International Atomic Energy Agency

INDC(NDS)-398

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

1st IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

September 24-25, 1998, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared by: R.K. Janev

February, 1999

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

INDC(NDS)-398

1st IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

September 24-25, 1998, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared by: R.K. Janev

February, 1999

Abstract

A brief description of the proceedings and the conclusions of the 1st Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies", held on September 24-25, 1999, at the IAEA Headquarters in Vienna, Austria, is provided. The conclusions of the Meeting regarding the data collection, assessment and generation priorities are also included in the report.

Reproduced by the IAEA in Austria
February, 1999

Table of Contents

1. INTRODUCTION

The 1st Research Co-ordination Meeting of the participants of the IAEA Co-ordinated Research Project (CRP) on "Charge Exchange Cross Section Data for Fusion Plasma Studies" was convened on September 24-25, 1998, at the IAEA Headquarters in Vienna, Austria. The objectives of the meeting were:

a) to review the available data on total and state-selective cross sections for electron capture processes in ion-atom (molecule) collisions of fusion relevant species;
b) to review the results obtained within the individual projects of the CRP during the first year of its existence;
c) to review the programmatic plans of CRP participants for the next period of the CRP duration;
d) to re-define the scope and objectives of the CRP to a realistic level that ensures that the essential needs for charge exchange data of fusion research community are met by the end of the CRP period; and
e) to agree on the strategy and methods of work co-ordination aiming at achieving the re-defined CRP objectives.

The meeting was attended by all chief scientific investigators of the individual CRP projects, except for Prof. A. Riera, Dr. R. Hoekstra and Dr. L. Gulyas. The list of Meeting Participants is given in Appendix 1.

2. BRIEF MEETING PROCEEDINGS

After the welcome address of the Scientific Secretary of the Meeting (R.K. Janev) and the adoption of Meeting Agenda (see Appendix 2), the meeting continued its work in four consecutive sessions.

The first session of the meeting (chaired by Prof. HP. Winter) started with the presentation of Prof. H.B. Gilbody on the recent cross section measurements of state-selective electron capture by slow multiply charged ions performed at Queen's University of Belfast. The results for a large number of collision systems studied recently at QUB by the TES method were presented. The ions and neutral targets involved in these studies include, among others, the fusion relevant species He^{2+}, C^{q+}, N^{q+}, O^{q+}, Ar^{q+}, Fe^{q+} and H, H_2, He, O, O_2, N_2, Ne, Ar. Prof. Gilbody also reported on the recent developments of the double TES (DTES) method at QUB, allowing an elegant and efficient resolution of the metastable ion beam fraction problem, and accurate state-selective electron capture cross section measurements by either ground state or metastable ions. Some examples and results of the use of DTES were also presented.

The second presentation in this session was given by Dr. W. Fritsch. Dr. Fritsch presented the results of his recent state-selective (and total) electron capture cross sections for the collision systems: Be^{2+} - H, He, N^{4+} - H and N^{7+} - H, He, and some preliminary results for B^{2+} - He. The calculations were performed by using the atomic-orbital expansion close-coupling method employing an adequately large basis set. The results were compared with the calculations of other authors and the experimental data, where possible. Dr. Fritsch outlined the plans for his future studies within the CRP, including more accurate calculations for the B^{2+} - He system.

The last presentation in this session was given by Dr. M. Kimura and was devoted to the electron capture processes from excited atoms and from heavy target atoms. Dr. Kimura presented state-selective and total cross sections for a large number of collision systems obtained by using the molecular-orbital expansion close-coupling method (in both its semi-classical and fully quantal versions). The molecular states used in the basis were obtained by the multireference single- and double-configuration interaction method. Cross section results were presented for the following systems: C^{2+} - H, H^+ - P, S, Be^{q+} - He, (q=2-4), Si^{2+} - He and H^+ - CH_4, C_2H_2. Dr. Kimura outlined the plans for his future work within this CRP.

