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IAEA CONSULTANTS' MEETING ON "ATOMIC DATA BASE FOR BE AND B"

Vienna, June 10-12, 1991

SUMMARY REPORT

Prepared by R.K. Janev

September 1991

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

This Summary Report contains the proceedings, conclusions and recommendations of the IAEA Consultants' Meeting on the "Atomic Data Base for Be and B" organized by the Agency's Atomic and Molecular Data Unit, and convened on June 10-12, 1991, at the IAEA Headquarters in Vienna, Austria. The existing collisional data base for these plasma impurities was thoroughly analyzed and critically evaluated at the Meeting. Many new, original results for both electron-impact and heavy-particle collisions of Be and B ions were reported at the Meeting, contributing significantly to the completion of the data base. The data analysis (including assessment of accuracies) and the recommendations of the Meeting regarding the best available collisional data for these impurities are given in two working Group Reports reproduced in this Summary Report. Analytic fits to the recommended electron-impact ionization cross sections, prepared by Dr. D.L. Moores after the meeting, are also included in the present Report.

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1. INTRODUCTION

Following a recommendation of the Subcommittee on Atomic and Molecular (A+M) Data for Fusion of the International Fusion Research Council, given at its 6th Meeting (October 1990), the IAEA A+M Data Unit convened on June 10-12, 1991, a Consultants' Meeting on "Atomic Data Base for Be and B" at the IAEA Headquarters in Vienna.

The Meeting objectives were:

1) to compile and evaluate the available data base for the Be and B plasma impurities, and
2) to identify the needs for additional data for completion of Be and B data bases.

The Be and B plasma impurities have attracted a great deal of attention in the recent fusion research, motivated by the spectacular improvement of plasma performance on JET and TEXTOR tokamaks after covering the plasma facing surfaces by Be and B, respectively.

The data analysis at the Meeting included the following categories of processes:

a) Electron-impact processes: excitation, ionization and dielectronic recombination;
b) Heavy-particle collision processes: excitation, ionization and electron capture in collisions of Be^{q+} and B^{q+} with H, H_2 and He.

A number of leading experts in the field were invited to participate in the Meeting (see Appendix 1: List of Participants). Some of the participants were asked prior to the Meeting to compile the existing data on specific categories of processes and perform a preliminary quality assessment of the data. Other participants were asked to perform extensive and highly accurate calculations on those classes of processes were the data base was known to be either defficient or inadequate. These preparatory tasks were fully accomplished by the participants, which substantially contributed to the success of the Meeting.

2. MEETING PROCEEDINGS

After adopting the Meeting Agenda (see Appendix 2), the meeting work proceeded in the following sessions:

1) Electron-impact collisions with Be- and B-ions;
2) Collisions of Be- and B-ions with H, H_2 and He;
3) Review and evaluation of existing data base and selection of best available data sets (work in parallel working group sessions);
4) Discussion of recommended data bases for Be and B.

Below we briefly describe the highlights of the presentations and discussions in the Meeting sessions.

In the session on electron-impact collision processes, K. Berrington presented a comprehensive review of the data base for excitation of Be- and B-ions in the low-energy region. The review included also data for transitions between excited states (available mostly for the H-, He- and Li-like ions). For each isoelectronic sequence an accuracy analysis of the data was presented, with recommendations of the best available data and suggestions for additional calculations for transitions where the existing data are either absent or of insufficient accuracy. Dr. Berrington presented also an extensive set of new R-matrix calculations for certain B-ions.

The electron-impact excitation data for B- and B-ions were reviewed by R.E.H. Clark. Dr. Clark also presented systematic sets of DWA and FOMBT (First Order Many-Body Theory) cross section data for the H-, He-, Li- and Be-like ions including transitions from the ground and first two excited state configurations. (Data for some transitions from BI have also been presented). The energy range of these calculation extends from the threshold to (10^2-10^4) x threshold. Dr. R.E.H. Clark also presented the data on dielectronic recombination rate coefficients for all Be- and B-ions performed by Drs. M.S. Pindzola and N.R. Badnell in the zero-electron-density limit by using a multiconfiguration, intermediate-coupling approximation for the atomic structure. The temperature range covered by these calculations is from 10^4K to 10^8K.

A comprehensive review of the existing data base for electron-impact ionization of Be^{q+} and B^{q+} ions was presented by D.L. Moores. The analysis included data generated after the 1982 UKAEA Report (CLM-R216) of K. Bell et al, as well as ionization from the $2^{1,3}S$ metastable states of He-like ions. Cross section data recommendations were suggested, accounting for the recent progress in the field, and cases were identified where improvement of the data accuracy is necessary.

In the session on heavy-particle collision, R.A. Phaneuf reviewed the data situation for excitation and ionization of H, H_2 and He by Be^{q+} and B^{q+} ions. The most accurate available data for these systems and processes have been compiled, prepared for evaluation and their accuracy discussed. A number of scaling relationships for the ionization were shown and their applicability discussed. H. Tawara presented the available data base for electron capture in collisions of Be^{q+} and B^{q+} ions with H, H_2 and He. Both total and state-selective electron capture cross section data were covered. All the collected data were represented in form of graphs, suitable for evaluation by the corresponding Working Group of the Meeting. A comprehensive set of cross section data for electron capture in collisions of Be^{2+}, Be^{3+}, Be^{4+}, B^{3+} and B^{5+} ions with H and H_2 in the energy range 0.05-100 keV/amu was reported by M. Kimura. The method employed in these calculations (MO+AO expansion with appropriate electron translational factors and a model representation of molecular potential) provides a very high accuracy of the reported results. These calculations will be extended in the near future to cover the other charge states (B^{+}, B^{4+}) and the He target. A similarly extensive set of new cross section data was reported at the Meeting by P.S. Krstic for the excitation, ionization and charge exchange processes in low-energy Be^{4+}, B^{5+} + H collisions. The adiabatic method with hidden crossings of molecular states was applied in these calculations. A large number (more than hundred) of molecular states were included in the calculations allowing cross section information for hydrogen excitation to n=2 states, hydrogen ionization from n=1 and n=2 and state-selective electron capture up to n'=6 on Be^{4+} and n'=8 on B^{5+}. A collection of total electron capture and ionization cross section data was reported by M.A. Mazing for all Be^{q+} and B^{q+} ions colliding with hydrogen atoms. The calculations were made by using the Kel'dish quasi-classical method (elaborated by D.B. Uskov and L.P. Presnyakov), which treats the electron capture and ionization processes on the same footing. Partial electron capture data generated by the same method were also reported in this presentation.

