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Summary Report of

Final IAEA Research Co-ordination Meeting

Atomic and Molecular Data for Plasma Diagnostics

Prepared by

R.E.H. Clark

IAEA Headquarters, Vienna, Austria

19-20 July 2004

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
PO Box 100
Wagramer Strasse 5
A-1400 Vienna
Austria

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Abstract

Detailed discussions were held to determine the outcomes of participants' research at the final Research Coordination Meeting (RCM) on "Atomic and molecular data for fusion plasma diagnostics" at IAEA Headquarters on 19-20 July 2004. Participants summarized the specific results obtained in the course of the Coordinated Research Project (CRP), and considered the impact of the data generated on the design and modelling of fusion devices. Areas for which data needs still exist were also identified, and hope was expressed that further research in these areas could be supported in the future. The discussions, conclusions and recommendations of the RCM are briefly described in this report.

February 2006

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1. Introduction

The final Research Coordination Meeting (RCM) dedicated to "Atomic and molecular data for fusion plasma diagnostics" was held on 19-20 July 2004 at IAEA Headquarters, Vienna,. The main purposes of this RCM were to review the research activities of the participants, summarize the outputs of the Coordinated Research Project (CRP), and identify additional data needs for plasma diagnostics that require continued study.

The ten participants are experts in the study and understanding of the various atomic and molecular processes used in diagnosis of fusion plasmas (Appendix 1). Each participant gave a detailed presentation of their research activities during the final phase of the CRP, and provided short written summaries (Appendix 2). Two CRP participants were unable to attend (M. Panov and P. Krstic), but provided written records of their contributions that are also included in Appendix 2. A summary of the various data outputs of the CRP was formulated during the RCM, and is outlined below.

2. Meeting Proceedings

N. Ramamoorthy (Director, NAPC) welcomed the participants on behalf of the International Atomic Energy Agency (IAEA). He stated that fusion research continues to be an important topic within the IAEA. There are many processes of importance to diagnostic method in fusion devices, and he was aware that this CRP has provided much new data. He also added that the IAEA is grateful to the hard work and dedication of the participants. R. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (Appendix 3).

2.1 Summary of current research activities

Each participant reviewed their research activities and data outputs through their individual presentations to the group during the course of the meeting. These presentations have been collected together electronically and distributed on CD; only brief summaries are given in this section.

A. Pospieszczyk presented recent work on the determination of rate coefficients for the excitation and ionization processes of atoms and molecules. Comparisons were made between experimental determinations and available theoretical methods. Cross sections for heavy particles with helium were determined through calculations and analysis of gas puff experiments. Some preliminary experiments were also carried out for boron, and compared with data from the ADAS database. There are few reliable theoretical cross sections for tungsten, and there seem to be significant uncertainties among available results that require further investigation. Overall, data for atoms were found to be acceptable. Heavy-particle collisions were found to be important for species with high ionization energies, while the data look surprisingly good for hydrogen molecules. Spectroscopy of the CD radical is the standard tool for the determination of CD_4 particle fluxes, but the conversion between photon and particle flux measurements by means of D/XB values is indirect and depends on the dissociation chain. The consistency of the used/measured D/XB values for CH/D from CH_4/D_4 is still not satisfactory. Surface and geometry effects seem to dominate the values, and therefore a better modelling process is critically important. During the course of the work, data that have undergone comparison and analysis have been collected into databases, and are available for plasma modelling studies.

Luo Zhengming reported on measurements of inner-shell ionization cross sections by e-impact. The group at Sichuan University has developed a self-supporting thin film method for measurements of inner shell ionization cross sections. A modification based on a thick, rigid substrate allows cross-section measurements of a more extensive range of elements, although the method requires careful corrections for substrate effects. Results have now been reported for many targets, including V, Sc, Co, Ni, Cu, Zn, W, Mo, Ag and Sn with impact energies of several keV to several tens of keV.

B. Gilbody summarized results for charge transfer (CT) processes, using translational energy spectroscopy (TES). Results have been obtained for excited state formation in CT by slow multi-charged ions of impurity species at the plasma edge at energies below 1 keV/u. Cross sections were measured for H- and He-like ions of C, N and O in collision with H and H_2. The main collision mechanisms were identified and their relative importance assessed. Investigations on dissociative and non-dissociative CT from autoionizing states were carried out, and discrepancies between theory and previous measurements identified. Measurements for H provided an extension of previous data to energies below 1keV/u. This work included studies of one-electron capture by slow multiply-charged ions in molecular targets. Measurements of one-electron capture collisions by He^{2+} ions in H_2O, CO_2, CH_4, C_2H_4 and C_2H_6 and one-electron capture by O^{6+} ions in H_2O, CO_2 and CH_4 were made at energies in the range from 250 to 2000 eV/amu.

H.P. Winter reported on the status of atomic databases of single ionisation and excitation cross sections for proton collisions with neutral helium atoms. The database has been reviewed for collision energies relevant to He beam diagnostics (5 - 200 keV), in which the main focus of the work was to compile quantum-mechanical and classical calculations performed over the previous ten years. Classical trajectory Monte-Carlo (CTMC-) calculations have also been made for single ionisation and excitation of ground-state helium atoms by protons in the impact energy region of 5 - 200 keV. These calculated data were compared with the available experimental data. Furthermore, cross sections for excitation and charge exchange in slow collisions of protons with He (1s, NLM) excited atoms (N = 2, 3, 4) have been calculated over the collision velocity range 10^6 to 10^8 cm/s using the molecular orbital close-coupling (MOCC) method, with analytically calculated coupling matrix elements in the asymptotic region of internuclear distance (there are no results from other sources for comparison). The respective cross-section data have been calculated for all excitation and charge exchange transitions from the initial states with N = 2, 3 to all {N'} = 2, 3 (excitation) and {n} = 2, 3 (charge exchange) manifolds of states, but only cross sections for transitions from {N} = 2 states to {N'} = 2 and {n} = 2 manifolds of states were presented, adding sources and the mode of access to the other data.

H. Summers reviewed the results of a number of activities dedicated to the generation of fundamental collision data, the development of elaborated models for the use of these data for spectroscopic diagnostic analysis of fusion plasmas, and the validation of experimental studies. Rare gas elements and diagnosis include:

1) helium as an electron temperature/electron density monitor for the plasma edge at low energy (gas puff);
2) neon and argon as charge exchange spectroscopy emitters in association with neutral deuterium beams;
3) argon and krypton as soft X-ray helium-like and lithium-like satellite line emitters;

4) krypton and xenon as heavy species for integrated radial transport analysis to give line-like and quasi-continuum emission in XUV, EUV and VUV and total radiated power.

L. Mendez reported on the calculation of state selective electron capture in ion collisions with atoms and molecules. Calculations have been carried out using molecular expansion that include a common translation factor (semi-classical treatment) or a common reaction coordinate (quantal treatment). Quantal calculations of electron capture cross sections for the benchmark collision He^{2+}+ H(1s) were carried out at centre-of-mass energy from 20 eV up to 1.6 keV, and the results showed good agreement with those obtained with the hyperspherical close-coupling treatment of Lin et al. An important advantage of the common reaction coordinate method is that this procedure can be easily generalized to many-electron systems and has been applied to the N^{2+} + H(1s) system.. The goals of the work were to evaluate partial cross sections, obtain cross section for charge transfer reactions from both ground and metastable states, and obtain cross section for charge transfer reactions from both types of states. Results for impact energies from 0.15eV/amu to 25keV/amu have been completed and published. Core plasma diagnostics require knowledge of partial electron capture cross sections for collisions of highly-charged ions with H. Large-scale close-coupling molecular and CTMC calculations with an improved initial distribution have been carried out over a large range of impact energies. Both methods have been applied to Li^{3+} + H collisions, and the results have been compared with existing theoretical and experimental data. New capture and ionisation cross sections for Ne^{10+} + H collisions have also been carried out and published. The techniques for *ab initio* three-centre potential energy surfaces and dynamical couplings for ion-molecule collisions have been improved. These techniques, in particular the treatment of a series of narrow avoided crossings, have been applied to calculate single and double (autoionizing) electron capture in N^{5+} + H_2 collisions that show good agreement with the experimental studies of Kearns et al. and Lubinski et al. Recently, H_2^+ + H collisions have been considered, and anisotropy effects have been found to be critical because of the symmetry selection rules that lead to vanishing capture cross sections for transitions in the triplet subsystem, and for collisions where the relative velocity and the H2+ internuclear vector are perpendicular.

R. Janev presented work on a coupled CR model for $H/H_2(v)$. Extensive efforts have been made to compile, critically assess and generate (when necessary and possible) cross-section data for the processes involving the plasma constituents (typical for the fusion divertor): e, H^+, H, H^-, H_2, H_2^+ and H_3^+. Processes involving electronically excited neutrals (H, H_2) and vibrationally excited molecular species (H_2, H_2^+, H_3^+) have also been included in the development of this database. Critically assessed cross sections for the above collision processes have been represented by suitable analytical functions, with proper physical behavior in the low- (or threshold) and high-energy regions. Well-established theoretical or semi-empirical cross section scaling relationships have been used to generate missing cross sections (mainly for the processes with electronically excited states) in order to make the database as complete as possible (e.g., for construction of a coupled H/H_2 collisional-radiative model). However, this approach can only partially fill the numerous gaps still existing in the ideal "complete" H/H_2 collision database. These studies served also to identify missing cross sections for processes that are involved in the collision scheme of H/H_2 divertor plasma kinetics. Specific efforts were made to generate the cross sections for electron impact (vibrationally resolved) excitation transitions in the triplet system of H_2. All resulting databases have been published, and are available for modeling purposes.

R, Hoekstra reported on studies of Lyman α emission from alpha particles that interact with molecules by investigating the subsequent photon emission. For alpha particles colliding on molecular hydrogen at energies well below 1 keV/amu, two-electron capture dominates over single-electron capture by up to orders of magnitude. The state selective measurements indicate that two-electron capture populates mainly excited states at low energies. Single-electron capture into excited states changes to capture into the ground state at energies below 1 keV/amu. The latter channel must leave the electron-donor molecule in an excited state which most likely leads to dissociation and the production of relatively energetic atomic hydrogen. As such processes might be of relevance to the modelling of alpha-particle and possibly (molecular) hydrogen transport in the divertor/edge region of fusion plasmas, the experiments were extended to a whole series of di- and tri-atomic molecules and hydrocarbons. For almost all molecules except the larger hydrocarbons, their behavior is by and large similar to molecular hydrogen. Thus, it should be possible to generate an approximate scaling of charge exchange cross sections for alpha particles interacting with molecules.

C. Biedermann reviewed work performed using high-resolution X-ray and EUV spectrometry to study ions produced in an electron beam ion trap (EBIT). These studies encompassed a wide range of wavelengths, and compared the EBIT spectra with the results from *ab initio* calculations using the relativistic HULLAC package. Initial work focused on xenon ions: spectra for several ion stages of xenon were observed, and there was good agreement between observation and calculations from the HULLAC codes. Some previously unidentified lines have also been resolved by means of this analytical procedure. Separate efforts focused on HULLAC calculation of atomic data, including energy levels, radiative rate coefficients for E1, E2, M1 and M2 transitions, and electron impact collision strengths. Data were calculated for tungsten ions with charge state q = 25 - 45, ranging from In-like W^{25+} to Cu-like W^{45+}.

N. Brooks described studies undertaken on the DIII D device. Significant progress had been made in the following areas:

1) identification of neutral atomic and molecular carbon data needed for spectroscopic studies of carbon sources in Tokamaks with graphite walls,
2) development of a numerical hydrocarbon (primarily methane) dissociation-transport model to study the effects of chemical sputtering and transport in Tokamaks with graphite walls,
3) determination of atomic data needs associated with deuterium recycling from graphite walls,
4) development of numerical models for lithium sputtering and transport at the target plates of a poloidally diverted Tokamak, and assessment of the atomic data required for these models,
5) assessment of fluorine charge exchange data for spectroscopic studies of transport processes in the pedestal region of high performance Tokamak plasmas, and
6) evaluation of a divertor CER diagnostic system for DIII-D using atomic data produced specifically for this purpose.

