https://doi.org/10.61092/iaea.t5at-c64q

INDC(NDS)-0800
Distr. Web

INDC International Nuclear Data Committee

Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling

Summary Report

IAEA Headquarters, Vienna, Austria
6 – 7 June 2019

Prepared by

C. Hill
International Atomic Energy Agency
Vienna, Austria

September 2020

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://nds.iaea.org/publications
or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to
NDS.Contact-Point@iaea.org
or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

September 2020

INDC(NDS)-0800
Distr. Web

Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling

Summary Report
IAEA Headquarters, Vienna, Austria
6 – 7 June 2019

Prepared by

C. Hill
International Atomic Energy Agency
Vienna, Austria

ABSTRACT

Beryllium is a major plasma-facing material in the ITER fusion energy research reactor, where 440 beryllium-coated panels form the first wall (FW) of the vacuum reactor vessel. It is expected that plasma–wall interactions will result in the creation of a complex mixture of atomic, ionic and molecular species containing He, Be and isotopes of H. The aim of this meeting was to advise the IAEA Atomic and Molecular Data Unit on the data required for modelling edge plasma processes in fusion devices and to recommend state-resolved data sets for electron-collision excitation, de-excitation and dissociative recombination of the relevant atomic and molecular species.

September 2020

Table of Contents

1. Introduction

Since beryllium was chosen as the first wall (FW) material for the ITER fusion energy research reactor, there has been much interest in its properties with respect to its interaction with the edge plasma of that device. The central issues are the production of impurity species after erosion and ablation under regular heat and particle loads from the plasma. The result of these interactions is the formation of a complex mixture of atomic, ionic and molecular species containing He, Be and isotopes of H. Furthermore, it has been proposed that beryllium granules may be deliberately injected into the edge plasma region to better control the Edge Localized Mode (ELM) cycle without degrading the plasma [1].

Some of the relevant issues were addressed in a Coordinated Research Project (CRP) organised by the Atomic and Molecular Data (AMD) Unit at the IAEA from 2009 – 2014: "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" [2]. Since the conclusion of that project, researchers involved in theoretical calculations of the electron–collision and spectroscopic properties of relevant species have further enhanced the global knowledgebase. The purpose of this meeting was to advise the AMD Unit on the availability and accuracy of these data and to recommend (particularly, state-resolved) data sets for the spectroscopy and electron–collision excitation, de-excitation and dissociative recombination of atomic, ionic and molecular species containing He, Be and isotopes of H. In collecting together such data within a searchable, online database, edge plasma modellers can benefit from a persistent, evaluated data resource to use in their codes.

[1] R. Lunsford et al., Supplemental ELM control in ITER through beryllium granule injection, *Nuclear Materials and Energy* **19**, 34 (2019): https://doi.org/10.1016/j.nme.2019.02.005.

[2] The final report for this CRP can be read as a Volume 576 of Journal of Physics: Conference Series (https://iopscience.iop.org/issue/1742-6596/576/1).

2. Proceedings

The meeting was opened by C. Hill, Head of the Atomic and Molecular Data (AMD) Unit. After some administrative formalities and introductions, the general meeting objectives were outlined and the agenda adopted (Appendix 2).

The first morning of the meeting was devoted to short (20 minute) presentations from each of the participants physically present at the venue (two further participants attended the second day through videoconferencing software).

Detlev Reiter (retired from Forschungszentrum Jülich and now at Heinrich Heine University, Germany) outlined the status of Be, BeH and BeH^+ electron and proton collision data used in fusion, with particular focus on the need for the fusion plasma modelling community to have access to coherent, reliable data with which to replace the obsolete data currently used by many models.

Jonathan Tennyson (University College London, UK) spoke on his group's application of R-Matrix methods to the calculation of state-resolved electron collision cross sections and recently-calculated spectroscopic line lists for BeH, BeD and BeT for emission modelling in Joint European Torus (JET) plasmas [1].

Yuri Ralchenko (National Institute for Standards and Technology, USA) provided a summary of recent important publications concerning state-resolved electron-impact excitation and ionization of Be I and Be II.

Ioan Schneider (Université du Havre, France) described the latest results from his research group on collisions between electrons and H_2^+ and its isotopologues, including comparisons with measured data.

János Zsolt Mezei (Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary) presented related research on Multichannel Quantum Defect Theory (MQDT) calculations of photofragmentation of H_2 and low-energy H^+/H^- collisions.

