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## Electron collisional broadening of 2s3s–2s3p lines in Be-like ions

Yu.V. Ralchenko<sup>a,\*</sup>, H.R. Griem<sup>b</sup>, I. Bray<sup>b</sup>, D.V. Fursa<sup>c</sup>

<sup>a</sup>*Faculty of Physics, Weizmann Institute of Science, Rehovot 76100, Israel*

<sup>b</sup>*Institute for Plasma Research, University of Maryland, College Park, MD 20742, USA*

<sup>c</sup>*Electronic Structure of Materials Centre, School of Physical Sciences,  
The Flinders University of South Australia, G.P.O. Box 2100, Adelaide 5001, Australia*

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### Abstract

We present quantum–mechanical calculations for the electron collisional Stark linewidths of the 2s3s–2s3p singlet and triplet lines of the beryllium-like ions from B II to O V. The impact approximation is used with the convergent close-coupling method, which is shown for inelastic cross sections to agree well with the Coulomb–Born-exchange approximation. Similar to previous comparisons, we find our calculated widths to be generally smaller than both measured and (most) theoretical linewidths from semiclassical calculations. A possible contribution from non-thermal Doppler widths is discussed as well. © 2001 Elsevier Science Ltd. All rights reserved.

*Keywords:* Collisional line broadening; Be-like ions; Impact approximation

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### 1. Introduction

The collisional broadening of isolated lines of multiple-ionized atoms in dense plasmas is primarily due to interactions between plasma electrons and radiating ions [1,2]. Consequently, important plasma characteristics, e.g., particle densities, are manifested in, and can be determined from, the collisional line widths. The implementation of these powerful diagnostic techniques should obviously rely upon a well-developed theory supported by precise benchmark measurements of linewidths from hot dense plasmas as recently reviewed in Ref. [3].

While the basic quantum–mechanical (QM) theory of the collisional line broadening was established long ago [4], the number of fully quantal calculations of the electron-impact line widths is still very limited. Normally such computations make use of fundamental atomic scattering parameters (*T*-matrix elements or cross sections and amplitudes), and it is not surprising

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\* Corresponding author. Tel.: +972-8-9343610; fax: +972-8-9343491.

*E-mail address:* frralch@plasma-gate.weizmann.ac.il (Yu.V. Ralchenko).

that the reliable calculation of quantal line widths have become possible only recently, after a number of sophisticated atomic collision codes were made available. The very first reliable calculations [5,6] showed, however, that the QM results underestimate the experimental line widths for the B III 2s–2p transition measured in a benchmark experiment on a gas-liner Z-pinch at Bochum [7] by as much as a factor of 2. Although an explanation of this discrepancy in terms of non-thermal plasma motions was proposed in Ref. [6] (see also the ensuing discussion [8–11]), the uncertainty of this situation was exacerbated by a good agreement between experimental and other theoretical (mainly semiclassical, including the non-perturbative) results. This ambiguity turned out to be more troubling after a similar disagreement was found also for the 2s3s–2s3p singlet and triplet collisional line widths in the Be-like ion Ne VII [12], and the latest results obtained with the modified non-perturbative semiclassical method [13] were shown to confirm the quantum calculations for the B III linewidth.

In view of these developments, a detailed comparison of benchmark experiments and accurate theoretical calculations becomes an urgent and important task. Fortunately, very recently a number of measurements of the electron collisional line widths in Be-like ions were conducted at different facilities, including a gas-liner Z-pinch [14] and low-pressure pulsed arcs [15,16]. In these experiments the Stark widths of the 2s3s–2s3p singlet and triplet lines were measured with a high accuracy of the order or better than 10%, providing thereby an appropriate testbed for the existing theoretical methods. The comparison of our new quantum–mechanical calculations with the above mentioned and other measurements [17,18] constitutes the subject of the present paper. The basic theory and related aspects, e.g., inelastic and elastic contributions, are discussed in Section 2. Comparisons with theoretical and experimental data and discussions of the results are presented in Section 3, which is followed by conclusions. Finally, we would like to mention that more attention is paid here to the triplet lines since, unlike the singlets, they were measured in all experiments.

