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IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions"

2-3 September 1996, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared by
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J.A. Stephens and R.K. Janev

April, 1997

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

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Abstract

Brief proceedings and a summary of the conclusions of the IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions", held on 2-3 September 1996 in the IAEA Headquarters in Vienna, Austria, are provided. The main emphasis in the database analysis is given to electron impact excitation of neutral and singly ionized beryllium for which new theoretical data became recently available. Also, the presently unsatisfactory situation for neutral boron is addressed and a course of action is suggested, in a timeframe conformal with the needs of present fusion research.

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April, 1997

TABLE OF CONTENTS

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1 Introduction

The IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions" was held on 2-3 September 1996 at the IAEA Headquarters in Vienna, Austria. The objectives of the meeting were to review and critically assess the existing cross section information on electron-impact excitation and ionization of Be and B atoms and ions, particularly that generated since the similar IAEA meeting held in 1992. The meeting was attended by two external consultants (Prof. K. Bartschat and Dr. K. Berrington) and two staff members of the IAEA Atomic and Molecular Data Unit (see Appendix 1). Dr. I. Bray (Flinders University) was also invited to participate in the meeting but was not able particularly to attend. However, the interaction with Dr. Bray was so active both before and during the meeting, and his input to meeting analyses, deliberations and results so significant, that the authors of the present report consider his contribution to the meeting as important as that of the actual participant and, therefore, (and with his consent) he was included among the co-authors of this report.

The critical assessment of electron-impact excitation and ionization cross section data base for Be and B atoms and ions was undertaken by the IAEA to respond to the demands of fusion research community for more accurate and up-dated data information on these processes in view of their role in the physics of several operating large tokamaks having significant amounts of Be and B plasma impurities, expected to be present also in the next generation fusion reactor devices (such as the International Thermonuclear Experimental Reactor). On the other hand, important new theoretical developments, accompanied by new cross section calculations, have taken place since the last IAEA critical assessment of Be and B collisional data in 1992, the results of which were published in vol. 3 of the IAEA series in "Atomic and Plasma-Material Interaction Data for Fusion" (1992). Some of the most recent cross section calculations and data assessments for electron-impact excitation and ionization of Be and B atoms and ions were published in the Topical Issue of "Physica Scripta", vol. **T62** (1996). The task of the Consultants' meeting was to review these new developments, complete and up-date the previous recommendations, and provide advice to the Agency regarding the course of action for further improvement of the Be and B collisional database.

In their preparation for the meeting, Prof. K. Bartschat, Dr. K. Berrington and Dr. I. Bray have also performed a significant amount of new cross section or effective collision strength calculations for the considered collision systems and processes, including calculations with the most recently developed theoretical methods. These new results were also reported and analyzed at the meeting.

2 Meeting Proceedings

After a brief outline of the meeting objectives by the Head of the IAEA A+M Data Unit, the meeting proceeded according to the adopted agenda (see Appendix 2).

During the first day of the meeting the status of the existing database for excitation and ionization of Be and B atoms and ions by electron impact was reviewed, with particular emphasis on the new results obtained after the last database assessment in 1992.

Prof. K. Bartschat reviewed the new theoretical results for neutral and singly ionized beryllium, obtained using the recently developed "R-matrix with pseudo-states" (RMPS) method [1,2] and the "convergent close-coupling" (CCC) approach [3,4]. The latter results were provided by Dr. I. Bray. The general properties of the RMPS and CCC methods in describing the electron-impact excitation physics were outlined, including their relative advantages and complementarity in obtaining highly accurate cross section results in various collision energy regions. Both methods have also the capability to provide a good estimate of the ionization cross section.

Dr. K. Berrington reported comparisons of effective collision strengths, calculated from the previously recommended database of Berrington and Clark [5], and emphasized the significant differences that may arise in the magnitude of effective collision strengths from changes in the adopted recommended cross section data.

The second day of the meeting was devoted to an analysis and upgrading the recommended database for excitation and ionization of Be and B atoms and ions in view of the most recent theoretical developments and results, and to formulate a course of action for further database improvements and completion.

The results of these analyses are described in the remainder of this Report.

