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2nd IAEA Research Co-ordination Meeting on
“Atomic and Molecular Data for Fusion Plasma Diagnostics”

16-18 June 2003, IAEA Headquarters
Vienna, Austria

SUMMARY REPORT

Prepared by: R.E.H. Clark

May 2004

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“Atomic and Molecular Data for Fusion Plasma Diagnostics”

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Abstract

This report briefly describes the proceedings, conclusions and recommendations of the 2nd Research Co-ordination Meeting (RCM) of the Co-ordinated Research Project (CRP) on “Atomic and Molecular Data for Fusion Plasma Diagnostics” held on 16-18 June 2003 at IAEA Headquarters, Vienna. During the course of the meeting the progress achieved to date was thoroughly reviewed. It was noted that during the course of the research several new areas of data needs were revealed. During detailed discussions proposals from all participants on ongoing data needs indicated that a one year extension of the CRP would be extremely valuable with an additional RCM to be held in 2004. A specific proposal for such an extension was formulated along with the summary of the results achieved to date.

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1. INTRODUCTION

The 2nd Research Co-ordination Meeting (RCM) of the Co-ordinated Research Project (CRP) on “Atomic and Molecular Data for Fusion Plasma Diagnostics” was held on 16-18 June 2003 at IAEA Headquarters, Vienna. The meeting was attended by representatives of the participating institutions. The list of participants is included as Appendix 1. During the course of the meeting each participant summarized the results achieved to date on work related to this CRP. A recurring theme was that there are more data to be generated and that collaborations achieved from this CRP are in a unique position to contribute greatly to data additional data needs in this area. Therefore, during the discussions of the results and conclusions of the RCM a proposal for a one-year extension of the CRP was formulated. Specific objectives of the extension were included and it was proposed that there be a final RCM to be held in 2004.

2. BRIEF MEETING PROCEEDINGS

The meeting was opened by the Scientific, Secretary, R. Clark, who welcomed the participants and introduced Dr. A. Nichols, Head of the Nuclear Data Section. The strong support of the Agency, the Division and the Section to fusion activities was noted. The importance of high quality data for diagnostics was emphasized. The appreciation for the time and effort spent on this project by the experts participating in the CRP was expressed.

Following the introductions, the agenda was reviewed and adopted by the meeting participants (see Appendix 2). The meeting was attended by ten participants from outside the IAEA.

During the course of the first day and a half, each participant gave a summary presentation of results achieved to date. Each participant gave a forty-five minute presentation, including questions. Much discussion resulted from the presentations and areas with need for further research were noted.

Following are short summaries of the current results achieved from each participant. For more detail from each participant, see Appendix 3.

Results Achieved to Date by CRP Participants:

A. Pospieszczyk:

Current status:

Measurements of ratios of excitation rates to ionization rates have been carried out. For O⁺ experimental and theoretical results have been compiled and compared to other theoretical results. Theoretical calculations have been carried out for B⁰⁻³⁺ and for He. For Si^{0,1+} old data were re-evaluated, both theoretically and experimentally. Work has been undertaken on providing data for H₂ for collisional radiative modelling.

L. Mendez:

Calculations have been carried out for cross sections for charge transfer for H with fully stripped argon and neon for beam diagnostics. Cross sections for H with O²⁺ at thermal energies for divertor spectral analysis have been calculated. Calculations have also been performed for cross sections for He²⁺ on H₂ in the energy range of 0.5-5 KeV/u. Cross

sections for Ar^{18+} , Ne^{10+} on H for the beam diagnostics, $\text{O}^{2+} + \text{H}$ at thermal energies for divertor spectral analysis (for ADAS) and $\text{He}^{2+} + \text{H}_2$, 0.5-5 keV.

H. Summers

For Ar^{16+} charge transfer data as well as effective emission coefficients have been accumulated. Data on $\text{Ar}^{15+,16+}$ soft X-ray processes have been collected with new collision data calculated with R-matrix theory. New data for $\text{Ti}^{15+,16+}$ have been obtained from Cadarache to be used in spectral analysis at Juelich Juelich. Efforts are underway to obtain new level-II dielectronic data for heavy species. He –electron impact excitation from comprehensive R-matrix pseudo-state calculations have been implemented for HELIOS diagnostics.

M. Panov:

Cross sections for He^{2+} on H_2 charge transfer, ionization, dissociation and two-electron processes have been obtained. Angular scattering of He, He^+ ions in ionization, dissociation and charge transfer with final state resolved has been calculated. N^{6+} , C^{5+} with He^+ (CT, final state resolved, excitation to different states of He^+ ion). Single electron charge transfer in H^+ collisions with the hydrocarbons CH_4 , C_2H_6 , C_3H_8 and C_4H_{10} into different channels of fragmentation have been studied as well as fragmentation of these hydrocarbons by He^{2+} and Ar^{6+} .

B. Gilbody:

Excited state formation in electron capture by slow multi-charged ions of plasma edge impurities is being studied at energies below 1 keV/u. Studies of one-electron capture by H- and He-like ions of C, N and O in collisions with H and H_2 have been completed in the energy range of 250-900 eV/u. The main collision mechanisms have been identified and in H_2 the dissociative and non-dissociative channels as well as two-electron capture into autoionizing states have been observed. Striking differences in behaviour have been observed. Measurements in H provide an important and useful extension of existing data to energies below 1000 eV/u.

Z. Luo:

Measurements have been carried out for inner-shell ionization cross sections by e-impact for V, Sc, Co, Ni, Cu, Zn, W, Mo, Ag, Sn over energies from several keV-several tens keV.

HP. Winter:

Total CT cross sections have been measured for impact energies in the range of 100-250 eV/amu for He^{2+} on H_2 , O_2 , and CO. Investigations have been made of the role of dissociative electron capture and of experimental conditions for correct measurement of the scattered He^+ projectile.

R. Radtke:

Measurements of W^{25-50+} X-ray and EUV spectra, line identification and measurement of intensities were undertaken for use in interpretation of impurity spectra from tokamaks. Line ratio measurements and EUV spectra for Ar were carried out. Measurements of channel specific cooling rates (for benchmark data to test theoretical calculations) and EUV spectra for Kr were made. Observations were made for EUV spectra of Xe.