## 2. Theory

In the impact approximation, which is almost always valid for lines from relatively low-lying excited states, the electron collisional linewidths can be calculated with the following general formula [4]:

$$w = N_e \int v f_M(v) dv \times \left( \sum_{k \neq l} \sigma_{lk}(v) + \sum_{k \neq u} \sigma_{uk}(v) + \int |f_u(v) - f_l(v)|^2 d\Omega \right), \quad (1)$$

where  $w$  is the line width (full-width at half-maximum),  $N_e$  is the electron density, and  $v$  is the electron velocity with  $f_M(v)$  being the Maxwellian electron energy distribution function. The atomic collisional characteristics entering Eq. (1) are the *inelastic* cross sections  $\sigma_{lk}(v)$  and  $\sigma_{uk}(v)$ , corresponding to transitions from the lower and upper states of the radiative transition in question into all possible channels, and the *elastic* (non-Coulomb) scattering amplitudes

$f_l(v)$  and  $f_k(v)$ . This formula not only provides a very clear separation of inelastic and elastic contributions to a linewidth, but also points out the parameters (inelastic cross sections) which can in principle be independently measured in other experiments. Although for the 3–3 transitions in Be-like ions direct measurement of the most important excitation cross sections is not easily performed, one can nevertheless hope that corresponding rate coefficients can indeed be measured, e.g., using the techniques described in Ref. [19].

According to Eq. (1), in order to calculate the electron-impact linewidths, it suffices to compute the inelastic cross sections and elastic scattering amplitudes. In the present work, such calculations were performed with the convergent close-coupling (CCC) method [20,21], which was also utilized in Ref. [12]. The basic procedure in the CCC is to make a close-coupling expansion on a large set of square-integrable basis states. The convergence of the expansion is checked by increasing the number of such states. It is particularly important for the elastic contributions to use good energy resolution. For the atomic wave functions the Hartree–Fock (HF) frozen-core approximation provides sufficient accuracy, which was verified by comparisons between full HF and frozen-core HF results using Cowan’s code [22]. Similarly, the validity of LS coupling in the CCC calculations for all ions involved here was confirmed by comparisons with the large-scale atomic structure calculations using Cowan’s code that accounted for configuration interaction and intermediate coupling.

The precision of the line width calculations ought to be checked not only against the atomic line widths, which are directly measured in plasma experiments, but also versus other atomic characteristics relevant to the specific ions and/or atomic transitions. The first indication of the calculational accuracy can be inferred from the oscillator strengths for electric-dipole transitions that have also been computed in the CCC runs. We have found that the HF frozen-core approximation provides very accurate oscillator strengths, differing only by a few ( $\lesssim 5$ ) percent from the NIST recommended data [23].

As will be shown below, the main contribution to the linewidths here comes from inelastic, both excitation and deexcitation, transitions between the 2s3l states. There is presently no experimental information for these cross sections, nor are any other theoretical calculations available. Therefore, to check the accuracy of the CCC results we performed an independent calculation of all 2s3l  $^1,^3L$ –2s3l'  $^1,^3L'$  cross sections with the Coulomb–Born-exchange (CBE) unitarized method using the code ATOM [24]. Some of the dipole-allowed cross sections, calculated by both techniques, are presented in Fig. 1. One can see that the overall agreement between the CCC and CBE results is good, although for the 3s–3p transition of C III the discrepancy reaches 50% near the reaction threshold. The accuracy of the CCC cross sections is considered to be superior to that of the CBE cross sections, and therefore use was made of the CCC data for all excitation and deexcitation cross sections involved in the present linewidth calculations. However, a comparison of elastic contributions to the linewidths cannot be performed, since the current version of ATOM does not produce elastic amplitudes.

The CCC elastic non-Coulomb cross sections 2s3s  $^3S$ –2s3s  $^3S$  and 2s3p  $^3P$ –2s3p  $^3P$  as well as the corresponding triplet elastic difference term (EDT)  $\int |f_u(v) - f_l(v)|^2 d\Omega$  entering Eq. (1) are given in Fig. 2 for all ions from B II to O V. Again, similar to the case of B III [6] and Ne VII [12], a strong cancellation in the difference of elastic amplitudes is obvious and especially pronounced for high energies, where details of atomic structure become unimportant and amplitudes are determined mainly by the ion size and charge. Because of this cancellation, even

