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Summary Report of the 3rd Biennial Technical Meeting

IAEA Headquarters, Vienna, Austria

6–8 May 2013

Prepared by

Hyun-Kyung Chung

July 2013

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Abstract

This report summarizes the proceedings of the third Technical Meeting of the International Code Centres Network held on 6-8 May in 2013. Ten experts from seven member states and four IAEA staff members attended the three-day meeting held at the IAEA Headquarters in Vienna to discuss issues on uncertainty estimates of theoretical atomic and molecular data. The report includes discussions on data issues, meeting conclusions and recommendations for the IAEA Atomic and Molecular Data Unit.

July 2013

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1. Introduction

Plasma modelling in fusion research often requires a complete data set, a comprehensive set of data for all the relevant processes and states of atoms and molecules of plasma constituents. It is almost impossible to generate such a full set of data without a large number of calculated data as a limited amount of data is available from literature or from databases. The international Code Centres Network (CCN) is coordinated by the IAEA A+M Data Unit in order to gather and provide access to computational codes and to calculated atomic, molecular and plasma-surface interaction (AM/PSI) data relevant for modelers in fusion and plasma sciences. Starting with a consultants' meeting on "Establishment of Atomic and Molecular computer Code Network" in 2005, the Unit has organized a series of meetings of code developers in the Code Centres Network (CCN) to address related issues including the accessibilities of physics codes. The following recommendation and conclusions were reached at the 1st meeting in 2008.

- An IAEA web page is created to include basic information from summaries of the current code capabilities and links directly to the centre web pages.
- The centres maintain their home pages with updates as capabilities change
- The group should begin utilizing the XSAMS format for data transmission/exchange
- Code authors will attempt to assess the accuracy of the calculations in a similar manner to the numerical database estimate.
- The Network will meet biennially at IAEA headquarters to monitor progress and identify future needs.
- The Network will constitute an informal federation to permit flexible membership.
- The Network should make the broader fusion community aware of the capabilities represented by this group (presentations at fusion-oriented conferences)

At the 2nd technical meeting in 2010, concerns were raised over the quality of data sets produced with online codes or downloadable codes by non-expert users. It was noted that there has been a growing demand in the user community for validated and verified data sets such as a recommended data library for fusion and other plasma applications. It motivated the Unit to collaborate with data centres, AM/PSI communities and users to explore various aspects of evaluating and recommending AM/PSI data sets. A series of meetings have been organized to discuss the road map towards the internationally agreed recommended data library for fusion applications. The discussion and recommendations can be found in the IAEA reports INDC(NDS)-600, INDC(NDS)-617, INDC(NDS)-622 and INDC(NDS)-627. The IAEA-NFRI (National Fusion Research Institute, Republic of Korea) technical meeting on data evaluation was held in Dae-jeon, Korea with more than 20 experts from 10 member states and IAEA and the proceeding papers from invited presentations were published in Fusion Science and Technology, Volume 63, Number 3 in 2013.

One of the recommendations from the series of meetings concerns the critical assessment and uncertainty estimates of theoretical data sets. While uncertainties of measurement, or "error bars" of experimental data are duly reported, theoretical data are seldom provided with such estimates. It is not immediately obvious how to give a quantitative number in the uncertainties of theoretically or numerically obtained values. In order to discuss the issue, the Unit invited experts in theoretical atomic and molecular physics codes to the 3rd technical meeting on the international Code Centres Network held at IAEA headquarters in May 6-8 in 2013. The 3rd meeting was originally planned to be in 2012 but was postponed to 2013 in order to accommodate the recommendations from the IAEA-NFRI technical meeting in September 2012 and the international conference on atomic and molecular data (ICAMDATA 2012, NIST, USA) in October 2012.

It had been agreed in the 2nd meeting that the CCN has a flexible membership and would expand to include experts in user communities and experiment communities as needed. In the 3rd meeting, the Unit invited 10 experts from seven countries including experimentalists and fusion modelling users in addition to code developers: D. Coster (Germany), Yu. Ralchenko (USA), P. Jönsson (Sweden), K. Bartschat (USA), C.-Z. Dong (China), E. Stambulchik (Israel), J. Tennyson (UK), V. Kokoouline (USA), G. Garcia (Spain) and N. Mason (UK). The IAEA staff members R. Capote Noy and N. Otsuka were invited to give overview presentations on the uncertainty estimates and data evaluation activities in nuclear data communities.

The timing of the CCN meeting was coordinated with the organizers of a new European COST Action network, eMOL, led by N. J. Mason of the Open University. This project was created to carry out group evaluations of electron-molecule collision data for 13 systems, and the development of evaluation methodology is an important part of their mandate. The eMOL work is coordinated with SUP@VAMDC and with that of members of the IAEA Data Centres Network following the IAEA-NFRI technical meeting in September 2012. The first eMOL group meeting organized by N. Mason was held in Vienna May 8-10 to evaluate data of electron-water molecules collisions. On the 8th of May, participants of eMOL group joined the CCN meeting at the IAEA headquarter to share the recommendations of the CCN meeting on uncertainty estimates of theoretical data and discuss data evaluation activities. The eMOL group participants at this meeting were F. Kupka (Austria), T. Rank-Lueftinger (Austria), P. Limao-Vieira (Portugal), Y. Itikawa (Japan), B. Marinkovic (Serbia), G. Karwasz (Poland), S. Matejcik (Slowakia), J. Tennyson (UK), V. Kokoouline (USA), G. Garcia (Spain) and N. Mason (UK).

The Code Centres Network meeting was opened by Dr R. Capote Noy (Deputy Section Head, Nuclear Data Section, Division of Physical and Chemical Sciences, IAEA) who welcomed all participants and emphasized the importance of the uncertainty estimates in data evaluation. He suggested future collaboration between atomic and nuclear communities on various problems. Dr B. Braams (Head, A+M Data unit) and the scientific secretary Dr H.-K. Chung (Atomic physicist, A+M Data unit) welcomed the participants during the introduction of participants. The agenda was adopted (Appendix 2).

This proceeding report contains an introduction, short summaries of presentations in Section 2 and discussions and recommendations in Section 3. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Presentations

The presentations at the meeting are available on the A+M Data Unit web site http://www-amdis.iaea.org/CCN via the link to Presentations for more detailed information. This report summarizes presentations given on uncertainty estimates and critical assessment of nuclear data, atomic data and molecular data as well as the current needs of data evaluation and uncertainty propagation in fusion and plasma sciences.

2.1 Meeting objectives, B. Braams (IAEA Nuclear Data Section)

A core task of the IAEA Atomic and Molecular (A+M) Data Unit is to compile and disseminate A+M collision data that have been evaluated and recommended by experts. However, although many plasma applications including fusion rely heavily on calculated data, uncertainty estimates of calculated atomic and molecular collision data are very scarce. (The situation is better for calculations of structure and spectra where many experimental benchmarks are available.) As a result, data made available through ALADDIN and other datasets on the Unit's web pages are in many cases not critically evaluated.

The present CCN meeting is part of the long-term effort of the Unit to provide an internationally recommended standard data library of A+M and plasma-material interaction data for fusion. At this meeting the Unit hopes to obtain recommendations towards uncertainty assessment of calculated A+M cross-section data. The Unit also wants to encourage the computational A+M data community to view uncertainty assessment as a part of their computational work and to value and reward A+M data evaluation work. Within the broad area of atomic and molecular collision data, this meeting will concentrate on technical aspects of electron scattering for atoms and molecules, leaving heavy particle collision processes to another occasion. The technical aspects include the propagation of uncertainties from structure data to scattering data and the development of tools within scattering codes to facilitate uncertainty assessment. In addition this meeting has recommendations for future actions by the IAEA and the community to improve uncertainty assessment and data evaluation.

2.2 Unified Monte Carlo: An evaluation method combining experimental and modelling uncertainties, R. Capote Noy (IAEA Nuclear Data Section)

An overview was presented on the data evaluation methodology employed by the nuclear data community with emphasis on methods by which covariances in uncertainty estimates are obtained. A typical situation is a set of measurements of a neutron reaction cross section as a function of energy. Each measurement is supplied with an uncertainty, but there is at first no information on the correlation structure of these uncertainties over the energy range and in addition there may be gaps in the covered energies. Based on Bayes theorem (1763) where the posterior is proportional to prior times likelihood, neutron reaction cross-sections (posterior) are evaluated by combining a properly weighted combination of experimental data (likelihood) with a well-defined theoretical model (prior). The theoretical model has unknown parameters to which some prior probability density is assigned. In a procedure that is referred to as Unified Monte Carlo (UMC) simulations are carried out varying the model parameters and each calculation yields a posterior probability (unnormalized at first) for the chosen values of the model parameters and thereby a probability, with detailed correlation structure, for the reaction cross section or for other quantities that may be obtained from the model.