3 Status of Electron-Impact Excitation Database for Be and B Atoms and Ions

The goal of the present report is to update the database previously recommended by Berrington and Clark [5]. All the changes are the results of new theoretical developments. These developments appear to be most significant for neutral and singly ionized targets. Briefly, the "R-matrix with pseudo-states" (RMPS) method [1] and the "convergent close-coupling" (CCC) approach [3] take into account the effect of the target continuum states in the close-coupling expansion. Compared to the results of traditional n-state (discrete) close-coupling (R-matrix) calculations, the cross sections for inelastic transitions are often predicted to be somewhat lower in the intermediate energy regime, approximately between one and five times the ionization threshold. These effects were not accounted for in the Berrington and Clark review [5].

At present, some new results are available for Be and Be^{+}. These will be summarized below. On the other hand, no ew experimental data for any atom or ion discussed in [5] have been produced.

3.1 Electron impact excitation of Be^{+}

Results for the electron impact induced 2s – 2p and 2s – 3d transitions in Be^{+} are shown in figure 1. The 2s – 2p transition is an example of good agreement between the new and the previously recommended theoretical data. The disagreement (approximately 10%) with the experimental data [6] for this transition has not been resolved. In light of the success of the RMPS and CCC theories for other systems, their level of sophistication, and the comparison with other elaborate calculations such as that of Mitroy and Norcross [7] indicates a need for further checking the calibration of the experimental results.

On the other hand, the RMPS and CCC results for the 2s – 3d transition differ substantially from the previous 9-state R-matrix calculation [5] (labeled RM9) in the intermediate energy region. The merge towards the first-order distorted wave results [5] does not occur until energies well above 50 eV, in contrast to the earlier indication of a merge near 20 eV. This is most likely due to important coupling effects to higher F states which are not accounted for sufficiently by only including the physical 4f-state in the 9-state R-matrix calculation. We strongly recommend the adoption of the new RMPS/CCC data sets, as well as further testing of the results for this transition in other Li-like ions.

3.2 Electron impact excitation of neutral Be

Results for the electron impact induced $(2s^2)^1S - (2s2p)^{3,1}P$ and $(2s^2)^1S - (2s3d)^1D$ transitions are shown in figure 2. In the calculation labeled "3-state", only the physical states $(2s^2)^1S$ and $(2s2p)^{1,3}P^o$ were included in the close-coupling expansion, but the states were expanded using pseudo-orbitals $3\bar{s}$, $3\bar{p}$ and $3\bar{d}$. Consequently, the results from this calculation exhibit a remarkable pseudo-resonance structure in the intermediate energy region. That structure can be greatly reduced by keeping states, which originate from the additional configurations, in the expansion. This has been done in the curve labeled "3+23-state" where all the states that can be generated from the configurations $2p^2$, $2s3\bar{s}$, $2s3\bar{p}$, $2s3\bar{d}$, $2p3\bar{s}$, $2p3\bar{p}$ and $2p3\bar{d}$ were also included.

A computationally efficient approximation to the latter procedure is a T-matrix averaging technique [8]. This method was applied in the previous 12-state R-matrix calculation by Fon [9] since keeping all the states arising from the many configurations in their work would have gone beyond the available computational resources. (These results were recommended in the Berrington and Clark report [5]). We note, however, that some broad structure remained even after the T-matrix averaging.

The curves labeled RMPS and CCC represent results from calculations that explicitly account for the effect of the target continuum states. The important conclusion to be drawn from figure 2 is the fact that the inclusion of the additional pseudo-states reduces the cross section results dramatically for incident energies in the region between the ionization threshold (9.32 eV) and about 70 eV. For the forbidden $(2s^2)^1S - (2s2p)^3P^o$ transition, the reduction factor around 30 eV incident energy is approximately 2 when compared to the results of Fon [9]. For the optically allowed $(2s^2)^1S - (2s2p)^1P^o$ transition the result is strongly influenced by contributions from high partial waves which are not as sensitive to the correlation effects. Consequently, the percentage reduction (up to 20%) is less in this case, but clearly the effect is not negligible.

It should also be pointed out that the small oscillations in the RMPS results are again due to pseudo-resonances. The most important reason for their visibility is the fact that the calculation was performed for about 200 energies on a narrow grid. Due to the small amplitudes, these oscillations could easily be smoothed out, but even the data presented here can be expected to yield smooth effective collision strengths as a function of temperature.