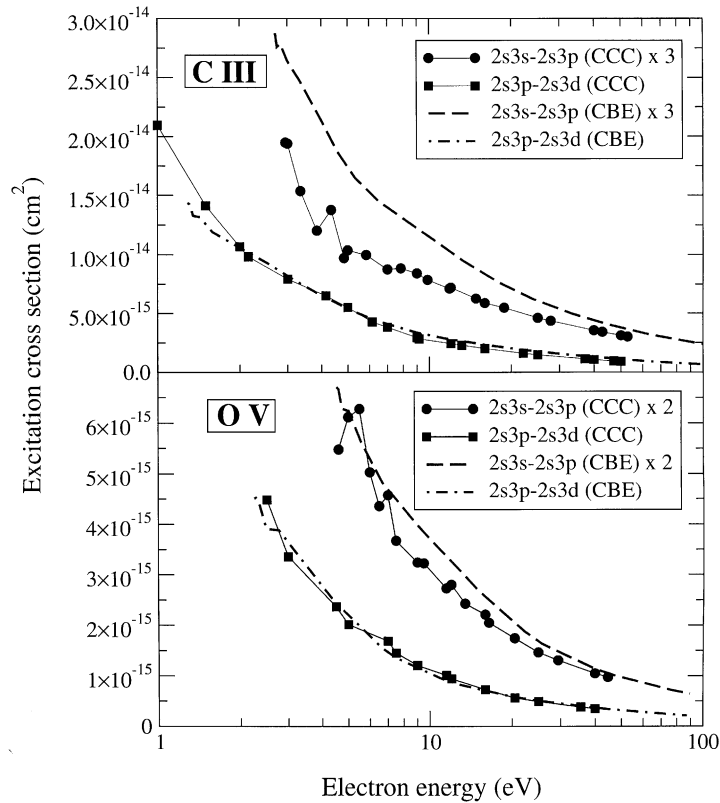


Fig. 1. Dipole-allowed excitation cross sections  $2s3s\ ^3S-2s3p\ ^3P$  and  $2s3p\ ^3P-2s3d\ ^3D$  ( $\text{cm}^2$ ) in Be-like ions C III and O V.

relatively small resonance structures in either of the elastic amplitudes lead to the appearance of prominent peaks in the EDT; this can be seen especially well for the O V data. It should be noted that any unresolved resonances may further contribute to the linewidths. However, this effect, as well as some uncertainty due to the above-mentioned strong cancellation in EDT, is unlikely to noticeably affect the final calculated linewidths, since the fraction of the EDT in the total linewidth is rather small for the electron temperatures of interest (see below). Note also that the average energy dependence of the EDT is steeper than that of the elastic cross sections, namely,  $\sim 1/E^{1.4-1.6}$  vs.  $\sim 1/E$ . This supports the energy dependence of EDT which was determined in our previous calculations [6,12].

The  $2s3s\ ^3S-2s3p\ ^3P$  linewidths for B II–O V, as functions of electron temperature, are presented in Fig. 3 and in Table 1, and the  $2s3s\ ^1S-2s3p\ ^1P$  linewidths for N IV and O V are given in Table 2. The electron density was taken to be  $N_e = 10^{18}\ \text{cm}^{-3}$  for all calculations, and the electron temperature was limited to the range  $T_e = [2-20]$  eV, which covers all available experimental data. The elastic contribution to the linewidth is shown by a dotted line, the inelastic part by a dashed line, and the total linewidth is presented by a solid line with open circles. First of all, there is a rather weak dependence of the linewidths on electron temper-

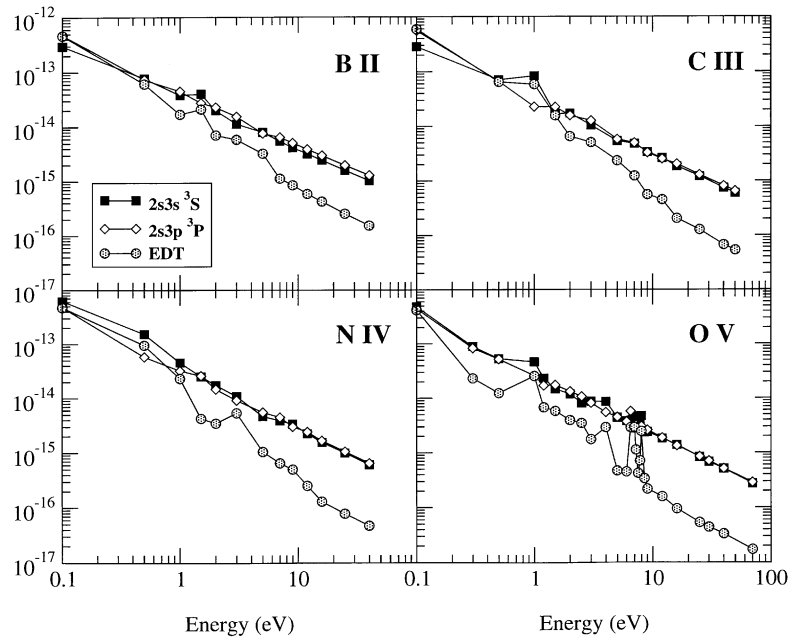


Fig. 2. Elastic scattering cross sections and elastic difference term ( $\text{cm}^2$ ) for the  $2s3s \ ^3S$ – $2s3p \ ^3P$  lines.