The second session of the meeting (chaired by Prof. H.B. Gilbody) was devoted mainly to the results of experimental CRP projects. The first speaker in this session was Dr. M.N. Panov who presented the results of his project during the first year of its duration. The experimental part of this project was confined to a detailed study of all processes occurring in the collision system He^{2+} - H_2 in the energy range 1-100 keV. The used experimental techniques allowed to separate all reaction channels (including the state- and charge-selective ones) and determine their cross sections on an absolute scale. The processes of single- and double-electron capture, dissociative capture, single- and double-ionization, dissociative ion-pair formation were studied in detail, including (for some of them) their differential characteristics. Dr. Panov also presented the results of the theoretical calculations for the He^{2+} - He, H^{2+} - H, He^{2+} - O^{2+} and He^{2+} - H_2 collision systems performed by the theoreticians of the project (Dr. Nikulin and Dr. Gushtshina) by using a molecular-orbital based close-coupling method.

Dr. K. Okuno was the second speaker in this meeting session. He reported extensive cross section measurements for single- and multiple-electron capture in collisions of He^{2+} and $Kr^{(7-9)+}$ ions with Ne, CO, N_2 and O_2 in the energy region below 1 keV/amu. The measurements were done by using a mini-EBIS and the OPIG and a double-coincidence TOF technique for three particle detection. The cross sections for single- and multiple-(up to four) electron capture show a systematic behaviour in the considered energy region which can be qualitatively explained (and described) by a combination of the orbiting and over-barrier transition models. In the case of molecular targets, the processes of dissociative (single- and multiple)-electron capture and dissociative transfer-ionization were also studied. An outline of the future research plan of the project group was also presented.

The presentation of Prof. HP. Winter, that followed, was related to the recent studies of his group at TUW of the electronic- and vibrational-state resolved single electron capture processes in slow collisions of C^{2+}, N^{2+} and O^{2+} ions with H_2, N_2, and CO. The method used in these studies was TES, coupled with the attenuation method for determining the metastable primary ion beam fractions. Translational energy spectra were shown for selected ion-molecule collision pairs indicating clearly the vibrational structure of the product molecular ion. The experimental TES cross section results for the C^{2+} - H_2 collision system were shown and the progress in the study of other systems described.

The work of the session was closed with the presentation of Dr. B. Zygelman who reported on the progress in the development of a fully quantal MO-close-coupling package for state-selective electron capture cross section calculations at low-energy ion-atom collisions. The method, as developed at the present moment, was tested in detail for the N^{4+} + H system and comparison of the results was made with the MO-CC cross section calculations of other authors and with the experimental data. The package needs further enhancement by including rotational coupling and electron translation effects.

The third session of the meeting (chaired by Prof. R. McCarroll) started with the presentation of Prof. R. McCarroll who, after outlining some elements of the MO-CC method, described the results of his (and his group's) earlier and most recent cross section calculations for state-selective (and total) electron capture in the collision systems C^{4+}, Si^{4+} - H, D; N^{2+}, Al^{3+} - H; Be^{3+}, Si^{3+}, Ar^{6+} - He; O^{2+} - H, He; O^{3+}, O^{5+} - H. The calculated cross sections covered the region of low collision energies overlapping in its lower part with the region where quantum-mechanical description of nuclear motion is required. The results of calculations (both for state-selective and total electron capture) were compared with the results of other MO-CC calculations and with the experimental data where available. Certain persisting discrepancies in the calculated and measured cross sections for some systems were discussed.

In the second presentation at this session Dr. C.C. Havener gave an overview of the recent experimental cross section measurements for state-selective and total electron capture in collisions of multiply charged ions B^{4+}, $C^{3,4+}$, $O^{(3-5)+}$ with H atoms, as well for the C^{+} + H and Cl^{7+} + D collision systems. The method used in these measurements was the merged-beams method which allows accurate cross section measurement in the energy range 0.02 -5000 eV/amu. The recently measured cross sections by the ORNL group have an accuracy in the low-energy region superior to all the previous measurements and provide a significant extension of the energy range (towards the low energies) in which the cross sections of the above mentioned collision systems were known until now. The experimental data were compared with the results of various theoretical calculations and, at the higher energies, with other experimental data. The future work of the ORNL group within this CRP will include electron capture studies involving metallic beams and the system Ne^{q+} + H.

The last presentation in this session was given by Dr. J.P. Hansen and was related to the excitation of 2p and 2s states in H(1s) + H(1s) collisions in the energy region below 100 keV. The method used in these studies was the two-centre AO-CC method (in its semi-classical version) employing a large basis set. It was pointed out in the discussion that the state describing the (H^+ - H^-) ion pair may be necessary to include in the basis, since this virtual (intermediate) channel may provide an effective excitation mechanism. Dr. Hansen has outlined the future plans for electron capture cross section calculations for collision systems of interest to fusion by using the two-centre AO-CC method.