Many refinements are taken into account in practical implementations including any known uncertainty correlations within and between experiments. Useful references include a report [1] and a paper [2].

References

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[2] Roberto Capote and Donald L. Smith, "An Investigation of the Performance of the Unified Monte Carlo Method of Neutron Cross Section Data Evaluation", Nuclear Data Sheets 109 (2008) 2768–2773.

2.3 Uncertainties in experimental nuclear reaction data - needs, concepts and documentation, N. Otsuka (IAEA Nuclear Data Section)

In order to design new reactor cores by considering both economics and safety, nuclear reaction data evaluators are required to provide evaluated cross sections with their uncertainties and covariances. Experimental cross sections are essential contributors to the evaluated uncertainties and covariances, and propagation of experimental data uncertainties to evaluated data uncertainties must be done in an appropriate manner.

In general, the total uncertainties of experimental cross sections are propagated from various sources of uncertainties (e.g., counting statistics, sample mass)[1,2]. Each source of uncertainty has different property of correlation between two data points (e.g., uncorrelated, correlated), and this property must be known when the experimental uncertainty is propagated to the evaluated data. Suppose there are two experimental data points A and B giving the same cross section with an uncertainty, 100 ± 5 mb and the 5% uncertainty (5 mb) quoted by each experimental data point is from two sources of uncertainties, 4% and 3% as $5= \sqrt{(3^2 +4^2)}$. If two sources of uncertainties are uncorrelated between

measurements of A and B, the weighted average of cross-section and calculated uncertainty using A and B data points is 100 ± 3.5 mb. The uncertainty of the cross-section is reduced by two measurements giving the same results. However, if one of the two uncertainty sources is correlated, for example, 4% uncertainty is uncorrelated and 3% uncertainty is correlated, then their weighted average becomes 100 ± 4.1 mb. This simple example shows an impact of correlation properties on evaluation.

An important task of the International Network of Nuclear Reaction Data Centres (NRDC) is to receive detailed information of experimental uncertainties from experimentalists, and compile it in the experimental nuclear reaction data library (EXFOR).

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[2] D.L. Smith and N. Otuka, "Experimental nuclear reaction data uncertainties: Basic concepts and documentation", Nucl. Data Sheets 113 (2012) 3006.

2.4 Standardising access to AMNS data within the EFDA Task Force on Integrated Tokamak Modelling, D. Coster (Max-Planck-Institut für Plasmaphysik, Germany)

The approach that the EFDA Task Force on Integrated Tokamak Modelling (ITM) is taking on standardizing access to Atomic, Molecular, Nuclear and Surface (AMNS) data was described. The ITM, involving ~200 scientists from across the EU, is working to combine codes to better understand and predict fusion plasma in present and future tokamaks. A number of these codes already use AMNS data and require new/better data, and new codes require AMNS data. For atomic data, the needs are for rate coefficients as well as for cross-section data, in both cases after collisional-radiative (CR) modelling. For molecular data, the need for CR pre-processing is probably even more important, again for both rate coefficients as well as for cross-sections. For nuclear data, beam-beam, beam-target and target-target data are needed, for the main fusion reactions as well as for diagnostics. For surface data, information about reflection and sputtering are needed, with information about rates, and distributions in energy and angle also required.

It is a challenging task for code authors (who are often not AMNS experts) to use data: the issues of finding data, evaluating data, working out how to use data, and then maintaining or adding data. For at least the first two of these challenges, the IAEA could play a key role. For the ITM the challenges include: multiple codes, many with their "own" AMNS data, have to work together; that it would be desirable that the codes use the same data; and that the data has been evaluated by experts. To meet these challenges, the ITM is building a framework that provides easy access to data and attempting to provide all of the necessary data through this framework. It is also attempting to track the provenance of any AMNS data used in a simulation so that older runs can be reproduced. Amongst the issues faced by the ITM are: that ITM codes are written in a number of different computer languages; that "legacy" data might need to be supported; and that ITM codes can be run in a distributed environment (HPC and/or GRID). An important issue that has been identified is the issue of data "robustness" - that AMNS data might be requested over an extreme range of parameters (in one case, from $6\text{x}10^{10} < n_e < 1\text{x}10^{23}$ m^{-3} and $1\text{x}10^{-5} < T_e < 2\text{x}10^{4}$ eV) and that either tables or physics based formulae should be used in preference to arbitrary polynomial fits.

To provide a solution, the ITM is leveraging the ITM developed methods for storing and accessing structured objects (called Consistent Physical Objects, or CPOs) for storing the AMNS data, and building a library that provides access to the data for physics codes.

The talk provided a number of examples in the use of AMNS data including cases: where available data was "wrong"; where changes in the included processes had changed the prediction of the peak flux to the outer target of ITER as a function of the average neutral pressure in the private flux region by more than a factor of two; the challenges of mixed target materials for sputtering; where the

sensitivity of plasma conditions to changes in the ionization rate were examined; where the use of data for looking at prompt redeposition of W near the target were used; and the provision of "filtered" total radiated power data in the AMNS system.

In summary, the fusion community needs data that are: complete; robust; and "correct". In some cases the fusion community will need guidance in how data should be used, and for some new areas, direct collaboration would be useful. As a challenge to the fusion community, the fusion modelling community needs to start thinking about how it could use uncertainty data from the AMNS data providers to identify the sensitivity of the simulations to AMNS data.

2.5 Some thoughts on data uncertainty propagation in collisional-radiative models, Y. Ralchenko (National Institute of Standards and Technology, USA)

Atomic data represent one of the most critical components of collisional-radiative (CR) models. The rate equations that are being solved within a CR model depend on the rates of various physical processes that affect populations of atomic states. The most important processes included radiative decay, electron-impact excitation, deexcitation, and ionization, photorecombination, three-body recombination, and dielectronic recombination. In CR models with explicitly included autoionizing states, the autoionization and dielectronic capture are to be included as well. Other processes may include heavy-particle-induced reactions (excitation, deexcitation, ionization, charge exchange) or photoinduced processes (e.g., photoexcitation and photoionization). For Maxwellian plasmas, the rates are obtained from the Maxwellian-averaged rate coefficients while in non-Maxwellian plasmas (e.g., those of electron-beam ion traps) the reaction cross sections are to be convolved with the non-Maxwellian electron energy distribution functions, such as Gaussians.

The number of papers devoted to analysis of data uncertainty propagation in CR models is very limited. In early 1980s, D. Salzmann performed first analytical and numerical calculations and showed that the relative ion population uncertainty increases away from the most abundant ionization stage. The more recent works from several groups (ADAS, Auburn, NASA, and others) apply both analytical and Monte Carlo approaches to analysis of data uncertainty propagation on the diagnostically most important line ratios G and R in He-like ions. However, these efforts are only in the initial phase.

A number of Monte Carlo (MC) simulations were performed to study variations in the mean ion charge $\overline{Z}$ and central moments (σ_2 and σ_3) due to variations in the input atomic data. The CR code NOMAD was modified to include the MC option and calculate the plasma kinetics parameters for Ne and C. The Ne runs were performed for ground states only. The log-normal distribution was used to modify all atomic rates; importantly, to preserve correct relations between direct and inverse processes, their rates were modified by the same factor. The simulation was performed for the following standard deviations σ in the log space: 0.05, 0.30, 2, and 10. The small values of σ resulted in only small deviations of $\overline{Z}$ and moments. The largest σ, however, clearly showed development of attraction points on the ($\overline{Z}$,σ_2) plane which correspond to cases when only two ionization stages are abundant. Similar behaviour was found for a single-T_e case. As for the C cases, the difference between two models was in inclusion of excited states. It was found that excited states tend to suppress propagation of data uncertainties as compared to the ground-state-only case. More MC simulations are planned for more complex systems with a larger number of states including autoionizing ones.

2.6 Evaluating the Accuracy of Theoretical Transition Data for Atoms, P. Jönsson (Malmö University, Sweden)

The process of estimating uncertainties of calculated transition data for atoms depends on the complexity of the atomic system as well as on the number of different states that are studied. Here we may distinguish between calculations for a few states and "spectrum" calculations for hundreds of states, which yield massive sets of transition data. The process also depends on the computational methods used.