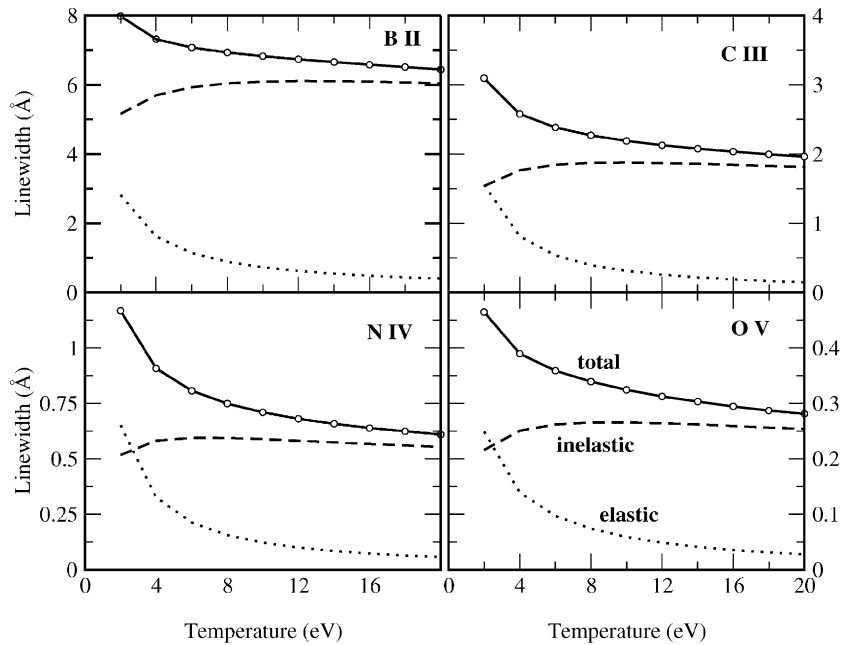


Fig. 3.  $2s3s \ ^3S$ – $2s3p \ ^3P$  collisional linewidths ( $\text{\AA}$ ) for the B II–O V ions: ( $\cdots$ ) elastic, ( $---$ ) inelastic, ( $—$ ) total.

Table 1

Elastic, inelastic and total linewidths ( $\text{\AA}$ ) for the  $2s3s\ ^3S-2s3p\ ^3P$  transitions in Be-like ions vs. electron temperature  $T_e$  (eV) for electron density of  $N_e = 10^{18}\text{ cm}^{-3}$

$T_e$	B II			C III			N IV			O V		
	El	Inel	Tot	El	Inel	Tot	El	Inel	Tot	El	Inel	Tot
2	2.82	5.16	7.98	1.56	1.54	3.09	0.651	0.517	1.17	0.249	0.216	0.470
4	1.62	5.70	7.32	0.811	1.77	2.58	0.326	0.582	0.907	0.139	0.251	0.390
6	1.15	5.93	7.07	0.538	1.85	2.38	0.212	0.595	0.807	0.097	0.262	0.359
8	0.891	6.04	6.93	0.398	1.87	2.27	0.156	0.594	0.749	0.074	0.266	0.339
10	0.733	6.09	6.83	0.314	1.88	2.19	0.122	0.588	0.710	0.059	0.266	0.324
12	0.625	6.11	6.73	0.258	1.87	2.13	0.100	0.581	0.680	0.049	0.264	0.313
14	0.547	6.11	6.65	0.218	1.86	2.08	0.084	0.574	0.658	0.041	0.262	0.303
16	0.487	6.09	6.58	0.189	1.85	2.03	0.072	0.567	0.639	0.035	0.259	0.295
18	0.440	6.07	6.51	0.166	1.83	2.00	0.064	0.560	0.624	0.031	0.256	0.287
20	0.401	6.04	6.44	0.148	1.81	1.96	0.057	0.553	0.610	0.027	0.254	0.281

Table 2

Elastic, inelastic and total linewidths ( $\text{\AA}$ ) for the  $2s3s\ ^1S-2s3p\ ^1P$  transitions in Be-like ions vs. electron temperature  $T_e$  (eV) for electron density of  $N_e = 10^{18}\text{ cm}^{-3}$