In two comprehensive talks, G. Peach discussed the physical basis and applicability of the CTMC method and first Born approximation for calculation of electron capture and ionization cross sections in collisions of incompletely stripped Be^{q+} and B^{q+} ions with one- and multi-electron targets. In the talk on CTMC, prescriptions were given for constructing the model- and pseudo-potentials needed to describe the electron-core interaction in a multi-electron system, including the Be^{q+}, B^{q+} + H, He systems ($q < Z$). It was shown that introduction of new canonical variables in the effective three-body system can reduce the number of Hamilton's equations (from 12 to 8), with random sampling of only four variables. In the talk on the Born approximation, G. Peach presented scaled ionization cross sections for both H and He targets.

During session 3, the meeting participants split into two Working Groups, to discuss separately and in detail the existing data bases for collisions of Be^{q+} and B^{q+} ions with electrons (the first group) and with H, H_2 and He (the second group). The tasks of these Working Groups were: (i) to perform a completeness analysis of the existing Be and B collisional data bases, (ii) to assess the quality of existing data bases, (iii) to select the best available data sets for use in fusion applications, and (iv) to identify the gaps and defficiencies in the data base where more accurate cross sections are required. The findings of the Working Groups are summarized in their Reports and reproduced in the next section.

3. WORKING GROUP REPORTS

3.1. Recommended Data for Electron Impact Excitation and Ionisation of Be^{q+} and B^{q+} Ions

K. Berrington, R.E.H. Clark and D.L. Moores

1. H-like ions BeIV, BV

(a) Excitation

For 1s → 2s and 1s → 2p we recommend the Callaway[1] formulas which are a fit to accurate close-coupling-pseudostate calculations for the He II isoelectronic sequence. There are no specific calculations for BeIV or BV. Resonances are not included but they only have a small effect on the collision rate. The accuracy is judged to be 5%.

For more general n → n' transitions, the Sampson and Zhang[2] formulas have been checked by Clark[3] and agree with distorted wave results to 10% except at low energies where the uncertainty may be up to 25%.

We recommend these formulas for BeIV and BV but there is a need for calculations to examine resonance effects.

(b) Ionization

We recommend the recent calculations of Moores[4] merged with the data of Peach[5] at energies above 100 times ionisation energy, for ground-state ionisation.

Accuracy is estimated to be better than 12%. For ionization from other states the Golden and Sampson[6] formulae should be used.

2. He-like ions BeIII, BIV

(a) Excitation

For BeIII Pradhan et al[7] provide good low energy data but there is some question about the high energy tail which they used to calculate their tabulated collision rates. We recommend using their low energy collision strengths and merging these with Clark's[8] new high energy data to recalculate the rates.

Either Badnell[9] or Clark[8] can be used above four times threshold energy. There is no sophisticated calculation (i.e. with resonances and channel coupling effects, which can be large, 30-40%) for BIV at low energies. Berrington is currently doing an R-matrix calculation for BIV and we recommend using these new data together with high energy data from Clark[8]. In this context "high energy" means above 5 times the excitation energy.

(b) Ionization

For ground-state ionization of BIV there is good agreement between a crossed beam measurement[10], Distorted-wave exchange calculations[11] and a semi-empirical formula. Bell et al[26] recommend a cross section based on these data. We recommend a cross section based on these data merged with the results of Peach above 100 times threshold. BeIII data should be obtained by scaling the recommended BIV results in the ratio of the ionisation energies squared. (Accuracy 10%).

For ionization of metastable states (1s2s $^{1,3}S$) Coulomb-Born-Exchange calculations have been performed by Attaourti et al[13] for the isoelectronic C,N,O ions. The O results differ by 25% from a calculation by Moores and Tully[14] using COBION[15]. We recommend scaling the CV results of Attaourti et al. Accuracy should be ~ 30%.

3. Li-like ions BeII, BIII

(a) Excitation

For BeII we recommend the theoretical cross sections of Mitroy and Norcross[16] and Parpia et al[17] despite the disagreement with experiment. For BIII we recommend the new R-matrix calculation for low energy and the new Clark[8] calculation at high energy: we aim to produce rate coefficients based on merging these data sets. We do not recommend the Cochrane and McWhirter $\bar{g}$ fits because of their omission of resonances.

(b) Ionization

For BeII we recommend the experimental data of Falk and Dunn[28], merged with Peach's[5] high energy result. The calculation by Younger[11] is a factor of 1.26 below experiment.

For BIII we recommend the experimental data of Crandall et al[19] at low energies merged with the high energy calculation of Peach[5]. In this case the Younger calculation is 10% higher than experiment. Accuracy of both recommendations is about 30%, or so. We note that autoionisation, though non-negligible for higher members of this isoelectronic sequence, is small for BeII and BIII.

4. Be-like ions BeI, BII

(a) Excitation

For neutral BeI we recommend the new R-matrix calculation[10] at low energies and Clark[8] at high energies: similarly for BII we recommend the new R-matrix calculation in progress[21] at low energy and Clark[8] at high energies. K. Berrington will merge these two data sets. Accuracy ~ 10%. For metastable states the recommendations are the same.