R. Janev:

For $H^+ + He$ ($n=2,3,4$) state selective excitation and charge transfer ($E_k=0.2-8$ keV/u) cross sections relevant to He-beam diagnostics were compiled. Triplet-triplet vibrationally resolved excitation transitions in $e - H_2$ collisions ($E_k = \text{threshold}-200$ eV) (relevant to Fucherbands diagnostics) were determined. A database for $e, H^+ + C_xH_y$ for $x=1,3; y=0,2x+2$ was established. (D/XB determination)

P. Krstic:

Fully quantal, initial and final vibrational state resolved $H^+ + H_2$ and $H + H_2^+$ collisions in range 0.5-10 eV: excitation, CT, dissociation, energy and angular spectra of dissociation fragments, collisionally assisted diatomic association.

It was agreed that a great deal of new data of high value for plasma diagnostics had been developed through this CRP. However, a number of data needs were noted that could be addressed. It was stressed that a number of very valuable collaborations have been developed during the course of the CRP and that with an additional one year extension of the CRP these collaborations would be able very effectively in adding more data. Each participant suggested specific proposed additional work that could be performed during a one-year extension.

Future Plans For CRP Participants:

A. Pospieszczyk:

Further work remains to be done to fulfil the needs from the TEXTOR machines for data on hydrocarbons, boron and hydrogen. Included in data needs are both experimental and theoretical cross sections for higher order hydrocarbons, hydrosilicons and for tungsten.

L. Mendez:

Calculations need to be carried out for charge transfer cross sections for the ions $Ar^{16,17+}$ and N^{2+} colliding with H. In addition there is a need to extend the cross sections for He^{2+} on H_2 to lower energies, as low as 50 eV and for similar cross sections for $H^+ + CH$ at energies in the range of 500-5000keV.

H. Summers:

Many more cross sections need to be calculated with the best possible calculational tools. It is proposed to continue R-matrix calculations to higher level series. In particular, calculations similar to the Li calculations should be carried out for Be and B. Extension of level 2 di-electronic series through the Ne-like stages should be undertaken. Extension of the He- and Li- like calculations should be carried out for a number of elements identified as important in ITER for soft X-ray spectral studies.

M. Panov:

Calculation of SEC total and partial cross sections of n-states of B^{3+} ions and excitation of He^+ ion in collisions will be undertaken. Theoretical analysis of vibrational excitation of hydrocarbon ion produced in the SEC process by H^+ , He^{2+} and Li^{3+} ions will be initiated. Measurements of absolute values of fragmentation channels of hydrocarbon molecules in processes of SEC in collisions with ions in the energy range of 0.5-30 keV will be made.

B. Gilbody:

Recent successful studies of excited state formation in one-electron capture collisions by multiply charged ions at energies below 1 keV/u will continue. Measurements in H and H_2

will be extended to lower energies and to other species relevant to the plasma edge. It is also planned to consider electron capture in H₂O and CH₄. Some deficiencies in the existing database of benchmark cross sections will be addressed.

Z. Luo:

A new electron probe will be used for improved measurements of inner-shell ionization cross sections for low-Z elements and higher Z elements. Accuracy of the measurements of the thickness of thin targets will be improved by using RBS. Work will be undertaken to develop a thick target method for elements such as C, O, N, F, Na, Cl and others. Extension of k-shell cross sections by electron impact to C, O, N, F, Na and Cl neutral atoms in the energy range of a few keV to 30 Kev will be undertaken.

HP. Winter:

This CRP represents an almost ideal source of knowledge on atomic data which are needed for the evaluation of plasma diagnostics by means of fast He beam spectroscopy. In the future CTMC calculations of proton induced He excitation and ionization cross sections will be carried out with proton impact energies in the 5-40 keV range, which are needed for modelling of He I line radiation profiles along the diagnostic beam. If time permits, experimental studies on the total SEC cross section for slow He²⁺ on H₂ for energies above 100 eV will be continued.

R. Radtke:

The Berlin EBIT was used to produce fusion related atomic data from highly charged ions, for example cooling rates for Kr as well as line ratios for Ar which serve as temperature diagnostics for hot plasmas. Further detailed investigation will continue on measurement of the EUV spectra from Kr and Xe, which are needed to predict the radiative cooling in the plasma. Investigation of charge transfer reactions between highly charged and neutral atoms to understand line emissions observed in charge transfer reactions will take place. These processes will be measured as a function of the impact velocity.

R. Janev:

Cross section calculations will be made for H₂⁺, H₃⁺ + H⁻ charge transfer and detachment. Cross sections for singlet-triplet electron impact of H₂, vibrationally resolved will be carried out. An establishment of a complete vibrationally resolved H/H₂, coupled collisional radiative model will be initiated. These activities have direct relevance to Fulcher-band and H₂ edge plasma diagnostics and neutral particle transport in edge plasmas and are needed for plasma modelling codes such as EIRENE.

P. Krstic:

Vibrational state resolved charge transfer, excitation, dissociation in H⁺+H₂ and H+H₂⁺ collisions, in energy range 20-100 eV, for various isotopic combinations (H, D, T).
Vibrational state resolved CT, excitation, dissociation in He²⁺+H₂ collisions.

On the basis of the very good achievements of the CRP participants and the detailed list of possible outcomes from an extension of the CRP, a detailed proposal for a one year extension was formulated. The extension proposal is included in Appendix 4.

3. RECOMMENDATIONS AND CONCLUSIONS

The results achieved to date from the CRP on “Atomic and Molecular Data for Fusion Plasma Diagnostics” have been summarized by the participants and are included in short form in this report. A number of areas have been identified that would greatly benefit from an extension of the CRP by one year. Specific tasks for each CRP participant have been listed. A detailed proposal for a one-year extension, to include a final RCM in 2004 was formulated and is included as Appendix 4 of this report. It is highly recommended that such an extension be undertaken to make the best use of the expertise gathered in this CRP.