$T_e$	N IV			O V		
	El	Inel	Tot	El	Inel	Tot
2	1.36	2.04	3.40	0.500	0.851	1.35
4	0.904	2.20	3.10	0.262	0.928	1.19
6	0.625	2.19	2.82	0.177	0.926	1.10
8	0.463	2.16	2.62	0.133	0.906	1.04
10	0.360	2.12	2.48	0.106	0.886	0.992
12	0.291	2.08	2.37	0.088	0.862	0.950
14	0.242	2.05	2.29	0.075	0.844	0.919
16	0.206	2.02	2.22	0.066	0.825	0.890
18	0.178	1.99	2.17	0.058	0.807	0.866
20	0.156	1.96	2.12	0.053	0.793	0.845

ature, the exponent for the  $1/T_e^\alpha$  fit being in the range  $\alpha = [0.05, 0.10]$ . Although the elastic contribution shows a stronger  $\sim 1/T_e$  behavior, it is more than compensated for by the inelastic width which is mainly due to excitation and deexcitation. Among all possible inelastic channels, the dipole-allowed  $3s-3p$  excitation and deexcitation and  $3p-3d$  excitation produce the overwhelming contribution, which reaches more than 90% of the total inelastic width for some temperatures. This is expected for the small energy thresholds for these transitions, which give rise to large values of cross sections and rate coefficients. The elastic part is seen to become less important with the increase in temperature and does not contribute more than 30% for the electron temperatures of interest ( $T_e = [5, 10]$  eV).

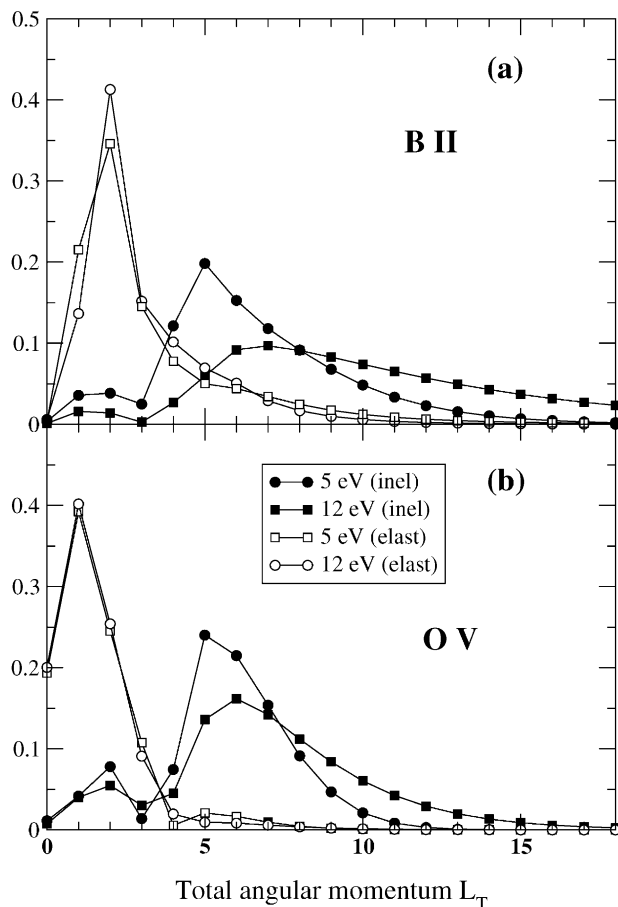


Fig. 4. Relative partial wave composition for inelastic  $2s3s\ ^3S-2s3p\ ^3P$  and elastic  $2s3s\ ^3S-2s3s\ ^3S$  cross sections in B II (a) and O V (b) for electron energies 5 eV (circles) and 12 eV (squares). The inelastic data are shown by solid symbols and the elastic data by open symbols.

We have previously emphasized the importance of the determination of partial wave (PW) contributions to the Stark linewidths. This provides both a clear indication of the significance of different impact parameters in electron-ion scattering and a convenient means for detailed comparisons with other theoretical results. As an example, Fig. 4 shows the relative PW contributions to the inelastic  $2s3s\ ^3S-2s3p\ ^3P$  and elastic  $2s3s\ ^3S-2s3s\ ^3S$  cross sections for the lowest-charge and highest-charge ions discussed in the present work, i.e., B II and O V. Two electron impact energies, 5 and 12 eV, were selected for the PW presentation. As one might have expected, the peak in inelastic PW composition shifts towards high total angular momenta  $L_T$  with the increase of electron impact energy. The major contribution at electron temperatures typical for the experiments discussed below comes from low and moderate  $L_T \lesssim 10$ . Even lower partial waves,  $L_T \lesssim 4-5$ , are important for elastic cross sections. Finally, the elastic partial wave contributions are seen to be almost independent of the electron energy, at least for the energy range relevant for the available experimental data.