(b) Ionization

For the Be-like C, N, O Jakubowicz and Moores[15] agree well with Younger[22]. Experimental data are in fair agreement but are affected by metastable ions. For BeI and BeII we recommend scaling the CIII calculations, though more work is required here. Accuracy is judged to be 25% - 30%.

For ionization out of the metastable $1s^22s2p\ ^3P$ state we recommend scaling Younger's[22] results for CIII.

5. Boron-like ions - B I

(a) Excitation

We recommend new R-matrix calculation[23] at low energy and Clark at high energies (above 5 times threshold). The calculations differ by small or large (factor of 2) amounts depending on the transition. Dr. K. Berrington will check all results. Given the disagreement with experiment of factor of 3-5, the accuracy of the recommended data may be low.

(b) Ionization

For isoelectronic ions CII and NIII good agreement is found between experiment[24] and theory[25]. We recommend scaling the CII results of Moores[25]. We note that for this sequence any calculation should include both

BI $1s^22s^22p \rightarrow$ BII $1s^2\ 2s^2$ 1S

$\rightarrow$ BII $1s^2$ 2s2P (1,3P)

Remark. All recommended ionisation cross sections in this report are intended to update and supersede the recommendations in the report by Bell et al[26] (1982).

Dielectronic Recombination. We recommend the rate coefficients for this process calculated for this meeting by Pindzola and Badnell[27] for the Be and B sequences in a zero-density limit.

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3.2. Collisions of Be^{q+} and B^{q+} Ions with H, H_2 and He

R.A. Phaneuf (Chairman), R.K. Janev, H. Tawara,
M. Kimura, P.S. Krstic, G. Peach and M.A. Mazing

1. Introduction

From the perspective of applications in fusion-energy research, the relevant heavy-particle collision processes involving Be^{q+} and B^{q+} ions are charge exchange, excitation and ionization in collisions with H, H_2 and He. The collision energy range considered is 10 - 10^6 eV per nucleon. The lower energies are relevant to modelling and diagnostics of the edge or scrape-off plasma, while the higher energies are important for diagnostics and energy-deposition in the plasma using energetic neutral beams of H or He. Collisions between Be and B impurity atoms and ions themselves are considered to occur too infrequently to play a significant role in such plasma devices. Such collisions are most often studied experimentally, by passing energetic ion beams through gaseous targets. Therefore, in the following discussion, Be or B ions will be referred to as the projectile and H, H_2 or He as the target.

The availability of data for charge exchange, excitation and ionization in collisions of Be^{q+} and B^{q+} ions with H, H_2 and He are summarized in Table 1, where "E" refers to experimental data and "T" to theoretical data. For excitation and ionization collisions, the subscripts "t" and "p" refer to target and projectile, respectively. For electron-capture collisions involving He or H_2, the subscripts "1" and "2" refer to the transfer of one or two electrons, respectively. New theoretical data which were presented at this meeting are also included in Table 1.

Semiempirical scaling relationships for heavy-particle collisions are often applied for higher-Z impurities. For example, such a formula for charge-exchange collisions [1] may be used quite reliably for impurities such as Fe or Ni in ionization stages higher than 5. This scaling formula is, however, generally not applicable to low-Z impurities such as Be and B, for which each collision system must be considered individually. One exception is the ionization of H, H_2 or He by Be^{q+} or B^{q+} ions at energies above 20 keV/amu, where scaling formulae based on the Bethe approximation [2,3] may be used with some reliability.

2. Charge Exchange

Charge-exchange (electron-capture) collisions between impurity ions and neutral H, H_2 and He are by far the most important heavy-particle processes occurring in fusion plasmas because of their relatively large cross sections at lower kinetic energies. This results from the exothermicity of such reactions involving multiply charged ions. At near-thermal energies such as those prevailing in the edge plasma, cross sections for charge exchange are very sensitive to the degree of exothermicity of a particular channel. Those which have appreciable cross sections generally leave the ion in an excited state and are exothermic by several electron volts, depending on the initial charge of the ion. Photon emissions from excited impurity ions are important for diagnostics involving the use of injected neutral beams of H or He.

The data for total and partial cross sections for electron transfer collisions of Be^{q+} and B^{q+} ions with H, H_2 and He have been recently compiled by Tawara [4] in preparation for this meeting. New coupled-state calculations were presented by Kimura [5] for Be^{q+} + H, Be^{q+} + H_2 (q=2,3,4) and B^{q+} + H, B^{q+} + H_2 (q=3,5). These are based on molecular orbitals (MO) with electron-translation factors at low energies, and the extended atomic-orbital method (AO+) at higher energies. New calculations for Be^{4+} + H and B^{5+} + H based on the "adiabatic hidden crossings" or "superpromotion" model were also presented by Krstic [6]. This method gives reliable partial cross sections for capture into a particular n shell down to 0.3 keV/amu. An intercomparison of the various theoretical methods that have been applied to the electron-capture process shows that the predicted cross sections for capture into specific states are very sensitive to the method applied, whereas the total cross sections are rather insensitive.

Be^{+} + H, Be^{+} + He:

Neither experimental nor theoretical cross-section data are available for these reactions. Since they are endothermic in all channels, the cross sections are expected to be very small for E < 1keV/amu.

Be^{2+} + H:

No experimental data are available. Theoretical perturbed-stationary-state (PSS) calculations of Wetmore et al [7] agree within 10% with the new coupled-state calculations (AO-MO) of Kimura [5], which include electron translation factors and a larger basis. The latter are recommended for the total cross section, and for capture to the 2s and 2p states. Data are needed at energies above 10 keV/amu.

Be^{3+} + H:

No experimental data are available. Molecular coupled-state calculations employing electron translation factors have been performed by Shimakura [8] for capture to the 2s, 2p, 3s, 3p, and 3d states, and for the total capture cross section. The accuracy of the total cross section is estimated to be 30-50% at energies above 25 keV/amu, and 20-30% at lower energies. The n=2 partial cross sections (dominant channels) are estimated to be accurate to 20-30% and the n=3 cross sections to 30-50%.

