound to them in both the initial and final channels [6]. Therefore the active electron evolves in a two center potential defined by these two model potentials. This allows for a more accurate description of the initial-target and final-projectile bound states and of the distortions in both channels. Here we give the main points in the generalization of the CDW theory and refer to [6, 7] for full details.

Let us consider the transfer of one electron from the target atom B to a projectile ion A. Z_B and Z_A denote the residual-target and projectile charge respectively. The potentials V_A (V_B) describes the interaction between the active electron and the projectile (residual target). In the pure three-body problem the continuum distorted waves are introduced as follows [3, 4]:

$$\begin{aligned} \xi_i^+ &= \varphi_i(\boldsymbol{x})\, E_{i,-\boldsymbol{v}}(\boldsymbol{r})\, N(\nu_A)\, {}_1F_1(i\nu_A; 1; ivs + i\boldsymbol{v}\cdot\boldsymbol{s}) \\ &= \varphi_i(\boldsymbol{x})\, E_{i,-\boldsymbol{v}}(\boldsymbol{r})\, D^+_{-\boldsymbol{v}}(Z_A, \boldsymbol{s}) \\ &= \varphi_i(\boldsymbol{x})\, E_{i,-\boldsymbol{v}}(\boldsymbol{r})\, \exp(i\boldsymbol{v}\cdot\boldsymbol{s})\, \psi^+_{-\boldsymbol{v}}(Z_A, \boldsymbol{s}) \end{aligned} \qquad (1)$$

$$\begin{aligned} \xi_f^- &= \varphi_f(\boldsymbol{s})\, E_{f,\boldsymbol{v}}(\boldsymbol{r})\, N(\nu_B)\, {}_1F_1(-i\nu_B; 1; -ivx - i\boldsymbol{v}\cdot\boldsymbol{x}) \\ &= \varphi_f(\boldsymbol{s})\, E_{f,\boldsymbol{v}}(\boldsymbol{r})\, D^-_{\boldsymbol{v}}(Z_B, \boldsymbol{x}) \\ &= \varphi_f(\boldsymbol{s})\, E_{f,\boldsymbol{v}}(\boldsymbol{r})\, \exp(-i\boldsymbol{v}\cdot\boldsymbol{x})\, \psi^-_{\boldsymbol{v}}(Z_B, \boldsymbol{x}), \end{aligned} \qquad (2)$$

with

$$E_{n,\boldsymbol{u}} = \exp\left[i\frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{r} - i\frac{1}{8}u^2 t - i\epsilon_n t\right], \qquad (3)$$

where $\boldsymbol{s}$, $\boldsymbol{x}$ and $\boldsymbol{r}$ denote the position vectors of the active electron with respect to a reference frame fixed at the target and projectile nucleus, and to the mid-point of the internuclear separation, $\boldsymbol{v}$ is the collision velocity, ${}_1F_1$ denotes the hypergeometric function and $\epsilon_{i,f}$ are the binding energies of the active electron in the initial and final states. In the present case, the bound φ and continuum ψ wave functions are obtained from the numerical solutions of the eigen equations:

$$\left(-\frac{1}{2}\nabla^2_{x,s} + V_X - \epsilon_{i,f}\right)\varphi_{i,f} = 0 \qquad (4)$$

$$\left(-\frac{1}{2}\nabla^2_{x,s} + V_X - v^2\right)\psi^{\pm}_{\boldsymbol{v}} = 0 \qquad (5)$$

where V_X is the model potential, $\nu = Z_X/v$ and $N(\nu) = \exp(\nu\pi/2)\Gamma(1 - i\nu)$ (X stands for A and B).

