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Evaluation and Uncertainty Assessment for Be, C and Ne Atomic Data

Summary Report of an IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria

13-15 July 2015

Prepared by

Hyun-Kyung Chung

October 2015

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Abstract

A Consultants' Meeting (CM) on Evaluation and Uncertainty Assessment for Beryllium, Carbon and Neon Atomic Data was held at IAEA Headquarters in Vienna, Austria, from 13 to 15 July 2015. Four experts from three countries participated in the three-day meeting to evaluate currently available electron collisional data for beryllium, carbon and neon atoms and ions and recommend the best possible data for electron-beryllium collision processes.

October 2015

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1. Introduction

A Consultants' Meeting (CM) on Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data was held at IAEA Headquarters in Vienna, Austria, from 13th to 15th July 2015. The objective of this meeting was to evaluate the current status of electron collisional data for Be, C and Ne atoms and recommend the best available data sets.

The Atomic and Molecular Data Unit (Unit) is interested in providing evaluated and recommended data for atomic, molecular and plasma-surface interaction processes relevant to fusion and other plasma applications. Beryllium is chosen as the plasma-facing material for the international collaboration project ITER being built in Cadarache, France and measurements of beryllium in the plasma are important for understanding the erosion and degradation of the first wall during machine operation. As the eroded beryllium atoms and ions flow into the main plasmas, the transport of Be is also an issue as it affects the control and confinement of plasmas. Carbon and neon atoms are also present in the tokamak as impurities and can play a role as well.

Spectroscopic measurements are often applied to quantify the erosion process and a complete set of electron collisional data is needed to interpret measured spectra. There are electron collisional data available in literature for Be, C, and Ne, however, they are neither complete nor consistent. Therefore it is required to evaluate available data and recommend the best possible data set for fusion researchers to use for spectroscopic interpretation.

In order to address this issue, four participants from three countries, K. Bartschat, C. Ballance, D. Fursa and Yu. Ralchenko were invited to evaluate currently available electron scattering data of Be as well as C and Ne atoms. As Be has only 4 electrons compared to 6 and 10 for C and Ne, the quality of available data is relatively better. The four participants worked together before the meeting to compile atomic data and they evaluated the compiled data during the meeting.

This report contains the proceedings of the meeting, conclusions and future work. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Proceedings of the Meeting

The Head of Atomic and Molecular Data Unit in the Nuclear Data Section, Dr B. Braams welcomed participants to the meeting and emphasized the importance of evaluation activities of Be, C, and Ne atomic data in the context of fusion applications.

Prof Bartschat described the most recent results of B-spline R-matrix with pseudo states calculations for electron-impact excitation and ionization of Be and the comparison with best available experimental results.

Prof Ballance presented the extensive work on generalized collisional-radiative rate coefficients produced by R-matrix/RMPS (R-matrix Pseudo States) method. The quality of calculated data depends on the treatments of pseudo states and convergence.

Prof Fursa gave an overview of electron cross-sections with beryllium and its ions by Convergent Close Coupling (CCC) calculations. Details of atomic structure and extent of continuum states can influence the quality of calculated data significantly.

Dr Yu. Ralchenko described the procedure of fitting electron collisional data for recommended data sets. Data for dipole allowed transitions and forbidden transitions should be fitted with different functions accordingly.

For electron-Be collisions, participants compared electron excitation and ionization cross-sections from B-spline R-matrix method and variants of CCC methods and found very good agreement for most data sets, including peaks and positions of resonances. CCC methods are well suited for intermediate-to-high energy ranges while B-spline R-matrix method for near-threshold to intermediate energy ranges. CCC methods were integrated into Maxwellian rate coefficients and later compared with generalized CR rate coefficients done by RMPS method and the agreement is very good.

As data was compared for neutral to ionized systems, the comparison between non-perturbative methods and the perturbative method of distorted wave method shows a better agreement for ionized systems. For neutral atoms and singly ionized ions, however, perturbative methods overestimate cross-sections at low energies as is well known.

Uncertainties of evaluated data were assigned by participants. For optically allowed transitions, the collisional excitation cross-section is related to the oscillator strength, which provides a measure of uncertainties of calculations. It also gives an indication on how well atomic structure calculations were performed inside the scattering calculations. For forbidden transitions, calculations using different methods give a range of uncertainties, which come out to be better than 10% for most transitions for Be.

3. Meeting Conclusions and Future Work

For electron-Be scattering data, three codes agree within less than 10% and agree with oscillator strengths for optically allowed transitions. It is concluded that the calculation methods are mature enough for Be atoms and ions and we are in a position to recommend the best e-Be collision data for use by the fusion community.

Dr Ralchenko and Prof Fursa will work together to produce the recommended data using the CCC method and to assess their uncertainties based on the comparison with results of B-spline R-matrix method and RMPS method calculations. The work will be submitted for publication in a suitable international journal shortly.

Data of C and Ne were investigated in much less detail partly because there were not enough data for detailed comparisons. Both elements are important for fusion applications and will be revisited in the near future.

Appendix 1

List of Participants

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Klaus Bartschat, Drake University, Department of Physics & Astronomy, 2804 Forest Avenue, DES MOINES, IA 53011, UNITED STATES OF AMERICA

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Appendix 2

IAEA Consultants' Meeting on

Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data

13-15 July 2015, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday 13 July 2015 **Meeting Room: M0E58**

09:30 – 10:00 Opening, Adoption of Agenda

10:00 – 10:30 K. Bartschat "B-spline R-matrix with pseudostates calculations for electron-impact excitation and ionization of beryllium"

10:30 – 11:00 C. Ballance "Report on R-matrix/RMPS calculations for Be, C and Ne"

11:00 – 11:20 *Coffee break*

11:20 – 11:50 D. Fursa "Electron collisions with beryllium and its ions"

11:50 – 12:20 Y. Ralchenko "Analysis and fits of collisional data"

12:20 – 13:50 *Lunch*

13:50 – 15:20 Review of electron collisional data for Beryllium (Be I, Be II)

15:20 – 15:40 *Coffee break*

15:40 – 17:00 Review of electron collisional data for Beryllium (Be III, Be IV)

Tuesday 14 July 2015

09:00 – 11:00 Recommendation of electron collisional data for Beryllium with uncertainties

11:00 – 11:20 *Coffee break*

11:20 – 12:20 Recommendation of electron collisional data for Beryllium with uncertainties

12:20 – 13:50 *Lunch*

13:50 – 15:20 Review of electron collisional data for Neon

15:20 – 15:40 *Coffee break*

15:40 – 17:00 Review of electron collisional data for C

Wednesday 15 July 2015

09:00 – 11:00 Discussion on atomic data for plasma kinetics modeling

11:00 – 11:20 *Coffee break*

11:20 – 12:20 Discussion on uncertainty assessment for atomic data

12:20 – 13:50 *Lunch*

13:50 – 15:20 Summary and Discussion on Future work

15:20 – *Adjournment of Meeting*

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