Be^{4+} + H:

No experimental data are available. Total and partial cross- section calculations have been performed by Fritsch and Lin [9] (AO) and by Kimura [5] (AO-MO). New low-energy calculations were presented by Krstic [6] based on the superpromotion model. In the 0.1-5 keV/amu energy range, all three calculations agree to within 5% for the total cross section, as well as for state-selective capture to the dominant channels (n=3). For the non-dominant (n=4) channels, the agreement is less satisfactory. Unitarized- distorted-wave (UDWA) calculations of Ryufuku [10] are available at energies above 10 keV/amu. The accuracy of the total and n=3 cross sections is estimated to be 10% at energies in the 0.1-5 keV/amu range, and 20% at higher energies. The accuracy of the n=4 and n=5 cross sections is estimated to be 20-50%. New low-energy total and partial cross-section data for capture from H^{*}(n=2) were presented by Krstic [6]. The accuracy of these data is unknown at the present time.

B^{+} + H:

Experimental total cross-section measurements using the ion-beam -gas-target method have been made by Goffe et al [11] at energies between 10 and 150 keV/amu. The estimated accuracy is 10-20%. Since all channels are endothermic, the cross section is expected to decrease at lower energies. No state-selective or theoretical data have been reported.

B^{2+} + H:
Total cross-section measurements based on the ion-beam - gas-target method have been reported by Goffe et al [11], McCullough et al [12], Crandall et al [13] and by Gardner et al [14]. These data are consistent and cover the energy range from 2-200 keV/amu. No state-selective or theoretical data are available. The estimated accuracy is 10%, except at the lowest and highest energies where it is estimated to be 20%.

B^{3+} + H:
Experimental total cross-section data have been obtained over the energy range 1-200 keV/amu using the ion-beam - gas-target method by Goffe et al [11], McCullough et al [12], Crandall et al [13] and Gardner et al [14]. Molecular-orbital coupled-state calculations by Olson et al [15] and by Wetmore et al [16] agree well with the experimental data and extend down in energy to 0.3 keV/amu. The uncertainty of the data is estimated to be 20-30% in the energy range 0.3-2 keV/amu and 10-15% from 2-200 keV/amu. Partial cross sections have been calculated Kimura [5] for capture to the 2s and 2p states, with estimated accuracies comparable to those of the total cross section for 2p and somewhat larger for the 2s state.

B^{4+} + H:
Experimental data based on the ion-beam - gas-target method are available for the total cross section at energies between 2 and 200 keV/amu from Goffe et al [11], Crandall [13] and Gardner et al [14]. Calculations by Olson and Salop [17] based on the classical trajectory Monte Carlo (CTMC) method in the energy range 10-150 keV/amu are in agreement with the experimental data. The estimated accuracy of the total cross section is 10-20%. No state-selective or low-energy total cross-section data are available.

B^{5+} + H:
Both total and state-selective cross-section data are available for this reaction. Experimental total cross-section data based on the ion-beam - gas-target method have been reported by Goffe et al [11], Crandall [13] and Bendahman et al [18] over the energy range 0.2-200 keV/amu, and are in good agreement with each other. Theoretical total cross-section data of Ryufuku [10] based on the UDWA approximation, Fritsch and Lin [9] based on the AO coupled-states method, and Krstic [6] using the superpromotion model agree well with experiment. The accuracy of the total cross section is estimated to be 10% for energies in the range 0.2-200 keV/amu. Total cross-section data are needed at energies below 200 eV/amu.
In the energy ranges where they overlap, partial cross-section calculations by Fritsch and Lin [9], Ryufuku [10] and Kimura [5] agree within estimated accuracies of 10% for n=4, 20% for n=3, and 30% for n=5. For the non-dominant channels (n=2,6,7,8), the cross sections are small, and only the UDWA calculation of Ryufuku [10] at higher energies and the superpromotion model calculation of Krstic [6] at lower energies are available. Since their energy ranges do not overlap, the uncertainty is difficult to assess for these channels. New total and partial cross-section calculations were also reported by Krstic [6] for capture from H*(n=2). The accuracy of these data is unknown at the present time.

$Be^+ + H_2$:

The only reported data are single-capture measurements by Sherwin [18] in the 1-3 keV/amu energy range. Their is difficult to assess.

$Be^{2+} + H_2$, $Be^{3+} + H_2$, $Be^{4+} + H_2$:
Experimental single-capture cross-section measurements of Takagi et al [19] based on the ion-beam - gas-target method are available in the 0.1-1 keV/amu energy range. Total cross sections have also been calculated for these reactions in the 0.1-9 keV/amu energy range by Kimura [5], and partial cross-section calculations are in progress. The accuracy of the total cross-section data is estimated to be 20%. Additional data would be useful at energies above 10 keV/amu.

$B^{+} + H_2$:
The only available data are single-capture cross-section measurements reported by Goffe et al [11] at energies between 10 and 150 keV/amu, to which the accuracy is estimated to be 10-20%. Additional data at lower energies would be useful.

$B^{2+} + H_2$:
Experimental data based on the ion-beam - gas-target method are available for the total single-capture cross section at energies between 0.3 and 200 keV/amu from Goffe et al [11], Crandall [13], McCullough et al [12] and by Gardner et al [14]. The data of Gardner et al appear to be low by 50%. An estimated accuracy of 20-25% is assigned to the data for this reaction. Since the cross section is unusually large for a doubly charged ion, and increases with decreasing energy, additional experimental and/or theoretical data at lower energies would be useful.

$B^{3+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11], Crandall [13], and by Gardner et al [14] over the energy range 1-200 keV/amu. New theoretical data were also presented by Kimura [5] in the energy range 0.1-10 keV/amu, which agree well with the measurements. The accuracy of the data for this reaction is estimated to be 20%. Double-capture measurements have also been reported by Gardner et al in the 1-5 keV/amu energy range. The double-capture cross section is unusually large relative to single capture in this case.

