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Recommended Data for Atomic Processes of Tungsten Ions

Summary Report of a Joint IAEA-KAERI Consultants' Meeting

KAERI, Daejeon, Republic of Korea

14-16 September 2015

Prepared by
Hyun-Kyung Chung

February 2016

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ABSTRACT

A Consultants' Meeting (CM) on Recommended Data for Atomic Processes of Tungsten Ions was held at Korea Atomic Energy Research Institute (KAERI) in Daejeon, Republic of Korea, from 14 to 16 September 2015. This meeting was jointly held by IAEA and KAERI Nuclear Data Center. Eight experts from China, Israel, Japan, UK and Japan as well as two staff members from IAEA participated in the three-day meeting to evaluate currently available dielectronic recombination data and recommend the best possible data for tungsten ions relevant to fusion applications.

February 2016

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1. Introduction

A Consultants' Meeting (CM) on Recommended Data for Atomic Processes of Tungsten Ions was held in Daejeon, Republic of Korea, from 14 to 16 September 2015. This meeting was hosted and jointly organized by KAERI (Korea Atomic Energy Research Institute) Nuclear Data Center. The objective of this meeting was to evaluate and recommend currently available atomic data for tungsten ions relevant to fusion applications.

The Atomic and Molecular Data Unit (AMD Unit) is interested in providing evaluated and recommended data for atomic, molecular and plasma-surface interaction processes relevant to fusion and other plasma applications. Tungsten is chosen as divertor material for the international fusion research reactor ITER being built in Cadarache, France and the transport of tungsten ions from colder region to core region has a great consequence in the tokamak operation, namely, control and confinement of plasmas in tokamak. The ionization and recombination rate coefficients, consequently, charge state distributions of tungsten ions as a function of electron temperature are of great interest in quantifying the radiation loss rates through tungsten ions in the hot core as well as tungsten spectroscopy in the divertor regions.

Currently, there is a rather reliable set of ionization rate coefficients available for the community calculated by elaborate and sophisticated R-matrix calculations, however, a consistent and comprehensive set of dielectronic recombination rate coefficients is not available for all charge states of tungsten. Recognizing the need, the evaluation of total Maxwellian averaged dielectronic recombination (DR) rate coefficients and a recommended data set from currently available data were pursued in this Consultants' Meeting in Korea.

Eight experts from five member states as well as two staff members from IAEA participated in the three-day meeting. Invited experts in the field of dielectronic recombination processes were Bowen Li of Lanzhou University, China, Xiaobin Ding of Northwest Normal University, China, Tomohide Nakano of Japan Atomic Energy Agency, Japan, Ehud Behar of Technion Israel Institute of Technology, Isarel, Connor Ballance of Queen's University of Belfast, UK, Simon Preval of University of Strathclyde, UK as well as Duck-Hee Kwon and Won-Wook Lee of Korea Atomic Energy Research Institute, Korea. Chris Fontes and James Colgan of Los Alamos National Laboratory, USA and Yuri Ralchenko of National Institute of Standards and Technology, USA didn't attend the meeting but instead sent their results before the meeting for review.

Available data were compiled before the meeting and compared during the meeting. Experts evaluated the current status of DR rate coefficients and proposed a recommended set of data. After the meeting, experts will collaborate to improve a few data sets, where the literature is significantly lacking.

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. Abstracts of presentations by participants are compiled in Appendix 3.

2. Proceedings of the Meeting

The Head of Atomic and Molecular Data Unit in the Nuclear Data Section, Dr B. Braams opened the meeting and emphasized the importance of evaluation and recommendation of atomic data. The local organizer Duck-Hee Kwon welcomed participants to the meeting on the first day and Dr Young-Ouk Lee, the director of KAERI Nuclear data Center delivered his welcome address on the next day due to his travel schedule. The meeting agenda was adopted and participants introduced themselves.

The meeting was followed by presentations and discussions of compiled data. Participants presented their work on dielectronic recombination (DR) coefficients and important physics.

Dr T. Nakano of Japanese Atomic Energy Agency of Japan presented a ratio of calculated W^{44+} ionization cross-section to calculated W^{45+} recombination cross-section derived from a ratio of W^{44+} spectral intensity to W^{45+} spectral intensity measured in a mono-energy plasma of Tokyo EBIT device. He also compared the experimentally derived cross-sections with calculations using FAC atomic code.