Using the straight line version of the impact parameter approximation, the transition amplitude for capture is given by:

$$T_{if}(\boldsymbol{\eta}) = -N(\nu_A)\, N(\nu_B)\, \boldsymbol{I}_A \cdot \boldsymbol{J}_B, \qquad (6)$$

where $\boldsymbol{\eta}$ is the transverse component of the momentum transfer, and $\boldsymbol{I}_A$ and $\boldsymbol{J}_B$ are defined as follows:

$$\boldsymbol{I}_A = \int \mathrm{d}\boldsymbol{s}\, \exp(i\boldsymbol{\rho}_A \cdot \boldsymbol{s})\, \varphi_f^*(\boldsymbol{s})\, \boldsymbol{\nabla}_s D_{\boldsymbol{v}}^+(Z_A, \boldsymbol{s}) \tag{7}$$

$$\boldsymbol{J}_B = \int \mathrm{d}\boldsymbol{x}\, \exp(i\boldsymbol{\rho}_B \cdot \boldsymbol{x})\, D_{-\boldsymbol{v}}^-(Z_B, \boldsymbol{x})\, \boldsymbol{\nabla}_x \varphi_i(\boldsymbol{x}) \tag{8}$$

with

$$\boldsymbol{\rho}_{A,B} = \pm\boldsymbol{\eta} - \left(\frac{v}{2} \pm \frac{\epsilon_i - \epsilon_f}{v}\right) \hat{\boldsymbol{v}} \tag{9}$$

where the +(−) sign corresponds to the label A (B). The integrals $\boldsymbol{I}_A$ and $\boldsymbol{J}_B$ can be evaluated numerically (see ref. [7] for details).

The total cross section is obtained as:

$$\sigma_{if} = (2\pi v)^{-2} \int \mathrm{d}\boldsymbol{\eta}\, |T_{if}(\boldsymbol{\eta})|^2 \tag{10}$$

We have applied this generalized CDW model for the calculation of the total cross sections for single electron capture from helium by bare projectile impact. The charge of the impinging ions range from 1-20 and the collision energies from 80 keV/amu to 10 MeV/amu. The interaction of the active electron with the $He+$ ion was represented by the Hartree-Fock-Slater potential [8]. The cross sections were calculated to selective (characterized by the quantum numbers n, l and m) final bound states and the sum of them over l and m are presented for a given n manifold in the tables. The sum of the state selective cross sections, calculated using the n^3 rule, are also given in the last line of a given table:

$$\sigma_{all} = \sum_{n=1}^{7} \sigma_n + 4.53\sigma_8, \tag{11}$$

provided that $\sigma_8 < \sigma_7 < \sigma_6$, where σ_n is the sum of the cross section for capture to each final bound state with principal quantum number n. All cross sections are given in cm^2. Dashes indicate entries which have been omitted because they are outside the domain of validity of the CDW model [1] defined by E(keV/amu) $\geq$ 80 sup($|\ \epsilon_i\ |$, $|\ \epsilon_f\ |$).

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Extension of model potential methods to treat charge transfer in open shell systems. Application to the Si^{3+}/He, He^{2+}/ He (2^1S) and He^{2+}/ He (2^3S) systems

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Abstract

Charge transfer reactions in ion-atom collisions are investigated theoretically for systems involving open-shell configurations. Both model potential and ab-initio methods are used to treat the adiabatic states of the collision complex. A quantum mechanical treatment of the collison dynamics is used. Electron capture cross sections for two representative systems (He^{2+} in collsion with either 2^1S or 2^3S metastable He and for Si^{3+} with ground state He) are calculated in the eV-keV energy range.