After each of the presentations there was an active discussion on the subject of the presentation, most of which oriented along lines of positive criticism and constructive suggestions.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

At the last session of the meeting (chaired by R.K. Janev), the meeting discussed the work priorities in the period of next two years of the CRP duration and the methods of work co-ordination within the CRP. The meeting participants first concluded that the charge exchange cross section data information is already quite significant (particularly for the total cross sections) and needs appropriate critical assessment. (For certain systems such assessment has also been done recently by some of the CRP participants). Nevertheless, the available data, particularly for state-selective electron capture and for the He and molecular targets, is far from sufficient for the fusion research needs. Most critical is the low-energy region (below 100 eV/amu) which is relevant for the fusion reactor divertor studies, holding presently a high priority in the fusion research. The analyses of the data availability and the most urgent needs for charge exchange data in the fusion community have resulted in identification of the species (projectiles and targets), the energy range, and the types of data required for specific groups of collision systems. This information is given in the table below. The participants have agreed to co-ordinate their work and undertake certain specific tasks to be carried out by the time of the next CRP meeting. The specific tasks and the participants who agreed to cooperate on them are also given in the table below.

At the end of its work, the meeting has recommended that R.K. Janev, after his separation from the Agency, be included as participant in the present CRP.

Table of important collision systems and specific activities

Impurity ions (as projectiles) A) Primary relevance: Be, B, C, N, O (all charge states); B) Second level relevance: Li, Ne, Mg, Si, Ar, Ti, Fe, Ni, Kr, Mo, W (all charge state for $Z \leq 10$, $q \leq 10$ for $Z > 10$)
Neutrals (targets) A) Primary relevance: H, H_2, He (all isotopic variants) B) Second level relevance: Li, Be, B, C, N, O, CO, N_2, O_2, C_nH_m
Energy range From thermal energies to several hundreds keV/amu
Processes 1) State selective electron capture for impurities and neutrals of primary fusion relevance (including vibrational level selectivity for molecular targets); 2) Total electron capture (for all ion-atom/molecule combinations); 3) Other many-electron transition processes involving electron transfer.
Specific tasks 1) Completion of the SSEC database for He^{2+}, Be^{4+}, B^{5+}, C^{6+}, O^{8} - H, He systems (Fritsch, Kimura, Janev, Panov); 2) Compilation and generation of data for total capture experimental cross sections of all relevant impurities colliding with primary neutrals (H.B. Gilbody, HP. Winter); 3) Compilation and generation of electron capture data for impurity ion collisions with neutrals of second level fusion relevance (Kimura, Okuno); 4) Generation of new cross section data in the thermal energy region (all relevant species) (McCarroll, Zygelman, Hansen, Havener, Okuno, Hoekstra, Gulyas, ...).

APPENDIX 1

1st IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

September 24-25, 1998, IAEA Headquarters, Vienna, Austria

List of Participants

CRP members

Dr. HP. Winter
Institut für Allgemeine Physik
Technische Universität Wien
Wiedner Hauptstrasse 8-10
A-1040 Wien, AUSTRIA
Fax: 43-1-586-4203
winter@iap.tuwien.ac.at

Dr. R. McCarroll
Laboratoire de Dynamique des Ions
Atomes et Molecules
Universite Pierre et Marie Curie
4, Place Jussieu
F-75252 Paris Cedex 05, FRANCE
Fax: 33-1-4427-7082
ron@diam.jussieu.fr

Dr. W. Fritsch
Hahn-Meitner Institut Berlin GmbH
Bereich Theoretische Physik
Glienicker Strasse 100
D-14109 Berlin, GERMANY
Fax: 49-30-8062-2098
fritsch@hmi.de

Dr. M. Kimura
Yamaguchi University
School of Medicine
UBE, Yamaguchi 755-8554
JAPAN
Fax: 81-836-22-2130
mineo@rikaxp.riken.go.jp

Dr. K. Okuno
Tokyo Metropolitan University
Graduate School of Science
Department of Physics
Minami-Ohsawa 1-1
Hachioji-shi Tokyo 192-03, JAPAN
Fax: 81-426-77-2483
okuno@phys.metro-u.ac.jp