Dr D.-K. Kwon of Korea Atomic Energy Research Institute, Korea presented her work on dielectronic Recombination of W^{45+} and W^{44+} where configuration mixing and channels were carefully investigated.

Dr S. Preval of University of Strathclyde, UK presented his work on the tungsten project: partial and total dielectronic/radiative recombination rate coefficients for W^{74+} to W^{56+} and his plan to provide a complete set of DR rate coefficients for all tungsten charge states.

Dr X. Ding of Northwest Normal University, China, presented work done by his collaborators at Northwest Normal University on the dielectronic recombination rate coefficients of W^{37+} to W^{45+} ions.

Dr B. Li of Lanzhou University, China, presented his work on dielectronic recombination computations of Rh-, Pd- and Ag-like W with the FAC code.

Prof. C. Ballance of Queen's University of Belfast, UK, presented his calculations using an R-matrix and AutoStructure distorted-wave approach for the dielectronic recombination of W^{35+} and W^{20+} .

Prof E. Behar of Technion Israel Institute of Technology, Isarel, presented his work on dielectronic recombination computations with the HULLAC code.

Dr H.-K. Chung of IAEA gave an overview of Internationally Coordinated Activities of Uncertainty Quantification of Atomic, Molecular and Plasma-Surface Interaction data for Fusion applications.

On the second and third day, participants discussed important physics issues in computing DR rate coefficients, compared available data sets and recommended DR rate coefficients for each charge state of tungsten ions. They also identified several charge states with no adequate DR rate coefficients and will work on the missing data sets in the future.

3. Meeting conclusions and future work

Important physics issues to be included in the total Maxwellian averaged dielectronic recombination (DR) rate coefficients calculations are identified as: 1) convergence in DR channels (autoionizing states) in terms of high principal quantum number (n) and angular momentum quantum number (l), 2) convergence in stabilization channels such as non-resonant stabilization (NRS) and decay to autoionizing levels followed by cascades (DAC), 3) correct treatment of $\Delta n=0$ DR channels including precise resonance positions and 4) details of atomic structure (fine structure or configuration average model, configuration mixing etc.).

A survey of total Maxwellian averaged DR rate coefficients as a function of electron temperatures from 73 charge states of tungsten ions from W^+ to W^{73+} was performed during the meeting. There are three categories of data sets: 1) experimental data, 2) calculated data sets with detailed atomic physics and 3) schematic data sets with scaled atomic data.

There are very few experimental data for total Maxwellian averaged DR rate coefficients available, only of W^{18+} and W^{20+} . For recommendation, experimental data sets were taken if available in conjunction with calculated data for high temperature range where experimental data are not available. Experimental data were also used to benchmark calculated data.

There were two classes of calculated data with detailed physics. More rigorously computed rate coefficients can be obtained from R-matrix calculations or non-perturbative methods. However, there are only a few results available, as it is computationally challenging for many electron atoms such as tungsten. The other data sets were obtained using distorted wave calculations using FAC (Flexible atomic codes, Gu 2003) or HULLAC (Hebrew University Lawrence Livermore Atomic Code, Klapisch et al. 1977, Bar Shalom et al. 1988, 2001). R-matrix calculations and distorted wave calculations tend to agree in a broad range of temperatures, but sometimes disagree in low temperature ranges where $\Delta n=0$ DR resonance positions are critical, and where it is hard to decide which results are more accurate without laboratory benchmarking. It was also stressed that the details of atomic levels whether fine structure levels or configuration average levels are used can make a distinct difference.

Calculated data were taken for recommendation if available. When multiple data sets were available, data sets with better atomic physics were recommended or participants collaborated during and after the meeting to provide the best possible data set. For more than 25 charge states, no calculated or experimental data sets exist except for schematic data sets based on scaling laws.

Three schematic data sets with scaled atomic data by A. Foster (ADPAK), T. Pütterich and H. Chung (FLYCHK) are available for all charge states. In a few cases, they agree with calculated data sets with detailed atomic physics for a certain range of electron temperatures within a factor of 2. However, they didn't agree at all at low electron temperatures due to the missing contributions from $\Delta n=0$ DR channels. When there are no calculated data available, schematic data sets hardly agree with each other in terms of the absolute values and shapes as a function of electron temperature, and it is concluded that there is need for more investigation before recommending schematic data for charge states with no experimental data or calculated data.