Vincenzo Laporta (CNR-Nanotec Bari, Italy) described calculations carried out by his group on fusion-relevant state resolved cross sections and rate coefficients for electron–BeH^+, –BeD^+ and –BeT^+ collisions.

The remainder of the meeting was devoted to discussion sessions in which the current knowledge base on relevant species was assessed, and recommendations made for the creation of an online data resource for use by plasma modellers. The discussion sessions were arranged into the following topics:

- Data priorities and formats;
- Review of available Be, Be^+ data for fusion;
- Review of electron-impact data for molecular hydrogen;
- Review of available state-resolved data for beryllium hydride, its isotopologues and ions;
- Review of available data on H, He and their ions.

The meeting concluded with the establishment of a set of priorities for the distribution and further calculation of these data (see Table 1) and the delegation of responsibility for their implementation.

[1] D. Darby-Lewis et al., Synthetic spectra of BeH, BeD and BeT for emission modelling in JET plasmas, *J. Phys. B: At. Mol. Opt. Phys.* **51**, 185701 (2018).

3. Discussions and Recommendations

Much of the data used in the field of plasma spectroscopy and collisional processes, particularly for beryllium-containing species, is, of necessity, calculated using a variety of theoretical techniques. In the five discussion sessions meeting participants evaluated the most recent theoretical calculations of relevant processes, outlined how uncertainties in these calculations

might be described, and discussed the most effective way they might be disseminated to the fusion plasma modelling community.

A summary of the conclusions, priorities and responsibility for further work (by initials of the meeting participants) in the creation of an online database for edge plasma modelling are given in Table 1. Processes involving tungsten hydrides (and their ions and isotopologues) have been included in this table, though work on such species is at a very early stage.

Table 1. Systems of interest for edge plasma modelling in fusion devices.
DR = Dissociative Recombination, DE = Dissociative Excitation, Pub. = Published data. Initials are those of the meeting participants responsible for a given system. Priorities are colour-coded: those rows in green represent data currently available to be included in the database; orange, red and purple denote, in decreasing order of priority, data that would be desirable for inclusion but require further work to prepare and/or are subject to the availability of suitable funding.

System	Process	Initials	Status
$H_2 + e^-$	Excitation / Ionization	DF	Pub.
$H_2 + e^-$	Vibrational excitation	DF	To come
$H_2 + e^-$ and isotopologues	Electron Impact Dissociation Resolved by product KE…	JT	Pub.
$H_2^+ + e^-$	Excitation	DF	Pub.
$H_2^+ + e^-$	DR / DE / Vibrational Excitation	IS / VL / JZM	Data avail.
$HD^+ + e^-$	DR / DE / Vibrational Excitation	IS / VL / JZM	Data avail.
$D_2^+ + e^-$	Excitation	DF	Pub(?)
$BeH + e^-$	**Excitation inc. vibs**	**JT/DDL**	**Data avail.**
$BeH + e^-$	**Ionization**	**JT to do BEB calculations; also available from 10.1140/epjd/e2012-30691-1**	**To come (15 mins)**
$BeH^+ + e^-$	**DR / DE / Vibrational Excitation**	**VL / IS / JZM**	**Pub.**
$BeD^+ + e^-$	**DR / DE / Vibrational Excitation**	**VL / IS / JZM**	**Pub.**
$BeT^+ + e^-$	**DR / DE / Vibrational Excitation**	**VL / IS / JZM**	**Draft, Pub.**

BeH / BeD / BeT	**spectrum – link to exomol.**	**JT**	**Pub.**
BeH_2	**spectrum / electron impact processes**	**JT**	**To be done (subject to funding)**
Be + e^-	**Excitation / Ionization**	**YR**	**Data avail.**
$Be^{(n+)}$ + e^-	**Excitation / Ionization**	**YR**	**To come**
H_3^+ + e^-	**DR: branching ration for H + H2 production known; the electronic state of H is not.**	**JT**	**??**
Be^+ + H_2	**BeH / BeH^+ formation**	**VL (for PE surface + …) / ask at ISIAC**	**To be done**
WH / WD / WT	spectrum	JT	To be done
WH	ionization	JT + summer student	To come?
WH^+ + e^-	Excitation / DR	??	??

The meeting made strong recommendations to collect and make easily available a set of data that is currently dispersed throughout the specialist academic literature in order to facilitate its inclusion in fusion plasma models. A set of priorities for the Atomic and Molecular Unit's development of this database were established and the database is expected to be made available online at the Unit's website over the next few months. At the time of writing, a prototype online service is available at https://db-amdis.org/.

