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Stark broadening of B I spectral lines

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ABSTRACT

We calculated widths and shifts due to collisions with electrons, protons, and He II ions for 66 multiplets of neutral boron, using the semiclassical perturbation theory. The range of temperatures is from 2500 to 50 000 K and electron density values are within the range 10^{11}–10^{19} cm^{-3}. The obtained Stark broadening parameters have been compared to other theoretical and experimental results.

Key words: atomic data – atomic processes – line: formation.

1 INTRODUCTION

For higher electron densities in high temperature plasmas broadening of spectral lines due to interaction with electric microfield of electrons and ions surrounding emitter/absorber (Stark broadening) is the most important pressure broadening mechanism. Such conditions are often found in astrophysical plasmas where data for Stark broadening of different spectral lines are of interest (see e.g. Beauchamp, Wesemael & Bergeron 1997; Popović et al. 2001; Dimitrijević 2003; Dimitrijević & Sahal-Bréchot 2014), as well as in laboratory plasma (see for example Blagojević et al. 1999; Konjević 1999; Torres et al. 2006) and for research of inertial fusion (see e.g. Griem 1992; Iglesias et al. 1998), lasers (see e.g. Wang et al. 1992; Csillag & Dimitrijević 2004; Dimitrijević & Sahal-Bréchot 2014) and laser produced plasma (for example Nicolosi et al. 1978; Gornushkin et al. 1999; Sorge et al. 2000). Strak broadening data may be of interest and for various plasmas existing in technology (Yilbas, Patel & Karatas 2015), used for example for welding, melting, and piercing of metals by lasers, but also to design and optimise plasma light sources (see for example Hoffman, Szymański & Azharonok 2006; Dimitrijević & Sahal-Bréchot 2014).

The principal users of Stark broadening data are astronomers. Such data are needed for abudance determinations, stellar spectra analysis, and synthesis, stellar atmosphere modelling, opacity, and radiative transfer calculations, determination of cosmic plasma parameters as well as for other subjects as for example stellar spectral type determination, modelling of subphotospheric layers, and monitoring of thermonuclear reactions in stellar interiors. Data on Stark broadenig of spectral lines are very important in the case of white dwarfs research. It has been demonstrated recently the importance of Stark broadening for DO (Dimitrijević et al. 2016; Dimitrijević & Chougule 2018; Dimitrijević et al. 2018), DB (Majlinger, Dimitrijević & Simić 2018; Majlinger, Dimitrijević & Srećković 2020a,b), and DA white dwarfs (Majlinger et al. 2020a,b), as well as for B subdwarfs (Hamdi et al. 2017; Chougule et al. 2020). Stark broadening data may be of interest and for A and late B stars (Majlinger et al. 2020a,b).

Observations of B I spectral lines using Goddard High Resolution Spectrograph (GHRS) of the *Hubble Space Telescope* (*HST*) have been reported in many papers. In Duncan et al. (1997), the object of study is a boron abundance of eight stars with metallicities ranging from [Fe/H] −0.4 to −3.0, one of them – the most metal-poor star ever observed for boron. The goal is a judgment of the quality of models for Galactic chemical evolution. The obtained results support the model where most light element production is due to low energy cosmic ray spallation of C and O nuclei on to protons and α-particles. Another investigation of the nature of LiBeB origin have been presented in Fields et al. (1999). BeB-OFe trends have been observed and analysed using Population II data on O/Fe-Fe. Detailed numerical calculation of LiBeB Galactic chemical evolution have been performed. In Duncan et al. (1998), boron abundances of two Hyades giants and one dwarf, have been measured. It serves to test the predicted evolution models of main sequence stars to giant branch. The same facility (GHRS of the *HST*) has been used to determine B abundances of nine F and G dwarfs in Population I (Boesgaard et al. 1998) and for the young Orion solar-type member BD - 05° 1317 (Cunha, Smith & Lambert 1999) by observing B I region near 2497 Å. The low boron abundance is unexpected in a near-solar metallicity star and there is no simple explanation according to the authors. They put the question on the decreasing of boron abundance in interstellar gas and young stars by factor of 4–5 since the formation of Solar system.

Three light elements lithium, beryllium, and boron fall in the range between elements produced in big bang nucleosynthesis (H, He), and elements produced by stellar nucleosynthesis (heavier than ^{12}C). Five stable nuclei of LiBeB trio originate from complex mechanism of many processes that require substantial data from observations and theory (Smith, Cunha & King 2001). The unique insight on the nature of non-thermal nucleosynthesis in our Galaxy is provided by beryllium and boron (BeB) light elements (Fields et al. 2000).

