Stark broadening of B IV lines for astrophysical and laboratory plasma research

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Abstract

Stark broadening parameters for 36 multiplets of B IV have been calculated using the semi-classical perturbation formalism. Obtained results have been used to investigate the regularities within spectral series and temperature dependence.

Keywords: atomic data; atomic processes; line: profiles; stars: atmospheres

1. Introduction

The study presents Stark broadening parameters (widths and shifts) of B IV spectral lines which have been determined using the semi-classical perturbation formalism (Sahal-Bréchot, 1969a,b). Data on boron lines are of interest in astrophysics, astrochemistry, and cosmology, in technological plasma research, for thermonuclear reaction devices, and for laser produced plasma investigations. For abundance determinations of boron and modelling, and analysis of stellar plasma it is necessary to have reliable atomic and spectroscopic data, including Stark broadening parameters. This enables to provide data on the astrophysical processes that can both produce and destroy this rare element. Namely, the light elements lithium, beryllium, and boron (LiBeB) are sensitive probes of stellar models due to the fact that the stable isotopes of all three consist of nuclei with small binding energies that are destroyed easily by (p, a) reactions at modest temperatures (Cunha & Smith, 1999). The origin and evolution of boron are of special interest because it is hardly produced by the standard big bang nucleosynthesis (BBN), and cannot be produced by nuclear fusions in stellar interiors (Tankošić et al., 2003). The cosmic abundance of $^{11}$B is of major importance for the model of Galactic chemical evolution (GCE) (Ritchey et al., 2011). Ritchey et al. (2011) concluded that a major portion of the cosmic abundance of $^{11}$B can be attributed to neutrino nucleosynthesis. Thus, it is necessary to accurately describe the stellar evolution, and the formation of elements, which are closely connected. To make progress in these developments chemical abundances are crucial parameters to be determined. This needs an accurate interpretation of the detailed line spectra of the stellar objects. In order to provide the data needed in astrophysics, laboratory-, technological-, fusion-, and laser produced-plasma research, our aim is to determine here Stark broadening parameters (full widths at half intensity and shifts) for 36 B IV multiplets. Obtained results will be also used for the consideration of regularities within spectral series and temperature dependence of Stark broadening parameters.

2. Theory of Stark broadening in the impact approximation

Pressure broadening of spectral lines arises when an atom, ion, or molecule which emits or absorbs light in a gas or plasma, is perturbed by its interactions with the other particles of the medium. Interpretation of this phenomenon is currently used for modelling of the medium and for spectroscopic diagnostics, since the broadening of the lines depends on the temperature and density of the medium. The physical conditions in the Universe are very various, and collisional broadening with charged particles (Stark broadening) appears to be important in many domains. For example, at temperatures around $10^4$ K and densities $10^{13} - 10^{15}$ cm$^{-3}$, Stark broadening is of interest for modelling and analysing spectra of A and B type stars: see e.g. Lanz et al. (1988), Popović et al. (2001a,b, 1999a,b), Tankošić et al. (2003), Simić et al. (2005), Sahal-Bréchot (2010). Especially in white dwarfs, Stark broadening is the dominant collisional line broadening mechanism in all important layers of the atmosphere (Popović et al., 1999b; Tankošić et al., 2003; Simić et al., 2006; Hamdi et al., 2008; Simić et al., 2009; Dimitrijević et al., 2011;
Dufour et al., 2011; Larbi-Terzi et al., 2012). The theory of Stark broadening is well applied, especially for accurate spectroscopic diagnostics and modelling. This requires the knowledge of numerous profiles, especially for trace elements, as boron in this case, which are used as useful probes for modern spectroscopic diagnostics. Interpretation of the spectra of white dwarfs, which are very faint, allows understanding the evolution of these very old stars, which are close to death. The results for Stark broadening parameters of 36 BIV multiplets have been calculated using the semi-classical perturbation formalism (Sahal-Bréchot, 1969a,b). Within this theory the full half width (W) and the shift (d) of an isolated line originating from the transition between the initial level i and the final level f is expressed as:

