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Uncertainty Assessment for Atomic and Molecular Data

Summary Report of an IAEA Consultants Meeting

IAEA Headquarters, Vienna, Austria

22-23 June 2015

Prepared by

H.-K. Chung and B. J. Braams

October 2015

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ABSTRACT

A Consultants' Meeting (CM) on Uncertainty Assessment for Atomic and Molecular Data was held at IAEA Headquarters in Vienna, Austria, from 22nd to 23rd June 2015. Three experts were invited to discuss a technical document addressed to the atomic and molecular physics community and outlining procedures for uncertainty quantification of theoretical atomic and molecular data. The proceedings of the meeting and the outline of the technical document are reviewed in this meeting report.

October 2015

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1. INTRODUCTION

The Atomic and Molecular Data Unit (AMD Unit) is interested in providing evaluated and recommended data for atomic, molecular and plasma-surface interaction (AM/PSI) processes relevant to fusion and other plasma applications. Since 2012, the Unit has organized a series of technical and consultants' meetings on the topic of data evaluation to promote the development of recommended AM/PSI data in the community. Particularly, the Unit recognized the urgent need to obtain community agreement on procedures to assess the uncertainties of calculated data in order to produce a complete set of evaluated and recommended data.

A Consultants' Meeting (CM) on Uncertainty Assessment for Atomic and Molecular Data was held at IAEA Headquarters in Vienna, Austria, from 22nd to 23th June 2015. The meeting was organized to follow up on the joint IAEA-ITAMP technical meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data held at the Institute of Theoretical Atomic Molecular and Optical Physics (ITAMP) in Cambridge, MA, USA, 7-9 July 2014. That TM assembled 25 participants to discuss issues of uncertainty estimates for theoretical atomic and molecular scattering data.

Three experts that had participated in the IAEA-ITAMP TM in 2014, K. Bartschat of Drake University (USA), J. Tennyson of University College London (UK) and A. Császár of Eötvös University (Hungary), were invited to discuss a technical document outlining the general strategies of uncertainty quantification (UQ) of theoretical electron-atom, electron-molecule and heavy particle collision data as well as related atomic structure and molecular electronic structure calculations.

This report contains short descriptions of the proceeding of this meeting in Section 2 and future work in Section 3. The document outlining the details of uncertainty quantification of theoretical collision data will be prepared for publication in a physics journal. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. PROCEEDINGS OF THE MEETING

The Head of the Nuclear Data Section, R. Forrest, welcomed participants to the meeting and emphasized the Unit's strong interest in uncertainty quantification (UQ) of theoretical atomic and molecular data and the importance of quantifying these uncertainties in an agreed systematic manner. The purpose of this meeting is to outline a technical document addressed to the atomic and molecular physics community to describe procedures for the UQ of calculated data for various atomic and molecular processes. Participants discussed where to publish the document and decided that a physics journal would be more suitable than an IAEA publication for a wider and more direct reach to the relevant physics community.

The two day meeting started with a brief presentation of K. Bartschat on his view of the UQ of electron-atom collision data followed by a presentation of A. Császár on the Focal-Point Analysis (FPA) approach applied to molecular electronic structure problems. Participants reviewed the draft of a technical document consisting of contributions from the participants of the joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and

Molecular Scattering Data held in July 2014. The draft, however, was found to be rather incoherent due to a different style and scope of each contribution and hence it was decided that the present group and a few experts who attended the TM should rewrite the document in a more coherent and organized fashion.

The scope of the document was discussed. The relevant processes include electron-atom collisions, electron-molecule collisions and heavy particle collisions, and all collision calculations rely in turn on calculations of atomic or molecular structure. Uncertainties in structure calculations and in calculations of these collision processes are in the scope of the document, and the document should address both how uncertainties are introduced and how they are propagated. The most important theoretical methods need individual attention. The relevance of various processes of atoms and molecules was identified depending on electron energies classified as very low, low, intermediate, high or relativistic energy range. For each electron energy range, dominant atomic and molecular processes were identified and the uncertainty components of each process were discussed.

3. SUMMARY AND FUTURE WORK

The outline of the technical document was agreed as follows with contributors identified:

1. Introduction – B. Braams
2. General considerations – A. Császár, J. Tennyson, K. Bartschat
3. UQ for structure computations
 - Atoms – H. Chung, G. Drake (University of Windsor)
 - Molecular electronic ground-state properties - A. Császár
 - Molecular electronic excited-state properties - A. Császár
4. UQ for electron scattering calculations
 - Electron – Atom/Ion Scattering – K. Bartschat
 - Electron - Molecule Scattering – J. Tennyson, V. Kokoouline (U. of Central Florida)
5. UQ for charge transfer collisions – T. Kirchner (York University)
6. Illustrations
 - Structure – A. Császár
 - Electron-Atom/Ion Collisions – K. Bartschat
 - Electron-Molecule Collisions – J. Tennyson, V. Kokoouline
 - Charge-Transfer Collisions – T. Kirchner
7. Summary, Conclusions, and Outlook – H. Chung, B. Braams and all

Participants in the CM and identified contributors will use electronic mail and discussions at upcoming workshops and conferences to make progress on the manuscript. The manuscript when completed will be submitted for a publication at a physics journal.

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**IAEA Consultants' Meeting on
Uncertainty Assessment for Atomic and Molecular Data**

22-23 June 2015, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, 22 June 2015

Meeting Room: M0E24

09:30 – 10:00	Opening: adoption of Agenda
10:00 – 11:00	Presentations: K. Bartschat, J. Tennyson and A. Császár
11:00 – 11:20	<i>Coffee break</i>
11:20 – 12:20	Discussion about the Accuracy of Electronic Structure Computations (FPA)
12:20 – 13:20	<i>Lunch</i>
13:20 – 15:00	Review of Issues in the draft version of Guidelines for Uncertainty Quantification (Publication, Document style, Document structures)
15:00 – 15:20	<i>Coffee break</i>
15:40 – 17:00	Discussion on Uncertainties associated with Models and Methods

Tuesday 23, June 2015

09:00 – 10:00	Discussion on the Structure of Guidelines for Uncertainty Quantification (What to include, where to include, how to include)
10:00 – 11:00	Discussion on the Structure of Guidelines for Uncertainty Quantification (continued) (Projectile, Target, General ideas of Models and Methods)
11:00 – 11:20	<i>Coffee break</i>
11:20 – 12:20	Work Distribution
12:20 – 13:20	<i>Lunch</i>
13:20 – 15:00	Revision of Guidelines for Uncertainty Quantification
15:00 – 15:20	<i>Coffee break</i>
15:40 – 17:00	Revision of Guidelines for Uncertainty Quantification (continued)
17:00 – 17:30	Summary and Discussion on Future work
17:30 –	<i>Adjournment of Meeting</i>

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