Finally, we note an overall reduction in the collision strength for the $(2s^2)^1S - (2p^2)^1D$ transition compared to the Fon [9] calculation presented in [5]. Most importantly, however, we note that the assignment of the $(2p^2)^1D$ and $(2s3d)^1D$ in the recent work of Clark and Abdallah [10] is reversed compared to the results presented in the Berrington and Clark report [5]. Despite the large discrepancy between the DWBA and the close-coupling results for this transition, we still believe the assignment given in [5] to be correct. In any case, we now recommend the adoption of the new RMPS/CCC results.

Excitation from the metastable $(2s2p)^3P$ state was not addressed by Berrington and Clark [5]. In figure 3, we present the new RMPS and CCC results for the collision strength of the $(2s2p)^3P - (2s3s)^3S$, $(2s2p)^3P - (2p^2)^3P$, and $(2s2p)^3P - (2s3d)^3D$ transitions, in comparison with the previous R-matrix results of Fon [9]. For the $(2s2p)^3P - (2s3s)^3S$ and $(2s2p)^3P - (2p^2)^3P$ transitions, the Fon [9] calculation appears to slightly (by about 10%) overestimate the collision strength around 30 eV, while otherwise the agreement is satisfactory. Finally, for the $(2s2p)^3P \rightarrow (2s3d)^3D$ transition, significant disagreement remains between all three predictions for energies between threshold and 100 eV. In principle, the CCC calculation should be the most accurate, but the present results are still preliminary and should be treated with caution. We therefore recommend further checking of the RMPS and CCC results against each other.

3.3 Electron impact excitation of neutral B

Berrington and Clark [5] showed that the theoretical data for electron impact excitation of neutral B were not consistent between the R-matrix calculation of Nakazaki and Berrington [11] and the DWBA results [5]. In addition, a big discrepancy was noted between the theoretical predictions and the only available experimental data of Kuchenev and Smirnov [11]. In light of the new results for e-Be scattering, we strongly recommend to first repeat the R-matrix calculation with the same orbitals and configurations as used by

Nakazaki and Berrington [11], but with the pseudo-states from all configurations explicitly included in the close-coupling expansion. This would give an immediate improvement to the theoretical data base, since the effect of pseudo-resonances would be drastically reduced [2]. Nevertheless, even more elaborate RMPS and/or CCC calculations will be necessary to establish an accuracy estimate as well as definitive results. However, such calculations will be very demanding and could take up to several years before completion.

3.4 Electron impact excitation of B^+

There are no new results available for this target. However, in light of the improvements emerging from the new calculations for neutral and singly ionized beryllium, we strongly recommend to perform RMPS and CCC calculations for singly ionized boron.

3.5 Electron impact excitation of the remaining ions of Be and B

There are no new results available for these targets. The recommendations by Berrington and Clark [5] still hold, but spotchecks using the new theoretical methods seem worthwhile, especially for the 2s $\rightarrow$ 3d transition B^{2+}.

4 Status of electron ionization database for Be and B atoms and ions

This topic has recently been reviewed by Moores [12]. We agree with the recommendation made in this review. Especially for neutral Be, however, new results for ionization should be extracted from the RMPS and CCC calculations. It is also noted that further theoretical development is necessary to extract this information for specific final states of the residual ion. However, this development is non-trivial and may take some time.

5 Meeting conclusions and recommendations in the preceding two sections

As mentioned, we strongly recommend to update the existing data base for neutral atoms and singly ionized ions by performing elaborate RMPS and CCC calculations for both Be and B impurities, and also to perform spotchecks at least for the doubly ionized targets. The new results are available electronically be sending a request to `I.Bray@flinders.edu.au` (CCC) and `kb0001r@acad.drake.edu` (RMPS). For higher ionic charges, the previously recommended data [5] are expected to be sufficiently accurate.

Compared to the amount of theoretical work for these collision systems, we are very concerned about the apparent lack of highly accurate experimental benchmark data. Consequently, we strongly encourage experimental efforts in this area, particularly for the neutral targets.

Finally, the use of the updated recommended data for all ionization stages of Be and B to calculate effective collision strengths is currently in progress. These results will be presented at the IAEA meeting on "Radiative Cooling Rates of Fusion Plasma Impurities" to be held in Vienna on 14-15 October, 1996.