Introduction

Model potential methods have proved very successful in the theoretical treatment of the dynamics of charge transfer by multiply charged ions A^{q+} from atomic H targets. Experiments show that these methods are excellent not only for closed shell ions such as C^{4+}, N^{5+}, O^{6+}, Al^{3+}, $Si^{4+}$and Ar^{8+}[1-6] but also for closed sub-shells such as N^{3+}, $Si^{2+}$and Ar^{6+} [7,8]. Basically, the reason is that charge transfer occurs at relatively large internuclear distances, primarily by electron capture into excited Rydberg states of $A^{(q-1)+}$. As a consequence, the ionic core A^{q+} plays a passive role and its effect can often be adequately described by an effective (or model) potential. This greatly simplifies the computation of the network of adiabatic molecular potentials (and non-adiabatic matrix elements) of the collision complex. For ions with charge q=2 charge units, such networks reveal a finite number of effective avoided crossings, which control the charge transfer process. And since the non-adiabatic coupling is dominant only in the vicinity of avoided energy crossings, a fairly small (usually less than 10) basis set of adiabatic states is sufficient to describe the charge transfer process (at least for q=6). With a simple modification [8], the model potential methods can also be adapted to deal with a restricted class of two active electron systems involving single electron capture from ground state He targets. Systems such as Si^{4+}/He and Ar^{6+}/He have been successfully treated in this way [8, 9]. In this presentation, we consider an extension of the model potential approach to treat systems in which either the ion or the neutral target has an open-shell configuration. We shall consider two such systems, which are representative of two different types of processes. The first involves capture by a structureless ion from a neutral target in an excited open-shell configuration, the second capture by an open-shell ion from a ground state neutral target.

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VIBRATIONALLY RESOLVED CHARGE TRANSFER AND IONISATION CROSS SECTIONS FOR ION-$H_2(D_2, DT, T_2)$ COLLISIONS

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ABSTRACT

In the CRP on charge exchange we presented theoretical semiclassical (*ab initio* and model potential) vibrationaly resolved cross sections for charge transfer in collisions between multicharged ions (A^{q+}) with H_2, using the Sudden and Franck-Condon approximations, for impact energies 40 - 2000 eV/amu. In some cases, a close-coupling vibronic expansion was also employed. At higher energies, the Classical Trajectory Montecarlo (CTMC) method was used to study single electron capture (SEC) and ionization (SI). The influence of metastable states in the ionic beam , and the effect of anisotropy have also been analyzed.

INTRODUCTION

Charge transfer cross sections in collisions of multicharged ions with molecules are of interest in the outer regions of the plasma in fusion devices, particularly near divertors. We have presented calculated cross sections for collisions of ions with H_2 (D_2, DT and T_2) for energies above 40eV/amu, using the semiclassical eikonal method for fixed H_2 target position, and nuclear rectilinear trajectories with impact parameter $\boldsymbol{b}$ and velocity $\boldsymbol{v}$, $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$, the sudden and the Franck-Condon (FC) approximations to treat the ro-vibrational motion of the diatom, [1]. The electronic wavefunction can be written in terms of *ab initio* triatomic AH_2^{q+} molecular functions, $\phi_k(r; \boldsymbol{R}, \rho)$, obtained with MELD [2],[3], and including a common translation factor (CTF) [4, 5] as:

$$\Psi(\boldsymbol{r},\rho,t) = \chi_0(\rho) Y_{JM}(\hat{\rho}) \sum_k a_k(\rho,t)\phi_k(\boldsymbol{r};\boldsymbol{R},\rho)\exp\left(-i\int_0^t \varepsilon_k \, dt'\right) \tag{1}$$

where $\chi 0(\rho) YJM(\hat{\rho})$ is the initial rovibrational wavefunction of H_2.

Probabilities for transitions from the vibronic state *{0i}* to *{vf}* are:

$$P_{vf}(v,\hat{\rho}) = \left| \int d\rho \chi_0 \chi_v \exp\left[-i\int_0^\infty dt(\varepsilon_f - E_f)\right] a_f(\infty,\rho) \right|^2 \tag{2}$$

and state-to-state vibrational cross sections

$$\sigma_{vf}(v) = \frac{1}{4\pi}\int d\boldsymbol{b} \int d\hat{\rho}\, P_{vf}(\boldsymbol{v},\hat{\rho}). \tag{3}$$

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[1] Also at Instituto de Estructura de la Materia CSIC, Serrano 113 bis, 28006 Madrid, Spain

have been calculated in collisions of Be^{4+}, C^{4+} [6], H^+ [7] and $C^{2+}(^3P)$ [8] with H_2 in the impact energy range 50eV/amu–2keV/amu. Significant deviations from the simple FC approximation were found.