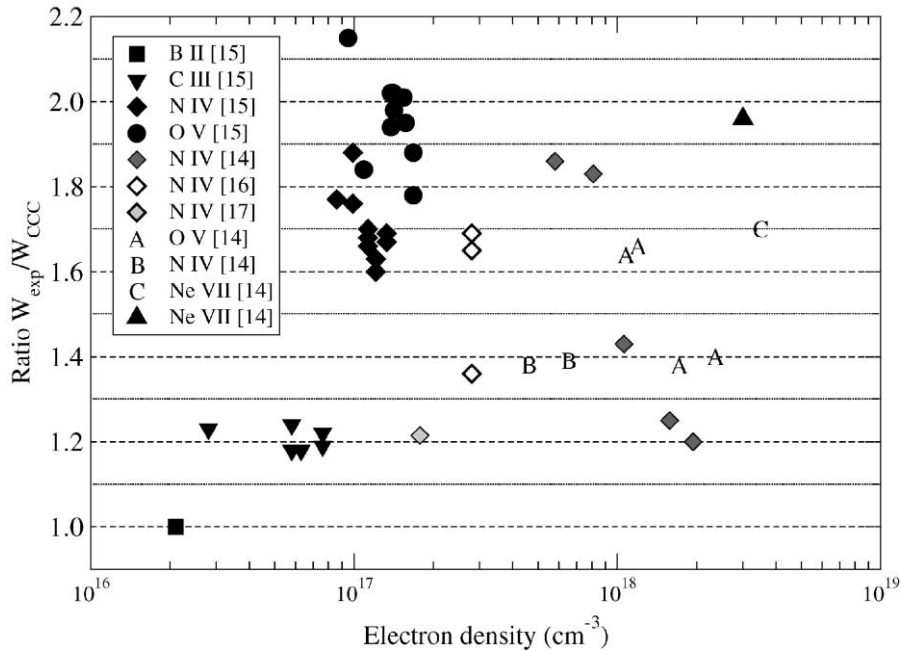


Fig. 5. Ratio of experimental linewidths to the CCC linewidths (present work) vs. electron density.

### 3. Comparisons and discussions

As was mentioned in the Introduction, a number of experimental results were published recently. Fig. 5 shows the ratios  $R$  of the measured [14–17] and CCC widths at the experimental electron temperatures, scaled linearly to the independently measured densities. Again, the singlet linewidths were measured only by the Bochum group [14]. Ion–ion collisions are not included here; according to semiclassical calculations [15] they should add not more than 10% to the electron collisional widths. As can be seen from Fig. 5, for all cases except for the B II triplet transition, the experimental results are higher than the CCC linewidths. A closer inspection of these results indicates some interesting peculiarities. First of all, the results of Bochum group were obtained at rather high electron densities of the order of  $10^{18} \text{ cm}^{-3}$ ; moreover, they cover a fairly large range of densities for some lines. The variation of O V and especially of N IV triplet experimental linewidths with electron density clearly demonstrate convergence to the CCC results with an increase in density. Such a behavior is likely to be due to an additional density-independent (or weakly dependent) contribution to the linewidth, which becomes more negligible compared to the Stark width. Consider in more detail the N IV triplet linewidths: the electron temperature for this line was measured to be between 7 and 9 eV with an experimental error of 10–30%, and the electron density varied from  $0.58 \times 10^{18}$  up to  $1.94 \times 10^{18} \text{ cm}^{-3}$  with an error smaller than 12%. The difference between the measured linewidth and our data

is slowly changing and takes the following values:

$$w_{\text{Bochum}} - w_{\text{CCC}} (\text{\AA}) = 0.39 (0.58), 0.49 (0.81), 0.33 (1.06), 0.29 (1.58), 0.29 (1.94), \quad (2)$$

where the electron density (in units of  $10^{18} \text{ cm}^{-3}$ ) is given in parentheses for each measurement. In our previous work on the lithium-like B III 2s–2p lines [6] and again in the paper on beryllium-like Ne VII 2s3s–2s3p lines [12] we had suggested that these narrow and relatively short wavelength lines may have experienced significant additional Doppler broadening from non-thermal motions, which are to be expected for the very large Reynolds number flows in the implosion phase of the gas-liner pinch. Further evidence for significantly non-thermal motions was reported [25] for very similar conditions in terms of a persistent (Doppler) splitting of the lithium-like C IV 2s–2p line. However, as in Ref. [14], the impurity peaks in the Thomson scattering spectra did not show any corresponding effects [26], given both the noise in the data and ambiguities in fitting to the relatively complicated theoretical Thomson-scattering line shapes (relative to those of the C IV emission lines). In any case, such non-thermal Doppler effects would also help to explain the trend toward lower  $R$ -values with increasing electron density.