Progress and results from these efforts have been well documented in published papers, and are summarized in an article within *Atomic and Plasma-Material Interaction Data for Fusion (APID)*.

3. Specific Outputs of the CRP

During the course of the Coordinated Research Project, new data were generated for a variety of processes impacting on a number of diagnostic procedures for fusion plasmas:

spectral observations near the strike zone and divertor (where alpha particles interact with molecules) require a variety of cross-section data that have been measured and calculated during the current work programme;

helium beam diagnostics from fast to thermal require cross-section data for both electron and proton impact have been generated;

data have been produced for use in the determination of species from light elements such as helium, boron and hydrocarbons, as well as heavy elements such as tungsten;

large amounts of data on spectral properties were generated to assist greatly in spectral analysis of plasma emissions;

X-ray emissions from impact on surfaces have been addressed;

data have been generated for use in hydrogen charge exchange spectroscopy for determination of the flow and temperature of impurities in the divertor region.

4. Concluding Remarks

The CRP on "Atomic and molecular data for plasma diagnostics" has been very successful in meeting all of the objectives established at the beginning of the project. All participants have published their work in refereed journals over the course of the CRP, are making their data available in electronic form, and have prepared summary articles for a dedicated issue of *Atomic and Plasma-Material Interaction Data for Fusion* (IAEA journal).

Appendix 1

Final IAEA Research Co-ordination Meeting on
Atomic and Molecular Data for Plasma Diagnostics

19-20 July 2004, IAEA Headquarters, Vienna, Austria

List of Participants

Dr. HP. Winter
Technische Universität
Institut für Allgemeine Physik
Wiedner Hauptstrasse 8-10
A-1040 Vienna, AUSTRIA
Tel.: +43-1-58801-5710
Fax: +43-1-5864203
E-mail: winter@iap.tuwien.ac.at

Dr. Luo Zhengming
Key Lab for Radiation Physics and
Technology of Education Ministry of
China and Center for Radiation Physics
Institute of Nuclear Science & Technology
Sichuan University
610064, Chengdu
CHINA
Tel.: +86-28-85410252
Fax: +86-28-85417822
E-mail: luozm@scu.edu.cn

Dr. Christoph Biedermann
Max-Planck-Institut für Plasmaphysik
Institut für Physik der Humboldt-
Universität zu Berlin
AG Plasmaphysik
Newtonstrasse 15
D-12489 Berlin
GERMANY
Tel.: +49-30-2093-7538
Fax: +49-30-2093-7549
E-mail: biedermann@ipp.mpg.de

Dr. A. Pospieszczyk
Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
GERMANY
Tel.: +49-2461-61-5536/513
Fax: +49-2461-61-3331
E-mail: a.pos@fz-juelich.de

Dr. Ratko K. Janev
Macedonian Academy of Sciences & Arts
Bulevar K. Misirkov, 2
P.O. Box 428
91000 Skopje
MACEDONIA
Tel.: +389-91-114200
Fax: +389-91-114685
E-mail: rjanev@manu.edu.mk

Dr. R. Hoekstra
Kernfysisch Versneller Institut
University of Groningen
Zernikelaan 25
NL-9747 AA Groningen
NETHERLANDS
Tel.: +31-50-363-3600
Fax: +31-50-363-3403
E-mail: hoekstra@kvi.nl

Dr. Luis Méndez
Universidad Autonoma de Madrid
Dempartmento de Quimica, C-9
Canto Blanco
28049 Madrid
SPAIN
Tel.: +34-91-3975259
Fax: +34-91-3974187
E-mail: i.mendez@uam.es

Dr. H.B. Gilbody
The Queen's University of Belfast
Department of Pure and Applied Physics
Belfast BT7 1NN
Northern Ireland
UNITED KINGDOM
Tel.: +44-1232-273508
Fax: +44-1232-438918
E-mail: b.gilbody@qub.ac.uk

Dr. H.P. Summers
Department of Physics & Applied Physics
University of Strathclyde
107 Rottenrow
Glasgow, Scotland G4ONG
UNITED KINGDOM
Tel.: +44-141-548-4196
Fax: +44-141-552-2891
E-mail: summers@phys.strath.ac.uk

Dr. Neil Brooks
MS 13-49
General Atomics
P.O. Box 85608
San Diego, CA 92186-9784
U.S.A.
Tel.: +1-858-455-3979
Fax: +1-858-455-4156
E-mail: brooks@fusion.gat.com

Dr. R.E.H. Clark
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21731
Fax: +43-1-26007
E-mail: r.e.h.clark@iaea.org

Dr. D. Humbert
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21729
Fax: +43-1-26007
E-mail: d.humbert@iaea.org

Appendix 2

Final IAEA Research Co-ordination Meeting on
Atomic and Molecular Data for Plasma Diagnostics

19-20 July 2004, IAEA Headquarters, Vienna, Austria

Agenda

Monday, 19 July **Meeting Room: B-05-45**

09:30 – 10:00 Opening, Adoption of Agenda, N. Ramamoorthy, R. Clark

Session 1: Progress Reports I

Chairman: C. Biedermann

10:00 – 10:30 A. Pospieszczyk
Determination of rate coefficients for atoms and molecules by gas blow experiments at TEXTOR and JET

10:30 – 11:00 *Coffee Break*

11:00 – 11:30 Luo Zhengming
The thick target method for measurement of inner shell ionization cross section by electron impact

11:30 – 12:00 H. Gilbody
Excited state formation in one-electron capture collisions of slow multiply charged ions with molecules

12:00 – 12:30 HP. Winter
Measurement of total cross sections for single- double electron capture in low-energy collisions of doubly charged He ions with atoms and molecules

12:30 – 14:00 *Lunch*

Session 2: Progress Reports II

Chairman: Luo Zhengming

14:00 – 14:30 H. Summers
Rare gases: Data and diagnostics for fusion

14:30 – 15:00 L. Méndez
Calculation of state selective election capture in ion-atom (molecule) collisions

15:00 – 15:30 R. Janev
Towards a complete coupled CR model for $H/H_2(v)$

15:30 – 16:00 *Coffee Break*

16:00 – 16:30 R. Hoekstra
Lyman-a emission from alpha particles interacting with molecules

16:30 – 17:00 C. Biedermann
Experiments with highly charged ions at the Berlin EBIT

17:00 – 17:30 N. Brooks
Feasibility studies for a charge exchange recombination diagnostics for measurement of impurity flows in the divertor of DIII-D

17:30 – 18:00 R. Clark
Summary of results from CRP members not able to attend

Tuesday, 20 July

Session 3: Review of Work Plan and Outcomes

Chairman: R. Janev

09:00 – 12:30 All
Comprehensive review of results obtained in support of the work plan for the CRP

12:30 – 14:00 *Lunch*

Session 4: Formulation of Meeting Conclusions and Reports

Chairman: H. Summers

14:00 – 17:00 All
Meeting conclusions formed, discussion of submission of reports for inclusion in APID journal and submission of data for inclusion in electronic databases

17:00 – *Adjournment of Meeting*

Appendix 3

Final IAEA Research Co-ordination Meeting on Atomic and Molecular Data for Plasma Diagnostics

19-20 July 2004, IAEA Headquarters, Vienna, Austria

Summaries from Participants

Experiments with highly charged ions at the BerlinEBIT

C. Biedermann

Institut für Physik der Humboldt-Universität zu Berlin, Lehrstuhl Plasmaphysik, Newtonstraße 15, 12489 Berlin, Germany, and Max-Planck-Institut für Plasmaphysik, EURATOM Association

Activities at the Berlin Electron Beam Ion Trap during the period June 2003 to July 2004 have been dominated by the change in the organization and infrastructure of the Berlin group. The Plasma Diagnostic branch of the Max-Planck-Institut für Plasmaphysik has been shut down at the end of 2003. The BerlinEBIT facility and staff have been relocated at the department of experimental plasma physics lead by Professor Fußmann at the Institut für Physik der Humboldt-Universität zu Berlin which recently has been concentrated at the science and technology park Adlershof (WISTA) in the south of Berlin. Due to the move and reconstruction of the EBIT device, beam line and peripheral laboratory inventory, the scientific work has been delayed. Nevertheless our program which concerns the investigation of EUV radiation of xenon ions could be accomplished.

Heavy noble gases like xenon are envisaged as to be injected as a radiating buffer in the high temperature fusion plasmas of JET and ITER. However, up to now, there is only sparse information available for the spectral features of radiating highly charged xenon ions, especially in the EUV region.

We have recently measured with our grazing-incidence spectrometer the extreme ultraviolet radiation of xenon ions with charge states 17+ to 26+ in the wavelength range 9 to 24 nm. Successively stepping the monoenergetic electron beam energy of EBIT in small increments over the ionization potentials of the ions we can clearly identify the lines observed in the spectra with a certain ionization stage. EBIT allows the selective production of a narrow, limited charge state distribution of ions which can be confined for long observation time. With the high-resolution grazing-incidence spectrometer about 33 individual lines have been registered in the present experiment. In the wavelength region around 10.7 nm a band-like structure for Xe^{17+} to Xe^{20+} ions was detected, which could be resolved as closely spaced individual lines, operating the spectrometer in 2^{nd} order reflection. The related transitions of the observed lines were identified with the help of elaborated atomic structure calculations with the HULLAC-suite of codes which are provided by collaboration with Prof. Schwob and Dr. Mandelbaum at the Hebrew University of Jerusalem. Good agreement is found for $^2P_{3/2}$ and $^2P_{1/2} - {}^2S_{1/2}$ transitions of Cu-like Xe^{25+} and the $^1P_1$ and $^3P_1 - {}^1S_0$ transition of Zn-like Xe^{24+} between the EBIT-data, observations at tokamaks and the HULLAC predictions. For Ga-like Xe^{23+} ions to Rb-like Xe^{17+} ions an increasing deviation between the predicted wavelengths and the observed line positions is noted. This fact stresses the complicated atomic structure of these ions, where due to the open 4p shell many configurations can couple and have to be included in the calculation. Some of the lines observed with EBIT have been previously seen but not identified at the TFR tokamak. With the EBIT technique we can now identify these lines and label the transition. It is intended to expand the wavelength and charge-state range in future investigations and refine the calculations.

Results from DIII-D

T.E. Evans and N. Brooks

General Atomics, San Diego, California, USA

Overview:

Activities at DIII-D related to the 2000-04 IAEA CRP on Atomic Data for Plasma Diagnostics have included: 1) identification of neutral atomic and molecular carbon data needed for spectroscopic studies of carbon sources in tokamaks with graphite walls, 2) development of a numerical hydrocarbon (primarily methane) dissociation-transport model for studying the effects of chemical sputtering and transport in tokamaks with graphite walls, 3) establishing atomic data needs associated with deuterium recycling from graphite walls, 4) developing numerical models of lithium sputtering and transport at the target plates of a poloidally diverted tokamak and the atomic data needed for these models, 5) assessment of fluorine charge exchange data for spectroscopic studies of transport processes in the pedestal region of high performance tokamak plasmas, and 6) the evaluation of a divertor CER diagnostic system for DIII-D using atomic data produced specifically for this purpose.

Summary of results:

2000-2003 Results – Results and progress on activities 1-5) were summarized in our June 15, 2003 progress report. Some of these results have been published in various journal articles or have been submitted for publication (e.g., R. C. Isler, et al., *Phys. Plasmas* **8** (2001) 4470; W. P. West, et al., General Atomics report GA-A23960, May 2002; and N. H. Brooks, et al., in press J. Nucl. Mater.) while others have been presented at conferences and workshops (e.g., November 2002 DPP-APS Meeting by W. P. West, et al.; October, 2002 IAEA Technical Meeting on Atomic and Molecular Data by T. E. Evans, et al.; November 2002 ALPS/APEX Workshop at PPPL, New Jersey by T. E. Evans; and April 2003 ALPS/APEX Workshop, Grand Canyon Meeting Center, Arizona by T. E. Evans, et al.,). Additional details on these results will be given in our final report for this CRP.