At high impact energies (9–625keV/amu for SEC and 9keV/amu–2.5MeV/amu for SI) classical trajectory and model potential calculations have been carried out [9]. When effective potentials are used , a two-electron interpretation is required to evaluate transition probabilities and cross sections. We have studied the accuracy obtained with the usual equivalent-electron independent particle model (IPM) approach, [10], and with the new IPM-SEC method.

RESULTS

$H^+ + H_2(X^1\Sigma_g^+, v)$

We have presented SEC vibrationally resolved cross sections using the sudden approximation [7]. At the lowest energies considered, a preliminar vibronic close-coupling calculation using 14 (7+7)states has been performed. The excelent agreement obtained with experimental data for capture of Gealy and van Zyl [11] shows the energy range where the Sudden approach is valid. We also calculated the capture to dissociative vibrational states (DC), total vibrational excitation (VE) and dissociative excitation (DE) cross sections, for H_2, D_2, DT, and T_2 targets.

$Li^+ + H_2$

A FC 5-electronic-state calculation for the system LiH_2^+ was performed [7]. Anisotropic effects are very important, and orientation averaged cross sections for SEC to Li(2s,2*l*)+ H_2^+ and excitation to $H_2(B\,^1\Sigma_u^+)$ were calculated.

$C^{2+} + H_2$

The influence of the presence of metastable $C^{2+}(2s2p;^3P)$ ions in the incident beam has been analyzed. Dynamical calculations using 13- and 16- states were performed for the ground $(2s^2;^1S)$ and metastable $(2s2p;^3P)$ states of C^{2+} using the FC and sudden approaches respectively ([12], [8]). In the later case, vibronic cross sections to were obtained for the process:

$$C^{2+}(2s2p;^3P) + H_2(X^1\Sigma_g^+, v=0) \rightarrow C^+(2s2p^2;^2D) + H_2^+(\Sigma_g^+, v'). \qquad (4)$$

and compared to the (improved) TES measurements of [13] at *E*=*1*keV. The very good agreement obtained for the vibrational distribution of H_2^+, confirms the accuracy of the sudden approximation method and of the experimental data.

$C^{3+} + H_2$

Preliminar calculations obtained using the FC approximation, collinear geometry and a basis of 8 electronic states, showed that DEC cross sections leading to Coulomb explosion, were competitive with SEC.

$C^{4+}+H_2$

A basis of 8 electronic molecular states and the sudden approximation were used ([6]) to calculate state-selected (vibrational and electronic) cross sections in SEC, as well as cross sections for transfer dissociation and vibrational excitation in collisions with H_2, D_2 and DT at impact energies below 1 keV/amu.

At higher energies (E≤6keV/amu), we have employed the FC IPM-SEC model approximation, (see [14]), to get partial SEC cross sections, using a basis set of 20 MOs and the CTF of ref. [5], obtaining a good comparison with experimental data and with the more accurate sudden calculations.

$N^{5+}+H_2$

A model potential FC IPM-SEC treatment with 8 molecular states has been used, with a more sophisticated two-center model potential to improve the representation of the *H2* target. An overall agreement with experimental data of [15], for the total SEC cross section to $N^{4+}(n=3)+H_2^+$ is obtained.

More elaborate *ab initio* (sudden) calculations are required at lower velocities, including double capture N^{3+}*(3l3l')* states, (not considered in our preliminar treatment).

CTMC calculations

SEC and single ionisation (SI) cross sections for H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+} in collisions with H_2, were presented using the improved impact parameter CTMC treatment (see [9]). The calculation employs the FC approximation and a model potential for the H_2 target. Comparison of our results with experimental and other theoretical data show a fair agreement.