The meeting was highly productive and successful. The recommended data sets and technical discussions will be published shortly in a physics journal for more access to the fusion community. Participants will work together on the DR rate coefficients for charge states where no recommendation was made. It was recommended for IAEA to organize a follow-up meeting in the future for a complete set of DR rate coefficients for all charge states of tungsten ions in the future.

A table of recommended data sets at the meeting is found in Appendix 4.

List of Participants

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Ehud Behar, Physics Department, Technion Israel Institute of Technology, Technion City HAIFA 32000, ISRAEL, on leave at the University of Maryland through a European Unions Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 655324.

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**Joint IAEA-KAERI Consultants Meeting on
Recommended Data for Atomic Processes of Tungsten Ions**
hosted by Korea Atomic Energy Research Institute (KAERI)
14-16 September 2015, Daejeon, Republic of Korea

Meeting Agenda

Monday 14 September 2015

- 09:30 - 10:00 Adoption of Agenda, Meeting objectives
- 10:00 - 10:40 **Tomohide Nakano**: Experimental evaluation of W^{44+} ionization and W^{45+} recombination cross-sections
- 10:40 - 11:20 **Duck-Hee Kwon**: Dielectronic Recombination of W^{45+} and W^{44+} : Configuration Mixing and Channels
- 11:20 - 11:50 Coffee Break
- 11:50 - 12:30 **Simon Preval**: The Tungsten Project: Partial and Total Dielectronic/Radiative Recombination Rate Coefficients for W^{74+} to W^{56+}
- 12:30 - 14:00 Lunch
- 14:00 - 14:40 **Xiaobin Ding**: The calculation on the Dielectronic recombination rate coefficients of W^{37+} to W^{45+} ions
- 14:40 - 15:20 **Bowen Li**: Dielectronic recombination computations of Rh-, Pd- and Ag-like W with the FAC code.
- 15:20 - 15:40 Coffee Break
- 15:40 - 16:20 **Connor Ballance**: An R-matrix and AutoStructure distorted-wave approach to the Dielectronic Recombination of W^{35+} and W^{20+}
- 16:20 - 17:00 **Ehud Behar**: Dielectronic Recombination Computations with the HULLAC code

Tuesday 15 September 2015

- 09:00 - 09:30 **Welcome address by Dr. Young-Ouk Lee**, Director of Korea Nuclear Data Center
- 09:30 - 10:00 **Hyun-Kyung Chung**: Internationally Coordinated Activities of Uncertainty Quantification of Atomic, Molecular and Plasma-Surface Interaction data for Fusion applications
- 10:00 - 12:30 Evaluation of Dielectronic Recombination Data (W^{0+} - W^{40+})
- 12:30 - 14:00 Lunch
- 14:00 - 17:00 Evaluation of Dielectronic Recombination Data (W^{41+} - W^{72+})

Wednesday 16 September 2015

- 09:00 - 12:30 Recommendation of Dielectronic Recombination Data
- 12:30 - 14:00 Lunch
- 14:00 - 17:30 Summary and Discussion on Future work
- 17:30 - Adjournment of Meeting

**Joint IAEA-KAERI Consultants Meeting on
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Abstracts

Experimental evaluation of W^{45+} recombination and W^{44+} Ionization cross-sections

Tomohide NAKANO

Japan Atomic Energy Agency, Naka-shi, Ibaraki-ken, Japan

This talk presents comparison of a ratio of calculated W^{44+} ionization cross-section to calculated W^{45+} recombination cross-section with a ratio of W^{44+} spectral intensity to W^{45+} spectral intensity measured in a mono-energy plasma of Tokyo EBIT device. One of the advantages of this method is cancellation of electron energy dependence of excitation cross-section from 4s to 4p level, enabling direct conversion of the intensity ratio of W^{44+} 4s-4p spectral line (6.1 nm) over W^{45+} 4s-4p spectral line (6.2 nm) to a density ratio of W^{44+} over W^{45+} by using a coronal model. The W^{44+}/W^{45+} density ratio can be expressed as a ratio of W^{45+} recombination cross-section over W^{44+} ionization cross-section under ionization equilibrium. For the W^{44+} ionization cross-section calculation, considered are direct ionization of 4s electron and excitation to autoionization levels ($3d^9 4s^2 nl$, etc), followed by auto-ionization to W^{45+} (excitation-autoionization). For the W^{45+} recombination cross-section calculation, considered are radiative recombination to W^{44+} and dielectronic recombination, which starts with electron capture by W^{45+} to doubly excited levels of W^{44+} . This work considers $3d^9 4s nl n'l''$ (n up to 16, n' up to 100, l and l' up to 12), $3p^5 4s nl n'l''$ (n up to 5), and $3s 4s nl n'l''$ (n up to 5) as the double excited levels. The calculated W^{44+}/W^{45+} density ratio is compared with the experimental W^{44+}/W^{45+} density ratio, showing difference by a factor of 2. The reason of this difference is not yet known.