In multiconfiguration methods the wave function for a state is expanded in configuration state functions (CSFs), where the CSFs are symmetry adapted and anti-symmetrized products of one-electron orbitals. Given approximate wave functions for the initial and final states, transition parameters such as line strengths can be evaluated in length and velocity gauges. For accurate wave functions transition parameters in the two gauges should be close to each other.

For multiconfiguration methods *the uncertainties of transition data can be inferred from convergence studies*. Define a model for generating CSFs from the one-electron orbital basis. Increase the one-electron orbital basis in a systematic way and monitor the convergence of the transition parameters. Establish converged values within the model. Relax the model and include more electron correlation effects. Again, increase the one-electron orbital basis in a systematic way and monitor the convergence of the transition parameters to establish converged values within the new model. Based on both the convergence of transition parameters within each model as well as between models the uncertainties can often be estimated. A major problem is that the number of CSFs in many cases grows so rapidly with respect to the orbital basis that it is not possible to establish converged values. Also, it may be difficult to go beyond models that account for valence and core-valence correlation.

When experimental energies are available the wave functions can be "fine-tuned" by shifting diagonal elements in the Hamiltonian to reproduce the energy separations. *In some cases the sensitivity of the transition parameters to the tuning may be used to say something about the uncertainties*. Fine-tuning is not available for fully relativistic calculations in *jj*-coupling, where off-diagonal elements in the Hamiltonian matrix may be large.

The accumulated experience from many studies indicates that *differences between the transition parameters calculated in the length and velocity gauges can be used as uncertainty estimates*. For LS allowed transitions Froese Fischer suggested [1] that the uncertainty $\delta A'$ in a transition rate A' may be estimated by

$$\delta A' = (\delta E + \delta S)\, A',$$

where $\delta E = |E(\text{obs}) - E(\text{cal})|/E(\text{obs})$ and

$$\delta S = |S(\text{length}) - S(\text{velocity})| / \max(S(\text{length}); S(\text{velocity}))$$

are, respectively, the uncertainties in the transition energy and in the line strength. The above uncertainty estimate cannot directly be applied to LS forbidden transitions. Different generalizations are, however, possible.

For "spectrum" calculations internal benchmarking can be applied to estimate uncertainties. Internal benchmarking amounts to performing very accurate and elaborate calculations for a few carefully selected transitions. The results from the less accurate "spectrum calculation" are then compared against values from the internal reference transitions.

References

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2.7 Uncertainty of Atomic Data: Electron-Atom Collisions, K. Bartschat (Drake University, USA)

An overview was presented of computational methods to generate atomic data for electron-atom collisions. Particular emphasis was placed on approaches whose results have been used extensively for plasma applications. They include

- special-purpose methods, such as the optical potential approach [1,2] with local potentials to treat the projectile-target interaction, including an approximate account of exchange effects, charge-cloud polarization, and loss of flux into inelastic channels,

- a polarized-orbital approach with non-local exchange, polarization, and absorption potentials,
- perturbative methods based on some variant of the Born-series such as the distorted-wave Born approximation [3] (which, for example, is the basis of the Flexible Atomic Code [4] and to some extent also for Kim's Binary Encounter f-scaling [5]), and
- non-perturbative approaches based on the close-coupling expansion. Among the latter, the convergent close-coupling method (CCC) [6], the R-matrix with pseudo-states (RMPS) approach [7] based on the well-known Belfast suite of codes with orthogonal one-electron orbitals [8], and most recently the B-spline R-matrix (BSR) approach with non-orthogonal orbitals [9] are widely used, although time-dependent close-coupling [10] and exterior complex scaling [11] have been employed in some benchmark studies.

It is undoubtedly *a very difficult task to generally assess the accuracy of theoretical predictions, due to the large number of parameters to consider*. Specifically, the accuracy will depend on the target, with atomic hydrogen and light quasi-one electron systems (Li-like, Na-like) as well as He and light quasi-two electron (Be-like) systems being the easiest cases to treat.

Furthermore, the difficulty generally increases with increasing nuclear charge, due to the different ways of treating relativistic effects (neglect them in LS-coupling, approximate them through recoupling of LS-results or using the Breit-Pauli perturbative approach, or employing a fully relativistic Dirac-based formulation). Open-shell elements are much harder to describe than closed-shell systems, neutral atoms are more difficult than positively charged ionic targets, and optically allowed transitions are generally more suitable for less sophisticated approaches than forbidden ones. The resolution (angle, energy, state) is important as well, and in particular resonance effects can play a critical role.

Finally, it is important to specify the observables of interest, i.e., whether macroscopic parameters such as the electron mobility or a diffusion coefficient in low-temperature plasmas are to be modeled (elastic scattering, momentum transfer, excitation, and ionization from the ground state are usually sufficient in that case) or whether one needs a detailed collisional-radiative model with state-to-state transitions also involving excited initial states. Clearly, the sensitivity of the results to the various ingredients of the model calculations for electron-atom collision processes, including the effect of the target structure description, needs to be checked in order before ultimately drawing conclusions.

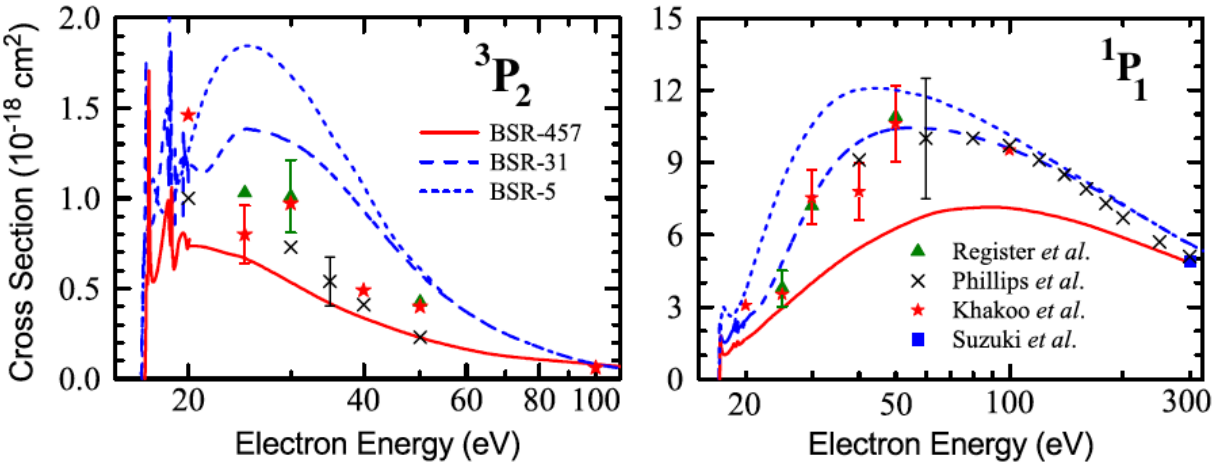

Fig. 1: Predictions from BSR models with 5 states, 31 states, and 457 states in the close-coupling expansion for electron impact excitation of two $3p^5 4s$ states in Ne. (Adapted from [12].)

Figure 1 shows an example from a BSR calculation [13] for electron-impact excitation of the $(3p^5 4s)^3P_2$ (metastable) and $(3p^5 4s)^1P_1$ states in Neon from the $(3p^6)^1S_0$ ground state. There is a strong effect of coupling to the ionization continuum, even for the optically allowed $^1S_0 - {}^1P_1$ transition. Consequently, distorted-wave approaches would likely be problematic in the low and intermediate energy range of incident energies up to a few times the ionization threshold.

Looking into the near future, *it seems advisable to agree on a few benchmark systems*, where predictions from the most sophisticated coupled-channel approaches can be compared to each other, to those from simpler Born-type methods, and in some cases to experimental data. The problems that come to mind are e-Be and e-Ne collisions. For the former, CCC and RMPS calculations have already been performed and are currently being further refined for benchmarking purposes, while BSR calculations could be carried out within the next few months. While the current CCC code is not ready to handle the e-Ne collision problem, presumably accurate BSR calculations are already available [12], and the results could be compared with RMPS predictions based on further extensions of the work reported by Ballance and Griffin [13]. Of course, DWBA calculations should be straightforward for these systems. Even though their accuracy is likely limited, particularly for optically forbidden transitions and low to intermediate energies, having such results available should assist in further quantifying the error estimates.