Calculated cross sections for SEC and SI allowed us to obtain scaling laws as functions of the charge q of the projectile and velocity v,

$$\sigma_{SI}^{scaled}(q,vq^{0.11})=\sigma_{SEC}(1,v)q \tag{5}$$

$$\sigma_{SI}^{scaled}(q,v)=\sigma_{SI}(1,v)q^{2\{0.92-\exp[-0.57(v-0.01q)]-\exp\left[-1.8(v^2-0.08_q)\right]\}} \tag{6}$$

Concluding Remarks

The combined implementation of the Quantum Chemistry SCF-MRDI MELD packet and of the sudden approach to describe the vibro-rotational motion of the diatomic target, leads to vibrationaly resolved charge exchange cross sections in ion-H_2 collisions with a similar accuracy to those of ion-atom. A detailed treatment of the anisotropy in the ion-target interaction has also been considered. Calculations involving projectiles in both ground and metastable states were carried out and compared with experimental data to asses the purity in the composition of the initial beams.

Acknowledgments

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SUMMARY

Title

Cross-section of electron capture by multiply charged ions from atoms and molecules of hydrogen and population of electronic state of created ions

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Period of Contract

1998 - July 2001

Scientific Background and Scope of Project

The purpose of experimental measurements and theoretical calculations within our Contract is to enrich the available data on the processes of Single–Electron Capture (SEC) and Double–Electron Capture (DEC) by alpha particles and multiply charged ions from hydrogen molecules and atoms, helium atoms and helium like and lithium like ions.

Experiment

The experiment includes measurements of absolute values of state selective cross-sections at collisions with alpha particles (the product of thermonuclear reaction) and multiply charged ions of Ar and Ne as possible additional artificial impurities to cool outer edge of thermonuclear plasma..

Data concerning ionization and dissociation of hydrogen molecules by alpha-particles and dissociation cross-sections of H_2^+ ions are needed for estimation of potentialities of method of determination of magnetic field direction and current density distribution over tokamak plasma column cross section (Q-factor) using hydrogen molecule diagnostic beams

Theory

The ion-ion collision system are less suitable for experimental study and there is increasing demand of appropriate data for nuclear-fusion research and astrophysics. The purpose of theory within the project was to calculate SEC and DEC including absolute values of state selective target excitation cross section at collisions of alpha particles with hydrogen molecules, He–like C^{4+}, N^{5+}, O^{6+} ions and with Li-like and Be-like C^{3+}, C^{2+} ions – the impurities released from tokamak surfaces.

Experimental and Theoretical Methods

Experiment

For measurements of cross-section of charge and electronic state change processes of particles we used well known methods of collision spectroscopy and scattering.

The initial ion beam goes through a gas target. Slow recoil ions are extracted by electric field and analyzed by magnetic field or TOF analyzer. Fast particles after interaction are analyzed in scattering angle with resolution about some angular minutes and in kinetic energy by electrostatic analyzer with resolution about 4000. Monoenergetic initial multiply charged ion beam had energy spread about 0,4 eV*z. Pulses produced by detectors of recoil and scattered particles with definite charge state formed in one binary ion-atom collision were registered in counting regime and analyzed by time delayed coincidence circuit to separate the process of charge state change.. Registration efficiency of detectors was defined experimentally.

Thus, this device allows us to measure absolute values of cross-sections of charge state change elementary processes and population of electronic states of ions with lower charge formed in the processes of one or two electron captured.

Theory

All theoretical results were obtained in the framework of close coupling equation method with quasimolecular states as a basis for each collision system using our program package for a study of inelastic atomic collisions. Many-electron states as well as the matrix elements of dynamic and potential couplings between them were calculated by using the basis set of screened quasidiabatic molecular orbitals.

Results obtained

Experiment

1-st.year

The absolute values of cross sections of different processes of charge states change of colliding particles at He^{+2} -H_2 interaction alpha-particles in kinetic energy range of 2 - 100 KeV have been measured. Final charge states of helium particles were 0, 1 and 2, final states of hydrogen system are H_2^+, H^0+ H^+ and H^++H^+.