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Scientific Secretary: R.E.H. Clark

Meeting Agenda

Monday 16 June

Meeting Room: F01-23

09:30-10:00 Opening, Adoption of Agenda, A. Nichols, R. Clark

Session 1: Progress Reports I

Chairman: P. Krstic

- 10:00-10:45 M. Panov
Single-electron capture and excitations in collisions of He⁺ with multiply ions N⁶⁺ and C⁵⁺ (theory) and interaction of H⁺, He²⁺ and Ar⁶⁺ ions with hydrocarbon molecules (experiment)
- 10:45-11:15 *Coffee Break*
- 11:15-12:00 L. Mendez
Calculation of state-selected electron capture cross sections in ion-H, H₂ collisions
- 12:00-12:45 H. Summers
Atomic data and modelling for argon as a reference plasma species
- 12:45-14:00 *Lunch*

Session 2: Progress Reports II

Chairman: R. Radtke

- 14:00-14:45 A. Pospieszczyk
Determination of rate coefficients for atoms and molecules (hydrocarbons & hydrogen) Problems and preliminary results
- 14:45-15:15 *Coffee Break*
- 15:15-16:00 B. Gilbody
Excited state formation in electron capture by slow H and He-like ions of C, N and O in H and H₂
- 16:00-16:45 Luo Zhengming
New method for measurements of inner-shell ionization cross sections of atoms by electron impact

Tuesday 17 June

Session 3: Progress Reports III

Chairman: A. Pospieszczyk

- 09:00-09:45 HP. Winter
Non-dissociative and dissociative single electron capture by slow doubly charged He ions from H₂, O₂ and CO
- 09:45-10:30 R. Radtke
Overview of the Berlin Electron Beam Ion Trap Project
- 10:30-11:00 *Coffee Break*
- 11:00-11:45 R. Janev
Status of database for collision processes of hydrocarbons
- 11:45-12:30 P. Krstic
Further progress in understanding vibrationally resolved ion-molecular collision processes of hydrogenic species
- 12:30-14:00 *Lunch*

Session 4: Review of work plan and outcomes

Chairman: HP. Winter

- 14:00-15:30 All
Discussion
- 15:30-16:00 *Coffee Break*
- 16:00-17:00 All
Discussion

Wednesday 18 June

Session 5: Formulation of meeting conclusions and reports

Chairman: L. Mendez

09:00-10:45 All
Discussion of reports and database additions

10:45-11:15 *Coffee Break*

11:15-12:30 All
Formulation of meeting conclusions

12:30-14:00 *Lunch*

Session 6: Proposal for extension of CRP

Chairman: B. Gilbody

14:00- All
Discussion and possible formulation of proposal to extend this CRP

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SUMMARIES OF WORK PERFORMED

T.E. Evans:

SUMMARY

Update on Atomic and Molecular Data Application for DIII-D Diagnostics

Work on this project since the first CRP meeting in November 2001 has focused primarily on identifying the types of atomic and molecular data needed to model impurity transport and to interpret spectroscopic signals from various DIII-D diagnostic systems. In addition, new atomic data provided by several other CRP participants (see below) has been applied to the analysis of impurity transport experiments in DIII-D.

Recent DIII-D experiments related to this CRP include:

1. Detailed spectroscopic studies of atomic and molecular carbon and hydrocarbon sources from various locations (including the upper and lower divertors and along the inner wall) during high power advanced tokamak operations. Results from our initial studies were reported in: R. C. Isler, R. J. Colchin, N. H. Brooks, T. E. Evans, W. P. West and D. G. Whyte, *Phys. Plasmas* 8 (2001) 4470 and extended in second paper ("Determination of carbon release mechanisms from analysis of CI spectral line profiles" by R. C. Isler, N. H. Brooks, P. C. Stangeby, T. E. Evans and W. P. West which is being submitted to *Physics of Plasmas*) where more details on the various contributions of atomic carbon and hydrocarbons to the core carbon concentration are given.
2. Methane injections experiments have been carried out to establish how hydrocarbon dissociation rates are affected by edge plasma parameters and source location. Results from these studies were reported at the November 2002 DPP-APS Meeting by W. P. West, et al., and at the October, 2002 IAEA Technical Meeting on Atomic and Molecular Data by T. E. Evans, et al.
3. Hydrogen neutral recycling studies of wall sources versus divertor sources were studied experimentally and compared to a simple 1D Monte Carlo neutral transport code in a paper on: "Atomic physics processes important to the understanding of scrape-off layer of tokamaks" by W. P. West, B. Goldsmith, T. E. Evans and R. J. Olson, General Atomics report GA-A23960, May 2002, published in the proceedings of the Third International Conference on Atomic and Molecular Data and Their Applications, Gatlinburg, Tennessee, April 24-26, 2002.
4. Lithium sputtering and transport modeling has been complete for a small solid/liquid sample inserted into the lower divertor strikepoint region of a low power L-mode plasma. These simulations were the first to combine the capabilities of the b2.5/DEGAS (fluid deuterium plasma / Monte Carlo deuterium neutral) background plasma code with the WBC (gyrokinetic Monte Carlo) sputtering/near surface transport code and the MCI (Monte Carlo Impurity) code by coupling code solutions near the divertor target plates and in the divertor SOL and outer region of the core plasma to predict the Li neutral and charge state distributions in each region of the plasma accessible to spectroscopic diagnostics on DIII-D. Recent high accuracy lithium ionization and recombination used in these simulations was supplied by the ADAS GCR project (H. Summers et al.). We are currently in the process of comparing LiI and LiII emission signals with code predictions and working with the atomic physicists at Auburn Univ., JET and the Univ.

of Strathclyde (members of the ADAS GCR project) to model the 2s-2p Li emission data from these experiments. Initial experimental and transport simulations results have been reported at the October 2002 ADAS Workshop in Cadarache, France, the November 2002 ALPS/APEX Workshop at the Princeton Plasma Physics Laboratory, Princeton, New Jersey and at the April 2003 ALPS/APEX Workshop at the Grand Canyon Meeting Center, Grand Canyon, Arizona. We are also in the process of preparing a paper for publication on these results.

5. We have also received ctmc charge exchange data for F9+ on H(1s) and H(n=2) between 5 - 100 keV/amu from R. Hoekstra et al., which we intend to use for the analysis of fluorine charge exchange studies with the DIII-D neutral beams.

If this CRP is extended we intend to complete the analysis of the methane injections experiments, the lithium transport studies and the fluorine charge exchange analysis. We also intend to investigate the use of a proposed lithium beam system in the DIII-D divertor for BES and CER measurements.

R. Radtke:

SUMMARY

Overview of the Berlin Electron Beam Ion Trap Project

The presentation gives an overview of the capabilities of the Berlin Electron Beam Ion Trap operated at the Max-Planck-Institut für Plasmaphysik, Bereich Plasmadiagnostik to produce general atomic and fusion related data from highly charged ions.