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According to Thomas et al. (1993) and Delbourgo-Salvador & Vangioni-Flam (1993), these nuclei are not produced significantly in the big bang or in stellar nuclear burning since they have low binding energy. In fact, they originate from spallation processes of energetic nuclei and neutrinos. Their nucleosynthesis is encoded in their abundances in Population II stars, the most primitive metal poor ones. The evolution of spallogenic BeB reveals the history of the accelerated particles in our Galaxy. Theoretical studies on the particle acceleration propose two components of non-thermal particles that lead to different BeB evolution. The observations show that B I lines are well intense in cool stars (Cunha et al. 1999).

Recently, we have started systematical research on Stark broadening of boron spectral lines: B IV (Dimitrijević et al. 2014, 2016) and B I (Christova & Dimitrijević 2019; Christova, Dimitrijević & Sahal-Bréchot 2019, 2020). These data are available in the STARK-B database (Sahal-Bréchot, Dimitrijević & Moreau 2015a) which is a part of VAMDC – Virtual Atomic and Molecular Data Center Dubernet et al. (2010), Dubernet et al. (2016), Albert et al. (2020).

Our aim in this work is to calculate Stark broadening parameters, widths, and shifts, due to collisions with electrons, protons, and He II ions for 66 additional multiplets of neutral boron, for a grid of temperatures and perturber densities, in order to complete Stark broadening data for spectral lines of this element important particularly in astrophysics.

2 THE IMPACT SEMICLASSICAL PERTURBATION METHOD

In order to calculate Stark broadening parameters of B I spectral lines, we have used the semiclassical perturbation formalism (Sahal-Bréchot 1969a,b, 1974). For ionized atoms only, see also Sahal-Bréchot (1991), Fleurier, Sahal-Bréchot & Chapelle (1977), Dimitrijević, Sahal-Bréchot & Bommier (1991), Dimitrijević & Sahal-Bréchot (1996), Sahal-Bréchot (2021).

The basic assumptions are recalled in a more modern writing in Sahal-Bréchot, Dimitrijević & Ben Nessib (2014). In that paper, all approximations used in the semiclassical perturbation treatment for isolated lines of neutral and ionized atoms perturbed by electrons and positive ions in the impact approximation are given, as well as all the formulae entering the numerical code. The FWHM – Full Width at Half intensity Maximum (W) and the shift (d) of an isolated spectral line of a neutral atom (no Feshbach resonances in the elastic collisions contribution) is expressed by:

$$W = N \int v f(v) \mathrm{d}v \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el} \right)$$
$$\mathrm{d} = N \int v f(v) \mathrm{d}v \int_{R_3}^{R_D} 2\pi\rho \mathrm{d}\rho \sin(2\varphi_p). \quad (1)$$

In this expression, i and f are inital and final level of the corresponding transition, i' and f' are their perturbing levels, N is perturber density, υ velocity of perturber, $f(\upsilon)$ the Maxwellian velocity distribution, and ρ the impact parameter of the perturber colliding with the emitting ion.

The inelastic cross sections $\sigma_{kk'}(\upsilon)$, $k = i, f$, are provided as an integration of the transition probability $P_{kk'}(\rho, \upsilon)$, over the impact parameter ρ as:

$$\sum_{k' \neq k} \sigma_{kk'}(\upsilon) = \frac{1}{2}\pi R_1^2 + \int_{R_1}^{R_D} 2\pi\rho \mathrm{d}\rho \sum_{k' \neq k} P_{kk'}(\rho, \upsilon). \quad (2)$$

The elastic collisions are included as:

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi\rho \mathrm{d}\rho \sin^2 \delta,$$
$$\delta = \left(\varphi_p^2 + \varphi_q^2\right)^{\frac{1}{2}}. \quad (3)$$

Here, σ_{el} is the elastic cross-section, φ_p (r^{-4}), and φ_q (r^{-3}), are phase shifts produced by the polarization and quadrupolar potential. More data are in Section 3 of Chapter 2 in Sahal-Bréchot (1969a). Also, the used symmetrization procedure and different cut-offs R_1, R_2, R_3, and R_D are presented in detail in Section 1 of Chapter 3 in Sahal-Bréchot (1969b).