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2.8 Evaluation of electron impact excitation data in RDW calculation, C. Dong (Northwest Normal University, China)

Electron impact excitation (EIE) is one of the most essential atomic processes, a large number of EIE data are necessary for both the understanding of atomic excited structures and the modelling of various plasma properties. To satisfy those requirements, various experimental techniques and theoretical approximations have been developed in the last few decades. Also there have been some available atomic databases for applications. However, the accuracy of these available data is often suspicious because different calculations using similar methods/codes sometimes differ by up to two orders or more of magnitude for some transitions.

On the basis of the GRASP92/2K and RATIP packages in the frame of Multi-Configuration Dirac-Fock (MCDF) method, a new relativistic distorted wave (RDW) program, named REIE06 has been developed in recent years. Some selected applications of this program are introduced in this presentation. A special attention has been paid on the systematic evaluation of EIE data in the present method. Such as *the electron correlation effects in calculation of target structure* can be considered systematically by increasing the active space sets, the contributions from high partial waves, Breit interaction and intermediate resonance states can be also included in the calculations. As a result, for highly ionized heavy ions, it is regarded as an easier and more effective method for producing a large amount data of cross sections and rate coefficients.

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2.9 Maintaining code accuracy across versions and upgrades, E. Stambulchik (Weizmann Institute of Science, Israel)

Detailed collisional-radiative (CR) models for laboratory and space plasmas typically comprise hundreds to thousands of atomic states and thousands to millions of radiative and collisional rates. Compiling such huge data bases from different data sources is a tedious and error-prone process with a high chance of inconsistency between different process types. Instead, researchers working in the field have developed automatic or semi-automatic procedures for generating the data bases in their entirety using universal (i.e., able to calculate all required types of atomic rates) codes. One such a code is Flexible Atomic Code (FAC), developed by M.F. Gu [1]. FAC is based on distorted wave approximation with relativistic potential and QED corrections, which makes it especially well-suited for highly-charged high-Z ions. Although the code is no longer maintained by the original author, its programming sources are freely available, allowing for modifications and further development by an interested party.

Making sources of scientific codes, used to produce published data, openly accessible is generally considered a necessity for ensuring reproducibility and verification of the published results [2]. However, *little is said about uncertainties associated with development of a code* over the course of its life. These uncertainties are actually *variations of the code's results, stemming from choosing different numerical algorithms or their implementations, switching to different computer architectures the code is run upon, change of compilers or real coding mistakes* ("bugs") which may remain unnoticed for a long time until a modification from the list above triggers them. In addition, data of scattering processes, such as the collisional ionization, are continuous entities (depend on the scattered electron energy etc.), but are output on a discrete grid of energy values. An external integration over a projectile energy distribution necessarily involves *interpolation or even extrapolation of the calculated data points*. This process further contributes to the uncertainties of the calculated results.

These issues were analyzed based on several versions of FAC and its modification (cFAC) developed for the last few years.

References:

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2.10 Evaluating uncertainties in experimental electron scattering data and exploring cross comparisons of experimental and theoretical data, N. Mason (Open University, UK)

Electron induced reactions in both the gaseous and condensed phases initiate and drive many of the basic physical and chemical processes in science and technology with applications from industrial plasmas to radiation damage in living tissue. For example, in contrast to previous hypotheses, collisions of very low energy secondary electrons with the components of DNA molecules (or to the water around them) has been shown to be a crucial process in inducing radiation damage in the DNA of living systems. Understanding electron interactions with larger biomolecules is therefore providing new insights to radiation damage and thence the development of new, alternative radiotherapies. In the technological field electron induced reactions underpin most of the multibillion dollar modern semiconductor industry since it is those reactive fragments produced by electron impact of etchant gases that react directly with the silicon substrate. Studies on electron scattering from molecules capable of improving the etch rate of surfaces are leading to development of new (environmentally

cleaner) plasma technologies. Electron induced processes are also of extraordinary importance for determination of structure and chemical reactivity of species adsorbed on surfaces.

Such research and technology is intricately linked to our knowledge of the key interactions between electons and atoms and molecules and thus a database is required for characterizing electron interactions with atomic and molecular species. However, the compilation of the electron collsion data required is rarely a coherent, planned research programme instead it is a parasitic process. Indeed today it is rare for researchers to be funded to measure fundamental collision processes since these are no longer regarded in themselves as 'cutting edge' research rather the field has developed to explore more exotic phenomena such as cold atoms; nanotechnology and chemical control.

The fundamental research community, the providers of such data, therefore need to assemble, update and police a set of approved databases. This is no longer as complicated as it was a decade ago. Most publications are accessible online and most authors place their data on home pages and in archives, Hence compiling databases is easier than it was in the past for example by using the General Internet Search Engine for Atomic Data (GENIE) developed as part of the International Atomic Energy Agency project. The current status of the electron scattering databases is reviewed, how they are assembled and updated and thus whether they are 'fit for purpose' or if not how they may be developed to meet the challenges of the 21st century Science and Technology. Ultimately it is for the community to develop a method for archiving and recommending sets of electron scattering data and propose methods by which this can and will be done.

A critical part of any such data review is the inclusion of calculated data since many of the targets can not be studied in experiments (e.g. data on free-radical or short-lived transient chemical species). Increasing semi-empirical theorems are used to estimate such data, but the limitation and validity of such data must be assessed. How such 'theoretical' data are assessed and how uncertainty estimates in such data are made remains a topic of debate but must be addressed as in future most data for the 'user community' will be derived from such theoretical calculations with experiments being used to benchmark such work.

The EU VAMDC project (www.vamdc.eu) provides a means to assemble, curate and disseminate such data but requires a series of protocols/guidelines on data validation that the Atomic and Molecular Data Unit of the IAEA could provide.

2.11 Uncertainties in electron - molecule collision calculations at low energies, J. Tennyson, (University College London, UK)

Electron collisions with molecules can lead to a variety of different processes. At low collision energies these are: elastic scattering, rotational excitation, vibrational excitation, electronic excitation, dissociative attachment or dissociative recombination, impact dissociation and impact ionization. Calculations are playing an increasingly important role in providing data on all of these processes but very little effort has so far been made to characterise the uncertainties in the results of these calculations. *Such uncertainties are almost entirely systematic and depend strongly upon the assumptions made in choosing and solving the model used to represent the collision process*. Some of these issues get easier at high collision energies where simplified treatments are known to give very reliable results. A further complication is that *no single method treats all processes simultaneously; this means that there are no complete, self-consistent computed data sets which encompass all the processes listed above*.

When comparing results from different research groups it is usual for people to label these results by the computational procedure used in the calculation. However *the results are determined not by the method of calculation but the model chosen*. Indeed intercomparison of the leading codes (R-matrix, Kohn, etc.) have demonstrated on several occasions that they give the same results for a given system and a given model.

Traditionally the most powerful model for treating low-energy collision has been based on the use of a close-coupling representation of the wave function. Work on electron-atom collisions has shown that a new class of methods based on the complete treatment of the close-coupling problem (i.e. allowing for the inclusion of the electron continuum in the close-coupling expansion) has meant that electron-neutral atom collision results can now be performed with accuracies approaching, or in some cases, exceeding those obtained by experiment. Two of these methods are now being applied to electron – molecule collisions: the R-Matrix with Pseudo-States method (RMPS) and Convergent Close-Coupling (CCC). So far the CCC method has only been applied to collisions with very simple molecular targets and this situation is likely to remain true for some time. However, the RMPS method provides a general procedure which can be applied to complex problems. However, the method is computationally very expensive and has, therefore, required the development of new computer algorithms to allow its application to problems of interest. So far the RMPS method has only been used sparingly and has not been used to systematically study all processes listed above. For example, while electron impact excitations cross sections have been a by-product of some RMPS calculations, a systematic study using the RMPS method has not yet been performed on how these cross sections behave as a function of model. Such studies are essential to establishing the uncertainties in the calculations.