- In the first section, a review of completed and published projects is summarized:
 1. The measurement of the radiative cooling function for krypton with a detailed list of the contributions of the different x-ray emission channels: bremsstrahlung, radiative recombination, dielectronic recombination and line emission radiation following electron-impact excitation. The experimentally determined total cooling rate at a plasma temperature of 4.7 keV shows that theoretical predictions underestimate the total cooling efficiency by about a factor of 2. Krypton is injected into the boundary layer of tokamak plasmas to control the energy release and reduce the load on plasma-facing components.
 2. The EUV radiation of tungsten ions with charges 21+ to 45+ was measured with a grazing-incidence spectrometer in the wavelength range of 4 to 7 nm. The detailed information provided by the spectra and EBIT's capability to successively scan the maximum ionization stage reveals the nature of the observed emission bands originating from 4p-4d and 4d-4f transitions. The explanation of the quasi-continua is supported by HULLAC calculations from the University of Jerusalem and clarifies the features observed at ASDEX Upgrade. The code also predicted magnetic dipole transitions in the 10 to 90 nm spectral range which have been experimentally confirmed. However, the agreement between the observed line positions and the calculated wavelengths is not fully satisfying for all transitions and requires inclusion of a large base of configurations to converge.
 3. The measurement of line ratios for helium-like argon which serve as a temperature diagnostic for hot plasmas, as is for example routinely employed at TEXTOR. High-resolution x-ray spectroscopy and varying EBIT's monoenergetic electron beam over a wide range of electron energies allows the separation of lines which commonly overlap in plasmas and the extraction of detailed line information. The intensity ratio of the dielectronic k satellite to the w resonance line is a steep function of electron temperature and well suited as a diagnostic in the range of 0.5 to 3.5 keV. Good agreement with HULLAC-predicted collisional excitation rates and results from tokamak facilities is obtained.
- Subsequently the following ongoing projects are described:
 1. The investigation of tungsten has been extended to higher charge states (W^{44+} to W^{50+}) radiating in the soft x-ray region at around 0.5 nm. By successive variation of EBIT's electron beam energy, the highest ionization state can be predefined and the lines are identified as $3l-4l'$ transitions of Ni-like to Cr-like ions with open M-shell configurations in good agreement with *ab initio* structure calculations from HULLAC. Lines for these ions have also been observed at the ASDEX Upgrade

tokamak in plasma discharges with electron temperatures of up to 5 keV in the spectral range of 0.5 to 0.8 nm and 1.5 to 1.9 nm. Comparison with HULLAC predictions where the strength of the transition is derived from a collisional radiative model show some discrepancy. By measuring excitation cross-sections we are planning to resolve this problem and allow a better determination of the tungsten concentration in fusion experiments.

2. With the grazing-incidence spectrometer a survey of EUV-lines from heavy noble gases has been performed. Approximately 60 lines for C- to Li-like argon (Ar^{12+} to Ar^{15+}) have been identified and some lines are measured to a precision of 0.6 pm in 36 nm. The wavelengths are in good agreement with predictions by Edlén from 1983. Several of the observed lines are tabulated in the solar line list. From the measurement of the line intensity ratio of certain intercombination and highly excited lines a plasma temperature can be determined. The comparison of theoretical predictions with measurements of the solar upper atmosphere have so far led to some discrepancy possibly due to incorrect assumptions regarding the atomic processes in the emitting plasma. The well-understood EBIT laboratory plasma can help resolve this problem and establish a diagnostic. The information gained is also of benefit to the measurement of the plasma temperature in the outer regions of present day fusion machines like ASDEX or TEXTOR.

The EUV spectroscopy is extended to highly charged krypton and xenon where up to now only sparse information has been available. While for krypton ions with charge state 20+ to 25+ individual line structures are observed in the spectral range 10 to 70 nm, the xenon spectrum is dominated by band-like emission structures for charge states up to 40+. These heavy noble gases are intended to be injected as a radiating buffer in the high temperature fusion plasmas of JET and ITER for which detailed spectral knowledge is needed. Another application currently explored is the use of xenon EUV radiation for lithography of nm-structures for chip-technology.

3. The Berlin Electron Beam Ion Trap facility has been extended with an extraction beamline and gas target station followed by a time-of-flight analyzer. With this setup collision experiments between low energy highly charged ions and neutral gas atoms have been started in order to investigate the electron capture process. Charge transfer reactions between highly charged ions and neutral atoms are of interest in the understanding of line emission observed from fusion plasmas found in JET, TFTR or DIII-D or non-terrestrial sources such as comets or solar flares. The Berlin EBIT beamline is equipped with a retardation unit to measure the charge transfer as function of collision velocity. After the collision the ejectile and/or target can be mass-to-charge analyzed by time-of-flight. During the charge transfer process an electron is captured to a highly excited n -state, which decays successively. The radiation emitted is analyzed by a low-energy x-ray detector with a large solid angle and a fibre-optic link to a UV-spectrometer. The pattern of the detected radiation provides information on the decay cascade and the initial principal and orbital angular momentum quantum number (nl). First experiments with bare and hydrogen-like argon colliding with argon atoms at 5 keV impact energy show the signature of a $n=2-1$ transition from the last step of the cascade. The lack of other features in the x-ray spectrum suggest initial capture into a large l -substate. Further and detailed investigation will be continued after the move of the Berlin EBIT to the Adlershof location of the Humboldt-Universität zu Berlin.

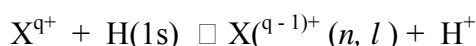
Publications

1. T. Fuchs, C. Biedermann, R. Radtke, E. Behar and R. Doron
Channel-specific dielectronic recombination of highly charged krypton
Physical Review A **58**, 4518 (1998)
2. C. Biedermann, T. Fuchs, P. Liebisch, R. Radtke, E. Behar and R. Doron
X-ray Spectroscopic Measurements of Dielectronic Recombination of Highly Charged Krypton Ions
Physica Scripta **T80**, 303 (1999)
3. R. Radtke, C. Biedermann, T. Fuchs, G. Fußmann and P. Beiersdorfer
Measurement of the radiative cooling rates for high-ionization species of krypton using an electron beam ion trap
Physical Review E **61**, 1966 (2000)
4. R. Radtke, C. Biedermann, J.L. Schwob, P. Mandelbaum and R. Doron
Line and band emission from tungsten ions with charge 21+ to 45+ in the 45-75 Å range
Physical Review A **64**, 012720 (2001)
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SUMMARY

Excited State Formation in Electron Capture by Slow Multiply Charged Ions

Translational energy spectroscopy (TES) is being used to study one-electron capture by slow multiply charged ions in both atomic and molecular hydrogen at energies below 1 keV amu⁻¹ where experimental data are often sparse or unreliable and the range of validity of current theoretical models is uncertain. It is well known that, for exothermic processes at low velocities the electron capture process may be dictated primarily by pseudo-crossings of the potential energy curves describing the initial and final molecular systems. Thus in the process



involving atomic hydrogen, electron capture may take place selectively into only a limited number of excited product states n, l . In the case of a molecular hydrogen target, the dissociative product channels can also play an important role. Indeed, our previous study [1] of one-electron capture by 0.5 – 2 keV amu⁻¹ He²⁺ ions in H₂ showed, rather surprisingly, that dissociative excitation channels (leading to mainly H($n = 2$) and He⁺(1s) products) provided the dominant contribution to electron capture. Our subsequent study [2] of one-electron capture by 0.2 – 1 keV amu⁻¹ He²⁺ ions in CO showed that dissociative electron capture channels associated with He⁺(1s) formation accounted for about 99% of the total cross section at the lowest impact energy considered.