The absolute values of cross sections of electron capture to the electron levels of He with n=1, 2 and 3 at He^{+2}-H_2 collisions have been measured at scattering velocities of alpha-particles (2 – 10) *10^7 cm/s. Cross sections of electron capture without dissociation of molecular ions increase monotonously for n=2 from 2*10^{-17} cm^2 to 8*$10^{-16}$$cm^2$; for n=3 from 1,3*$10^{-18}$ to 8*10^{-17} cm^2; and for n=1 from 2*10^{-19} to 1*10^{-17} cm^2. At electron capture with dissociation H_2 the He^+ ions are created in ground electron state 1s. The value of cross section at v= 1,5*10^7 cm/s reaches 7*10^{-16} cm^2.

2-ed year

The absolute values of electron capture cross sections by He^{+2}, Ar^{+z} (z= 3 – 6) and Ne^{+z}(z=3 and 4) from hydrogen atoms to different electronic states including ground states have been measured. The measurements have been done in collision velocity range of projectile ions:
He^{+2} -v= 5,13 – 13,9 *10^7 cm/s; Ne^{+3} v=1,7 – 5,84 *10^7 cm/s; Ne^{+4} v= 1,96 – 6,74 *10^7 cm/s; $Ar^{=4}$ v= 0,98 – 4,79 *10^7 cm/s; Ar^{+5} 1,1 – 5,35 *10^7 cm/s; Ar^{+6} v= 0,8 – 5,87 *10^7 cm/s.

3-d year.

The installation for separate measurement of population degenerated 2p and 2s state of He^+ ions formed in one electron capture by alpha-particles from helium atoms has been constructed and assembled. The measurements are under study now

.

Theory

1-st.year

New data on DEC processes in He^{2+} – H_2 collision at the energies of alpha-particles 4 – 80 keV and besides some partial and angle differential SEC cross sections were obtained.

2-ed year.

SEC, DEC and excitation cross sections in collisions between He^{2+} projectile and C^{4+}, N^{5+}, O^{6+} target ions were calculated in the energy range 50 keV – 3, 4, 5 MeV (The different high energy limits of He^{2+} kinetic energy for and C^{4+}, N^{5+}, O^{6+} target depended on whether the velocity of the projectile is lower than that of target electrons).

The maximum values of SEC cross sections were obtained equal to ~ 2.10^{-18}, 6.10^{-19} and 3.10^{-20} cm^2 for C^{4+}, N^{5+} and O^{6+} ions respectively. The maximum values of DEC and total excitation cross sections were obtained equal to 4.10^{-20}, 2.10^{-21}, 7.10^{-22} cm^2 and 4.10^{-16}, 2.10^{-16}, $1,5.10^{-22}$ cm^2 respectively.

3-d year

a) Reliable data on total and state-selective cross sections of SEC and for the first time on excitation processes in collision of alpha-particles with Li-like C^{3+} ions were obtained at collision c.m. energies 2 –200 keV.
b) Data on SEC and neutralization of alpha-particles in their collision with Be-like C^{2+} ions were obtained for the first time at c.m. energies from 0.1 keV to 60 keV.

Conclusions

The calculated total SEC, DEC and excitation cross sections in He^{2+} – H_2 collisions and for ion-ion collisions He^{2+} – C^{2+}, C^{3+}, C^{4+}, N^{5+}, O^{6+} may be used in modeling of processes involving alpha particles in thermonuclear plasma.

i) Publications on Work done under Contract

1. V.K.Nikulin and N.A.Guschina, «Two-electron description of excitation and charge-transfer in ion-ion He^{2+}– C^{4+}, N^{5+} , O^{6+} collisions». Preprint of Ioffe Physical-Technical Institute N 1740, St. Petersburg, 2000, 27 p.
2. V.K.Nikulin and N.A. Guschina, Electron Capture and Excitation in Ion-Ion Collision of Alpha-particles with He-like HCI. X Int. Conf. on the Physics of Highly Charged Ions, Book of Abstract, Berkley 2000.
3. V.K.Nikulin and N.A. Guschina, Multistate Quasimolecular Basis Treatment of He^{2+} – $C^{3+}(1s^2 2s)$ Collisions. Differential and Total Cross Sections. XXI ICPEAC, Japan, 1999, p. 586

4. V.K.Nikulin and N.A. Guschina, «Multistate molecular treatment of He^{2+}– H, $^3C^{3+}(1s^22s)$ collisions in impact parameter approximation. Differential and total charge-exchanged cross section'. Preprint of A.F.Ioffer Physical-Technical Institute N1712, St. Petersburg, 1998, 12 p.
5. N.A. Guschina and V.K.Nikulin, «The program package for inelastic process computation in slow ion-atom collisions'. Preprint of A.F.Ioffer Physical-Technical Institute N1717, St. Petersburg, 1998, 66 p.