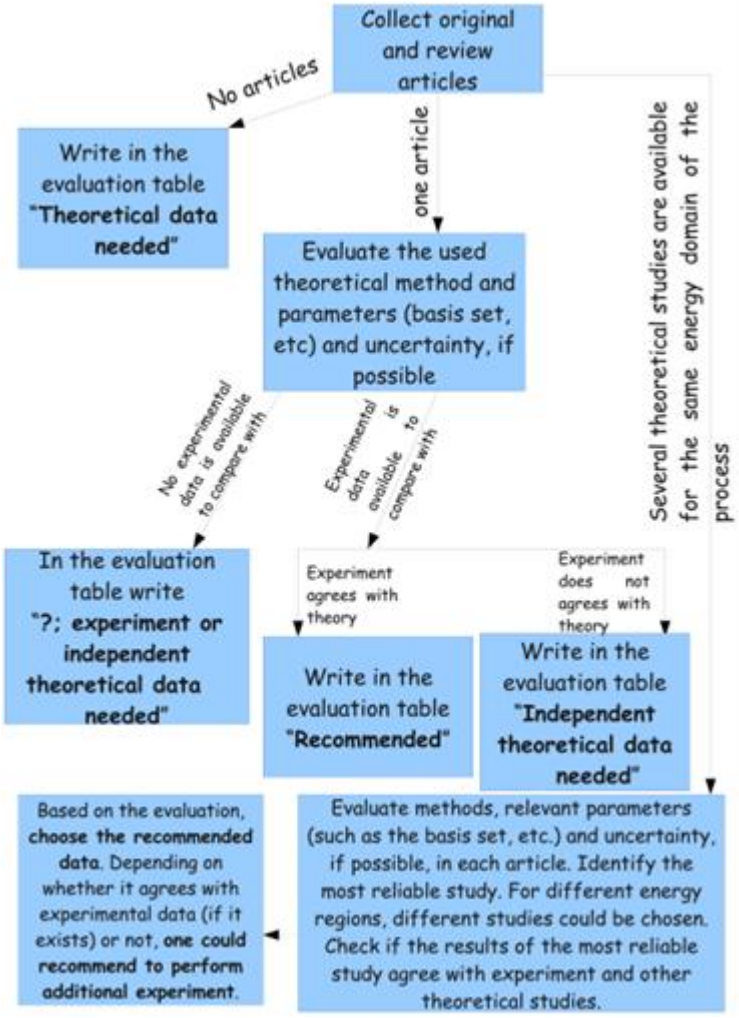
As electron-molecule collision calculations move from trying to model and interpret experimental measurements towards being a primary data source, there is an urgent need for these calculations to start giving uncertainties. To do this it is important that protocols for characterising these uncertainties are developed. Traditionally the quality of a calculation has been established simply by comparison with experimental measurements. However, uncertainties are needed for calculations on systems for which no measurements are available such as radicals or triterated species.

While we are not in a position to design a complete protocol at this stage, it is possible to make a number of recommendations on how studies should proceed. In particular:

- *Target properties* (excitation thresholds, dipoles) can be very well characterised using modern quantum chemistry codes. Even if the best wave functions are too complex to be used in scattering treatments, target properties should still be given with uncertainties. Some of these uncertainties (for example in the dipole moment) feed directly through to uncertainties in scattering observables (such as the elastic cross section at low-energy).
- *Resonance positions* (and to a lesser extent widths) behave somewhat similarly to target energies and should be presented with uncertainty estimates.
- *Reproducibility* of results is an important issue and historically has not always been achievable because of problems with full specification of inputs in journal articles (and in some cases changes with codes over time). Code inputs (and code specification) should be published to allow reproducibility (e.g. as supplementary material).
- To establish a protocol for giving uncertainties it would be very helpful to have *a case study where the electron molecule collision processes listed above are studied in a systematic manner by more than one method.* The aim of this study would be to not only obtain high quality (benchmark) results but also to properly characterise the uncertainties in these results. The procedure used to obtain these uncertainties should be fully documented and published (e.g. in Physical Review A). It was agreed that the electron – N_2 problem would be a good choice for this.
- Data validation procedures such as the ones being undertaken by the eMOL collaboration, should also aim to produce validated theoretical models (with uncertainties) so that these models can be used to perform further calculations such as on triterated isotopologues or higher-lying rotation-vibration states.

2.12 Uncertainty assessment of theoretical data on electron-molecule collisions: Examples of H_3^+ and CH_4, V. Kokoouline (University of Central Florida, USA)

In consideration of published theoretical studies on electron-molecule collisions, theoretical approaches and the corresponding computed cross sections are evaluated for the dissociative recombination of H_3^+ and elastic and various inelastic processes starting from e^--CH_4 collisions. The evaluation led to a scheme, which could be used to evaluate other similar theoretical data. The scheme is shown below.



2.13 Simulation tools to evaluate and estimate uncertainties of electron and positron scattering data for molecules, G. García (Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Spain)

A review was given on a modelling procedure to simulate single electron and positron tracks in molecular media, which could be useful to evaluate input cross section data by comparison with specific experimental arrangements. The model is focused on low energy processes, i.e. below 10 keV, paying special attention to those occurring close to the final thermalisation of the electrons and positrons in the medium. It is linked to a general purpose Monte Carlo simulation programme (GEANT4) in order to cover the initial interaction of the high energy primary particles. Once low energy secondary particles (electrons, positrons or radicals) are created our modelling programme simulate the track of those particles trough an event by event Monte Carlo procedure using as input

parameter the interaction and energy loss distribution functions derived from experimental and theoretical interaction cross section data.

The main experimental and theoretical data sources used in the model were reviewed. Estimated uncertainties for each considered process: elastic, ionization, electronic excitation, vibrational excitation, rotational excitation, positronium formation and electron attachment, were discussed. Based on an independent atom representation in combination with our screening corrected additive rule (IAM-SCAR) [1] a procedure to translate required collisional data from the gas phase to the condensed phase was proposed. It is a general procedure to use the most accurate experimentally obtained cross section data, i.e. grand total and ionization cross sections, our calculated differential and integral elastic scattering (once verified by comparison with differential experimental cross sections at selected angles) being data corresponding to the remaining inelastic channels taken from the literature. Following this procedure a complete data set has been published for representative molecules [2-6] in order to be used for modelling purposes.

Finally, some validation experiments are proposed in which solid substrates (gold, tantalum) having condensed molecules on their surfaces (water, DNA components) are irradiated with high energy photons. Using the complete set of photon and electron interaction data bases for the whole energy range covered by the experiment the energy and angular distribution of secondary particles (electrons and charged radicals) will be simulated and then compared with those experimentally observed.

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2.14 eMOL: Evaluating electron- molecule scattering data, N. Mason (Open University, UK)

The problem of assessing and presenting recommended datasets for electron–molecule cross sections has been discussed within the Electron scattering community for many years. The major conclusions were;

- It is important
- Only the community itself can do this job
- No single group or person can do this or receive support to do this (other than odd review every few years)

The eMOL (electron molecule) has been established to establish the process by which such data will be reviewed, validated and recommended data sets published. In particular eMOL seeks to suggest whether any particular data set be used as a primary or secondary source of data for the wider community. Primary would mean that is judged to the best representation of that particular interaction/cross section and therefore be used as a ‘recommended‘ value for users.

eMOL will operate through an eMOL Board drawn from the leading members of the international electron molecules scattering community (experimental and theoretical). This Board undertakes to work in sub-teams to review data and recommend specific data sets using guidelines for reviewing the data that are developed by eMOL in collaboration with other agencies (such as IAEA and VAMDC). These final recommendations will be placed on a dedicated server and the ‘complete set’ of cross sections for any molecule be reviewed for ‘completeness’ and internal consistency (e.g. if all the

individual cross sections add up to exceed the total cross section we will need to review this!). The data presentation should be compatible with VAMDC project architecture (www.vamdc.eu). Furthermore as new papers are published the Board will review data and recommend whether it replaces a recommended data set.

Initially it is proposed to undertake such a review for a dozen 'common' molecules (to be completed in 2013-16). For many of these molecules a current (recommended/reviewed) data set can be chosen to act as a basis upon which to base discussion. New papers that came out since the review will need to be reviewed and compared with data in the database and self-consistency checks made (as not all current reviews do this). A few (biomolecular) targets have also been selected for which no review has been undertaken. This programme has just begun with a review of electron-water scattering cross sections in Vienna in May 2013.

Subsequent meetings are now being planned to be held at international meetings where members of the eMOL community are expected to attend.

2.15 Further experimental works suggested and where we are now, Y. Itikawa (Institute of Space and Astronautical Science, Japan)

In the review paper by Itikawa and Mason [1] on the cross sections for electron collisions with water molecules, further experimental works were suggested. Following those suggestions, several new experiments have been done. In the present talk, those experiments are introduced and it is shown what new results are available now. Considering the results, an update of the recommended data is necessary at least for (1) elastic scattering, (2) momentum transfer, (3) vibrational excitation, (4) excitation of electronic state, and (5) dissociative electron attachment.