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Appendix 1

IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions"

2-3 September 1996, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions"

2-3 September 1996, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Monday, September 2

09:30 - 10:00 :	- Opening - Adoption of Agenda	Room: A-23-43
10:00 - 12:00 :	Review of the status of electron-impact excitation and ionization database for Be and B atoms and ions	
12:00 - 14:00 :	Lunch	
14:00 - 18:00 :	New recent theoretical developments and cross section calculations for Be and B atoms and ions	

Tuesday, September 3

09:00 - 12:00 :	Needs and course of action for upgrading the excitation and ionization database for Be and B atoms and ions
12:00 - 14:00 :	Lunch
14:00 - 16:00 :	Analysis continued
16:00 - 18:00 :	Formulation of Meeting conclusions and recommendations

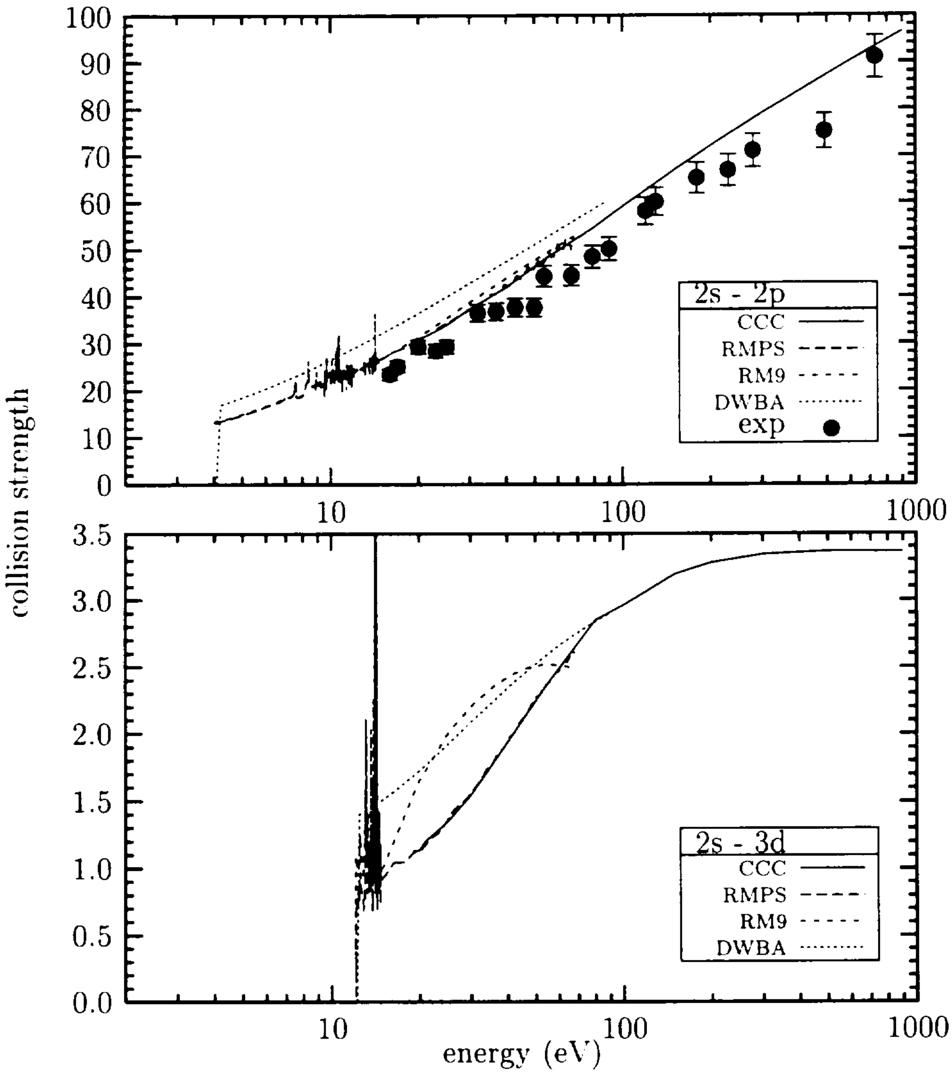

Figure 1: Collision strength for the 2s – 2p (top) and 2s – 3d (bottom) transition in Be^{+}. The individual curves are: CCC [4], RMPS [2], RM9 [5], and DWBA [5]. The experimental data (exp) are from Taylor *et al.* [6].