2003-2004 Results – Additional progress on activities 1-5) made during this period will be summarized in our final report. Below we summarize results from activity 6) on: Feasibility studies of a charge exchange recombination diagnostic for measurement of impurity flows in the divertor of the DIII-D tokamak.

A new diagnostic approach for measuring impurity flows in the divertor of a tokamak was evaluated through a combination of experimental measurements and code modeling. Basic atomic physics calculations played a central role in the modeling: rate coefficients from the ADAS database were employed for assessing the background emission from the thermal background plasma [1], and CTMC calculations were used for estimating the state-selective charge exchange recombination emission in the path of a diagnostic neutral beam [2].

Fluid-flow models of the scrape-off layer and divertor regions of tokamak plasmas predict complicated two-dimensional flow patterns, with some regions of the divertor exhibiting flow away from the target plate (reverse flow) under some conditions. To have confidence in the extrapolation of modeling results to ITER-like divertor conditions, fluid codes such as the LLNL's UEDGE need to be validated against experimental measurements in current devices.

This need for validation drives a search for methods to measure impurity flows and ion temperatures throughout the DIII-D divertor, with particular interest in the boundary zone between scrape-off layer and divertor. Charge Exchange Recombination has been proposed as means to obtain V and $T_{I.c}$ near the elevation of the divertor X-point, with the centimeter-scale spatial resolution necessary to map the strong spatial gradients predicted in the flow patterns.

Passive spectroscopic techniques have been used successfully to measure temperatures and flow velocities of impurity ions in the DIII-D divertor [3, 4, 5]. One notable success of this effort was the confirmation of an elongated region of reverse flow predicted by the UEDGE fluid model. However, the impurity species accessible by visible spectroscopy are limited to low charge states generally concentrated near the divertor targets. Though thermal charge exchange (CX) was successfully used to access the He-like ion of carbon, its CX line was measurable only when deuterium gas was puffed so strongly that both divertor legs detached [6].

Active charge exchange offers a means to detect the dominant ion in the divertor and to measure its temperature $T_{I.c}$ and flow velocity V in the vicinity of the X-point. Through a combination of modeling [7,8] and measurement, the most promising impurity elements and charge states were identified: for lithium and beryllium, these are the fully stripped ions; for boron and carbon, the He-like charge states. Injected lithium has been ruled out for ACX measurements, because a piggyback experiment conducted on DIII-D revealed that its CX lines overlap those of intrinsic boron. Beryllium was rejected, because of the onerous safety requirements associated with use of this toxic material. Boron and carbon are already present in DIII-D: the former as a thin surface layer accumulated by repeated "boronizations" of the vessel; the latter as the graphite armor which form the plasma-facing wall. By puffing their dust into the SOL continuously, the abundance of the non-recycling impurities boron and carbon can be enhanced in the divertor without raising core concentrations significantly.

A low signal-to-background ratio is the central challenge facing ACX measurements in the divertor. This is the result of a spatially extended region of cool plasma in the divertor: it gives rise to background emission by electron impact excitation of the daughter charge state (and dielectronic recombination to the daughter charge state) which is much larger than that typical of the core. Measurement of the C IV (7-6) transition in the path of a DIII-D heating beam at the vessel midplane shows an ACX signal-to-background ratio of roughly unity; in the divertor, the signal-to-background can be expected to be much lower. Divertor modeling calculations of the C IV ACX signal, combined with measurements of the background signal in the divertor, predict a signal-to-background ratio in the range 10^{-2} to 10^{-3}. Digital lock-in techniques utilizing a modulated diagnostic beam were evaluated for extracting a weak signal from a strong background, but photon noise on the individual pixel elements sets the limit of detection when the line profile is spread across a multichannel detector with sufficient spectral dispersion to fit the multi-peaked profile of the candidate CER lines from Li-like daughter charge states.

It should be noted that the high spectral dispersion required in the case of CER lines from Li-like daughter ions is an unavoidable consequence of the large wavelength separation between the multiple $\Delta = 1$ transitions comprising a given Δn transition; in the case of H-like daughter ions, such as Li^{+2} and Be^{+3}, the Zeeman splitting in a tokamak is much larger than the separation associated with different $\Delta = 1$ transitions. This means the spectral profile of the CER line formed by the envelope of the Doppler-broadened, Zeeman components is symmetric. On machines such as JET, which routinely use beryllium for wall conditioning, a divertor CER diagnostic based on beryllium might be feasible. Providing the spectral region

of the CER line is free of contaminating spectral features, Doppler shifts can be measured with a system comprised of just two detectors outfitted with sawtooth –shaped, spectral transmission filters [9]. Concentrating all the light on just two spot detectors dramatically reduces the statistical noise and permits the full power of lock-in detection to be realized.

References:

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Excited state formation in electron capture by slow multiply charged ions

H.B. Gilbody and R.W. McCullough

Queen's University Belfast, Belfast, UK

SUMMARY OF WORK COMPLETED IN PERIOD JUNE 2003 – JULY 2004

In the final phase of this CRP we have extended studies based on translational energy spectroscopy (TES) to obtain data on one-electron capture by slow multiply charged ions in molecular targets. Our previous studies in H_2 [1, 2, 3, 4] have shown that dissociative product channels can play an important and often dominant role.

We have carried out measurements of one-electron capture collisions by He^{2+} ions in H_2O, CO_2, CH_4, C_2H_4 and C_2H_6 and one-electron capture by O^{6+} ions in H_2O, CO_2, and CH_4 at energies within the range 250 - 2000 eV amu^{-1}. Total cross sections, where available, are known to be very large at low energies and, as in our previous work, it was of interest to identify the main excited product channels and determine the relative importance of dissociative and non-dissociative mechanisms in the selective capture process.

In the case of one-electron capture by He^{2+} ions in H_2O, while non-dissociative capture leading to $He^+(n = 2)$ is dominant at the highest energies, dissociative processes involving transfer-ionization leading to $He^+(n = 1)$ ions become very substantial at the lower energies. Our measurements for He^{2+} ions in CO_2 and CH_4 exhibit a similar behaviour. A rather different pattern is observed in the case of one-electron capture by He^{2+} ions in C_2H_4. While non-dissociative capture leading to $He^+(n = 2)$ is dominant at 2000 eV/ amu, dissociative capture also leading to $He^+(n = 2)$ formation increases with decreasing energy and is dominant at our lowest energy of 215 eV/ amu. For He^{2+} ions in C_2H_6, electron capture channels leading to $He^+(n = 2)$ are dominant in the energy range considered. Although information on the fragmentation modes is limited in this case, it appears that dissociative capture leading to $C_2H_4^+$ is the main product channel at our lowest impact energy of 200 eV/amu.

Known total one-electron capture cross sections for He^{2+} ions in H_2O and CO_2 and values measured in this work for He^{2+} ions in CH_4, have been used to normalise our TES data and thereby derive cross sections for the main excited product channels in these three cases. Tabulated values are available.

Our TES studies of one-electron capture by He-like O^{6+} ions in collisions with the molecules H_2O, CO_2, CH_4 at energies below 2000 eV/amu differ from the corresponding data for He^{2+} impact. Total capture cross sections for these cases are unavailable. It is found that non-dissociative electron capture channels are dominant with contributions from dissociative capture channels increasing in relative importance as the impact energy increases. In all cases, selective capture takes place into O^{5+}(4d) states through non-dissociative capture and $O^{5+}(n = 3)$ states through dissociative capture. It is interesting to note that, in our earlier TES studies of one-electron capture by O^{6+} in H_2 for energies up to 900 eV/amu, the only significant excitation process observed was non-dissociative capture leading to $O^{5+}(n = 4)$ formation.

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Results accomplished during CRP

R. Hoekstra

KVI Atomic Physics, Rijksuniversiteit Groningen, Zernikelaan 25, NL 9747 AA Groningen, the Netherlands

The emphasis of the work at KVI was on charge exchange by alpha particles, in particular we investigated the subsequent photon emission. For alpha particles colliding on molecular hydrogen, it was found that at energies well below 1 keV/amu two-electron capture dominates over single-electron capture, up to orders of magnitude. Our state selective measurements indicate that at low energies two-electron capture populates mainly excited states. Single electron capture swaps from capture into excited states to capture into the ground state at energies below 1 keV/amu. The latter channel must leave the electron-donor molecule in an excited state which most likely leads to dissociation and the production of relatively energetic atomic hydrogen.

As such processes might be of relevance for the modelling of alpha particle and maybe even (molecular) hydrogen transport in the divertor / edge region of fusion plasmas, the experiments were extended to a whole series of di- and tri-atomic molecules and hydrocarbons. In collaboration with the group of McCullough (Queen's University Belfast), our photon emission spectroscopy experiments have been complemented with socalled TES measurements which give access to the final states of the molecules. For almost all molecules except for the larger hydrocarbons the behavior is by and large the same and their behavior is similar to molecular hydrogen. Thus it should be possible to generate an approximate scaling of charge exchange cross sections for alpha particles interacting with molecules.

Generation, compilation and evaluation of atomic and molecular data for fusion plasma diagnostics

R.K.Janev

Macedonian Academy of Sciences and Arts, Skopje, Macedonia

An extensive effort has been undertaken to compile, critically assess and generate when necessary and possible the cross section data for the processes involving the following plasma constituents, typical for the fusion divertor: e, H^+, H, H^-, H_2, H_2^+ and H_3^+. The processes involving electronically excited neutrals (H, H_2) and vibrationally excited molecular species (H_2, H_2^+, H_3^+) have also been included in the scope of the database. More specifically, the following processes have been considered:

- Electron – neutral H, H_2 collisions (from the ground and excited states):
  - excitation (including vibrational), ionization, dissociation, radiative attachment;
- Electron – proton collisions:
  - radiative and three-body recombination;
- Electron – molecular ion (H_2^+, H_3^+) collisions:
  - vibrational excitation, dissociative excitation, ionization and recombination;
- Proton – neutral H, H_2 collisions (from ground and excited states):
  - excitation (including vibrational), ionization, dissociation, charge exchange;
- Neutral – (excited) neutral collisions:
  - excitation transfer, resonant, Penning and associative ionization, dissociation;
- H^- collision processes with e, H, H^+, H_2^+, H_3^+ :
  - detachment, charge exchange (resonant on H, quasi-resonant on H^+, dissociative on H_2^+ and H_3^+);
- H_2 collisions with H_2, H_2^+ and H_3^+ :
  - vibrational transfer, charge exchange, proton (atom) transfer, dissociation.

The critically assessed cross sections for the above collision processes have been represented by suitable analytic fit functions, with proper physical behavior in the low- (or threshold) and high-energy region. This greatly facilitates the implementation of data information in plasma application codes. In order to make the database as complete as possible (e.g. for construction of a coupled H/H_2 collisional-radiative model), well established theoretical or semi-empirical cross section scaling relationships have been used to generate the missing cross sections in the literature (which is mainly the case for the processes with electronically excited states). This procedure, however, could only partially fill the numerous gaps still existing in the ideally "complete" H/H_2 collision database. From this point of view, this effort served also to identify the still missing cross sections for processes that are involved in the collision scheme of H/H_2 divertor plasma kinetics. The assessment of the present data situation for constructing a complete collisional-radiative H/H_2 model is given in the publications [1, 2], while the presently assembled database, discussed above, is published in [3, 4]. A specific effort was undertaken to generate the cross sections for electron impact (vibrationally resolved) excitation transitions in the triplet system of H_2 [5].