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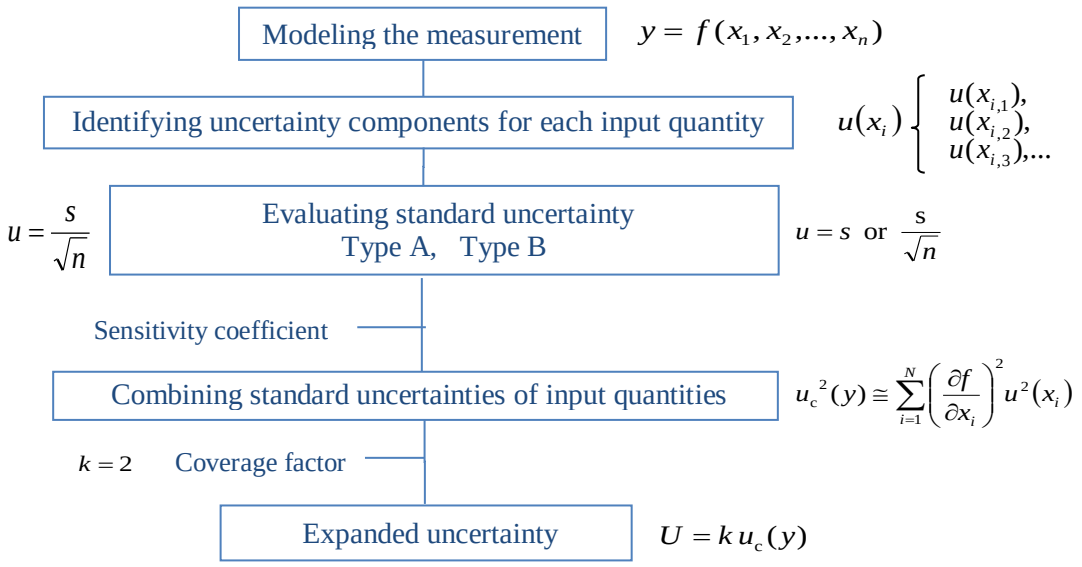
2.16 IAEA activities on data evaluation, H.-K. Chung (IAEA Nuclear Data Section)

Conclusions and recommendations of a series of IAEA meetings on data evaluation for atomic, molecular and plasma-surface (AM/PSI) data for fusion applications were summarized on the topics of the consensus of communities on data evaluation, theoretical and experimental data evaluation, propagations of uncertainties of fundamental data to the observable quantities. The proceeding papers with detailed discussions can be found in the special issue of Fusion Science and Technology [1].

International science and technology communities developed the internationally agreed terminologies for measurements based on VIM3 (International Vocabulary of Metrology, BIPM) [2] and GUM (Guide to the Expression of Uncertainty in Measurement) [3]. The definition of measurement is the "process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity". The value is defined as the number and reference together expressing a magnitude of a quantity. Traditionally, the value of the measurand (quantity intended to be measured) was a considered to be the "true" value. However, the modern concept ("uncertainty approach") defines the value to be a "measured" value with an uncertainty range in which the true value is likely to exist. Therefore, *the goal of a measurement is not to find the "true value" but to reduce the uncertainty range of the "measured value"*. The 5 steps in uncertainty evaluation are schematically shown in the figure.



The uncertainty quantification of theoretical data plays a critical role in data evaluation and hence the consensus to establish guidelines or suggestions for uncertainty estimates of theoretical data in the community is highly desirable.

References

[1] Fusion Science and Technology volume 63, number 3 (2013)
[2] International Vocabulary of Metrology – Basic and General Concepts and Associated Terms, JCGM 200:2012
[3] Evaluation of measurement data – Guide to the expression of uncertainty in measurement JCGM 100:2008

3. Discussions

An "error bar" of experimental data is a familiar concept to physicists as experimental measurements are subject to statistical variations and systematic "errors" or uncertainties associated with components of a measuring system. On the other hand, an uncertainty in theoretical data is difficult to conceptualize, let alone to evaluate. This rather new concept comes from the necessity to evaluate theoretical data in the modern framework of metrology beyond the traditional way of comparisons with experimental observations. It is not impossible if a code to produce theoretical data is considered to be a "measuring system" composed of many components such as a series of assumptions and input models which inherently have associated uncertainties. Then the quest comes down to identify the components and their uncertainties.

It is noted that an "error" of a measurement is defined as the difference of the measured value from the true value. However, the true value is rarely known and in some cases unknowable. Strictly speaking, the use of an "error bar" to describe the dispersion of measured values is not correct unless the true value is already known. Without the knowledge of true value, a measurement can only give the "measured" value and an "uncertainty" of the measurement. In a sense, experimental or theoretical pursuit to find the "true" values of atomic and molecular (A+M) data comes down to reducing uncertainties of (experimentally or theoretically) measured values by increasing our understanding of the physics.

Participants agreed that an evaluation of uncertainties associated with theoretical A+M data is a complex problem and the guidelines cannot be produced in this meeting. A consensus was reached, however, that this meeting can make a valuable contribution to theoretical A+M structure and collision studies by taking a first step towards the establishment of the guidelines. In addition the meeting will

raise awareness in the community of the importance of estimating uncertainties associated with theoretical data and will help to engage colleagues in the field.
Much attention was paid to the identification of the components and assumptions used by the code and strategies to quantify their associated uncertainties. Initial work programs were defined and agreed. Discussions summarized here were presented to the joint meeting of the CCN participants and the eMOL group on the 3rd day.

3.1 Guidelines for the uncertainty estimates of atomic data

Evaluating uncertainties of theoretical atomic data is a very complex problem. As the first step, three aspects are identified to be considered in developing a strategy or guideline to evaluate an uncertainty of data of interest.

Target: The maturity of physics and calculation procedures vary depending on the target system of the data. A guideline should be established based on the physics "models" appropriate for the target.

- H and quasi-one electron systems (Li-like, Na-like etc.): Theories are well defined and in a fully mature state.
- He and quasi-two electron systems (Be-like etc.): Theories are in a good shape and agree well with experiments with a few exceptions.
- Light vs. heavy (LS, recoupling, Breit-Pauli, Dirac): Physics changes as Z increases, and so should the theory. A treatment of assumptions such as relativistic effects becomes a key element in uncertainty evaluation.
- Transition (open-shell) elements: It is a difficult problem with many issues such as convergences.
- Neutral or charged: (Positively) charged particles tend to be easier to treat due to decreasing electron correlation effects.
- Type of transition (allowed, forbidden, inner electrons): Rates of allowed transitions are better understood and scaling laws or asymptotic behaviors exist for allowed transitions. Calculations for forbidden transitions, especially of small magnitudes have seen more disagreement with experimental data than those for allowed transitions.

Resolution: As in the case of laboratory measurement, a quantity of interest, whether an atomic level energy or a cross-section, depends on the resolution of measuring system. In some cases, calculated data with most details are needed and in other cases, averaged data are adequate for applications. A guideline should be developed based on the resolution of calculated data.

- State-resolved: Uncertainties of energies and transition/collisional rates will be evaluated in a different fashion for fine-structure states or configuration-average levels.
- Angle-resolved and energy-resolved: Uncertainties of angular or energy differential cross-sections will be evaluated in a different way.
- Resonances (positions, widths) vs. background: It would require some thoughts to quantify uncertainties of resonances. Considerations should be given for the peak intensities, positions and widths as well as the on and off resonances.

Observable of interest: Guidelines should be categorized based on the applications.

- Energy levels and oscillator strengths.
- Cross sections or rate coefficients: A collisional-radiative (CR) model requires cross-sections if the given electron energy distribution function is not the Maxwellian.

- Macroscopic phenomena (electron mobility, diffusion coefficient).
- Sensitivity of results to ingredients of the model.

Ideas and suggestions to quantify uncertainties were exchanged for atomic structure calculations and electron-atom collision calculations.

Atomic structure calculations: It is desirable to identify code components that make it possible to assess uncertainty estimates without significant computation.

- Descriptions of initial and final states, and then operators should be checked.
- Vary basis size (within reason) and basis parameters (within reason)
  - For CI models, uncertainties associated with basis set changes should be documented.
  - The selection of basis functions, nature of basis functions and complexity of the model (e.g. valence electron correlation) should be documented.
- Check sensitivity – for transition parameters
  - One should consider publish results both in the length and velocity gauges when sensible. The results should agree for accurate wave functions.
  - It is a problem when both results do not exist. Even if they agree with each other, it does not necessarily mean that they are right. One needs to identify the necessary and sufficient condition.
  - Matrix elements will be a better quantity for comparison and publication.
- A benchmark system to test methods is not yet identified.