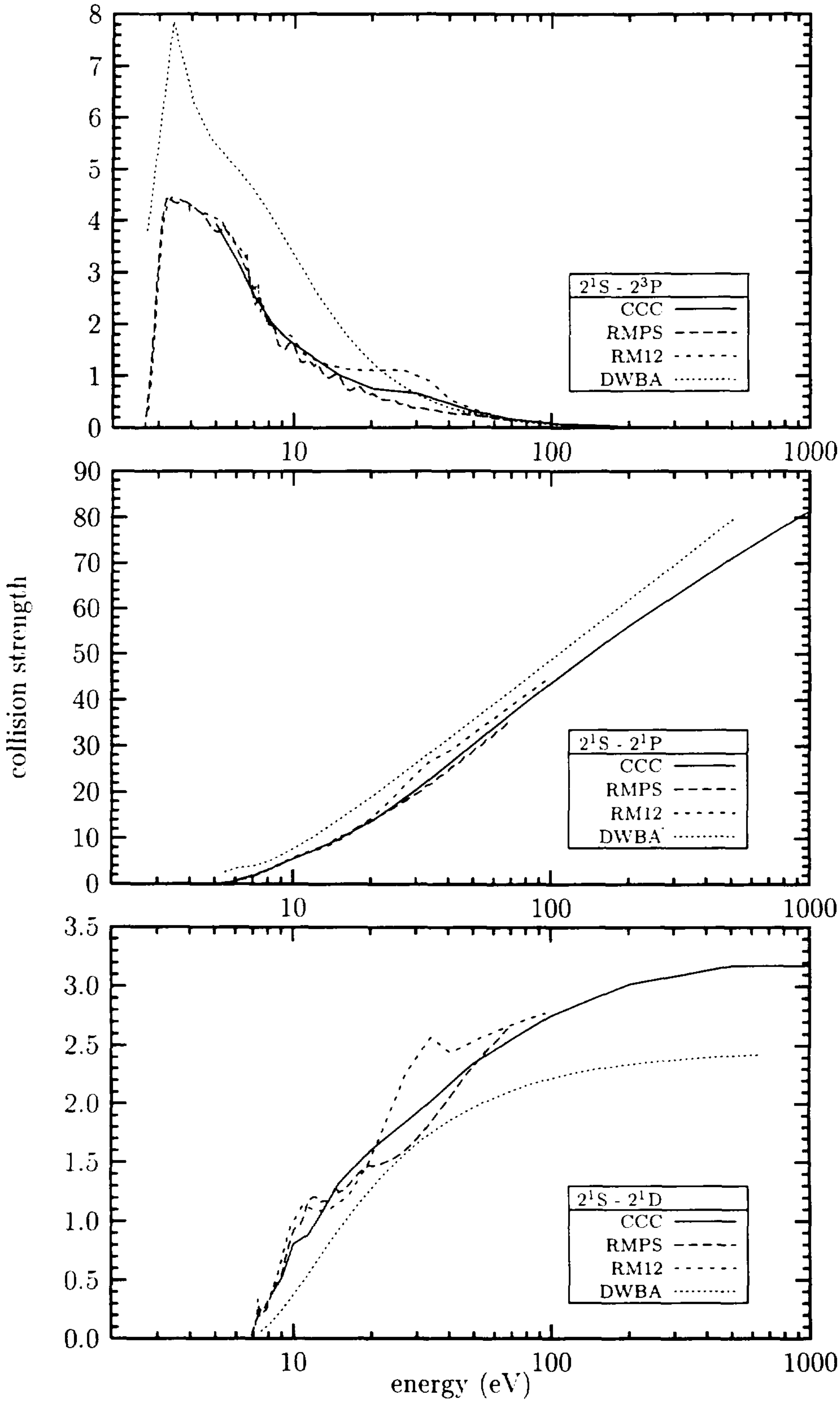

Figure 2: Collision strength for the $(2s^2)^1S - (2s2p)^3P$ (top), $(2s^2)^1S - (2s2p)^1P$ (center), and $(2s^2)^1S - (2p^2)^1D$ (bottom) transitions in Be. The individual curves are: CCC [4], RMPS [2], RM12 [5], and DWBA [5].