Dielectronic Recombination of W^{45+} and W^{44+} : Configuration Mixing and Channels

Duck-Hee KWON and Wonwook LEE

Nuclear Data Center, Korea Atomic Energy Research Institute, Daejeon, Korea

We have calculated dielectronic recombination (DR) cross sections and rate coefficients for W^{45+} and W^{44+} by the flexible atomic code (FAC) based on independent process, isolated resonance (IPIR), and distorted wave (DW) approximation. We have investigated effects of configuration mixing (CM) involving double electron core excitation as well as single electron core excitation on DR. Effects of Non-resonant stabilizations (NRS) and decays to autoionizing levels possibly followed by cascades (DAC) have been also investigated. DR rate coefficient is very sensitive to CM specially at low energy region. NRS and DAC effect is relatively smaller than the CM effect. Particular attention to $\Delta n_c = 0$ core excitation from 4s to 4l has been paid which dominates low energy DR. $\Delta n_c = 1$ core excitations $4s \rightarrow 5l$, $3d \rightarrow 4l$, and $3p \rightarrow 4l$ have been also calculated. $\Delta n_c = 2$ core excitations $4s \rightarrow 6l$, $3d \rightarrow 5l$, and $3p \rightarrow 5l$ and 3s electron promotion have been calculated. However the contributions are very small and not added to total Maxwellian DR rate coefficient. As a result, our newly calculated total DR rate coefficient for W^{45+} shows differences with the recombination data on the ADAS database obtained using a simple semi-empirical formula by over order of magnitude at low energy region and by about 30-50% at 2-7 keV.

In the future, we will complete the total DR rate coefficient calculation for W^{44+} and extend our calculation method to DR of W^{46+} and W^{40+} .

The Tungsten Project: Partial and Total Dielectronic/Radiative Recombination Rate Coefficients for W^{74+} to W^{56+}

Simon PREVAL

Department of Physics, University of Strathclyde, Glasgow, UNITED KINGDOM

The Calculation on the Dielectronic Recombination rate coefficient of W^{37+} to W^{45+} ions

Yanbiao Fu, Xiaobin Ding, Chenzhong Dong

Key Laboratory of Atomic and Molecular Physics & Functional Materials of Ganus,
College of Physics and Electronic Engineering,
Northwest Normal University, Lanzhou, China

Dielectronic Recombination is one of the basic atomic processes in both astrophysical and experimental plasma. It plays an important role in determination of the level population and charge state balance of highly ionized plasma. Tungsten will be used as a plasma-facing material within the divertor region of the ITER due to its favorable physical and engineering properties. For plasma modeling and radiative cooling studies, accurate atomic data for highly charged W ions are significant, especially data on recombination processes that are vital in the determination of radiation losses. The DR processes of W^{37+} to W^{45+} ions were calculated and analyzed in detail to provide some useful fundamental atomic data. The energy levels, radiative transition rates and autoionization rates were calculated by using relativistic configuration interaction method with the implementation of Flexible Atomic Code (FAC). All the $\Delta n=0,1,2$ channels were included in the present calculation. In the excited channels, all the contribution through the resonant configuration with $l' > 8$ were found to be negligible. For the captured electron, the principal quantum number was estimated up to 15 and extrapolation until 100. In most case, the $n=4$ shell excitation gives the most important contribution in the whole temperature region. In the low temperature, the $\Delta n=0$ excitation gives most important contribution to the total rate coefficients. According to a recent survey on the DR rate coefficients of W^{29+} ions, the effects of non-resonant stabilization (NRS) and decays to autoionizing levels followed by radiative cascade (DAC) contribution about 5% in the high temperature region. These DR rate coefficients could be used in further plasma modeling.

Reference:

- [1] Z.W. Wu et.al., Eur. Phys. J. D., (2015) **69**,140
- [2] M.J. Li et.al., Plasma Science and Technology, (2014) **16** 182
- [3] X.Z. Ma et.al., Nuclear Physics Review, (2013) **30** 214
- [4] Y.Z. Zhang et.al., High Power Laser and Particle Beams, (2011) **23** 1087
- [5] M.F. Gu, Canadian Journal of Physics, (2008) **86** 675.