Collision calculations: There are two categories of electron-atom collisional codes: highly accurate and computationally intensive codes (benchmark status calculations) and production codes to provide a complete set in a short time with an acceptable accuracy to a user.

- e-H, e-He, e-Be, e-Be^+ are already good benchmark cases, for which sophisticated theories (CCC, RMPS-ortho, BSR-RMPS) agree within about 10% for total cross-sections of all transitions involving n=1,2,3 and ionization – should give the same answers and they do. Theories agree well with experiments. For low value cross-sections in the differential cross-sections, the quoted uncertainty of 10% may not be realistic.
- In order to give a realistic number of uncertainties, a code comparison is the first step:
  - Good candidate for further benchmarking is e-Ne (neutral and ionized, e.g. Ne^{4+}).
  - Balance and Griffin (2004) results and the most recent results (2013) agree with each other and a convergence with basis sets seems to be reached.
  - Belfast RMPS (Auburn, Balance et al.) vs. BSRMPS (Drake, Zatsarinny et al.) could check each other. However, current CCC code cannot handle these.
  - For Ne^{4+}, one could "measure" how well the widely used FAC (Flexible Atomic Code) does compared to the much more sophisticated methods. Other (R)DW calculations might be useful as well. – It is a different way to check FAC code.
  - For this system, theories tend to agree, but not with experimental results.
- CCC calculations work well near threshold energy. It is noted that the cross-section peaks in the intermediate energy range of 1-5 times ionization potential where the sophisticated calculations converge to distorted wave or Born approximations.
- A consistency is an important check for scattering calculations not only for molecules but also for atoms. In the case of atoms, the insufficient account of continuum states in the CCC calculations leads to overestimation of excitation processes and underestimation of ionization processes. The approach of the FAC code that the same radial wave functions and potentials are used for all atomic processes has been considered to provide a "consistent" data set by users. One should be aware that the consistency of this approach will not always ensure the correct distribution among excitation and ionization channels.

The distorted wave calculations should be set up correctly to conserve unitarity of the system for reasonable answers.

3.2 Guidelines for the uncertainty estimates of electron-molecule collisional data

While scattering codes for atoms may treat almost all possible channels in one model, there is no single method to treat all channels and processes simultaneously in electron-molecule scattering. It means that there is no complete and self-consistent data set produced by a single calculation. Each channel and process of a scattering event is treated with a relevant model piece by piece and all pieces should sum up to the total cross-section which is observable. A difficulty is attributed to the large numbers of channels to consider; in most cases, much larger than a code can handle.

Electron-molecule scattering experiments are extremely challenging. One needs a protocol to characterize uncertainties of theoretical data beyond just experimental comparison so that uncertainties can be provided for systems for which no measurements are available. There are similarities between the uncertainty estimates of electron-atom scattering data and electron-molecule scattering data. Uncertainties (or "errors") are mostly systematic though it is not always the case. It is not yet clear how to characterize uncertainties of electron-molecule scattering data. Here is a list of suggestions to explore.

Target properties: Modern quantum chemistry is well developed and hence the target properties such as excitation thresholds, dipoles should be given with uncertainties. Even if the best wave functions are too complex to be used in scattering treatments, target properties should still be given with uncertainties. Some of these uncertainties (for example in the dipole moment) feed directly through to uncertainties in scattering observables (such as the elastic cross section at low-energy). Issues such as correlation along the curves or rotation corrections should be investigated. Approaches taken for atomic structure calculations to obtain uncertainty estimates may be adapted for the case of molecular potential curves.

Resonance positions and widths: Uncertainty estimates should be provided. Currently it is not in the community culture. Some thoughts are required on how to put an uncertainty for resonances close to threshold when they are either on or off.

Case studies: To establish a protocol for giving uncertainties it would be very helpful to have *a case study where the electron molecule collision processes are studied in a systematic manner by more than one method.* The study would seek to obtain agreed high quality (benchmark) results but the primary aim of the study would be to properly characterise the uncertainties in these results. The procedure used to obtain these uncertainties should be fully documented and published (e.g. in Physical Review A).

It was agreed that the electron – N_2 scattering problem would be a good choice for a series of sensitivity analyses. N_2 is an important species for fusion and atmospheric sciences and the physics of dissociation is complicated enough for comprehensive tests. Dissociation and break-up dynamics has similarity to H_2 and D_2 which are main constituents of fusion plasmas. The entire atomic and molecular processes of the break-up of N_2 molecules to N and N^+ ions and beyond are of interest to fusion modelling.

Data validation procedures: Cross-sections of all processes (elastic scattering, rotational excitation, vibrational excitation, electronic excitation, dissociative attachment or dissociative recombination, impact dissociation and impact ionization) should be sum up to the total cross-section. This consistency check should be used as a validation procedure. Validation procedures and uncertainty estimates are not unrelated. The procedure should also aim to produce validated theoretical models (with uncertainties) so that these models can be used to perform further calculations such as on triterated isotopologues or higher-lying rotation-vibration states.

Advantages and disadvantages of Hartree-Fock approaches for potential curves were discussed in terms of consistencies between ro-vibrational energies and electron scattering calculations. A methodology was discussed to tune calculated data with experiments and model resonances.

3.3 General remarks

Participants shared ideas on broader topics on general validation procedures and considerations of applications.

Reproducibility and version control: It is an important issue to have a mechanism to ensure reproducibility of results when a code is widely distributed for community use.

- One should keep master versions of codes that are widely distributed.
- One should archive input data sets of test cases so that a user can check for reproducibility and consistency. The inputs should be tested for new versions or modified codes.
- A full specification of inputs should be published to allow reproducibility when a code result is published (e.g. as supplementary material). For example, inputs such as potential surfaces to produce spectroscopic properties should be specified as a part of results.

Benchmark experiments: A validation of theoretical data would be hardly complete without measured data. There are systems such as tungsten where no data are available and theory is hard to evaluate or systems such as lead where it took more than 20 years to produce theoretical data anything close to experimental data. Unfortunately, experiments for both electron-atom and electron-molecule scattering physics are extremely challenging. Data produced experimentally tend to be more reliable, however, it is not always true and there are many cases where theoretical data should provide guidance. Evaluations of theoretical and experimental data should be regarded as complementary.

- There are known issues with measured data:
  - Issues with low and high angle scattering
  - Issues with what is being measured (e.g. cascade, target populations)
  - Issues with correction factors
  - Heavily biased sample: Closed-shell atoms and molecules

- If measured data are available, theory will develop.
  - More than one data point is necessary for validation purposes.
  - There are cases where data are presented with small uncertainties but completely different values among different groups. Such a discrepancy should be understood.
  - In EU collaboration, it is common that different experimentalist groups publish jointly by combining each measurement or do measurements in other group's laboratory.
  - An established network of experimentalists is highly desirable. As an example, a network of small tokamak research coordinated by IAEA Physics section is composed of 12-15 university and small laboratory groups with devices and agreed to do experiments on other tokamaks. The network has coordinated research projects for many years and normally the IAEA pays travel support and shipping costs of diagnostics necessary for the project.

Benchmark test cases to build guidelines of uncertainty estimates for theoretical data: It seems to be a sensible approach to use high quality theoretical data as a benchmark for the purpose of evaluation of uncertainties. Some data may be in a position to obtain uncertainty estimates. It is

understood that comparing benchmark codes is not enough to develop the methodology for uncertainty in theoretical data. For example, physics learned from one electron system will have a missing part of physics for other systems. Nevertheless it is important to try these ideas out first and learn if and where they are feasible.

An independent check of the S-Matrix by comparing with line shape theory and scattering may be considered as additional test.

Similar to the radial-vector matrix elements being preferable over the oscillator strengths, the collisional strengths seem better than the cross-sections for comparisons, since the latter include the 1/E factor which a) introduces additional uncertainty and b) results in non-monotonic dependence on E. Obviously, interpolation of a non-monotonic sequence is prone to larger uncertainties.

Code comparison workshops have so far provided useful opportunities to understand different codes, and particularly, assumptions used in the various codes. Organization is such that code results are submitted for carefully specified problems before the workshop. Code developers discuss the results during the workshop with help of analysis tools developed to compare input and output parameters in the codes. The understanding of assumptions improves all codes involved in the workshop and a new set of problems for the next workshop is defined based on the knowledge.

Consideration of applications: Understanding data requirements of applications is the first step to develop the guidelines of uncertainty estimates. In general, there are two types of users, spectroscopists who are interested in specific transitions and modelers who need the complete data sets for collisional-radiative (CR) modelling.