$B^{4+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11], Crandall [13], and by Gardner et al [14] over the energy range 2-200 keV/amu. The accuracy of the data for this reaction is estimated to be 20%. Double-capture measurements have also been reported by Gardner et al in the 2-5 keV/amu energy range. The double-capture cross section is negligibly small relative to single capture in this case.

$B^{5+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11] and by Crandall [13] over the energy range 5-200 keV/amu. New theoretical data were also presented by Kimura [5] in the energy range 0.1-10 keV/amu, which are consistent with these measurements. The accuracy of the data for this reaction is estimated to be 15-20%.

$Be^{+} + He$:
The only data for these reactions are angular differential total cross-section measurements by Ostgaard Olsen et al [19] in the 200-500 eV/amu energy range, and by Gay et al [20] at 56.25 keV.

Be^{2+} + He:
No experimental or theoretical cross-section data are available for this reaction.

Be^{3+} + He:
Theoretical Landau-Zener calculations have been reported by Boyd and Moiseiwitsch [21] for capture into the 2^3S, 2^3P and 2^1P states in the energy range 0.1-1000 eV/amu. No experimental data are available.

Be^{4+} + He:
Only theoretical data are available for this reaction. Total single-capture cross sections have been calculated by Olson [22] using the CTMC method, and by Suzuki et al [23] using the exponential distorted-wave approximation. These calculations are consistent with one another at energies where they overlap and cover the range 1-400 keV/amu. The accuracy is estimated to be 15-20%. Partial cross sections for single and double capture have also been reported by Martin et al [24] in the 0.25-20 keV/amu energy region.

B^{+} + He:
The only data are total cross-section measurements by Nikolaev et al [25] at energies in the 10-100 keV/amu range. Data are needed over a wider energy range.

B^{2+} + He:
Experimental single-capture data have been reported by Sherwin [18], Gardner et al [14], and by Nikolaev et al [25], covering the energy range 0.5-400 keV/amu. There is a large (order-of-magnitude) discrepancy between the data of Sherwin and those of Gardner et al at energies below 5 keV/amu. Above 40 keV/amu, the uncertainty is estimated to be 20%. There is a gap in the data between 4 and 40 keV/amu. Additional data are required at energies below 40 keV/amu.

B^{3+} + He:
Experimental total single-capture cross-section data have been reported over the energy range .04-400 keV/amu by Crandall [13], Gardner et al [14], Nikolaev et al [25], Zwalley and Cable [26] and Iwai et al [27]. Theoretical coupled-state calculations have also been reported by Shipsey et al [28] over the energy range .03-6 keV/amu. With the exception of the measurements of Gardner et al [14], these data are very consistent with one another, and an accuracy of 10-20% is estimated. Shipsey et al also reported partial cross section calculations for capture into the 2s and 2p states, whose ratio is confirmed by Matsumoto et al [29]. An accuracy of 10-20% is estimated for these partial cross sections as well. Double-capture cross-section measurements reported by Crandall [13] show an unusual energy dependence. The cross section is small relative to single capture, and likely unimportant for applications.

B^{4+} + He:
Experimental data have been reported for the total single-capture cross section by Gardner et al [14], Nikolaev et al [25] and by Iwai et al [27]. These data span the energy range 0.5-800 keV/amu, but a significant gap exists between 8 and 200 keV/amu, where further data are needed. No theoretical or partial cross-section data are available. An accuracy of 20-30% is estimated in the energy ranges 0.5-8 keV/amu, and 200-800 keV/amu.

B^{5+} + He:

Experimental data have been reported for the total single-capture cross section by by Iwai et al [27], Nikolaev et al [25] and Guffey et al [30]. Theoretical data based on the CTMC method by Olson [22] tie in well with the measurements. While these data span the energy range 0.5-800 keV/amu, a significant gap exists between 2 and 100 keV/amu, where further experimental and/or theoretical data are needed. The accuracy is estimated to be 20% at energies below 2 keV/amu and above 100 keV/amu.

4. Excitation

Data on excitation of H, H_2 and He (targets) by multicharged (projectile) ion impact are extremely limited. A small number of theoretical calculations have been reported for excitation of ground-state hydrogen atoms by bare Be and B ions; these are outlined below. No such data exist for partially-stripped Be or B ions, although a charge and energy scaling relation has been developed for multicharged ion impact on He. No data exist for excitation in collisions of Be^{q+} or B^{q+} ions with H_2. Dissociative excitation of H_2 could play an important role in fusion plasmas. Excitation of fine-structure ($\Delta n=0$) transitions in $H^+ + Be^{q+}$ and $H^+ + B^{q+}$ collisions can have relatively large cross sections and play an important role for partially stripped Be and B impurities.

$Be^{4+} + H(1s)$:
The two-state dipole-close-coupling approximation (DCC) has been applied by Janev and Presnyakov [31] to n=1 -> n=2,3,4 excitation of H by Be^{4+} ion impact at energies ranging from 2-100 keV/amu. Fritsch [32] has recently performed extended atomic-orbital close-coupling (AO+) calculations for n=1 -> n=2 excitation of H by Be^{4+} impact at energies ranging from 6 to 50 keV/amu. New theoretical data in the 1-30 keV/amu energy range based on the superpromotion model were also presented by Krstic [6]. The latter results are recommended with an estimated accuracy of a factor of 2. These data are consistent within a factor of 3 or better with the AO+ calculations, and to within an order of magnitude with the DCC calculation. Data are needed for for excitation from n=1 -> n=3,4 and n=2 -> n=3,4.

$B^{5+} + H(1s)$:
The unitarized distorted-wave approximation (UDWA) has been applied by Ryufuku [33] to the total excitation cross section (summed over excitations to all n). New theoretical data in the 1-30 keV/amu energy range based on the superpromotion model were also presented by Krstic [6] for n=1 -> n=2 excitation. These latter data are recommended with an estimated factor-of-two accuracy. Again, data are needed for for excitation from n=1 -> n=3,4 and n=2 -> n=3,4.