The line profile is determined if we know Stark width and shift, since the line profile is:

$$F(\omega) = \frac{W/(2\pi)}{(\omega - \omega_{if} - \mathrm{d})^2 + (W/2)^2}. \quad (4)$$

Here

$$\omega_{if} = \frac{E_i - E_f}{\hbar},$$

where E_i, E_f are the energies of initial and final atomic energy level, respectively. As we can see, if we know Stark broadening parameters it is easy to obtain the line profile.

3 STARK BROADENING PARAMETER CALCULATIONS

In order to perform calculations, the semiclassical perturbation theoretical approach (Sahal-Bréchot 1969a,b) has been used. As usual, we have calculated Stark broadening parameters in the case of electron-, proton-, and helium ion-impacts with neutral boron atoms, namely full width at half maximum of intensity (FWHM - W) and shift (d). We performed calculations for temperatures of 2500, 5000, 10 000, 20 000, 30 000, and 50 000 K and for a grid of perturber densities from 10^{11} to 10^{19} cm^{-3}.

Needed atomic energy levels have been taken from a critical compilation of energy levels and spectral lines of neutral boron (Kramida & Ryabtsev 2007). Concerning the needed oscillator strengths, they have been calculated using the method of Bates & Damgaard (1949), together with the tables of Oertel & Shomo (1968). In the cases when for very excited states the mentioned method of Bates & Damgaard (1949) is not convenient, the method of Van Regemorter, Hoang Binh & Prud'homme (1979) has been used.

We obtained Stark broadening parameters for 66 multiplets of neutral boron and they are presented online, as the supplementary material, in Tables S1– S9 in electronic, computer readable form, for a grid of perturber densities (10^{11} cm^{-3}, Table S1 – 10^{19} cm^{-3}, Table S9) and temperatures (2500–50 000 K). An example of the content of Tables S1– S9, is shown in Table 1, in order to show how the data in supplementary material are presented.

We also draw attention that the wavelengths given in Tables 1 and S1 – S9 are calculated from atomic energy levels and may differ from the experimentally determined. For some purposes, it is better to express Stark broadening parameters in angular frequency units. Namely, if expressed in angular frequency units, they depend on relative positions of atomic energy levels, and not on their absolute positions. One can transform Stark width in Å in angular frequency with the help of the following formula:

$$W(\text{Å}) = \frac{\lambda^2}{2\pi c} W(s^{-1}), \quad (5)$$

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Table 1. This table gives electron-, proton-, and helium ion-impact broadening parameters for B I lines. Calculated wavelength of the transitions (in Å) and parameter C are also given. This parameter, when divided with the corresponding Stark width, gives an estimate for the maximal pertuber density for which the line may be treated as isolated. The Stark broadening parameters for 66 B I multiplets are available in its entirety in machine-readable form in the online journal as additional data. Results for perturber densities 10^{11} cm^{-3}–10^{19} cm^{-3} are in Tables S1– S9 in additional data. In all Tables, temperatures are from 2500 to 50 000 K. A positive shift is towards the red part of the spectrum. A portion, for a perturber density of 10^{15} cm^{-3} is shown here for guidance regarding its form and content.

Transition	T(K)	Electrons Width(A)	Shift(A)	Protons Width(A)	Shift(A)	Ionized Width(A)	Helium Shift(A)
B I 3s - 3p	2500.	0.185E-01	0.920E-02	0.943E-02	0.236E-02	0.937E-02	0.193E-02
	5000.	0.199E-01	0.956E-02	0.948E-02	0.267E-02	0.941E-02	0.219E-02
11664.0 A	10000.	0.242E-01	0.930E-02	0.955E-02	0.301E-02	0.945E-02	0.248E-02
C= 0.84E+19	20000.	0.325E-01	0.661E-02	0.964E-02	0.339E-02	0.950E-02	0.279E-02
	30000.	0.393E-01	0.542E-02	0.970E-02	0.363E-02	0.954E-02	0.299E-02
	50000.	0.483E-01	0.453E-02	0.980E-02	0.396E-02	0.960E-02	0.326E-02
B I 3s - 4p	2500.	0.242E-01	0.151E-01	0.101E-01	0.398E-02	0.987E-02	0.323E-02
	5000.	0.278E-01	0.176E-01	0.103E-01	0.457E-02	0.100E-01	0.374E-02
5634.7 A	10000.	0.323E-01	0.188E-01	0.106E-01	0.521E-02	0.102E-01	0.427E-02
C= 0.70E+18	20000.	0.385E-01	0.180E-01	0.109E-01	0.590E-02	0.104E-01	0.485E-02
	30000.	0.429E-01	0.154E-01	0.112E-01	0.634E-02	0.106E-01	0.521E-02
	50000.	0.492E-01	0.128E-01	0.115E-01	0.692E-02	0.108E-01	0.569E-02

Table 2. This table gives the comparison of electron-impact widths and shifts in this work and those published by Griem (1974). The electron density is 10^{16} cm^{-3}.