- **Level of details:** Some applications require as detailed as possible data, for example, angle or energy differential cross-sections or state-resolved (electronic, vibrational or rotational) cross-sections and others require as averaged as possible such as configuration-average cross-sections and rate coefficients, or even super-configuration cross-sections and rate coefficients.
- **Resonances:** Astronomers deal with extremely low density plasmas at coronal equilibrium; much lower density than most laboratory plasmas and the resonances in cross-sections have a significant impact on the observables of interest. On the other hand, for high density laser-produced plasmas a collisional-radiative model is used to describe the non-local thermodynamic equilibrium and cross-sections used in the model should not include resonances as the resonant states (or autoionizing states) are explicitly treated as pseudo-bound states.
- **Relevant energy ranges:** At a given temperature, charge state distributions are found to be dominated by ions with ionization potentials (IP) of a few times the temperatures. Considering the Maxwellian electron distributions at the given temperature, excitation and ionization cross-sections near threshold electron energies contribute more to the rate coefficients than those at large energies in the case of ground state transitions. For metastable and excited states which have ionization energies much lower than the IP of the ion, the rate coefficients are much higher and hence the separate treatments of these states from the ground state may affect critically the simulations of observables.
- **Spatial and temporal behaviors:** A consideration of non-local transport of particles and radiation is important in determining the data needs of plasma modelling and spectroscopy.
- **Sensitivity of models:** A method to quantify the propagation of uncertainties of fundamental data to the observables of interest should be developed. A sensitivity analysis to identify most affected transitions is useful for applications.

Broader impacts of uncertainty estimates: All agreed that it is good to discuss uncertainties now. It is very difficult to write down guidelines to characterize uncertainties of theoretical data, but it is worthwhile to change the current culture in publication and the way that we do computational A&M science.

The sensible scope of guidelines will be ideas or suggestions that a referee should ask authors to describe associated uncertainties instead of just giving an error bar. The guidelines should not be too complicated and a summary of a few pages may suffice. This kind of information, a guideline is needed for referees and scientists, code producers and users. It is crucial to involve publication policies and the policy of the Physical Review A to ask uncertainty estimates for high precision atomic structure calculations is a good step towards the cultural change.

4. Recommendations

Broader topics were discussed and recommended for the future activities of IAEA A+M Data Unit. It was strongly suggested that IAEA with help of communities such as SUP@VAMDC should support follow-up meetings to address the issues in establishing the guidelines of the uncertainty estimates of theoretical data.

IAEA to encourage cultural changes: The most important aspects of uncertainty estimate and critical evaluation of theoretical data have to do with the changes of attitude in the community. It takes long time to change culture and requires a constant and steady operation. Participants recommended that the IAEA should coordinate activities to influence scientists, journal editors and national agencies in accepting the cultural changes.

- IAEA should develop and promote benchmark/test cases to develop and maintain guidelines for uncertainty estimates of theoretical data.
- IAEA should develop a collaboration network of theorists for code comparison workshops: a sustainable funding for network should be available.
- IAEA should have a coordinating role for on-going data evaluation group meetings so that they all work on the same principles and guidelines: eMOL group, SUP@VAMDC, NFRI group meeting.

Proposed meetings:

- The development project of XSAMS (XML Schema for Atoms, Molecules and Solids) coordinated by IAEA since 2003 is a good example of how the IAEA A+M Data Unit can create the momentum to change the way of exchanging data among the databases in the communities. The XSAMS project played a big role in the creation of the VAMDC (Virtual Atomic Molecular Data Centre) project supported by the EU. A development project of guidelines for uncertainty estimates and critical evaluation of theoretical data coordinated by IAEA can have a similar impact and create the momentum for the community.
- SUP@VAMDC aims to write a roadmap in 2014-2015 for collaboration and dissemination within the international atomic and molecular community, which includes the assurance of data quality. It is highly desirable to collaborate between SUP@VAMDC and IAEA as in the case of the XSAMS development.
- A smaller meeting between experimentalist and theorists on a specific topic in A&M data is highly desirable and this kind of framework is important for evaluation activities.

- Proposals on electron-atom scattering on e-Be and e-Ne and electron-molecule scattering on e-N_2 should be pursued in close collaboration with IAEA.
- IAEA-ITAMP (Institute of Theoretical Atomic and Molecular Physics, Cambridge, MA, USA) workshops are considered on uncertainty propagation in scattering calculations for electron-atom, electron-molecule and heavy particle collisions.

Appendix 1

List of Participants

Stephan Denifl (Observer), University of Innsbruck, Institute for Ion Physics and Applied Physics, Innsbruck, AUSTRIA

Friedrich Kupka (Observer), Faculty of Mathematics, Vienna University, Vienna, AUSTRIA

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Klaus Bartschat, Professor of Physics, Department of Physics and Astronomy, Drake University, Des Moines IA, UNITED STATES OF AMERICA

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Agenda

Monday, 6 May **Meeting Room: A0531**

09:30 Opening and welcome address by R. Capote Noy
Introduction of participants
Adoption of agenda by H. Chung

Session 1: Overview (Chair: B. Braams)

09:40 **B. Braams:** Meeting objectives

10:00 **R. Capote Noy:** Unified Monte Carlo: An evaluation method combining experimental and modelling uncertainties

11:00 *Coffee*

11:20 **D. Coster:** Standardising access to AMNS data within the EFDA Task Force on Integrated Tokamak Modelling

12:00 **Yu. Ralchenko:** Uncertainties and error propagation in collisional-radiative models

12:40 *Lunch*

Session 2: Uncertainty Estimates of Atomic Data (Chair: N. Mason)

14:00 **P. Jönsson:** Evaluating the accuracy of theoretical transition data

14:40 **K. Bartschat:** Electron-atom collisions: benchmark comparisons between experiment and theory

15:20 *Coffee*

15:40 **C. –Z. Dong:** Evaluation of electron impact excitation data in RDW calculation

16:20 **E. Stambulchik:** Maintaining code accuracy across versions and upgrades

19:00 *Social dinner (outside VIC)*

Tuesday, 7 May

Session 3: Uncertainty Estimates of Molecular Data (Chair: Yu. Ralchenko)

09:00 **J. Tennyson:** Errors in low-energy electron-molecule collision calculations

09:40 **V. Kokoouline:** Uncertainty assessment of theoretical data on electron-molecule collisions: Examples of H_3^+ and CH_4

10:20 *Coffee*

10:40 **G. Garcia :** Simulation tools to evaluate and estimate uncertainties of electron and positron scattering data for molecules

11:20 **N. Mason:** Evaluating uncertainties in experimental electron scattering data and exploring cross comparisons of experimental and theoretical data

12:00 *Lunch*

Session 4: Guidelines for Uncertainty Estimates of Atomic Data (Chair: K. Bartschat)

13:20 **All:** Discussions

Session 5: Guidelines for Uncertainty Estimates of Molecular Data (Chair: J. Tennyson)

14:20 **All:** Discussions

15:20 *Coffee*

Session 6: Internationally Agreed Guidelines for Uncertainty Estimates (Chair: B. Braams)

15:40 **All:** Action items – Internationally agreed guidelines for uncertainty estimates

Wednesday, 8 May (jointly with eMOL group meeting)

Session 7: Overview of IAEA Data Evaluation Activities (Chair: B. Braams)

09:30 Introduction of participants
Adoption of Agenda by H. Chung

09:40 **H. Chung:** IAEA activities on data evaluation

10:00 **N. Otsuka:** Experimental nuclear reaction data uncertainties - needs, concepts and documentation

11:00 *Coffee*

11:20 **K. Bartschat:** Guidelines for the uncertainty estimates of atomic data

11:40 **J. Tennyson:** Guidelines for the uncertainty estimates of molecular data

12:00 **All:** Action items – Internationally agreed guidelines for uncertainty estimates

13:00 *Lunch*

Session 8: Introduction to the Data Evaluation for Water Molecules (Chair: N. Mason)

14:00 **N. Mason:** Introduction to the Data Evaluation for Water Molecules

14:20 **Y. Itikawa:** Further experimental works suggested and where we are now

15:00 **All:** Discussions on guidelines of data evaluation

15:40 *Coffee*

16:00 **J. Tennyson:** Evaluation of electron-water collision data

Session 9: Conclusions and Recommendations (Chair: B. Braams)

16:30 **All:** Recommendations for IAEA

17:00 *Close of Meeting*

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