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Vibrationally resolved processes in slow ion-molecule and atom-molecular ion collisions of hydrogenic species

P.S. Krstić

Oak Ridge National Laboratory, Physics Division, P.O. Box 2008, Oak Ridge, TN 37831-6372, USA

Due to low temperatures and high densities of neutrals, with presence of molecules, in the tokamak divertor plasmas, all vibrationally resolved processes in H^++H_2(v) and H+H_2^+(v) collision systems are of potential importance for divertor plasma modeling and diagnostics: charge transfer, vibrational excitation, dissociation, chemical reactions, association, elastic. The charge transfer processes are critically important for Molecule Assisted Recombination. Only scattered data existed in literature (for the range 1-100 eV) for vibrational excitation and charge transfer, mainly with the ground vibrational initial state of H_2 for H^++H_2 collisions, and almost no data were available for scattering of hydrogen on hydrogen molecular ion.
We performed a series of comprehensive studies [1-4] for the scattering of a proton on H_2(v) and of a hydrogen atom on H_2^+(v), for all vibrational excited states, v, of the relevant molecules. Final state resolved cross sections for charge transfer, excitation [1], and dissociation [2] have been calculated in the range of the center-of-mass collision energies 0.5-10 eV, using a fully quantal, coupled-channel approach. An extensive vibrational basis set, defined in a large configuration space of the reactants, is used, including a large number of dicretized vibrational continua (dissociation states), to account for the transitions through the "closed" channels as well as for the nuclear rearrangements. A detailed picture is produced of all inelastic processes that involve two lowest, nonadiabatically coupled electronic surfaces of the H_3^+ molecule. The rotational dynamics of diatomic targets were treated with the sudden approximation (IOSA). The cross sections obtained are in reasonable agreement with the sparse data available from literature, mostly for the ground vibrational state.

The dominant dissociation mechanisms in the studied three-nuclear collision system were identified and their effectiveness analyzed for different collision geometries. The energy and angular spectra of the dissociating fragments are also calculated and analyzed and fitted to the analytical forms [2].

In addition, important plasma transport related moments of the elastic scattering cross sections, the momentum transfer and viscosity cross sections, were also calculated for all vibrationally excited states (of H_2 and H_2^+) of the considered collision systems [3]. These compare well with the elastic cross sections previously and independently calculated [4] from the ground vibrational states of H_2 and H_2^+.

In three-body collisions involving two hydrogen atoms and a proton, two atoms (or atom and ion) can form a diatomic molecule (H_2 or H_2^+) while the third, scattering, particle carries away the excess of energy and momentum. This process, collisionaly assisted diatomic association (also known as three-body recombination) was studied [5] for the first time, to assess its relative importance in the fusion tokamak divertor plasma. The association rate coefficients, resolved in final vibrational states, are calculated and show that the production of H_2^+ is significantly faster (factor of 2) than that of H_2 due to strong charge transfer between the corresponding continue and a favorable distribution of highly excited vibrational states in case of H_2^+. The total association rate coefficients are about $5x10^{-32}$ to $6x10^{-34}$ for plasma temperatures in the interval 200-20,000K, and decrease (approximately) as 1/T as temperature

increases. This indicates that these processes are not playing a significant role in the divertor volume plasma recombination in the presence of more powerful competing processes (such as three-body recombination in $e + H^+ + e$, for instance).

In addition to the previous, fully quantal, a new method was developed to treat vibrationally (initial and final state) resolved processes at higher collision energies, from about 20 eV to hundreds of eV [6]. This is based on the direct, numerical solution of the time-dependent Schroedinger equation on the numerical lattice, and assumes classical motion of the projectile, while treating vibrational and electronic motion quantum mechanically. The newly developed method uses the split-operator technique for construction of the iteration procedure in time. Preliminary results are a reasonable continuation of the excitation, charge transfer and dissociation cross section from vibrationally excited states dependences obtained fully quantum-mechanically at lower energies.

All calculated, initial and final vibrational-state resolved cross sections for vibrational excitation, charge transfer and dissociation in range of collision energies 0.5-100 eV (more than a thousand integral cross sections) are available from the ORNL-CFADC www site, in tabular and graphical form **(www-cfadc.phy.ornl.gov)**, and are transferred to IAEA for use through AMDIS engine.

The available data for one of the most frequently studied collision process, charge transfer in collision of alpha particle with hydrogen, are quite scattered at low collision energies (< 1000 eV/amu). The dispersion of data increases toward low energy end, reaching several orders of magnitude. Having in mind relative importance of this system fin the fusion plasma diagnostics we have performed a highly accurate calculation, using hidden crossing coupled channel technique [7]. The results are in very good (within a few %) with three other sets of data, obtained independently by other authors. On the other hand, below 100 eV/amu, these deviate from the current recommendation by orders of magnitude, while at higher energies the deviation decreases, reaching a factor of about 2 at 700 eV. These all indicate that the IAEA recommended cross section for charge transfer in $He_2^+ + H$ collision requires update at energies from threshold to e few keV. For such an update, for energies below 400 eV/amu, we recommend the data in reference [7].

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Work carried out in 2004

LUO Zheng-ming

Key Laboratory of Radiation Physics and Technology of Ministry of Education and Institute of Nuclear Science and Technology, Sichuan University, Chengdu 610064, PRChina

I. Improved measurement technique

1. Improved the accuracy of target thickness determination

In the past year, we made use of the RBS technique to measure the thin target thickness. The 2 MeV $^4He^+$ ions were provided by an electrostatic accelerator with maximum terminal voltage of 2.5 MV. The incident particles were impacted vertically on the thin targets. The backscattered particles were detected at a scattering angle of 150º by a Si surface-barrier detector with depletion depth of 300 μm. The backscattering spectra were analyzed using a computer program GISA3.3 [1]. The thickness of each thin target was measured at least twice by RBS. The uncertainty of thin target thickness determined by RBS is estimated to be about 5%.

2. Improved efficiency calibration in the lower energy region:

The efficiency calibration of this system in the energy region down to 0.58 keV was performed using the thick carbon target bremsstrahlung by 19 keV electron impact [2-4]. The shape of the efficiency calibration curve was determined from the ratio of experimental and theoretical thick carbon target bremsstrahlung spectra, and the absolute value for the efficiency calibration was obtained from the use of ^{241}Am radioactive standard source. The accuracy for the efficiency calibration in the lower energy region with the method described here was estimated to be about 5-6%. The details of this calibration method have been given elsewhere. The method used gives a continuous calibration curve down to 0.58 keV in the lower energy region, not simply discrete points obtained only from the use of standard sources. In addition, in general, it is very difficult for the only use of standard sources to obtain the efficiency calibration below 3.3 keV because the adequate sources are not generally available. Therefore, the method we used here is also very useful for the ionization cross-section measurements of K-shell for lower Z elements and of L and M-shell for medium and higher Z elements, which are in progress in our laboratory.

3. Transport correction based on the bipartition model

Due to the zigzag track of the electrons in the thin target, their actual path length is larger than the geometric path determined by $d/\cos\theta$, where d and θ are the thickness of the target and the incident angle of the incident electrons respectively. In this study, the mean track length s of the incident electrons, transmitted through the thin targets with depth d was calculated using a bipartition model. From the transport theory we have a formulae of path-length correction as follows:

$$s = \int_0^d \phi_0(z)/\phi_1(z)dz \qquad (1)$$

where ϕ_0 is the electron total fluence at depth z. ϕ_1 is the electron total current at depth z. These transport quantities can be calculated by using the bipartition model of electron transport [5]. The correction will be applied to the measurements of inner shell ionization cross sections for heavy elements by electron impact.

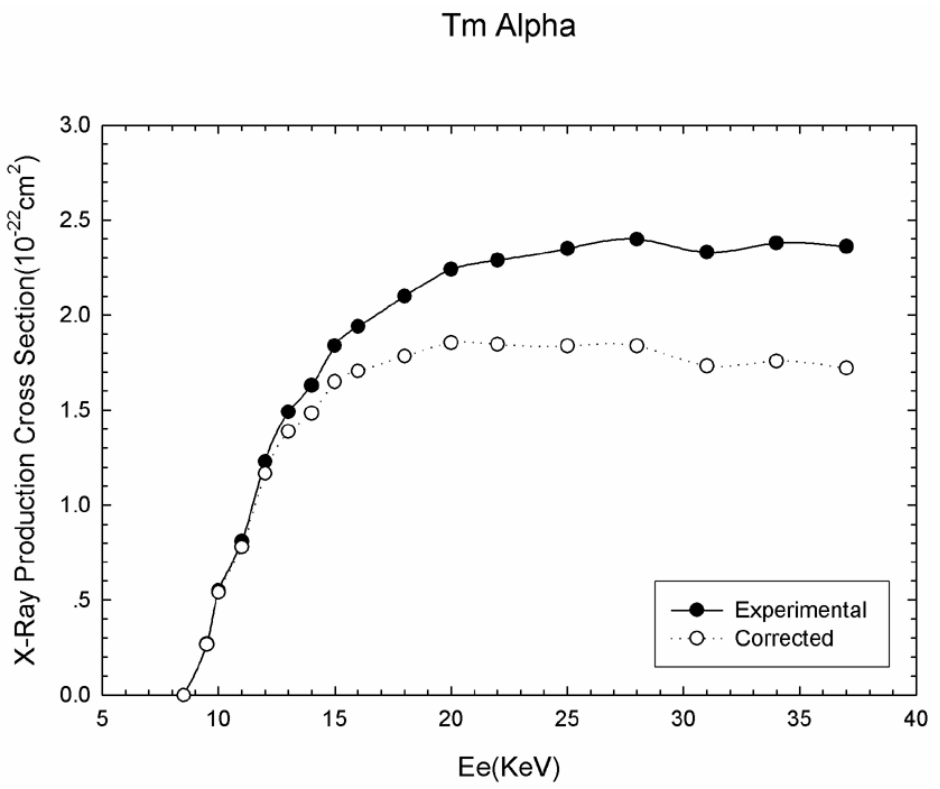
II. Carrying out the measurement of L-shell ionization cross sections for some heavy elements by electron impact

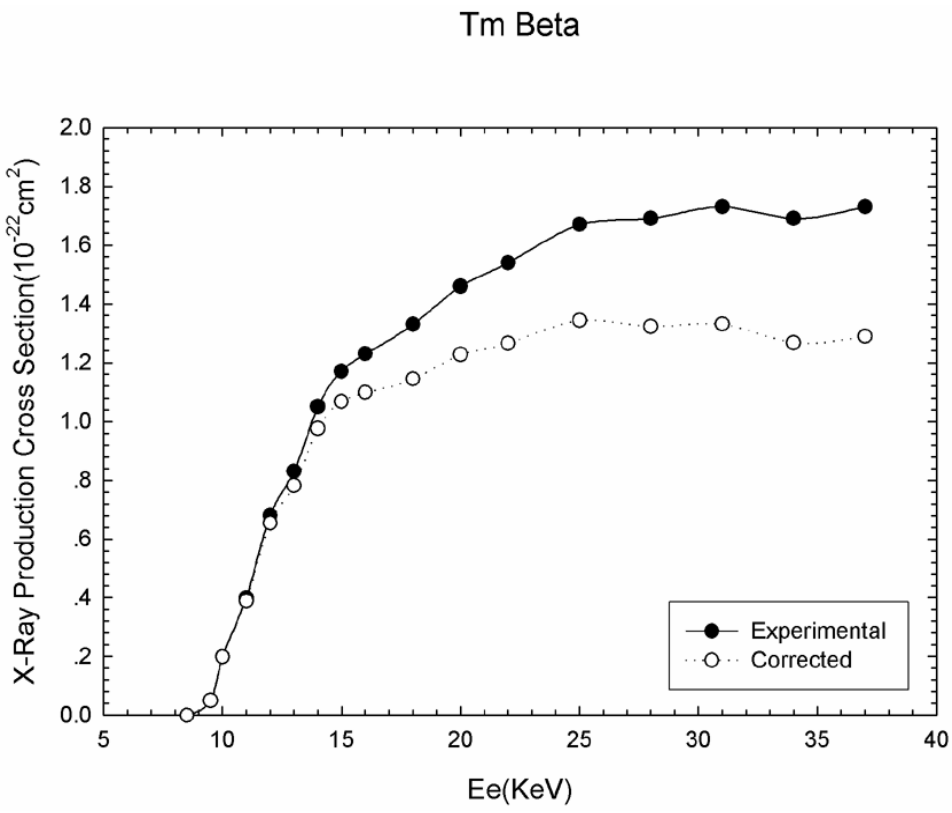
Since last year our group has systematically measured L-shell cross sections for heavy elements by electron impact. Until now we have completed primary measurement of L-shell ionization or x-ray production cross sections for Au, Ir, Hf and W. Some experimental results have been summarized in two papers one of which has published in Chinese Physics Letters.[6, 7] Reprint of the published papers have been sent to IAEA at CRP meeting in this summer. In this research progress report we give out some new measurement results of L-shell ionization cross sections for some heavy elements by electron impact. The final X-ray production cross section σ_{Li} for a given X-ray line L_i is given by