Appendix 1

Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling

6 – 7 June 2019

Meeting room: M0E24

LIST OF PARTICIPANTS

Hyun-Kyung CHUNG, Innovation Strategy Division, National Fusion Research Institute, 169-148 Gwahak-ro, Yuseong-gu, DAEJEON, 34133, REPUBLIC OF KOREA

Vincenzo LAPORTA, Consiglio Nazionale delle Ricerche (CNR/Bari), Via G. Amendola 122/D, 70126 BARI, ITALY

János Zsolt MEZEI, Hungarian Academy of Sciences, Institute of Nuclear Physics, Bem ter 18/c, P.O. Box 51, 4026 DEBRECEN, HUNGARY

Yuri RALCHENKO, National Institute of Standards and Technology, 100 Bureau Drive, Mailstop 8422, GAITHERSBURG, MD 20899-8422, USA

Detlev REITER, Heinrich Heine University Düsseldorf, Arbeitsgruppe Prof. Pretzler, Universitätstraße 1, 40225 DÜSSELDORF, GERMANY

Ioan F. SCHNEIDER, University of Le Havre, 25, rue Philippe Lebon, POB 540, 76058 LE HAVRE CEDEX, FRANCE

Jonathan TENNYSON, Department of Physics and Astronomy, University College London, Gower Street, LONDON WC1E 6BT, UNITED KINGDOM

Dmitry FURSA, Department of Physics and Astronomy, Curtin University, G.P.O. Box 1987 U, PERTH, WA 6845, AUSTRALIA – remote participation via videoconference

Liam SCARLETT, Department of Physics and Astronomy, Curtin University, G.P.O. Box 1987 U, PERTH, WA 6845, AUSTRALIA – remote participation via videoconference

Appendix 2

Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling

IAEA Headquarters, Vienna, Austria

6 – 7 June 2019

Meeting room: M0E24

AGENDA

Thursday, 6 June 2019

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

Session 1: Presentations

Chair: Christian HILL

10:00 – 10:20 **Detlev REITER**, *Heinrich Heine University Düsseldorf, Germany*
Status of Be, BeH and BeH^+ electron and proton collision data used in fusion

10:20 – 10:40 **Jonathan TENNYSON**, *University College London, United Kingdom*
Molecular data for fusion (and other) plasmas

10:40 – 11:00 **Yuri RALCHENKO**, *National Institute of Standards and Technology (NIST), United States of America*
Electron-impact collisions with Be^+

11:00 – 11:20 Coffee Break

11:20 – 11:40 **Ioan F. SCHNEIDER**, *Université du Havre, France*
Electron – H_2^+ (and isotopomers) collisions: theoretical cross sections and rates, and comparison with measured data

11:40 – 12:00 **János Zsolt MEZEI**, *Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary*
Photofragmentation of H_2 and low-energy H^+/H^- collisions

12:00 – 12:20 **Vincenzo LAPORTA**, *CNR Bari, Italy*
Cross sections and rate coefficients for electron–BeH^+ scattering

12:20 – 12:40 **Hyun-Kyung CHUNG**, *National Fusion Research Institute (NFRI), South Korea*
Uncertainty estimates for theoretical atomic and molecular data

12:40 – 13:00 **Christian HILL**, *IAEA, Austria*
Atomic and Molecular Data services at the IAEA

13:00 – 14:00 Lunch

Session 2: Discussion Session: Overview

Chair: Christian HILL

14:00 – 15:30 Discussion (all): Data priorities and formats

15:30 – 16:00 Coffee Break

Session 3: Data Evaluation I: Atomic Data

Chair: Yuri RALCHENKO

16:00 – 17:30 Discussion (all): Review of available Be, Be^+ data for fusion

Friday, 7 June 2019

Session 4: Data Evaluation II: Molecular and Molecular Ion Species

Chair: Ioan F. SCHNEIDER

09:00 – 10:30 Discussion (all): Review of electron-impact data for molecular hydrogen

10:30 – 11:00 Coffee Break

11:00 – 12:30 Discussion (all): Review of available state-resolved data for beryllium hydride, its isotopologues and ions

12:30 – 13:30 Lunch

Session 5: Data Evaluation III: Atomic Hydrogen and Helium

13:30 – 15:00 Discussion (all): Review of available data on H, He and their ions

15:00 – 15:30 Coffee Break

15:30 – 16:00 Concluding remarks; Close of meeting

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

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org