In our current work, we have completed out detailed TES studies [3] of electron capture by 214 - 857 eV amu⁻¹ N⁵⁺ ions in both H and H₂. These show that non-dissociative electron capture leading to the N⁴⁺($n = 3$) states is the main product channel at the higher impact energies with smaller contributions to the N⁴⁺($n = 4$) states. While this has also been observed in previous studies based on photon emission spectroscopy (PES), there are substantial differences in both magnitude and energy dependence between the TES and PES results. Theoretical predictions for $n = 3$ formation are also in poor accord with experiment. Unlike previous PES measurements, our TES study has been able to identify the presence of dissociative one-electron capture channels and two-electron autoionizing capture channels both leading to N⁴⁺($n = 2$) formation. Two-electron autoionizing electron capture is the dominant main collision mechanism leading to N⁴⁺ ions at the lowest energies considered.

Our measurements of one-electron capture in N⁵⁺ + H(1s) are in excellent accord with previous higher measurements based on PES and now provide a useful extension to energies below 1 keV amu⁻¹. In this case, only the N⁴⁺($n = 4$) and N⁴⁺($n = 3$) product channels are observed with contributions from the latter becoming insignificant at our lowest energies.

We have now also completed TES studies [4] of one-electron capture by H and He-like ions of C, N and O in both H and H₂ within the range 250 – 900 eV amu⁻¹. The main collision mechanisms leading to state-selective electron capture have been identified, their relative importance assessed and compared, where possible, with theoretical predictions and with any previous measurements based on PES. For one-electron capture in H₂, the relative importance of contributions from non-dissociative and dissociative capture as well as from two-electron capture into autoionizing states is found to be strikingly different for the cases considered.

Unlike N^{5+} in H_2 where both dissociative one-electron capture and two-electron autoionizing capture channels are very important [3], in the case of one-electron capture in $O^{6+} - H_2$ and $C^{4+} - H_2$ collisions, non-dissociative electron capture channels are found to be dominant. For H-like ions, in the $O^{7+} - H_2$ system non-dissociative and dissociative electron capture are found to be of about equal importance. However, for N^{6+} in H_2 there is no evidence of dissociative electron capture. In contrast, for C^{5+} in H_2 contributions from dissociative electron capture channels are substantial and increase in relative importance with decreasing energy when evidence of a two-electron autoionizing capture mechanism also appears.

Our TES studies of one-electron capture by H and He-like ions of C, N and O in atomic hydrogen [4] provide an important extension of previous measurements to energies below 1000 eV amu^{-1} . In all the cases considered, as the impact energy decreases, electron capture becomes more selective until only a single n product channel is significant. These main product channels are well predicted by reaction windows calculated using a Landau-Zener approach. However, the same approach applied to the more complex energy change spectra in H_2 is less successful in predicting the main product channels.

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R.K. Janev:

SUMMARY

Generation, Compilation and Evaluation of Atomic and Molecular Data for Fusion Plasma Diagnostics

The following work has been carried out and accomplished on the project:

1. State-selective excitation, de-excitation and electron capture in slow collisions of protons with excited helium atoms in $nl\ ^{1,3}L_J$ states. A restricted molecular expansion (MO) close-coupling method was used to describe the collision dynamics of all $nl\ ^{1,3}L_J$ states of the $n=2,3,4$ manifolds on He^* and hydrogen atom. Cross sections for transitions between all these states were calculated in the energy region below 10 keV. The results of this work were published in [1] and [2].
2. Cross sections for electron-impact excitation of $B^1\Sigma_u^+$ and $C^1\Pi_u$ states of D_2 , DT and T_2 from their vibrationally excited ground electronic state were calculated from threshold to 300 eV. The impact parameter method adapted to electron – molecule collisions was used. The scaling properties of the cross sections with respect to initial state vibrational energy, and the target mass have been revealed. The results were published in [3]. In addition, cross section calculations have been performed by the same method for the $a \rightarrow c$, d , and $g \rightarrow h$ triplet-triplet electron impact induced transitions in molecular hydrogen. The results have been submitted for publication [4].
3. Electron capture and particle exchange cross sections were calculated for slow collisions (below 10 eV) of protons with vibrationally excited hydrogen molecules within the general IOSA (frozen rotations) approximation. A close-coupling computational scheme has been employed on an adiabatic vibronic basis containing all the discrete vibrational states of H_2 and H_2^+ systems, and about 850 states from the discretized continua of these systems. The results are published in [5].

The same method (and expansion basis) has been used to calculate the state-selective and total dissociation cross sections in $H^+ + H_2(v)$ and $H + H_2^+(v)$ collisions, as well as the cross sections for diatomic association in $H^+ + H + H$ three-body collision systems. The results are published in Refs. [6] and [7].
4. An extensive cross section compilation and evaluation of all inelastic electron impact processes involving vibrationally excited hydrogen molecules and ions, and their isotopic variants, was accomplished. The results are published in [8].
5. An extensive cross section data compilation, evaluation and generation effort was undertaken for the electron and proton impact processes with hydrocarbon molecules (C_xH_y) and their ions. A complete cross section database has been prepared for all the families of hydrocarbons with $x=1,2,3$ and $0 \leq y \leq (2x+2)$. The results are published in [9,10] and in the reports [11-14].

The results obtained under 1 and 2 above are relevant for the He-beam and Fulcher band emission diagnostics of fusion edge/divertor plasmas. The results obtained under 3 and 4 are

relevant for the H_α edge plasma diagnostics, while the database established under 5 above is relevant for the diagnostics of hydrocarbon erosion fluxes entering the divertor region.

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P. Krstic:

SUMMARY

Vibrationally Resolved Processes in Slow Ion-molecule and Atom-molecular Ion Collisions of Hydrogenic Species

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 1-10 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 discretized 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. The cross sections obtained are in reasonable agreement with the sparse data available from literature, mostly for the ground vibrational state.