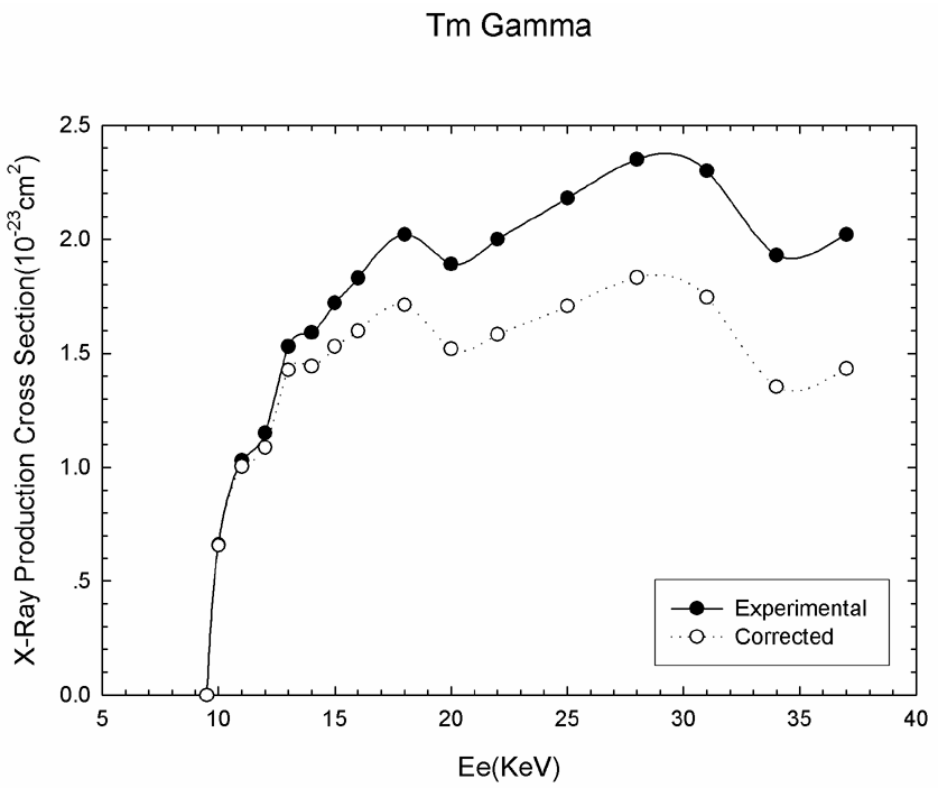
$$\sigma_{Li}(E) = \frac{4\pi N_{Li} A}{N_A N_e s n \varepsilon \Omega} - \int_0^E \Phi_{ref}(E')\sigma_{Li}(E')dE' \qquad (2)$$

where the subscribe i indicates α, β and γ, and E is the energy in units of keV for the incident electrons. N_{Li} is the number of detected X-ray events in the given line corrected for dead-time effects if necessary. A is the atomic weight of the target atoms. N_A is the Avogadro constant. N_e is the number of electron hitting in the target. s is the mean path length of electrons undergoing multi-scattering. n is the target density in units of atom/cm^3. ε is the efficiency of the detector. Ω is the solid angle subtended by the beam spot to the effective detector area. $\Phi_{ref}(E)$ denotes the energy spectrum of the electrons reflected from the substrate. The symbol $\sigma_{Li}(E)$ represents the X-ray production cross sections induced by the electrons with energy E. In order to correct the effect of the reflected electrons from the substrate, we need knowledge of the spectrum of the electrons reflected from the substrate. In this study, the reflected energy spectrum was calculated by use of the bipartition model of electron transport.

The following figures demonstrate the measured L-shell ionization cross sections for the heavy element Tm by electron impact


Tm Alpha
X-Ray Production Cross Section($10^{-22}cm^2$)
Ee(KeV)
Experimental
Corrected
3.0
2.5
2.0
1.5
1.0
.5
0.0
5
10
15
20
25
30
35
40


Tm Beta
X-Ray Production Cross Section($10^{-22}cm^2$)
Ee(KeV)
Experimental
Corrected
2.0
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
0.0
5
10
15
20
25
30
35
40



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Calculation of state-selective electron capture cross sections in ion-atom (molecule) collisions

L. Méndez

Laboratorio asociado al CIEMAT de Física Atómica y Molecular en Plasmas de Fusión. Departamento de Química. Universidad Autónoma de Madrid, 28049 Madrid, Spain

In the last year of the CRP, we have studied low energy atomic collisions by employing a molecular expansion which includes a common translation factor (semi-classical treatment) or a common reaction coordinate (quantal treatment). We have performed quantal calculations of electron capture cross sections for the benchmark collision He^{2+}+ H(1s), at centre-of-mass energy from 20 eV up to 1.6 keV [1]. Since experimental data are not available, we have compared our results in this publication with those obtained with the hyperspherical close-coupling treatment of Lin et al.. The good agreement between both methods allows us to ensure the accuracy of the calculations.

An important advantage of the common reaction coordinate method is that it can be easily generalized to many-electron systems. In this respect, we have considered the collision N^{2+} + H(1s). The aims of this work were:

1. To evaluate partial cross sections, required in plasma diagnostics. To check the accuracy and to cover a large energy range, we have performed quantal and semi-classical calculations.
2. To obtain cross section for charge transfer reactions from both ground ($2s^2 2p\ ^2P^o$) and metastable ($2s2p^2\ ^4P$) N^{2+} ions, which are in principle present in beam experiments.
3. To compare the cross sections with experimental data from Belfast and Oak Ridge laboratories.

Results for impact energies from 0.15 eV/amu to 25 keV/amu have been presented in a recent publication [2].

Core plasma diagnostics require the knowledge of partial electron capture cross sections for collisions of highly charged ions with H. In particular, cross sections for Ne^{10+} + H and Ar^{18+} + H collisions are needed in CXRS diagnostics in ASDEX-U and JET. To cover a large range of impact energies ($1 < E < 500$ keV/amu), we have carried out [3, 4] both large-scale close-coupling molecular calculations and CTMC calculations with an improved initial distribution (see [4]) for capture and ionization. In order to study the usefulness of both methods, we have applied them to Li^{3+} + H collisions, where we can compare our results with existing theoretical and experimental ones. New capture and ionisation cross sections for Ne^{10+} + H collisions have been published in Ref. [3]. In this work we have evaluated capture cross sections for population of Ne^{9+}(nl) states up to n = 8; this data together with further extension to n = 9 - 14 are currently employed in new CXRS measurements in ASDEX-U in the project *Improvement of the CXRS density diagnostics for impurity elements with $Z \geq 10$* (Summers et al.). We are performing similar calculations for ionisation and capture in Ar^{18+} + H. In this case, very large molecular expansions are needed to obtain the high-n partial (n = 14 - 17) cross sections involved in the CXRS experiments. Results for this collision will be presented in the Highly Charged Ions Conference (HCI2004).

With respect to ion-molecule collisions, we have improved our techniques for evaluating *ab initio* three-centre potential energy surfaces and dynamical couplings [5]. These techniques, in particular the treatment of series of narrow avoided crossings, have been applied to calculate single and double (autoionizing) electron capture in $N^{5+} + H_2$ collisions [6] which show good agreement with experimental works of Kearns et al. (J. Phys. **B35**, 4335) and Lubinski et al. (J. Phys. **B33**, 4763). In a recent work, we have considered $H_2^+ + H$ collisions [7], where we have found that anisotropy effects are critical because of the symmetry selection rules that lead to vanishing capture cross sections for transitions in the triplet subsystem, and for collisions where the relative velocity and the H_2^+ internuclear vector are perpendicular.

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Cross-sections of charge and electronic states change of particles at ion-ion and ion-molecule collisions

M.N. Panov, V.V. Afrosimov, A.A. Basalaev, N.A. Guschina, V.K. Nikulin.

A. F. Ioffe Physical-Technical Institute, St. Petersburg, Russian Federation

I. Interaction of protons and alpha-particles with hydrocarbons

At the last RC meeting of 2003 it was reported that schema of fragmentation of hydrocarbon molecules after their ionization did not depend on the type of ionizing fast particles removing the electron, but depend on the number of these electrons. This could mean that the process of fragmentation had taken place after ionization and was dependant only on the excitation energy of the produced ion.

In analyzing the experimental data it is of interest to compare the measured relative probabilities of different fragmentation channels obtained experimentally with calculated fragmentation energies.

Therefore a quantum-mechanical computation of the electronic structure of all hydrocarbons from methane to butane (for example the C_2H_6 case has been given in this Progress Report, Figs 1-3) and its fragment ions was performed in the Hartree-Fock RHF/UHF approximation using a GAMESS program (General Atomic Molecular Electron Structure System) [1] with a 6-31 G[ld] basis [2]. The correlation energy was taken into account within the framework of MP2 perturbation theory. The structural parameters of the hydrocarbon molecules and their charged and neutral fragments were calculated in two cases: in the geometry of the parent molecule or of the relaxation states. The direction of the change of particle charge or atom number of fragments is indicated by arrows in Fig.4. The fragments with the geometry of the parent particles are indicated by the brackets. The difference of the full energy of the same fragments in and out of brackets gives us the vibration excitation energies of the fragments at the moment of creation. Additional Mulliken effective charges (in electron charge units) of atoms in the fragments have been calculated.

The calculations show that removing one electron from the ethane molecule without electronic excitation produced a single charged molecular ion in vibration state with binding energy of hydrogen atoms, some decimal eV. As results we obtain $C_2H_6^+$ and $C_2H_5^+$. Additional fragmentation of hydrocarbon needs electronic excitation of produced single charged ions.

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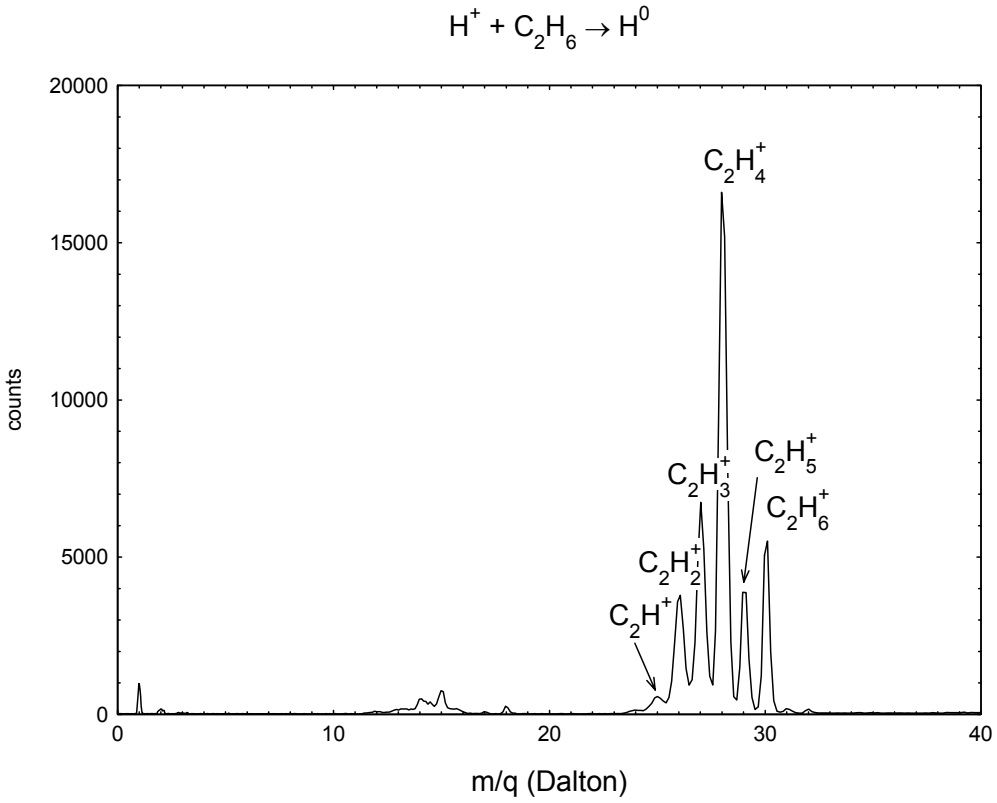