TRANSITION	T(K)	WSCP(A)	dSCP(A)	WG(A)	dG(A)
B I 3s - 3p	5000.	0.199	0.948E-01	0.123	0.107
11664.0 A	10000.	0.242	0.927E-01	0.164	0.107
	20000.	0.325	0.660E-01	0.222	0.960E-01
	40000.	0.444	0.500E-01	0.287	0.774E-01
B I 2p - 3s	5000.	0.624E-02	0.537E-02	0.426E-02	0.507E-02
2498.2 A	10000.	0.746E-02	0.630E-02	0.487E-02	0.582E-02
	20000.	0.841E-02	0.708E-02	0.556E-02	0.628E-02
	40000.	0.900E-02	0.710E-02	0.631E-02	0.617E-02
B I 3p - 4s	5000.	1.57	1.13	1.29	1.52
15632.1 A	10000.	1.74	1.24	1.50	1.63
	20000.	2.01	1.25	1.72	1.59
	40000.	2.31	0.984	1.91	1.41
B I 3p - 5s	5000.	1.58	1.17	1.48	1.74
8670.5 A	10000.	1.70	1.23	1.71	1.81
	20000.	1.87	1.21	1.93	1.71
	40000.	2.12	0.973	2.05	1.47
B I 3p - 3d	5000.	0.769	0.303	0.455	0.374
16247.7 A	10000.	0.923	0.294	0.600	0.353
	20000.	1.20	0.228	0.793	0.305
	40000.	1.57	0.188	1.00	0.245

where c is the speed of light. In the case that we have say Stark width of the multiplet and want to scale it to the width of a particular line within this multiplet we can do this (and similarly for the shift) using the relation:

$$W_{cor} = \left(\frac{\lambda_{\rm exp}}{\lambda}\right)^2 W. \quad (6)$$

Here, W_{cor} is the corrected width, λ_{exp} is the wavelength of the needed line within multiplet, λ the wavelength of multiplet, and W the width from Tables in this paper.

In order to show the limits of validity of our results we included in Tables S1– S9 and 1 the quantity C (Dimitrijević & Sahal-Bréchot 1984). This quantity divided by the corresponding width (W) shows the maximal perturber density when the line may be considered as isolated. We also checked the validity of impact approximation calculating the value of NV, where V is the collision volume and N the perturber density. If $NV < 0.1$, the impact approximation is valid (Sahal-Bréchot 1969a,b).

We excluded from tables the cases when $NV > 0.5$, since then the impact approximation is not valid. When the violation of impact approximation is more or less tolerable, for $0.1 < NV \leq 0.5$ we put an asterisk before the corresponding Stark broadening parameter in order to draw attention that this value is on the limit of validity of impact approximation.

Since ion perturbers are heavier, the impact approximation is more often questionable for them. When it is not valid, a formula of Griem (1974), Sahal-Bréchot (1991) within the quasi-static approach may be used. We note also that in the case of intermediate conditions

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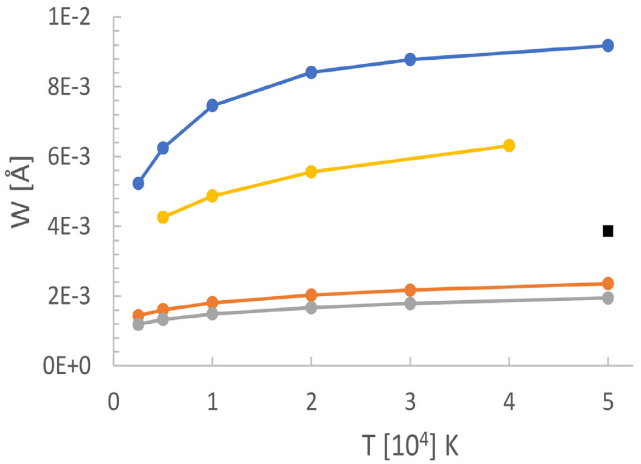

Figure 1. Stark widths for multiplet B I $2p^2P^o$ - $3s^2S$ (2498.2 Å) versus temperature due to collisions with: Electrons – blue line; protons – red; ionized helium ions – grey. Electron-impact width calculated by Griem (1974) (in yellow) and width measured by Djeniže et al. (1992) (black square) are added also. Electron density is 10^{16} cm^{-3}.