The dominant dissociation mechanism 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 [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 the considered collision systems [3].

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, collisionally assisted diatomic association (also known as three-body recombination) was studied [4] 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 than that of H_2 due to strong charge transfer between the corresponding continua and a favorable distribution of highly excited vibrational states in case of H_2^+ . The total association rate coefficients are about 5×10^{-32} to 6×10^{-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).

To vary the isotopic content in the above treatment of inelastic processes, in the energy range where the nuclear rearrangement processes are still present (a few eV), would require full involvement of the rotational dynamics of the diatomic targets, which is beyond the scope and numerical capabilities of the described method.

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 20 eV to several hundreds eV. 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. Preliminary results are a reasonable continuation of the excitation, charge transfer and dissociation cross section dependences obtained fully quantum-mechanically at lower energies. This method is capable for treating of various isotopic combinations of hydrogenic species in $H^+ + H_2$ and $H + H_2^+$ collisions, since the nuclear rearrangements are absent in the higher energy range.

All calculated, initial and final vibrational-state resolved cross sections for vibrational excitation, charge transfer and dissociation are available from the ORNL-CFADC [www site](http://www.cfadc.phy.ornl.gov), in tabular and graphical form (www.cfadc.phy.ornl.gov).

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H.P. Summers:

SUMMARY

Generation of Selected Collisional-radiative Coefficient Data of Atoms and Ions for the Support of Beam, Core Plasma and Divertor Models and the Reduction of Experimental Spectral Data

A new, comprehensive, dielectronic recombination database within the generalized collisional-radiative (GCR) framework is in process of assembly^[1]. This *level 2* approach, executed in intermediate coupling, is concerned with the need to handle medium and heavy species in both fusion and astrophysics and to handle more extreme environments. Thus in this approach, we work with levels rather than terms and use an intermediate coupling scheme, based-on the use of the Breit-Pauli Hamiltonian (Badnell 1997). It parallels *level 1* calculations, in LS coupling, generated in the early nineties. The resolution and precision of the data are tuned to spectral analysis and so are sufficient for prediction of the dielectronic recombination contributions to individual spectral line emissivities. The fundamental data are structured according to the format prescription *adf09* of the Atomic Data and Analysis Structure (ADAS). The He-like, Li-like, Be-like, B-like, C-like, N-like O-like iso-electronic sequences have been completed and include explicitly the appropriate ions of the elements. He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, Ca, Ti, Cr, Fe, Ni, Zn, Kr, Mo and Xe.

Special attention has been given to extending the validity of the data to GCR application at very high density by allowing a mechanism for ion impact and/or microfield redistribution effects to be introduced for the doubly excited resonance states. This is by use of support functions built on the simpler Correspondence Principle approach to high level dielectronic recombination (the BBGP method) which are normalised to the high precision *level 2* data at zero density. Simultaneously with *level 2* production, compatible parameters (threshold partial collision strengths, dipole polarizabilities etc) have been generated which enable the BBGP approximation. These brief 'driver' datasets (ADAS format *adf28*) can be used to generate dielectronic data at a simpler level (and reduced precision) by workers for whom the *level 2* approach is too sophisticated.

Electron-impact excitation collision strengths for transitions among doubly-excited levels up to the $n=3$ shell (excluding the $1s3l3l'$ configurations) of lithium-like argon and iron^[2] have been calculated using a radiation and Auger damped, intermediate coupling frame transformation, R-matrix approach. Collision strengths have also been calculated for transitions between all singly-excited levels up to the $n=5$ shell for the same systems. The Maxwell-averaged effective collision strengths are estimated to be accurate to within 20% at temperatures 5×10^4 - 5×10^8 K for Ar^{+15} and 10^5 - 10^9 K for Fe^{+23} . These results are of substantially improved precision compared to previous studies. The data relate to the analysis of soft x-ray helium-like spectra in both astrophysical and fusion thermal plasmas and parallel previous work on the helike sequence^[3]. The new data are matched to experiment in current spectral analysis procedures. The calculations are currently being extended to a wide range of elements through to xenon. These data are archived for population (and satellite line) modelling in ADAS format *adf04*.

Configuration-average distorted-wave calculations have been carried out for electron-impact single ionization of all ionization stages of krypton^[4]. Contributions to the cross sections are included from both direct ionization and excitation-autoionization. Good agreement with experimental crossed-beams measurements is found for many of the moderately-charged ionization stages. Maxwellian-averaged rate coefficients have been calculated for each ionization stage and then archived for future use in studies of ionization balance in astrophysical and laboratory plasmas (ADAS formats *adf23* and *adf07*). These calculations provide a starting point for extended use of the CADW ionization calculations to provide metastable resolved and excited state ionization data for medium/heavy species for GCR modelling. These large scale calculations are in progress.

The current production of high grade resonant e^- impact x-sect. Data has coincided with a need to address non-Maxwellian electron distribution functions in modelling excited populations of ions in plasmas. A specification has been set-up for reducing the complete R-matrix outputs to intermediate ‘interval averaged’ collision strengths suited to subsequent non-Maxwellian averaging. These data, archived in ADAS format, *adf04-type1*, are transferred semi-automatically to *adf04_type4* where they enter revised population modelling. A complete handling chain has been put in place. The diagnostic use in line ratio and emission studies survives intact. The H-like, He-like and Li-like x-sect. data describe earlier work processed through this chain and a paper is in preparation^[5].

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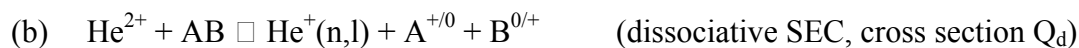
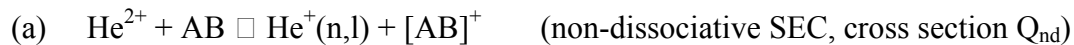
SUMMARY

Dissociative and Non-dissociative Single Electron Capture by Slow He²⁺ from H₂, O₂ and CO

Improvements for tokamak fusion plasma confinement are quite probably correlated with steeper density- and temperature gradients in the outer plasma region (H mode development, formation of internal transport barrier). Plasma profile steepening is supported by local enhanced cooling due to plasma impurity radiation. In this context it is of great interest to study the change in density- and temperature profiles in the outer plasma region with suitable diagnostic methods as, e.g., He beam emission spectroscopy [1,2]. A fast (30 – 120 keV) neutral He beam injected into the plasma gives rise to HeI line emission which will be detected along the He beam direction. From such HeI emission profiles the plasma properties can be evaluated by some modeling procedures, taking into account all relevant collisional excitation and ionisation processes for He atoms in the given plasma environment. For this purpose reliable data on the relevant collision processes are needed.