Dr. J.P. Hansen
University of Bergen
Institute of Physics
Allegaten 55
N-5007 Bergen, NORWEY
Fax: 47-5558-9440
janpetter.hansen@fi.uib.no

Dr. M. Panov
Ioffe Physical Technical Institute of
the Russian Academy of Sciences
Atomic Collision Physical Lab.
Polytechnicheskaya Str. 26
St. Petersburg 194021
RUSSIAN FEDERATION
Fax: 7-812-247-1710
m.panovv@pop.ioffe.rssi.ru

Dr. H.B. Gilbody
The Queen's University of Belfast
Department of Pure and Applied Physics
Belfast BT7 1NN
Northern Ireland, UNITED KINGDOM
Fax: 44-1232 438918
b.gilbody@qub.ac.uk

Appendix 1 Contd.

Dr. C. Havener
Oak Ridge National Laboratory
Bldg. 6003, MS 6372
Physics Division
P.O. Box 2008
Oak Ridge, Tennessee 37831-6372
U.S.A.
Fax: 1-423-574-4745
havener@mail.phy.ornl.gov

Dr. B. Zygelman
University of Nevada
Department of Physics
4505 Maryland Parkway
Las Vegas, Nevada 89154-4002
U.S.A.
Fax: 1-702-895-0804
bernard@bohm.physics.unlv.edu

IAEA AMDU staff

Dr. R. K. Janev
Atomic and Molecular Data Unit
International Atomic Energy Agency
Wagramerstrasse - 5, P.O. Box 100
A-1400 Vienna, AUSTRIA
Fax: 43-1-26007
janev@ripcrs01.iaea.or.at

Dr. J. Stephens
Atomic and Molecular Data Unit
International Atomic Energy Agency
Wagramerstrasse - 5, P.O. Box 100
A-1400 Vienna, AUSTRIA
Fax: 43-1-26007
j.stephens@iaea.org

APPENDIX 2

1st IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"

September 24-25, 1998, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Thursday, September 24 **Meeting Room: C-07-IV**

09:30 - 10:00	- Opening - Adoption of Agenda	
Session 1:	*Recent Experimental and Theoretical Results:*	
Chairman: HP. Winter		
10:00 - 10:30	H.B. Gilbody:	Recent measurements of state-selective electron capture by slow multiply charged ions
10:30 - 11:00	W. Fritsch	Close-coupling studies for the Be^{2+} - H, N^{4+} - H and N^{7+} - H, He collision systems
11:00 - 11:30	*Coffee break*	
11:30 - 12:00	M. Kimura	Electron capture from excited targets and from heavy atom targets
12:00 - 14:00	*Lunch*	
Session 2:	*Recent Experimental and Theoretical Results: II*	
Chairman: H.B. Gilbody		
14:00 - 14:30	M. Panov:	Collisions of He^{2+} with H_2: experiment and theory
14:30 - 15:00	K. Okuno:	Electron capture processes in collisions of He^{2+} and Kr^{q+} (q=7-9) with diatomic molecules
15:00 - 15:30	HP. Winter:	Electron- and vibrational state-resolved single electron capture in slow collisions of doubly charged ions (C,N,O) with simple molecules (H_2, N_2, O_2, CO).
15:30 - 16:00	*Coffee break*	
16:00 - 16:30	B. Zygelman:	Ab-initio studies of charge transfer at low collision energies

Friday, September 25 **Meeting Room: C-07-IV**

Session 3: *Recent Experimental and Theoretical Results: III*

Chairman: R. McCarroll

09:30 - 10:00	R. McCarroll:	Model studies of charge transfer at thermal-eV energies
10:00 - 10:30	C. Havener:	Low energy total and state-selective cross sections for multiply charged ions colliding with atomic hydrogen
10:30 - 11:00	*Coffee break*	
11:00 - 11:30	J.P. Hansen:	Excitation in H-H collisions
12:00 - 14:00	*Lunch*	

Session 4: *Co-ordination of the CRP work; definition of specific CRP objectives*

Chairman: R.K. Janev

14:00 - 15:30	Discussion of a set of more specific CRP objectives and of the methods of work co-ordination
15:30 - 16:00	*Coffee break*
16:00 - 17:00	Meeting Conclusions
17:00 -	*Adjourn of the Meeting*