$Be^{q+} + He$, $B^{q+} + He$:
A charge-scaling relation has been derived from experimental data by Reyman et al [34] for excitation of a He target by a variety of multicharged ion projectiles with charges ranging from 6 to 44 and energies from 120 to 1000 keV/amu. This scaling relation is estimated to be reliable in predicting the He excitation cross sections to within a factor of 2 at 100 keV/amu, and better at higher energies. Experimental and theoretical cross-section data for projectile 2s-2p excitation of Be^+ in collisions with He have also been reported by Andersen et al [35] and Nielsen et al [36] respectively, over the energy range .05-40 keV/amu. Such data may be useful for diagnostic purposes.

5. Ionization

The only experimental data for ionization of H, H_2 or He by Be^{q+} or B^{q+} impact are measurements by Haugen et al [37] for single ionization of He by B^{3+}, B^{4+} and B^{5+} at energies ranging from 190 to 2310 keV/amu. These have an estimated accuracy of 20%. Andersen [38] has also reported double ionization cross sections for these same reactants and energy range, and has investigated their scalings with ionic charge.

The CTMC method has been employed by Olson [39] and by Pfeifer and Olson [40] to Be^{4+} + He and B^{5+} + He collisions at energies in the 100-500 keV/amu range. New theoretical data were also presented by Krstic [6] based on the superpromotion model for ionization of H(n=1) and H(n=2) by Be^{4+} and B^{5+} impact at energies ranging from 0.4-30 keV/amu. The accuracy of these data are difficult to assess. Nikolaev et al [41] have also reported calculations based on the Bethe-Born approximation for Be^{2+} + H and Be^{2+} + He collisions at energies ranging from 6 keV/amu to 25 Mev/amu. Goffe et al [42] have also reported projectile ionization or stripping cross-section measurements for B^{+} and B^{2+} colliding with H and H_2 at energies in the 10-200 keV/amu range.

In general, for ionization of H, H_2 or He by Be^{q+} or B^{q+} ions at energies above 50 keV/amu, where ionization dominates electron capture, scaling formulae of Gillespie based on the Bethe approximation [2,3] may be used to predict the target single- ionization cross section with an estimated accuracy of 10-30%. At lower energies, where the ionization cross sections become very small, and the capture process dominates, theoretical methods and scaling laws are generally unreliable. Tabata et al [43] have modified the Gillespie scaling relations to better represent what low-energy data are presently available, but experimental data are needed for all these collision systems at energies $E/q < 50$ keV/amu to establish the low-energy behavior of the ionization cross sections. These and additional data at higher energies are needed to provide important tests of such scaling relations.

6. Two-Electron Processes

For collisions involving H_2 and He, two-electron collision processes must also be considered. Examples are double electron capture, transfer-ionization at lower energies, and double ionization at higher energies. Cross sections for these processes are generally an order of magnitude smaller than those for single-electron processes. Relatively less attention has been devoted to such processes.

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Table 1. Availability of Data for Collisions of Be^{q+} and B^{q+} Ions with H, H_2 and He

Target (t)	H					H_2					He				
Projectile (p)	TC	SSC	ANG	EX	ION	TC	SSC	ANG	EX	ION	TC	SSC	ANG	EX	ION
Be^{+}						E_1							T_1 E_1	T_p E_p	
Be^{2+}	T	T			T_t	T_1 E_1	T_1								T_t
Be^{3+}	T	T				E_1	T_1					T_1			
Be^{4+}	T	T		T_t	T_t	E_1	T_1				T_1				T_t
B^{+}	E				E_p	E_1					E_1				
B^{2+}	E				E_p	E_1				E_p	E_1 E_2				
B^{3+}	T E	T				E_1 E_2	T_1				T_1 E_1 E_2	T_1 E_1			E_t
B^{4+}	T E					E_1 E_2					E_1				E_t
B^{5+}	T E	T	T_t	T_t	T_t	T_1 E_1					T_1 E_1 E_2				T_t E_t

TC = total electron capture (summed over final states)
SSC = state-selective electron capture
ANG = data on angular distribution of products of electron-capture collisions
EX = excitation of projectile (p) or target (t)
ION = ionization of projectile (p) or target (t)
E = experimental data
T = theoretical data
1,2 = single or double electron capture

4. MEETING CONCLUSIONS AND RECOMMENDATIONS

In summarizing its work on the collisional data base for Be^{q+} and B^{q+} ions, the Meeting at its last session draw the following conclusions:

1) The data base for electron-impact processes for Be^{q+} and B^{q+} ions is fairly complete, as far as the processes involving the ground state are concerned. With the exception of H-like ions, where appropriate scaling relationships both for excitation and ionization exist, and the metastable states 1s2s $^{1,3}S$ of He-like ions, the data for processes involving transitions between and from excited states are rather sparce. For the ionization of BeI and BII the data are of inadequate quality and additional work is required. This is also true for the excitation of BI where discrepancies of a factor of two exist for some transitions.

2) For the collisions of Be^{q+} and B^{q+} ions with H, H_2 and He targets, only the charge transfer data base (mostly total cross sections) is in form which can partially meet the basic fusion needs. Even for this process more data are needed in the intermediate and high energy regions, particularly for the low charge states and for state-selective electron capture. With the exception of Be^{4+}, B^{5+} +H systems, the excitation processes in Be^{q+}, B^{q+} collisions with H, H_2 and He are very poorly documented, despite the fact that the cross sections may have significant values in the energy region of interest (up to several tens of keVs). Generation of cross section information on these processes is a highly urgent task. The data base for ionization in these collision systems is also incomplete, particularly for the lower charge states. For the higher charge states and the fully stripped ions, ionization data for H and He exist from several methods, but their disagreement is still large. For $q \gtrsim 2$ the Gillespie scaling for ionization of H, H_2 and He may be adopted. For the two-electron targets (H_2, He), some two-electron processes (transfer ionization, double electron capture) may have large cross sections for certain ion charge states and need to be investigated.