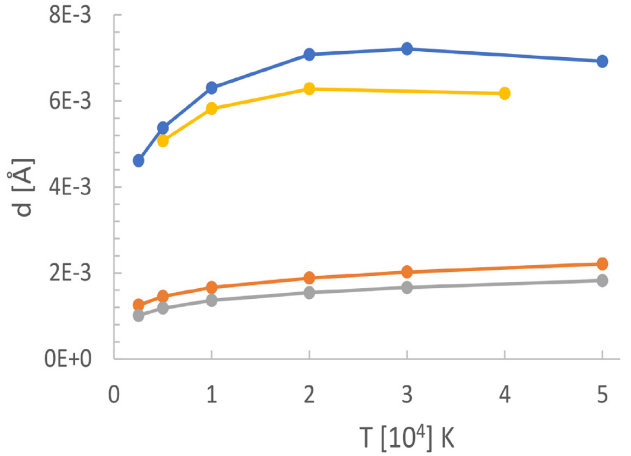

Figure 2. Stark shifts for multiplet B I $2p^2P^o$ - $3s^2S$ (2498.2 Å) versus temperature due to collisions with: Electrons – blue line; protons – red; ionized helium ions – grey. Electron-impact shifts calculated by Griem (1974) (in yellow) is added also. Electron density is 10^{16} cm^{-3}.

between the impact and quasi-static approximation, we recommend the use of unified-type theories, as for example of Barnard, Cooper & Smith (1974).

The validity and accuracy of the semiclassical perturbation method was analysed in detail in various Workshops on Spectral Line Shapes in Plasma Code Comparison (Sahal-Bréchot et al. 2018). Since the spectrum of neutral boron is not complex, we consider that the error bars of Stark widths are within the limits of 20 per cent. For the shifts, where different contributions have different signs and mutual cancellations can occur, we consider that the error is within the limits of 20 per cent of the width value.

In Table 2, our results for Stark widths and shifts are compared with those published by Griem (1974). One can see that the agreement is better for widths than for shifts. Our results for widths are higher than those of Griem (1974). For shifts the agreement is better for small temperatures and for higher temperatures become worse.

Stark broadening parameters as a function of the temperature for the B I multiplet $2p^2P^o$ - $3s^2S$ (2498.2 Å) are illustrated in Figs 1 and 2. One can see that the width increases for low temperatures. This is due to the fact that the inelastic excitation cross-sections are zero before and at the threshold, and begin to increase as the velocity of the incident electron increases (Seaton 1962a, b) and then decrease at high energies as given by the Born or semi-classical expressions (Sahal-Brechot et al 2014). So, depending on the temperature and on the importance of the different cross sections entering the calculation of the line width, we can have an increase or a decrease of the width.

In Fig. 1, our results for electron-impact width (FWHM) are compared with the semiclassical results of Griem (1974) and experimental Stark width of Djeniže et al. (1992), at an electron density of 10^{16} cm^{-3}. Additionally, Stark widths due to collisions with protons, and He^+ ions are compared with the width due to impacts with electrons. Electron-impact width predominates both others. Its values are 3–4 times greater from both other contributions, in the whole examined range of temperatures. The semiclassical data from Griem (1974) are lower than ours. We found only one experimental result for this multiplet (Djeniže et al. 1992), which is smaller from both calculations. The ratio of experimental and theoretical widths is 0.63 for the semiclassical result of Griem (1974) (see Konjević et al. 2002) and 0.42 for our result. Fig. 2 displays the Stark shifts for the same multiplet. All shifts are positive, red shift. Electron-impact shift is a dominant and slowly decreases for temperatures above 30 000 K. Griem's (1974) values are closer to them.