In fusion reactor-relevant D-T plasmas (e.g., ITER), He is a reaction product („He ash“) and constitutes an impurity of particular interest for cooling in the edge- and divertor plasmas. Collisions of alpha particles (He²⁺) with neutral species (e.g., H₂, O₂) may produce radiation from excited He⁺ states via single electron capture (SEC), and it is of interest to study such SEC reactions in some detail.

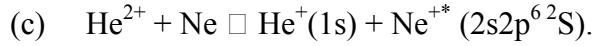
Within the present IAEA Coordinated Research Program on „Atomic and Molecular Data for Fusion Plasma Diagnostics“, we have investigated by means of translational energy spectroscopy (TES; for experimental details cf. [3, 4]) state-selective SEC in low-energy collisions of He²⁺ (impact energy ≤ 1 keV) with H₂, O₂ and CO molecules. In addition, total SEC cross sections have been measured for He²⁺ impact energies up to 20 keV. As apparent from the state-selective measurements, in our low impact energy range SEC from O₂ can proceed both via "non-dissociative" (a) and "dissociative" (b) channels, whereas for H₂ and CO only dissociative SEC could be identified:



The total SEC cross sections Q_{t} are then the sum of respective cross sections Q_{d} and Q_{nd} .

We remark that the ratio $Q_{\text{d}}/Q_{\text{nd}}$ between dissociative and non-dissociative SEC cross sections depends critically on the ion impact energy. Generally, this ratio seems to increase with decreasing impact energy, as shown in [5] for SEC from H₂ and CO, which may be understood from two-electron transitions needed for dissociative SEC.

In our measurements for state-selective SEC from different molecular target species the translational energy gain/loss scale and the relative importance of the SEC channels (a) and (b) have been calibrated with translational energy spectra for He²⁺-Ne collisions, using defined 20%:80% Ne-molecular gas mixtures:



For ≤ 1 keV He^{2+} impact energy with Ne as the target gas, only the SEC channel (c) is observed in our TES measurements and its cross section is therefore equal to the total SEC cross section. Consequently, from the comparison of the relative TES peak heights for SEC from Ne and a molecular target AB we can evaluate the total SEC cross sections Q_t for our molecular target species.

In our TES measurements the acceptance angle for collecting the charge-exchanged $\text{He}^{+(*)}$ projectiles is rather critical for determination of the relative importance of SEC channels (a) and (b). For SEC from O_2 our ratios Q_d/Q_{nd} differ considerably from other data [6], most probably because of the difference in acceptance angles for the two experiments. To understand this influence of the acceptance angle in more detail, we have carried out classical model calculations for SEC in collisions of He^{2+} with H_2 and O_2 , taking into account the appropriate polarization attraction on the incoming trajectory until the capture of the „active electron“ occurs at a given crossing radius R_c . These calculations indicate that for our TES acceptance angle of $\pm 0.5^\circ$ the dissociative SEC from H_2 will not be fully observed if the electron capture occurs at $R_c \leq 2.5 a_0$ ($4 a_0$) for He^{2+} impact energy of 1 keV (250 eV). On the other hand, MO potential curves from ab-initio exact full CI calculations [7] show crossings of the incoming He^{2+} - H_2 MO potential curve with numerous He^+ - H_2^{+*} MO potential curves at $4 a_0 \leq R_c \leq 6 a_0$. For dissociative SEC from O_2 the minimum R_c for full coverage would be about $3 a_0$ ($5 a_0$), whereas the non-dissociative SEC can already proceed at much larger R_c .

The precise nature of the dissociative SEC observed by our TES measurements is not yet clear. Most probably it involves the capture of an electron accompanied by the production of various highly-excited states of the singly ionized target molecule (see above). Consequently, the TES energy gain from dissociative SEC is rather broadly distributed (as observed for all three target species), in contrast to the narrow TES peak indicating non-dissociative SEC (only observable for O_2). Double electron capture into autoionizing projectile states, which could also give rise to final singly ionized He projectiles in the TES, involves rather large endothermicity and is thus highly improbable.

A qualitative interpretation of our experimental results can be given within the concept of the SEC "reaction window" based on multichannel-Landau-Zener calculations, or from the classical over-the-barrier model for the respective collisional quasimolecules [3,4].

For more quantitative interpretation we have carried out some explorative five-body classical-trajectory Monte-Carlo (CTMC) calculations for SEC in He^{2+} - H_2 collisions. However, such calculations proved only reasonable for He^{2+} impact energies above 20 keV. The respective total SEC cross section Q_t is obtained by summing over all transfer ionization, dissociative and non-dissociative SEC events. It was derived at 20 keV impact energy and compared reasonably well with our directly measured total SEC cross section.

Despite its comparable simplicity, SEC in slow collisions of He^{2+} with H_2 is rather difficult to be studied both experimentally and theoretically. Given the considerable practical interest for this collision system in various fields of research, further work on it would well be justified.

Acknowledgments

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2nd IAEA Research Co-ordination Meeting on
“Atomic and Molecular Data for Fusion Plasma Diagnostics”

16-18 June 2003, IAEA Headquarters, Vienna, Austria



International Atomic Energy Agency
INTEROFFICE MEMORANDUM

To: All Members of the RCC-NA
Subcommittee

Date: July 17, 2003

Reference
:

Through: W. Burkart
DDG-NA
D.D. Sood
DIR-NAPC
D.W. Muir
Head, NDS-NAPC

From: R.E.H. Clark
Head, A+M Data Unit

Tel: 21731

Subject: **Proposal to extend a Co-ordinated Research Project (CRP)**

1. Title of CRP: Atomic and Molecular Data for Fusion Plasma Diagnostics

2. Background Situation Analysis

The CRP F4.30.11 on “Atomic and Molecular Data for Fusion Plasma Diagnostics” is scheduled to come to a conclusion in 2003. This CRP had its second RCM on June 16-18, 2003. This CRP has been extremely successful in producing a wealth of new data for a variety of processes needed for diagnostics of plasmas found in nuclear fusion energy machines.