3) The meeting itself has provided a substantial contribution to the improvement of the Be^{q+} and B^{q+} collisional data bases. The major contributions have been in the following areas:

   - low-energy electron-impact excitation (R-matrix calculations);
   - intermediate- and high-energy excitation (a complete DWA data base);
   - dielectronic recombination rate coefficients for all Be^{q+} and B^{q+} ions;
   - high-energy ionization cross sections (CBX and Born);
   - low-energy electron capture involving H and H_2 and incompletely and fully stripped ions (MO+AO close coupling; adiabatic hidden crossings method);
   - excitation and ionization of H(n=1,2) by Be^{4+} and B^{5+} (adiabatic hidden crossings method);
   - intermediate- and high-energy electron capture and ionization (the quasi-classical Keldish and Born methods)

4) The sets of cross sections selected by the Meeting participants form a solid basis for a recommended data base for fusion applications. The most important gaps identified in the data base could be filled-in by performing additional calculations either by Meeting participants (see sections 3.1. and 3.2.) or in collaboration with some other groups.

The Meeting participants have recommended to the IAEA Atomic and Molecular Unit to:

1) Carry on the necessary technical work for implementation of the data assessments performed by the Working Groups and their data recommendations into an integrated collisional data base for Be^{q+} and B^{q+} ions;

2) To collect the data which will be additionally generated by Meeting participants and other groups after the meeting and introduce them into the integrated data base after their prior evaluation by selected experts.

3) Publish the Working Group Reports and other presentations at the Meeting (if the authors choose to do so) in the Supplement to Nuclear Fusion "Atomic and Plasma-Material Interaction Data for Fusion" vol. 3 (to appear late in 1992 or at the beginning of 1993).

5. POST-MEETING ACTIVITIES

1) Dr. D.L. Moores has merged the low- and intermediate-energy data on electron-impact ionization with the high-energy (Born) data generated by Dr. G. Peach and fitted the resulting cross sections to appropriate analytic expressions containing a limited number of parameters. The expressions and the values of the fitting parameters are given in Appendix 3 (prepared by Dr. Moores).

2) Dr. P.S. Krstic has visited the IAEA after the Meeting and started the collection of all the data recommended by the Meeting and their introduction into the Agency ALADDIN data base. In the course of this work new sets of R-matrix electron impact data and first Born ion-impact ionization data have been received from Dr. K. Berrington and Dr. G. Peach, respectively. The activity on the recommended data collection and their ALADDIN formatting will be continued by Dr. Krstic in Belgrade until the completion of the data base.

Appendix 1

IAEA Consultants' Meeting on
"Atomic Data Base for Be and B"

10 - 12 June 1991, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

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Appendix 2

IAEA Consultants' Meeting on
"Atomic Data Base for Be and B"

10 - 12 June 1991, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

MONDAY, June 10

09:30 - 09:45 - Opening (Room: C07-VI)
- Adoption of Agenda

Session 1: Electron-impact collision processes with Be and B ions

Chairman: D.L. Moores

09:45 - 10:30 K. Berrington: Electron-impact excitation of Be^{q+} and B^{q+} ions: An evaluation of low energy data

10:30 - 11:15 R.E.H. Clark: Electron-impact excitation cross sections for Beryllium and Boron

11:15 - 11:30 Coffee break

11:30 - 12:15 M.S. Pindzola: Dielectronic recombination rate coefficients for ions of the Be and B isonuclear sequence (presented by R.E.H. Clark)

12:15 - 14:00 Lunch

Session 1: Cont'd

Chairman: R.E.H. Clark

14:00 - 14:45 D.L. Moores: Electron impact ionization cross sections for Be and B ions

14:45 - 15:15 General Discussion on the completeness and quality of electron-impact collision database for Be and B

15:15 - 15:30 Coffee break

Session 2: Collisions of Be^{q+} and B^{q+} ions with H, H_2 and He

15:30 - 16:15 R.A. Phaneuf: Database assessment for excitation, and ionization in collisions of Be^{q+} with H, H_2 and He

16:15 - 17:00 H. Tawara: Total and partial electron capture data for collisions of Be^{q+} and B^{q+} ions with H, H_2 and He

17:00 - 17:45 M. Kimura: Theoretical determination of total and partial electron capture cross sections in collisions of $Be^{(2-4)+}$ and $B^{3,5+}$ with H and H_2

TUESDAY, June 11

Session 2: (Cont'd)

Chairman: R.A. Phaneuf

09:00 - 09:45	P.S. Krstic:	Excitation, ionization and electron capture cross sections in low-energy collions of Be^{4+} and B^{5+} with H(n=1,2)
09:45 - 10:30	G. Peach:	Classical collisions between atoms and atomic ions
10:30 - 10:45	Coffee break	
10:45 - 11:30	M.A. Mazing:	Charge exchange in Be^{q+}, B^{q+} +H collisions
11:30 - 12:15	G. Peach:	Application of the Born approximation to the ionization of atoms and atomic ions
12:15 - 14:00	Lunch	

Session 3: Review and evaluation of existing database and selection of best available data sets

14:00 - 15:45 Work in parallel sessions:

A) Working Group on electron-impact processes (Room: C-0743)

B) Working Group on Be^{q+}, B^{q+} - H, H_2 He (Room: C-07VI) collisions

Completeness analysis of existing Be and B databases and accuracy assessment

15:45 - 16:00 Coffee break

16:00 - 18:00 Work in parallel sessions:

Selection of best available data sets and establishment of recommended databases

WEDNESDAY, June 12

Session 3: Cont'd

09:00 - 10:30 Work in parallel sessions:

Selection of best available data sets and establishment of recommended datbases

10:30 - 10:45 Coffee_break

10:45 - 12:15 Preparation of Working Group Reports on recommended databases for Be and B

12:15 - 14:00 Lunch

14:00 - 15:45 Preparation of Working Group Reports on recommended databases for Be and B

15:45 - 16:00 Coffee_break

Session 4: Discussion of recommended databases for Be and B (Room: C-VI)

Chairman: R.K. Janev

16:00 - 18:00
- Discussion of data evaluation and selection results
- Discussion of Working Groups Reports

18:00 - Adjourn of the Meeting

Appendix 3

Analytic Fits of the Recommended Electron Impact Ionization Cross Sections for Be and B Ions and Atoms

Prepared by

D.L. Moores
Department of Physics and Astronomy
University College London

For the H-like ions B V and Be IV the recommended data are a merger of the calculations by Moores[1] below X=5 with those of Peach[2] above X=150.

For the He-like ion B IV, for ground-state ionisation, the data recommended by Bell et al[3] below X=5 have been merged with the calculations of Peach[2] above X=150. The Be III data were obtained by scaling the B IV results in the ratio of the ionization energies squared.

For the ionisation of the metastable states 1s2s ^{1,3}S the low energy data of Attaourti et al[4] have been similarly scaled and merged with the Burgess and Chidichimo[8] formula above X=150. The results are shown in Table 3.

For the Li-like ions B III and Be II the calculations of Younger[5] at low energies have been merged with those of Peach[2] above X=150.

For the Be-like ions B II and B I the prescription given by Younger[6] cannot be extrapolated below Z=6. Instead, Younger's C III results have been scaled. This applies to ionisation from both the $2s^2$ and 2s2p ^{3}P initial states.

The above cross sections have been fitted in each case to the formula:

$$XQ(X) = AlnX + \frac{C_0}{X}lnX + \sum_{i=1}^{N} C_i(1 - \frac{1}{X})^i \tag{1}$$

where Q(X) is the cross section in cm^2 and X is the incident energy divided by I, the ionisation energy. The coefficients A and C_i are given in Tables 1 and 3.

For B I we recommend the scaled C II calculations of Moores[7]. In order to avoid unnecesary work the cross sections have been parametrized in the same form as in that paper

$$XQ(X) = AlnX + \sum_{i=0}^{N} \frac{\alpha_i}{X^i} \tag{2}$$

instead of the form (1). Coefficients A and α_i are given in Table 2.

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Table 1

SPECIES	I(eV)	A	Co	C1	C2	C3	C4	C5	REMARKS	ACCURACY
BV	340.22	1.5275-19	–	2.1678-19	–4.9163–19	2.2145-18	–2.8808–18	1.6432–18		12%
BeIV	217.71	3.7027–19	–	4.9003–19	–1.0595–18	4.8960–18	–6.2381–18	3.6395–18		12%
BIV	259.37	6.8418–19	–	–9.7357–20	4.0760–20	5.7328–18	–8.4384–18	4.9724–18		12%
BeIII	153.89	1.9435–18	–	–2.7656–19	1.1579–19	1.6285–17	–2.3971–17	1.4125–17		12%
BIII	37.93	8.4971–18	–	9.6681–18	1.5560–17	–1.0150–17	–2.1487–17	5.3676–17		30%
BeII	18.21	3.3039–17	–	9.0589–17	–8.8416–17	3.4311–16	–4.1859–16	2.6885–16		30%
BII	25.15	3.9682–17	–3.0639–16	3.6726–16	–1.1683–16				(a)	30%
	20.53	4.2350–17	–2.7128–16	3.5826–16	–1.1887–17				(b)	40%
	26.52	1.9621–17	–1.2940–16	1.5677–16	–5.1186–17				(c)	40%
BeI	9.32	2.8896–16	–2.2311–15	2.6743–15	–8.5077–16				(a)	30%
	6.60	4.0978–16	–2.6249–15	3.4665–15	–1.1501–15				(b)	40%
	13.28	7.8250–17	–5.1599–16	6.2520–16	–2.0413–16				(c)	40%

(a) $2s^2\ ^1S \rightarrow 2s\ ^2S$ **(b)** $2s2p\ ^3P \rightarrow 2s\ ^2S$

(c) $2s2p\ ^3P \rightarrow 2p\ ^2P$

Table 2

SPECIES	I(eV)	A	αo	α1	α2	α3	α4	α5	REMARKS	ACCURACY
BI	8.30.	4.2820–16	1.1049–15	–2.6816–15	8.3591–16	3.4155–15	4.1763–15	1.5015–16	(a)	Factor of 2
	12.93	3.4867–16	1.3375–16	6.7887–16	–8.4807–16	–9.3416–16	2.5971–15	–1.3600–15	(b)	Factor of 2
	17.40.	6.4165–17	2.4614–17	1.0032–16	–1.5607–16	–1.7191–16	4.7795–16	–2.5028–16	(c)	Factor of 2

(a) $2s^2 2p\ ^2P \rightarrow 2s^2\ ^1S$

(b) $2s^2 2p\ ^2P \rightarrow 2s2p\ ^3P$

(c) $2s^2 2p\ ^2P \rightarrow 2s2p\ ^1P$

Parameters of formula (2) for electron impact ionisation of BI

Table 3

SPECIES	STATE	I(eV)	A	Co	C1	C2	ACCURACY
BIV	21S	56.4	1.4870–17	3.0520–17	–3.1517–17	1.4244–17	30%
BeIII	21S	32.0.	4.6194–17	9.4808–17	9.7908–17	4.4244–17	30%
BIV	23S	60.8	9.7412–18	–1.6292–17	1.4620–17	–1.2500–17	30%
BeIII	23S	35.3	2.8908–17	–4.8347–17	4.3384–17	–3.7093–17	30%

Electron Impact Ionisation from metastable states 2^1S, 2^3S of He-like ions