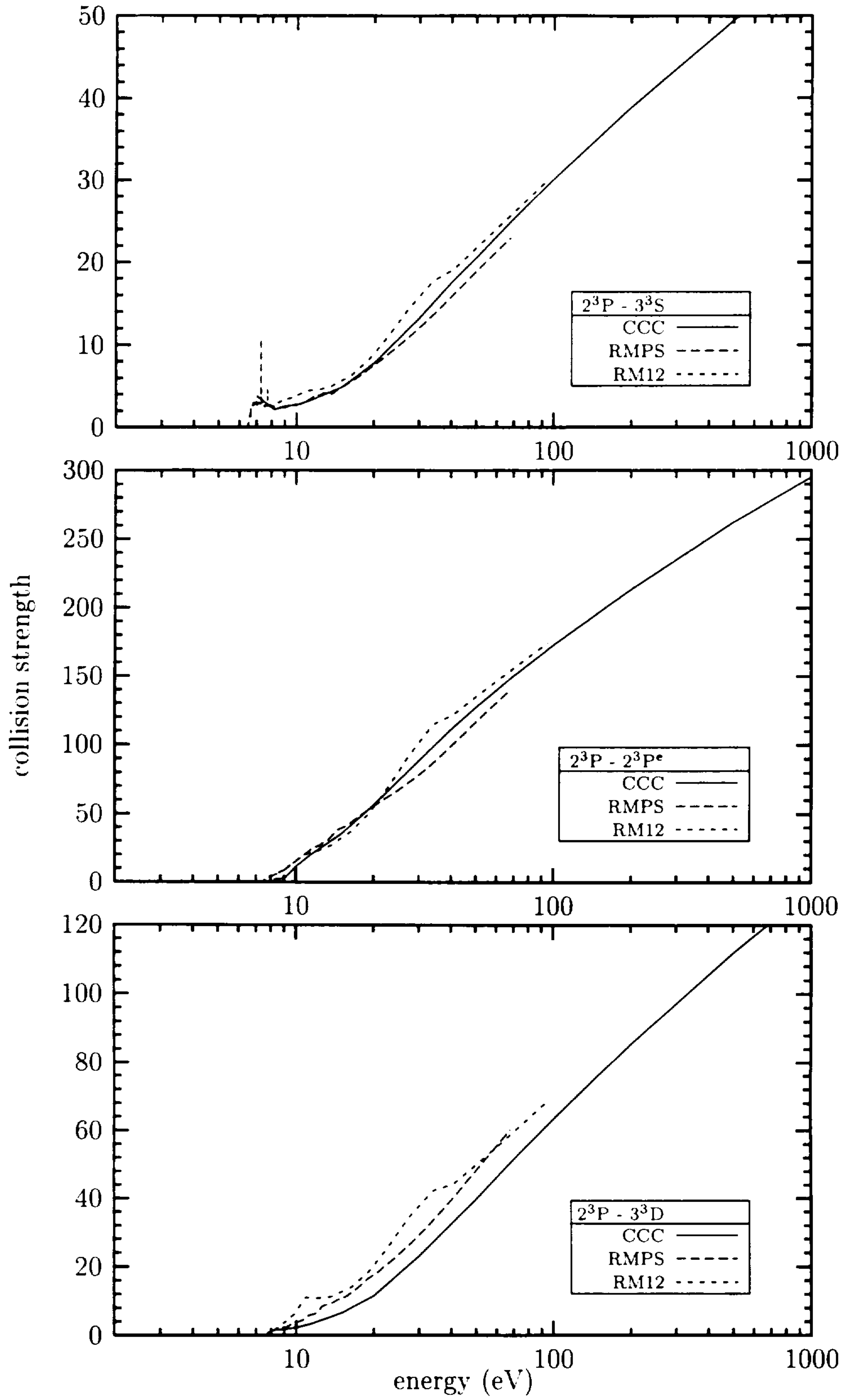

Figure 3: Collision strength for the $(2s2p)^3P$ – $(2s3s)^3S$, (top), $(2s2p)^3P$ – $(2p^2)^3P$ (center), and $(2s2p)^3P$ – $(2s3d)^3D$ (bottom) transitions in Be. The individual curves are:CCC [4], RMPS [2], and RM12 [5].