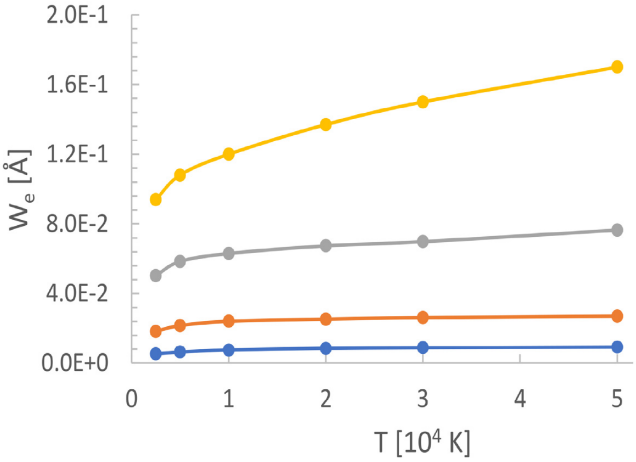

Figure 3. Electron-impact widths for multiplets of B I 2p – ns series versus temperature: 3 s – blue; 4 s – red; 5 s – grey; 6 s – yellow. Electron density is 10^{16} cm^{-3}.

Electron-impact widths for multiplets of B I 2p - ns (n = $3P^o$–6) series versus temperature are given in Fig. 3. The width increases 5 times for lower temperatures up to 7 times for higher T-values within a series. The behaviour of electron-impact shift for the same spectral series is examined on Fig. 4. All shifts are positive. There is a weak increase – from 2500 to 10 000 K, which is notable for multiplets originated from higher energy levels, and in particular for n = 6. For initial energy levels with small principal quantum numbers, the shifts are almost constant for temperatures above 10 000 K, while for others – a weak decrease is observed.

4 CONCLUSION

Using the semiclassical perturbation theoretical approach (Sahal-Bréchot 1969a,b), we have calculated new Stark widths and shifts in the case of electron-, proton-, and helium ion-impacts for 66 B I multiplets for temperatures from 2500 up to 50 000 K and for

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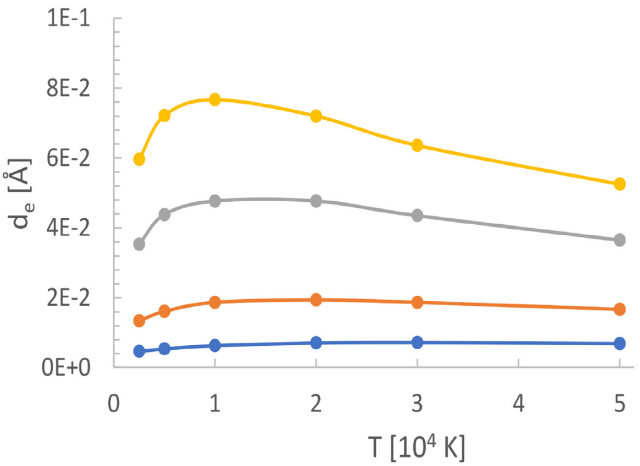

Figure 4. Electron-impact shifts for multiplets of B I 2p – ns series versus temperature: 3s – blue; 4 s – red; 5 s – grey; 6 s – yellow. Electron density is 10^{16} cm^{-3}.

perturber densities from 10^{11} to 10^{19} cm^{-3}. The obtained results are compared when possible with theoretical results of Griem (1974) and with experimental results of Djeniže et al. (1992) but these results exist only for several spectral lines and there is no others.

The obtained Stark broadening parameters for spectral lines of neutral boron results are of interest particularly for astrophysical problems like analysis and synthesis of stellar spectra, modelling of stellar atmospheres, radiative transfer calculations etc. These data are also of interest for laboratory plasma investigations and diagnostics.

Stark widths and shifts for B I spectral lines presented here will be included in the STARK-B database (Sahal-Bréchot 2010; Sahal-Bréchot, Dimitrijević & Moreau 2012; Sahal-Bréchot et al. 2015a,b), which enters in [VAMDC - (Dubernet et al. 2010; Rixon et al. 2011; Dubernet et al. 2016; Albert et al. 2020)]. A link to STARK-B is also in the Serbian Virtual Observatory [SerVO, http:servo.aob.rs, Jevremović et al. (2009), Jevremović et al. (2012)].

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DATA AVAILABILITY

The data underlying this article are available in the article and in its online supplementary material.

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SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

Table S1.
Table S2.
Table S3.
Table S4.
Table S5.
Table S6.
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