The low-pressure pulsed arc experiment of the Belgrade group [15] was carried out at lower densities near  $10^{17} \text{ cm}^{-3}$ , i.e., would be even more susceptible to any additional broadening mechanism. However, the density spread for each of the triplet lines was much smaller than in the Bochum experiment, and therefore no density dependence can be discovered here.<sup>1</sup> Nevertheless, the measured linewidths do show a deviation which is monotonically increasing along the *isoelectronic sequence*: for B II the ratio of the Belgrade linewidth to our calculated width is approximately unity, while for C III it increases up to 1.2, for N IV this ratio reaches 1.6–1.7, and finally for O V it becomes almost 2. Such a behavior may again be explained by some quasi-constant additional broadening which is independent of the ion. Neglecting the small ion–ion collisional linewidth, one can determine the absolute difference between the CCC and averaged experimental [15] widths for  $N_e \simeq 10^{17} \text{ cm}^{-3}$ :

$$w_{\text{Belgrade}} - w_{\text{CCC}} (\text{\AA}) = 0 (\text{BII}), 0.05 (\text{CIII}), 0.055 (\text{NIV}), 0.035 (\text{OV}). \quad (3)$$

Thus, these experimental results for *different elements*, obtained for similar plasma conditions, seem to favor the presence of some extra broadening. B II is the only exception, probably because its Stark width at a given density is larger by a factor of about 3 or more than that of the other ions, and because the additional broadening is not Lorentzian.

The measurement of the collisional linewidths requires not only a very accurate determination of the linewidth itself but in addition a reliable measurement of the electron temperature and density, especially the latter. The electron density in the Belgrade experiment was inferred [15] for most of the data from the measured width of the He II Paschen- $\alpha$  line, using its comparison with gas-liner pinch Thomson-scattering data [27] as calibration. However, inspection of Fig. 4 of Ref. [27] shows that for a given measured halfwidth the actual electron density could

<sup>1</sup> The C III line was measured for very low densities  $N_e = (2.8 - 7.6) \times 10^{16} \text{ cm}^{-3}$ .

be higher by about 20%. Additional difficulties in experimental procedures might have appeared because of the very small amount of Be-like O V at the measured electron temperatures. For instance, the linewidths for O V are given in Ref. [15] for  $T_e$  as low as 4.7 and 5.3 eV. We carried out collisional–radiative (CR) calculations, using the CR model of Ref. [28], of the oxygen level populations accounting for all major kinetic process, such as electron impact excitation, deexcitation and ionization, radiative transitions, and 3-body, radiative and dielectronic recombination. For these temperature and an electron density of  $N_e = 1 \times 10^{17} \text{ cm}^{-3}$  the relative equilibrium populations of the upper level  $2s3s \ ^3P$  were found to be about  $9 \times 10^{-13}$  and  $9 \times 10^{-11}$ , respectively, of the total oxygen ion density. At the experimental conditions of Ref. [15], these relative populations are equivalent to only  $10^2$  and  $10^4$  excited ions per  $\text{cm}^3$ , and a reliable determination of line profiles for such small particle densities is at least at the very edge of modern spectroscopic techniques, if not beyond it.

The low ratio for N IV near  $N_e = 1.8 \times 10^{17} \text{ cm}^{-3}$ ,  $R \approx 1.2$ , was also measured in a linear pinch discharge plasma [17], with the electron density in this case determined by laser-interferometry and using nitrogen rather than helium as a carrier gas. Even this independent density diagnostic may be subject to systematic errors [29] because of the tendency of low-density discharges to spiral, such that the effective length for the probe beam becomes less than the inter-electrode distance. This effect would yield erroneously low electron densities for the emitting regions, i.e., cause  $R$ -values which are too high. It may also have been responsible [29] for anomalously large widths of the He II Paschen- $\alpha$  line measured by Pittman et al. [30] at similar densities and temperatures.

To summarize this discussion of the various experiments, neither additional Doppler broadening from non-thermal motions nor systematic errors in the electron density determination can be excluded. Their inclusion may well lead to a better agreement with the CCC calculations, but clearly more experiments under well-defined conditions are needed to verify this tentative conclusion.