Dielectronic recombination computations of Rh-, Pd- and Ag-like W with the FAC code.

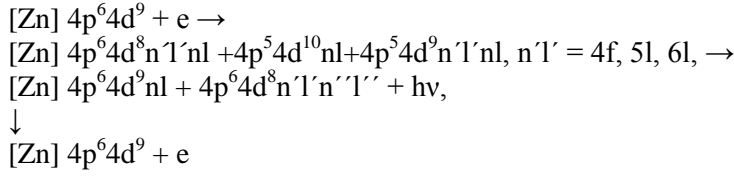
Bowen LI

School of Nuclear Science and Technology, Lanzhou University, Lanzhou, CHINA

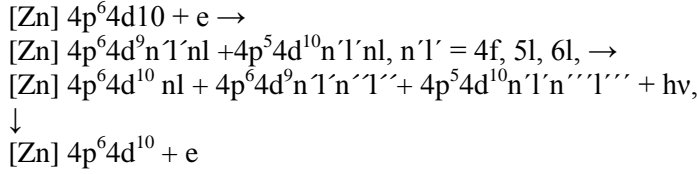
The dielectronic recombination (DR) process plays an important role in high-temperature plasmas, where it affects both the ionization balance and radiative energy losses. Tungsten is being considered as a plasma-facing material in magnetically confined fusion devices, such as ITER, because of its low sputtering rate, high temperature characteristics and low tritium absorption. Considerable effort has been made to obtain reliable atomic data to enable identification of reference lines for plasma diagnostics and to reliably estimate radiative cooling rates and a significant number of publications on

DR processes have been published. DR rate coefficients for Rh-, Pd- and Ag-like tungsten have been studied by using the Flexible Atomic Code (FAC).

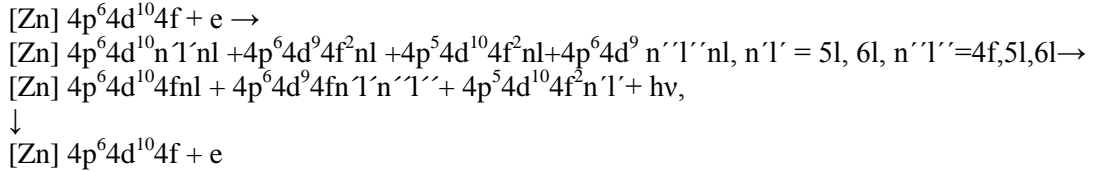
A. Rh-like W



B. Pd-like W



C. Ag-like W



Energy levels, radiative transition probabilities and autoionization rates were calculated using the Flexible Atomic Code up to $n=18$. The contributions from higher- n states were extrapolated up to $n = 1000$ using an empirical scaling formula.

The data obtained are expected to be useful for modelling plasmas for fusion applications

An R-matrix and AutoStructure distorted-wave approach to the Di-electronic Recombination of W^{35+} and W^{20+}

Connor BALLANCE
Queen's University Belfast, University Road Belfast, UNITED KINGDOM

Dielelectronic Recombination rate coefficients of W^{35+}

The total Maxwellian averaged DR rate from both the ground-state and a statistically weighted averaged of levels from the ground-state complex were presented. This was achieved by three independent calculations including the level resolved Dirac R-matrix codes (DARC)[1], configuration-averaged AUTOSTRUCTURE[2] and the configuration-averaged DRACULA code (Di-electronic Recombination Averaged Configuration using the Local Approximation potential) based upon the Cowan suite of codes. The level resolved DARC result, the only non-perturbative method differed only from the other two methods at the lowest temperatures and all three methods converged at the high temperature asymptotic limit. Therefore the configuration averaged result which did not differ substantially from the level resolved one was merged with delta $n=0$ zero DARC calculation to provide the recommended data set for this ion stage. The paper also provides the well-known fitting co-efficients for the total rates used within astrophysics.

Dielectronic Recombination rate coefficients of W^{20+}

Calculations based upon standard theoretical expressions for DR are unable to represent the very low temperature rate coefficients from the experimental paper [3], which represents the experimental measurements of the Schippers/Mueller group. The theoretical calculations for this open f shell system were carried out with AUTOSTRUCTURE with level resolved calculations still being over an order of magnitude less than experiment. Theoretical calculations based many-bodied perturbation suggest that the chaotic nature (the heavy mixing of such energetically closely spaced states) [Flaumbaum] that a statistical theory may better reproduce the experimental values. Given the complexity of this system, our recommendation was the experimental result combined with the theoretical top-up from AUTOSTRUCTURE to account for high n shell contributions missing from their measurement.