This CRP has been providing data directly relevant to the needs of the diagnostics of core and edge plasmas. With regard to core plasma diagnostics, data on inner shell ionization and on excitation of heavy elements are of high importance. Participants of the CRP have produced significant data on these processes. In addition, spectral measurements have been made which contribute to better understanding of line emission from impurities under fusion

relevant conditions. With regard to edge plasma diagnostics needs, important results have been achieved for He-beam diagnostics, H₂, hydrocarbons and other molecular diagnostics. Such data are also important for detailed studies and better understanding of plasma-wall interaction and are in the process of being implemented in computer modelling codes.

In the course of this CRP a number of extremely valuable collaborations have developed, particularly between experimentalists and theorist. Several agreements have been reached to undertake experiments and calculations on some specific, important processes where there are serious discrepancies between theory and experiment. In addition all of the participants are connected to modelling activities in support of active fusion research devices, such as TEXTOR, ASDEX-Upgrade, DIII-D and JET, as well as ITER. Data from the CRP are already being used in such systems as EIRENE and ADAS.

Although the research carried out to date has been of great benefit to the modelling of fusion plasmas, it has also identified further needs and deficiencies in existing databases. These include cross sections, rate coefficients and spectral line data. Summaries of the participants research are attached as is a brief overall statement on future plans produced in the last RCM. Also attached is the evaluation of the CRP to date, giving a more detailed summary of the accomplishments of the participants.

3. Overall Objectives

The overall objective of this extension would be to provide data for diagnostic processes in fusion plasmas for direct use in fusion energy projects.

4. Specific Research Objectives (purpose)

The specific purpose of the proposed extension to the CRP is to provide as much data as possible in areas where gaps exist in current databases for plasma diagnostics. This will include additional measurements and calculations of cross sections for excitation, ionization and charge exchange for atoms and molecules and their ions where such data are needed but do not yet exist, as well as expanding the energy ranges in some cases. In addition, data on radiative processes will be measured to support spectral line diagnostics.

5. Expected Research Outputs (Results)

The outputs from this CRP will be:

New data for the calculation of plasma impurity emission, alpha particle diagnostics, beam spectroscopy, and charge exchange cross sections will be generated. Results from this CRP will be published in recognized scientific journals by the individual participants.

The new data will undergo a critical assessment and recommended sets of data will be published as an Agency technical report, or as an issue of the IAEA series *Atomic and Plasma-Interaction Data for Fusion*.

The recommended data will be added to the Agency's on-line database, available through the A+M Data Unit home page.

Other outputs

Progress Reports will be prepared by the Research Contract holders each year.

Summary Reports will be prepared after each RCM.

In the Summary Report of the final RCM a detailed report of the work and accomplishments will be given and Final Reports of all CRP participants will be included.

6. Action Plan for the CRP on Atomic and Molecular Data for Fusion Plasma Diagnostics

<i>Activity</i>	<i>2004</i>
4. Organize final RCM to review data and prepare final report.	X
4. Prepare CRP Final Report	X
6. Inclusion of recommended data in IAEA AMDIS database	X

7 Inputs

(a) *Financial Resources required (\$)*

<i>Item</i>	<i>2004</i>
Research Contracts	12,000
RCM	18,000
Printing	10,000

Total for the CRP:\$40,000

8. Assumptions

No outside factors which could negatively influence the implementation of the proposed CRP can be foreseen.

9. Logical Framework of the CRP on Atomic and Molecular Data for Fusion Plasma Diagnostics

<i>Narrative Summary</i>	<i>Objective Verifiable Indicators</i>	<i>Means of Verification</i>	<i>Important Assumptions</i>
<p>Overall Objective: To identify the needs for A+M data for the diagnostics of core and edge plasmas and for the diagnostics of the velocity distribution of fusion alpha particles.</p>	NA	NA	NA
<p>Specific objectives: To identify the specific processes for diagnostics for which data are most urgently needed and to generate such data. These will include new additions to the data-bases for cross section data on collisional processes and for beam spectroscopy</p>	Data for plasma diagnostics are required in fusion reactor design programs and in the interpretation of tokamak experiments	Computer codes for fusion reactor design and for analysis of plasma experiments	None
<p>Outputs:</p> <ol style="list-style-type: none"> 1) Identify the specific processes that are important for diagnostics of fusion plasmas 2) To provide data for some of these processes 3) Publish CRP result in the Final Report 4) Add recommended data to online database 	<ol style="list-style-type: none"> 1) Number of systems studied 2) Amount of data generated 3) Hard copy of IAEA publication 4) Data files included in AMDIS system 	<ol style="list-style-type: none"> 1) Articles in scientific journals and other publications 2) Access to AMDIS via the web 3) Publication Committee approval 4) Access to the AMDIS system 	<ol style="list-style-type: none"> 1) None 2) None 3) None 4) None
<p>Activities</p> <ol style="list-style-type: none"> 1) constituting the CRP - selection of participants 2) Organize 1st RCM to coordinate work plans 3) Organize 2nd RCM to review CRP results 4) Prepare CRP Final Report 5) Organize CM for editing Final Report manuscript 6) CRP Final Report publication 7) Inclusion of recommended data in AMDIS 		<ol style="list-style-type: none"> 1) Twelve RA and 3 RC anticipated 2) 1st RCM planned for 2001 3) 2nd RCM planned for 2003 4) Written contributions to be collected in 2003 5) CM planned for 2004 6) Manuscript submitted for publication 7) AMDIS data files exist 	<ol style="list-style-type: none"> 1) Anticipating approval of 9 RA and 3 RC 2) None 3) None 4) None 5) None 6) None 7) None

10. Brief Summary for the Agency's Bulletin

The Co-ordinated Research Project on “*Atomic and Molecular Data for Fusion Plasma Diagnostics*” is being organized to establish a recommended numerical database for processes that are likely to be important in the diagnostics of nuclear fusion reactor plasmas. In the core region there is a need to use soft x-ray spectroscopy as well as optical spectroscopy for diagnostics. Heating beams are used to raise the core temperature and doped beams are used for diagnostic purposes. Thus, beam spectroscopy is an important consideration in the core region. Radiation from impurities in the edge region is very important in understanding the formation of advanced discharge regimes. Processes such as charge exchange can be important for diagnostic purposes and will be included in this CRP. Data generated in this CRP will undergo an evaluation process and recommended data will be added the electronic database available through the world wide web.

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“Atomic and Molecular Data for Fusion Plasma Diagnostics” (2001-2003)**

- | | |
|--|---|
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RIPL for FTP file transfer of RIPL.
NDSOVL for FTP access to files sent to NDIS "open" area.

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