Comparisons with other theoretical, semiclassical and semiempirical calculations, in terms of a ratio  $R_c$  of the various calculated values and our CCC results for the triplet linewidths, are plotted in Fig. 6 against the electron temperature. (The graph is split into two parts for a better visibility.) The modified semiempirical method of Dimitrijević and Konjević [31] (open symbols in Fig. 6a) generally agrees with our CCC results within 20%. This good agreement between two methods was already noticed both for the B III  $2s-2p$  and Ne VII  $2s3s-2s3p$  linewidths [6,12]. The semiclassical calculations by Hey and Breger [32,33] as well as the recent results by Hey [34] (open and shadowed symbols in Fig. 6b) are also consistent with our calculations, and the difference is again within 20%. As for the two other sets of theoretical semiclassical calculations, the linewidths calculated with Eq. (526) of Ref. [1] (solid symbols in Fig. 6b) and cited in [15] are about 50–60% higher than our results, and furthermore this difference remains practically the same for all ions considered here. The other, new semiclassical theoretical results presented in Ref. [15] (solid symbols in Fig. 6a) deviate even more, and the corresponding  $R_c$  values reach  $\sim 1.8$  for the O V linewidth.

So far, the non-perturbative semiclassical (NPSC) method of Alexiou has only been applied to calculations of the  $3-3$  linewidths in Ne VII [18]. As in several other cases, the NPSC results agreed within experimental errors with the Bochum data, and the difference with our quantum-mechanical results of Ref. [12] was about a factor of 2. However, the latest version

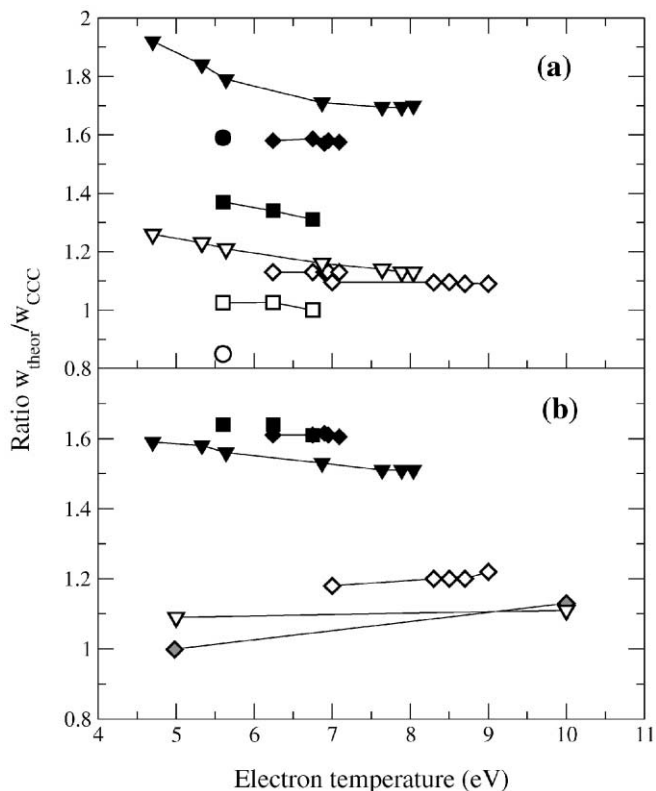


Fig. 6. Ratio of theoretical linewidths for the  $2s3s\ ^3S-2s3p\ ^3P$  transitions to the CCC linewidths (present work) vs. electron temperature. Designation of elements: B II—circles, C III—squares, N IV—diamonds, O V—triangles. (a) solid symbols—Ref. [15], open symbols—Ref. [31] (as cited in Ref. [15]); (b) solid symbols—Ref. [1] (as cited in Ref. [15]), open symbols—Refs. [32,33] (as cited in Ref. [15]), shadowed diamonds—Ref. [34].

[13] of the NPSC method, modified by dropping the long-range approximation and allowing for penetrating collisions, in fact accurately reproduces the quantal results for the B III  $2s-2p$  linewidth which *disagreed* by a factor of 2 with the experiment [7]. This new development not only exemplifies the obscurity of the present state of affairs in Stark broadening of isolated ion lines but also suggests new NPSC and other semiclassical and/or semiempirical calculations for Be-like ions.

#### 4. Conclusions

The detailed comparison of the new quantum-mechanical collisional linewidths with the available experimental and theoretical data shows that there are strong indications of the presence of (quasi-)constant extra broadening in the experimental linewidths. Besides, the measured widths may well suffer from plasma inhomogeneities. On the other hand, the existing theoretical results produced with semiclassical, semiempirical and quantum-mechanical methods show a wide

spread, which can only be studied via comprehensive step-by-step comparison of different contributions to collisional linewidths. Moreover, we would like to emphasize that the correctness of theoretical calculations should be checked not only by comparing theoretical and experimental linewidths but also by evaluating other calculated parameters, such as oscillator strengths and excitation cross sections, against recommended and/or high-quality atomic data. For example, for the B III 2s–2p line, the dominant inelastic cross section can be compared with merging beam measurement [35]. Thus, not only more experiments but also more careful calculations and analyses are required to determine the correct procedures for calculating Stark width of isolated lines.

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