Error propagation

It was suggested, that assuming that the lowest temperature DR rate coefficients may be affected by the positions of a few resonances, that one simple error uncertainty could be the difference in total rates between pure theoretical model and one in which the target levels are shifted to known NIST values. Uncertainty in the DR rate coefficients is one component when propagating the uncertainty for particular plasma diagnostic. This uncertainty must be integrated with the uncertainty in the atomic structure and other collisional processes such as electron-impact excitation and ionization.

References

1. P H Norrington and I P Grant, J Phys B: At Mol Phys , 10 , pg 4869 (1987)
2. N R Badnell, J Phys B, 19, pg 3827 (1987)
3. S Schippers, D Bernhardt, A Mueller, C Krantz, M Grieser, R Repnow, A Wolf, M Lestinsky, M Hahn , O Novotny and D W Savin, Phys Rev A 83, 012711(6) (2011)

Dielectronic Recombination Computations with the HULLAC code

Ehud BEHAR

Physics Department, Technion Israel Institute of Technology, HAIFA, ISRAEL

Methods for harnessing the Hebrew University Lawrence Livermore Atomic Code (HULLAC) for DR rate coefficients were described. The role of low-lying resonances was discussed. The importance of Non-Resonant Stabilizations (NRS) and Decays to Autoionizing levels possibly followed by Cascades (DAC) was demonstrated. The limitations of HULLAC and similar codes in accurately describing these contributions were also discussed. The effect of quantum interference between direct radiative and dielectronic recombination was shown to be small in most computed cases.

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A list of recommended total Maxwellian averaged dielectronic recombination rate coefficients of tungsten ions

Charge states	Recommended data	References
W ¹⁺	S. Preval + C. Ballance	Private communications
W ²⁺ - W ⁴⁺	No recommendation	
W ⁵⁺	U. I. Safronova et. al.	J. Phys. B 45, 085001 (2012)
W ⁶⁺	U. I. Safronova et. al.	Phys. Rev. A 85, 032507 (2012)
W ⁷⁺ - W ¹⁷⁺	No recommendation	
W ¹⁸⁺	K. Spruck et. al.+ FLYCHK scaling	Phys. Rev. A 90, 032715 (2014)
W ¹⁹⁺	No recommendation	
W ²⁰⁺	S. Schippers et. al.+ S. Preval	Phys. Rev. A 83, 012711 (2011)
W ²¹⁺ - W ²⁶⁺	No recommendation	
W ²⁷⁺ - W ²⁹⁺	B. Li et al.	Private communications
W ³⁰⁺ - W ³⁴⁺	No recommendation	
W ³⁵⁺	C. P. Ballance et al.	J. Phys. B 43, 205201 (2010)
W ³⁶⁺	No recommendation	
W ³⁷⁺ - W ³⁹⁺	Z. Wu et al.	Atoms, 3, 474 (2015)
W ⁴⁰⁺	No recommendation	
W ⁴¹⁺ - W ⁴²⁺	Z. Wu et al.	Atoms, 3, 474 (2015)
W ⁴³⁺	X. Ding et al.	Private communications
W ⁴⁴⁺	Z. Wu et al.	Atoms, 3, 474 (2015)
W ⁴⁵⁺	D. Kwon et al. + T. Nakano	J. Quant. Spectrosc. Radiat. Transfer 170, 182 (2016) + Private communications
W ⁴⁶⁺	E. Behar et al.	Eur. Phys. J. D7, 157 (1999)
W ⁴⁷⁺	F. Meng et al.	J. Quant. Spectrosc. Radiat. Transfer 109, 2000 (2008)
W ⁴⁸⁺ - W ⁵⁵⁺	No recommendation	
W ⁵⁶⁺	A. Peleg et al.	Phys. Rev. A 57, 3493 (1998)
W ⁵⁷⁺ - W ⁶³⁺	S. Preval et al.	S. Preval et. al. Submitted
W ⁶⁴⁺	S. Preval et al. + E. Behar et al.	S. Preval et. al. Submitted + Phys. Rev. A 59, 2787 (1999)
W ⁶⁵⁺ - W ⁷³⁺	S. Preval et al.	S. Preval et. al. Submitted

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