$H^+ + C_2H_6 \rightarrow H^0$
20000
15000
10000
5000
0
counts
0
10
20
30
40
m/q (Dalton)
$C_2H_4^+$
$C_2H_3^+$
$C_2H_5^+$
$C_2H_6^+$
$C_2H_2^+$
C_2H^+

Fig. 1

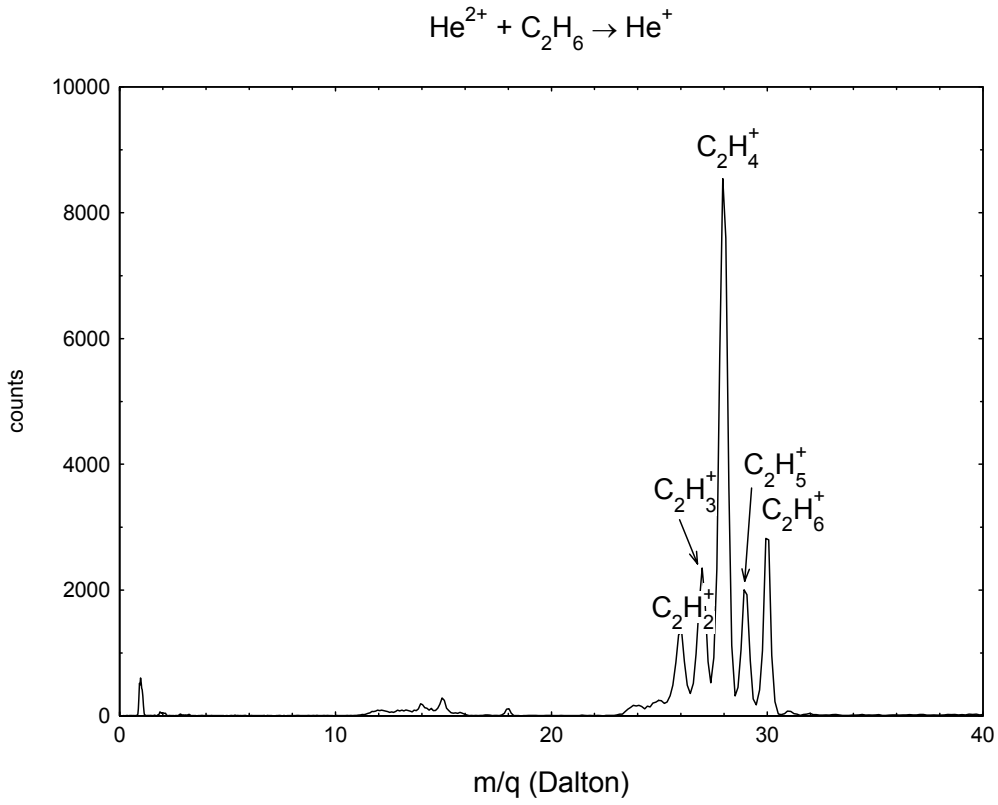

$He^{2+} + C_2H_6 \rightarrow He^+$
10000
8000
6000
4000
2000
0
counts
0
10
20
30
40
m/q (Dalton)
$C_2H_4^+$
$C_2H_3^+$
$C_2H_5^+$
$C_2H_6^+$
$C_2H_2^+$

Fig. 2

Name: Ethane
Formula: C_2H_6
MW: 30 CAS#: 74-84-0 NIST#: 61308 ID#: 1916 DB: mainlib
Other DBs: Fine, TSCA, RTECS, HODOC, EINECS, IRDB
Contributor: D.HENNEBERG, MAX-PLANCK INSTITUTE, MULHEIM, WEST GERMANY
10 largest peaks:
28 999 | 27 362 | 26 258 | 30 232 | 29 212 |
15 65 | 25 51 | 14 48 | 13 19 | 2 12 |

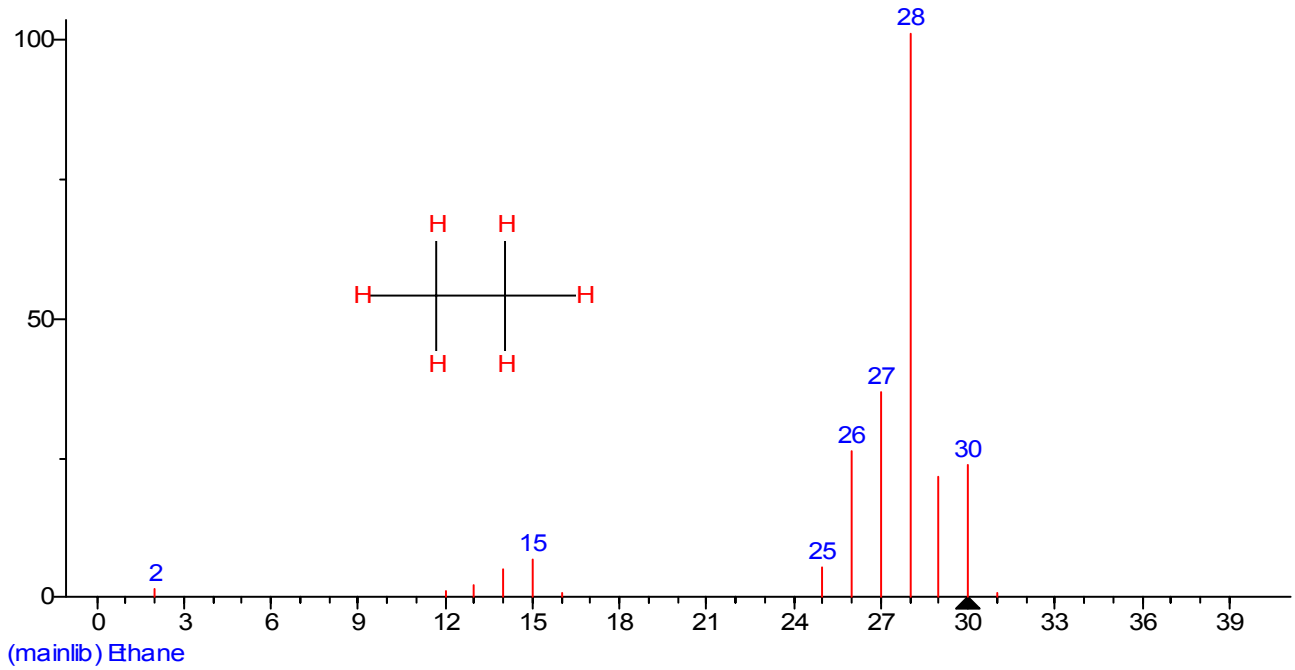
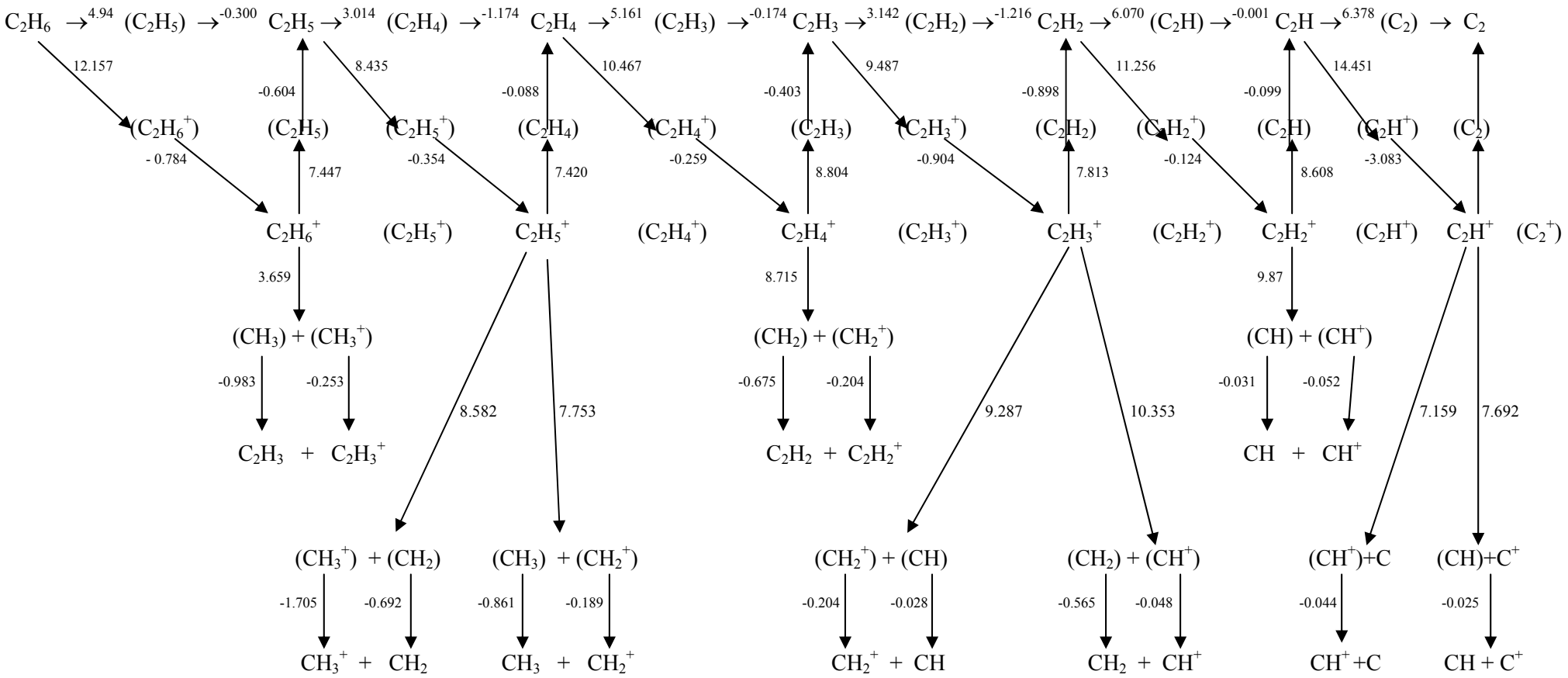


Fig. 3

Fig. 4. Differences of full potential electronic energies (eV) of neighbouring fragments for the ethane molecule.



Fragments indicated in brackets have unrelaxed geometry of parent fragments.

II. Cross sections for electron capture and excitation processes in collisions between the hydrogen-like He^+, B^{4+} and O^{7+} ions.

1. Description of research carried out

The purpose of the theory within this project during the period under review was to get for the first time new data on Single-Electron Capture (SEC) and Excitation Processes (EP) in collisions of $He^+(1s)$ ions with hydrogen-like impurity ions $B^{4+}(1s)$ and $O^{7+}(1s)$ in the energy range for He^+ ions from 0.2 MeV to 3.0 MeV:

$$^4He^+(1s) + B^{4+}(1s) \rightarrow {}^4He^{2+} + B^{3+}(1snl) \quad (1)$$
$$n=2-5$$
$$\rightarrow {}^4He^+(nl) + B^{4+}(1s) \quad (2)$$
$$n=2-3$$
$$^4He^+(1s) + O^{7+}(1s) \rightarrow {}^4He^{2+} + O^{6+}(1snl) \quad (3)$$
$$n=2-5$$
$$\rightarrow {}^4He^+(nl) + O^{7+}(1s) \quad (4)$$
$$n=2$$

The calculations were carried out by using the method of close-coupling equations with basis sets of eleven and ten quasimolecular two-electron states for reactions (1, 2) and (3, 4), respectively (entrance channel, seven charge transfer channels, three or two single excitation channels).