Summary Report of Dr. Fritsch

Within the CRP on Charge Exchange Cross Section Data for Fusion Plasma Studies, theoretical studies have been performed for slow Be2+ - H, N4+ - H, N7+ - H, and N7+ - He collision systems. These studies have been done within the semiclassical close-coupling method, with atomic orbitals and atomic-orbital-like pseudostates representing the motion of the one or two active electrons in those systems. Studies within this method are known to allow the reliable prediction of transition cross sections for electron transfer and electron excitation, including the distribution of these cross sections over the final states of the ion or atom. An assessment of ionization cross sections in slow collisions is also possible.

For Be2(1s**2)+ - H collisions, electron transfer into the Be+(1s**2 nl) states (n=2-4) and electron excitation to the H(2l) states has been determined between 0.1 and 50 keV/u projectile energies. The transfer process populates predominantly the 2l states in the Be+ ion, the calculated cross sections agree there with a simple PSS study (Wetmore et al. 86) and also with unpublished cross sections by Kimura. The recommended cross sections in the tabulation by Janev et al. (95) however turn out to be a factor of ten too low.

R.K. Janev, HP. Winter, W. Fritsch, Chapter 13 in Atomic and Molecular Processes in Fusion Edge Plasmas, ed. R.K. Janev, Plenum, New York 1995, p. 341

The situation for Be2+ - H collisions is reminiscent of that for Be2+ - He collisions. There a two-electron study with atomic basis sets (Fritsch 96) predicts transfer cross sections that are up to a factor of ten (at 2 keV/u) larger than a MO calculation (Shimakura 96) predicts. The two-electron study blends smoothly with a one-electron model calculation (Wang 96) at the higher energies.

W. Fritsch, Physica Scripta T62 (1996) 59.
N. Shimakura, S. Suzuki, Y. Murakami, J.P. Gu, G. Hirsch, R.J.
Buenker, M. Kimura, I. Shimamura, Physica Scripta T26 (1996) 39.
Y.D. Wang, N. Toshima, C.D. Lin, Physica Scripta T26 (1996) 63.

The N4+ - H system has been studied between 0.06 and 10 keV/u with a two-electron model that describes the motion of the two active electrons, one initially in the 2s state of the N4+ ion and the other in the 1s state of H. Electron transfer cross sections have been determined separately for the singlet and the triplet final states of N3+(3l3l'). The results agree with existing data sets if they are assigned larger error bars than the authors do – a plausible procedure which is also suggested by the scatter of within the data themselves. Structures in the energy dependence of total transfer, which are believed to be real by some experimentalists, are in the percent range in these calculations.

E.Y. Sidky, W. Fritsch, C.D. Lin, Phys. Rev. A 59 (1999) 1994.

Electron transfer in N7+ - H collisions has been studied between 10 and 70 keV/u for the N6+ n=5-10 final states. This has been the first study for this system that includes the full set of final states and all respective intercouplings. Also the transfer cross sections for collisions with an excited H(2s) target have been determined. For those however it would be desirable to have even higher excited final states in the basis as all the n=8-10 shells turn out to be dominantly populated.

In the N7+ - He system, the two-electron calculation predicts the N6+ n=4 shell to be dominantly populated in the collisions. Cross sections have been determined also for the N6+ n=5-7 shells between 7 and 90 keV/u.

The cross sections for the N7+ - H/He systems have not been published yet.

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Web: http://www-nds.iaea.or.at