2. Results obtained

The partial and total cross sections of SEC into singlet (Figs. 5 and 6) and triplet 1snl states of B^{3+} and O^{6+} ions for n = 2 – 5 were calculated. There is only a slight difference between the SEC cross sections into singlet and triplet states of B^{3+}, O^{6+} ions. The results for electron excitation $1s \rightarrow 2p_{0,\pm1}$, $3d_0$ of He^+ ions are given in Figs. 7 and 8. The dominant contribution to the excitation cross section of $He^+(1s)$ ion was found to be $1s \rightarrow 2p_{\pm1}, 3d_0$ excitations in $He^+(1s) + B^{4+}(1s)$ collisions and $1s \rightarrow 2p_0$ excitation in $He^+(1s) + O^{7+}(1s)$ collisions at the energy E > 1 MeV. The results for electron excitation $1s \rightarrow 2p_{0,\pm1}$, $3d_0$ of He^+ ions are given in Figs. 7 and 8. The dominant contribution to the excitation cross section of $He^+(1s)$ ion was found to be $1s \rightarrow 2p_{\pm1}, 3d_0$ excitations in $He^+(1s) + B^{4+}(1s)$ collisions and $1s \rightarrow 2p_0$ excitation in $He^+(1s) + O^{7+}(1s)$ collisions at the energy E > 1 MeV.

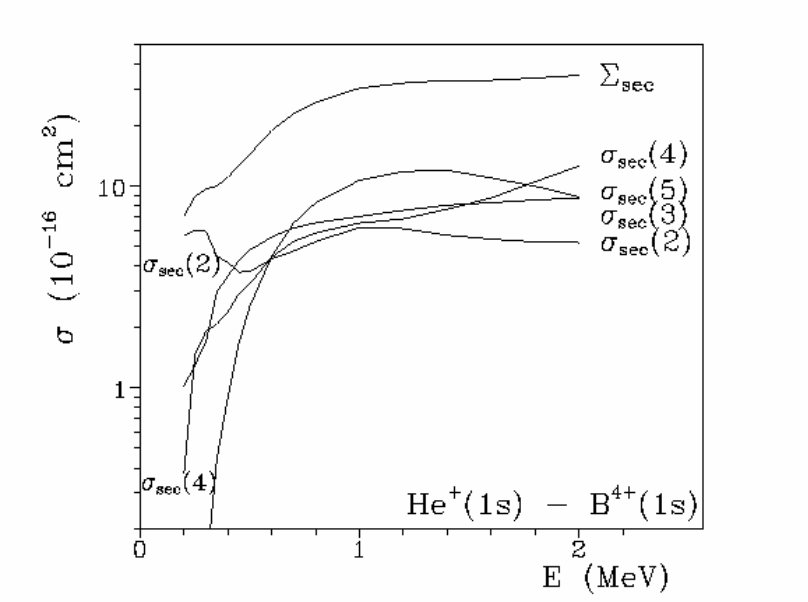


Fig. 5 The total Σ_{SEC} and partial σ_{SEC} (n) cross sections of the single-electron capture into singlet 1snl states of B^{3+} ions: $\Sigma_{SEC} = \Sigma_{n=2-5}\, \sigma_{SEC}$ (n);
σ_{SEC} (2) $=\sigma_{SEC}$ ($2p_0$) + σ_{SEC} ($2p_{\pm1}$), σ_{SEC} (3) $=\sigma_{SEC}$ ($3d_0$) + σ_{SEC} ($3d_{\pm1}$), σ_{SEC}(4)= σ_{SEC} ($4f_0$)+ σ_{SEC} ($4f_{\pm1}$), σ_{SEC} (5) $=\sigma_{SEC}$ ($5g_0$)

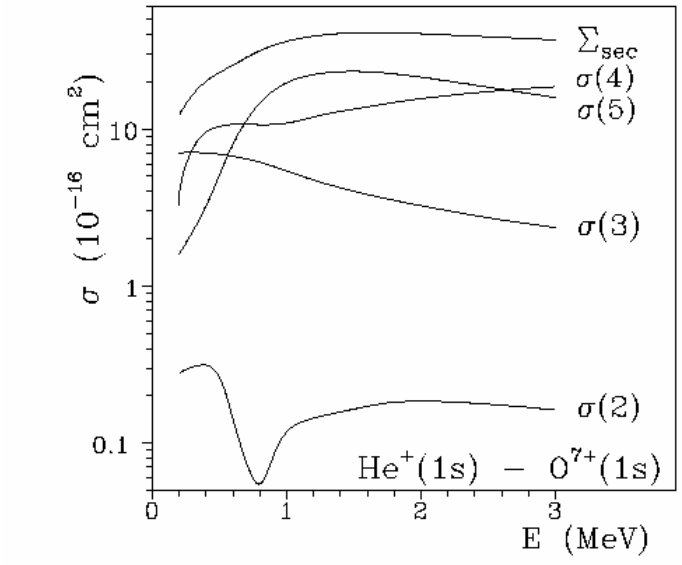


Fig. 6 The total Σ_{SEC} and partial σ_{SEC} (n) cross sections of the single-electron capture into singlet 1snl states of O^{6+} ions: $\Sigma_{SEC} = \Sigma_{n=2-5}\, \sigma_{SEC}$ (n); σ_{SEC} (2) $=\sigma_{SEC}$ ($2p_0$),
σ_{SEC} (3) $=\sigma_{SEC}$ ($3d_0$) + σ_{SEC} ($3d_{\pm1}$), σ_{SEC}(4)= σ_{SEC} ($4f_0$)+ σ_{SEC} ($4f_{\pm1}$),
σ_{SEC} (5) $=\sigma_{SEC}$ ($5g_0$) + σ_{SEC} ($5g_{\pm1}$).

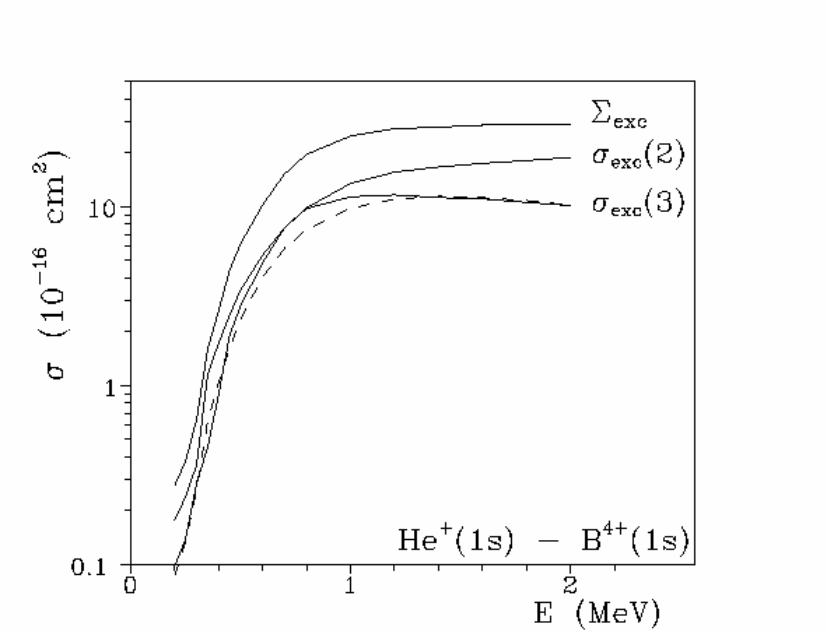


Fig. 7 The total Σ_{EXC} and partial $\sigma_{EXC}(n)$ excitation cross sections of $He^+(1s)$ ions in $He^+(1s)$ + $B^{4+}(1s)$ collisions: $\Sigma_{EXC} = \sigma_{EXC}(2) + \sigma_{EXC}(3)$; $\sigma_{EXC}(2) = \sigma_{EXC}(2p_0) + \sigma_{EXC}(2p_{\pm1})$, $\sigma_{EXC}(3) = \sigma_{EXC}(3d_0)$; (broken line – the partial $\sigma_{EXC}(2p_{\pm1})$ excitation cross section

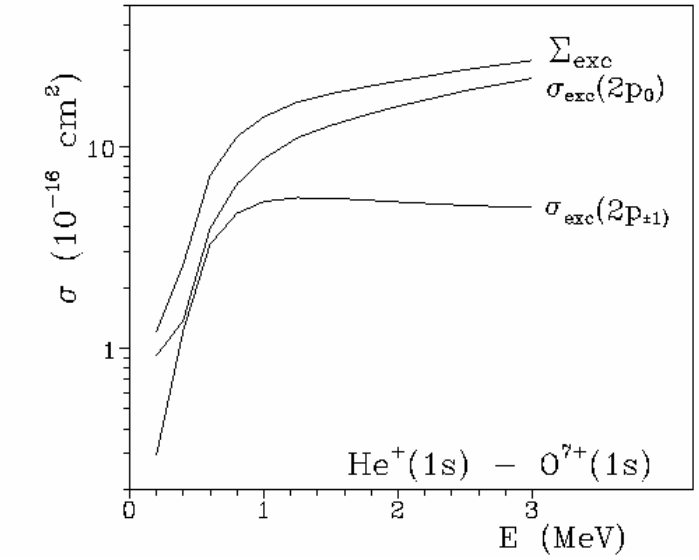


Fig. 8 The total Σ_{EXC} and partial $\sigma_{EXC}(n)$ excitation cross sections of the $He^+(1s)$ ions in $He^+(1s)$ + $O^{7+}(1s)$ collisions: $\Sigma_{EXC} = \sigma_{EXC}(2p_0) + \sigma_{EXC}(2p_{\pm1})$.

III. Conclusions

The calculated SEC and excitation cross sections for ion-ion He^+ – B^{4+}, O^{7+} collisions may be important for diagnostic and modeling of alpha-particles in plasma.

Publications (third year of contract):

1. V.K. Nikulin and N.A. Guschina, Zhurnal Techn. Fiz. **74**, no. 12 (2004) to be published; Tech. Phys., **49** (2004) N 12 (translated from Russian).
2. V.K. Nikulin, N.A. Guschina and Yu.N. Tsarev "Theoretical Study of Electron Capture and Excitation Processes in Collisions between He^{+} and B^{4+}, C^{5+}, N^{6+}, O^{7+} Hydrogen-Like Ions", preprint of A.F. Ioffe Physical-Technical Institute, N 1772, St. Petersburg, 2004.

Determination of rate coefficients for atoms and molecules (hydrocarbons and hydrogen with its isotopes) by measurement and modelling in the plasma boundary of TEXTOR.

A. Pospieszczyk, D. Borodin, S. Brezinsek, A. Huber, A. Kirschner, Ph. Mertens, G. Sergienko, B. Schweer, I. Beigman, L.Vainshtein

Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster, D-52425 Jülich, Germany

I. Helium, Boron

The modelling of experimental emission line profiles from neutral helium was again performed by taking into account the influence of proton collisions on the population of the excited states. It was found that these collisions can lead to enhanced electron density values up to a factor of 2 when fitting the observed emission profiles with the new ones with input from the code ATOM-IMP. The reason for this is the increased ionisation probability of the excited levels by the protons. The values for the electron temperatures remained unchanged.

A similar campaign for boron as for oxygen (see 2003 report) was planned and started including a preliminary modelling and a choice of the suitable spectral lines. The experiments were carried out in November last year but suffered from an insufficient knowledge of the plasma boundary parameters. These will be re-determined in an additional experimental campaign this summer. Preliminary experimental results (e.g. ratios of adjacent B II lines) and a comparison of modelled S/XB data for 10 lines with those from ADAS are provided.

D.Borodin et al., *Spectra of B II in the boundary plasma of TEXTOR: Diagnostic of the boron influx*, Spring meeting of the German Physical Society, Kiel, Germany, 2004.

II. Tungsten

Modelling of the S/XB-value for the 400.9nm line of W I has been performed. For this purpse transitions between following terms were considered:

$$5d^4(^5D)6s^2\ ^5D, \quad 5d^5\ (^6S)6s\ ^7S, \quad 5d^4\ (^5D)6s\ (^6D)6p\ ^7P, \quad 5d^5\ (^6S)6p\ ^7P$$

The energies for states mentioned were calculated by Cowan code and code GRASP-92 . The results were compared with data from Moore tables. A one configuration approximation is quite inadequate. In the calculations 4 even and 2 odd configurations were included. The oscillator strengths were calculated by Cowan (5 even and 3 odd configurations) and Grasp (4 even and 2 odd configurations). Configurations included in the Cowan calculations are:

$$5d^46s^2\ ,\ \ 5d^56s,\ \ 5d^6\ ,\ 5d^46p^2,\ \ 5d^36s6p^2,\ \ 5d^46s6p\ ,\ \ 5d^56p\ ,\ 5d^36s^26p$$

There is strong influence of the configuration mixing and deviation from SL-coupling. Cowan and Grasp gf values differ up to a factor of 2. The Cowan results are in better agreement with the experiment than Grasp. The largest gf values are in the range 290nm, the next are in the range 400nm.

The excitation cross sections and rate coefficients for transitions

$$5d^5(^6S)6s\ ^7S\ \rightarrow\ 5d^4\ (^5D)6s\ (^6D)6p\ ^7P,\ \ 5d^5\ (^6S)6p\ ^7P$$

were calculated by the Normalized Born method. From the data for oscillator strengths one can see that a direct calculation by ATOM is not appropriate. Therefore, a semiempirical approach based on the assumption that the cross section is proportional to the oscillator strength was used. The corrected cross section is then:

$$\sigma\,(\mathrm{corr}) = \sigma\,(\mathrm{ATOM}) * f(\mathrm{exp})/f(\mathrm{ATOM})$$

The ionization cross sections and rate coefficients were calculated for the ground level $5d^4\,(^5D)6s^2\ ^5D_0$ and metastable state $5d^5\,(^6S)6s\ ^7S_3$, and contributions from 5d and 6s shells were included. The contribution from the shell $4f^{14}$ is very small. The cross section for the metastable states is about 30% greater than for the ground state. σ(5d) is 3 times the one for σ (6s) of about 3 times.

The calculations for the S/XB values were done for the following model:
The states $5d^4\,(^5D)6s^2\ ^5D_0$, $5d^5\,(^6S)6s\ ^7S_3$ are in LTE and excited levels included are:
$5d^4\,(^5D)6s\,(^6D)6p\ ^7P_J$, $5d^5\,(^6S)6s\ ^7P_J$ (J=2,3,4), $\Delta S \neq 0$ transitions are excluded.

The agreement with experimental values from IPP-Berlin and IPP-Garching was surprisingly good

III. Hydrogen molecules

For the evaluation of experiments carried out on JET in order to determine the molecular contribution to the total hydrogen flux via Fulcher-α- band spectroscopy the collisional radiative model (CRMOL) by Thornton Greenland was used. On TEXTOR the conversion factor D/XB taken from CRMOL and relating the number of molecular losses per photon was verified in gas injection experiments. The latest version of the code contains also vibrationally resolved D/XB values and provides reasonable molecular atom to molecule ratios for JET conditions.

P.T. Greenland, The CRMOL-Manual, Jül-Report 3858 (2003).
A. Pospieszczyk, S. Brezinsek, G. Sergienko, P.T. Greenland, A. Huber, A. Meigs, Ph. Mertens, U. Samm, M. Stamp and S. Wiesen, J. Nucl. Mater. **337–339** (2005) 500.

IV. Hydrocarbons

Spectroscopy of the CD radical is the standard tool for the determination of CD_4 particle fluxes. But the conversion between photon and particle flux measurements by means of D/XB values is indirect and depends on the dissociation chain.

Several attempts have recently been performed in order to both measure and model the CD-production and its emission on TEXTOR, JET and ASDEX by gas blow experiments into the boundary plasma and divertor surrounding. However, it was found that consistency of the used/measured D/XB values for CH/D from CH_4/D_4 is still not satisfactory. Surface and geometry effects seem to dominate the values and, therefore, a better modelling by an ERO-code is urgently needed, which includes all rates for normal and higher order hydrocarbons as far as possible. However, the measured D/XB values for C_2 look consistent with laboratory experiments.

S. Brezinsek, A. Pospieszczyk, A. Kirschner, G. Sergienko, A. Huber, V. Philipps, Ph. Mertens, U. Samm, M.F. Stamp, A. Meigs and P.T. Greenland, Physica Scripta **T111** (2004) 42.

Atomic data for diagnostic analysis of fusion plasmas using rare gases

H. P. Summers, M. G. O'Mullane, A. D. Whiteford

University of Strathclyde, UK

Work completed as part of the Collaborative Research Project spans generation of fundamental collision data, development of elaborated models for the use of these data for spectroscopic diagnostic analysis of fusion plasmas and the validation in experiments. Rare gas elements and diagnostic contexts include helium as an electron temperature/electron density diagnostic for the plasma edge as a low energy (gas puff); neon and argon as charge exchange spectroscopy emitters in association with neutral deuterium beams; argon and krypton as soft X-ray helium-like and lithium-like satellite line emitters; krypton and xenon as heavy species in integrated radial transport analysis giving line-like and quasi-continuum emission in the XUV, EUV and VUV and total radiated power.

For electron impact with neutral helium, extended R-matrix with pseudostate calculations, emphasizing improvement of the resonance region below ionisation threshold and continuity with CCC calculations above ionization threshold, were completed. These data were merged with previous studies to provide a new comprehensive collision strength dataset of sufficient precision for production of rate coefficients with arbitrary Maxwellian and non-Maxwellian free electron distributions. The data were used in an integrated spatial model of a weakly collimated helium gas puff penetrating tokamak edge plasma. The evolution of the He $1s^2\ ^1S$ ground and He 1s2s ^3S metastable states were described in the full generalized collisional radiative picture and line of sight emissivities in relevant visible spectrum lines predicted. The model was oriented to global optimized fitting of observed intensities for determination of parametric representations of the edge plasma temperature/density profiles. The analysis methodology was tested in dedicated experiments with the HELIOS system on the MAST tokamak and further validation of the diagnostic will take place on ASDEX-U.

Charge exchange spectroscopy with neon as the bare nucleus receiver from neutral deuterium was revisited. This was in the light of revision of CTMC calculations of sub-dominant capture to take account of flaws in the microcanonical representation of the deuterium donor ground state used in older work. New preferred state selective charge exchange data sets were prepared merging these data with CCMO data at lower beam energies and then used to generate effective emission coefficients for all relevant visible charge exchange lines. The methodology was extended to Ar^{+18} as a receiver, for which the revision of CTMC has much larger effect. Preparation of comprehensive data (over all energies) proved difficult in the key 40keV/amu region, so the new data sets prepared cannot be considered finalized yet. The work carried out recognized that Ar^{+18}, Ar^{+17} and Ar^{+16} must be considered together and linked to radial transport and ion location in charge exchange spectroscopy for current fusion machines and for ITER. Experiments were prepared on ASDEX-U and JET to validate the new CXS data. The experimental programmes for both machines have experienced large delays due to technical issues. The critical experiments are now expected from February to June, 2006. It is also noted that along side the new atomic data preparation, a new shared analysis for charge exchange spectral analysis has been initiated in Europe, implemented by the atomic physicists associated with this CRP, which is now in early testing at JET, TEXTOR and ASDEX-U. This work will be taken to Japan in early 2006.

The increasing emphasis on argon in fusion and the extension to interest in krypton has made a fresh look at the familiar soft X-ray helium-like and satellite line emission timely. New calculations in the radiation and Auger damped R-matrix method for inner and outer shell electron impact excitation were carried out for Ar^{+16} and Ar^{+15} and for Fe^{+24} and Fe^{+23}. These have been combined with resonance capture, and dielectronic data to give complete datasets for the collisional-radiative modeling of the singly and doubly excited states. These data have been used in detailed assessments of spectra from TEXTOR and TORE-SUPRA. Agreement is excellent and the new data has now become the preferred form. A systematic programme has been set up to generate data to these standards along whole iso-electronic sequences - in particular spanning also krypton. This exploits massively parallel systems and automatic running and assembly through scripts. Several sequences are underway with helium-like and lithium-like for the present purpose completed. Unification around a single diagnostic implementation of the helium-like soft X-ray analysis within the associated laboratories of EURATOM is in progress but remains incomplete.

Krypton and xenon have been treated as representatives of the very heavy species which are now a focus of attention for ITER. A systematic approach has been set up to enable heavy species and their spectroscopy study to be addressed in a manner analogous to that for light species. This has required special methods to handle and reduce the effect in practice of the complexity of very-many-electron complex ions. Concepts introduced include previews, layers of sophistication in atomic modeling –'baseline', 'level 1' and 'level 2', feature emissivity coefficients for quasi-continuum standing alongside ordinary emissivity coefficients for line-like emission, exploitation of configuration average and special parametric forms to supplement more refined methods, natural partitions and superstages to enable complex 2-d and 3-d transport codes to function with heavy impurity species. Krypton and xenon have been the test beds. Very large scale scripted computations on parallel machines have again been used. The final collisional-radiative coefficient datasets are extensive. In addition, special fully relativistic R-matrix calculations at the top layer of sophistication have been demonstrated for the key line-like emitter Xe^{+26} as part of this CRP. Our view is that this heavy species modeling approach is an appropriate one for progress towards ITER. The methodologies summarized here have now been used quite extensively and have proved effective in EFDA-EURATOM tasks for the design and performance assessment of proposed spectrometers for ITER.

Atomic data for H^+ + He($1s^2$), He(NLM) collisions: single ionisation, excitation and charge exchange cross sections

K. Dimitriou[1], F. Aumayr[1], K. Katsonis[2], H.P. Winter[1],
M.I. Chibisov[3], R.K. Janev[4], X. Urbain[5] and F. Brouillard[5]

[1]*Institut für Allgemeine Physik, TU Wien, Wiedner Hauptstraße 8-10, A–1040 Wien, Austria*

[2]*Laboratoire de Physique des Gaz et des Plasmas, Universite de Paris-Sud, 91405 Orsay, France*

[3] *Russian Research Center "Kurchatov Institute", Moscow, Russia*

[4] *Macedonian Academy of Sciences and Arts, 1000 Skopje, Macedonia*

[5]*Department de Physique, Universite Catholique de Louvain, Louvain-la-Neuve, Belgium*

In the present work, the status of the atomic database of single ionisation and excitation cross sections for proton collisions with neutral helium atoms is reviewed for collision energies relevant to He beam diagnostics (5 - 200 keV). We have mainly focused on the compilation of quantum-mechanical and classical calculations performed during the last ten years. In addition, classical trajectory Monte Carlo (CTMC-) calculations have been made for single ionisation and excitation of ground-state helium atoms by protons in the impact energy region of 5 - 200 keV. These calculated data are compared with the available experimental data. For ionisation they are in close agreement, while for excitation the calculated data are larger by up to a factor of two. For excitation into higher quantum numbers we observe a n^{-3} scaling law for our CTMC calculations.

Furthermore, cross sections for excitation and charge exchange in slow collisions of protons with He(1s, NLM) excited atoms (N = 2, 3, 4) have been calculated in the collision velocity range 10^6 – 10^8 cm/s by using the molecular orbital close-coupling (MOCC) method, with analytically calculated coupling matrix elements in the asymptotic region of internuclear distance. There are no results from other sources for comparison. The respective cross section data have been calculated for all excitation and charge exchange transitions from the initial states with N = 2, 3 to all {N'} = 2, 3 (excitation) and {n} = 2, 3 (charge exchange) manifolds of states, but only cross sections for transitions from {N} = 2 states to {N'} = 2 and {n} = 2 manifolds of states have been presented here, adding sources and the way of access to the other data.

Cross section data obtained from our CTMC and MOCC calculations are presented in graphical and tabular form.

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1)26007
cable: INATOM VIENNA
telex: 1-12645
telephone: (43-1)2600-21710