\[
W = n_e \int_0^{\infty} v f(v) dv [\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el}],
\]

\[
d = n_e \int_0^{\infty} v f(v) dv \int_{R_1}^{R_2} 2\pi \rho d\rho \sin 2\phi_p,
\]

where \(i'\) and \(f'\) are perturbing levels, \(n_e\) and \(v\) are the electron density and the velocity of perturbers respectively, and \(f(v)\) is the Maxwellian distribution of electron velocities.

The inelastic cross sections \(\sigma_{ii'}(v)\) (respectively \(\sigma_{ff'}(v)\)) can be expressed by an integration of the transition probability \(P_{ii'}\) over the impact parameter \(\rho\):

\[
\sum_{i' \neq i} \sigma_{ii'}(v) = \frac{1}{2} \pi R_1^2 + \int_{R_1}^{R_2} 2\pi \rho d\rho \sum_{i' \neq i} P_{ii'}(\rho, v).
\]

The elastic collision contribution to the width is given by:

\[
\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 8\pi \rho d\rho \sin^2 \delta + \sigma_{r},
\]

\[
\delta = (\phi_p^2 + \phi_\Omega^2)^{1/2}.
\]

The phase shifts \(\phi_p\) and \(\phi_\Omega\) are due to the polarization and quadrupole potential respectively. The cut-off parameters \(R_1, R_2, R_3\), the Debye cut-off \(R_D\) and the symmetrization procedure are described in the above mentioned papers. The contribution of Feshbach resonances, \(\sigma_r\), is described in Fleurier et al., (1977). In the following, the collisions of emitters with electrons, protons and ionized helium are examined, and the contribution of different perturbers in total Stark broadening parameters are discussed.

3. Results and discussion

In this paper, Stark broadening widths (FWHM) and shifts for 36 BIV multiplets have been calculated using the semiclassical perturbation formalism (Sahal-Bréchot, 1969a,b) and presented in Table 1. Since the Stark broadening widths and shifts are the same for spectral lines within a multiplet when expressed in angular frequency units for a simple spectrum like the B IV one, it is easy to obtain their values in Angströms or nanometers (see e.g. Eqs. 7 and 8 in Hamdi et al. (2013)). In particular, the spectral line broadening due to interactions of the emitters with electrons, protons and singly charged helium ions as perturbers has been examined.

Calculations have been performed using experimental values of energy levels in Kramida et al. (2008). The oscillator strengths have been calculated using the Coulomb approximation method Bates & Damgaard (1949) and the tables of Oertel & Shomo (1968), while for higher levels, the method described by Van Regemorter et al. (1979) has been applied. The asterisks in Table 1 indicate that the impact approximation reaches the limit of validity.

The temperature dependences of Stark widths and shifts for the 1s2p\(^1\)P\(^o\) – 1s3s\(^1\)S, 1s2p\(^1\)P\(^o\) – 1s3d\(^1\)D, 1s3p\(^1\)P\(^o\) – 1s4s\(^1\)S and 1s3p\(^1\)P\(^o\) – 1s4d\(^1\)D transitions at an electron density of \(10^{17}\) cm\(^{-3}\) have been presented in Fig. 1 and Fig. 2, respectively. The first two transitions have the same lower energy level 2p where both, the width and shift of 2p – 3s are larger than the Stark parameters of 2p – 3d. For the other transitions with the same 3p lower energy level, 3p – 4d transition has larger width, while 3p – 4s has larger shift. For all of them, the width and shift due to electrons decrease slowly for temperature values above 100 000 K.

In Fig. 3 and Fig. 4, the temperature dependences of proton-impact widths and shifts, respectively, are shown. One can see that both widths and shifts slowly increase with the temperature. For proton-impact broadening for B IV 3p – 4d transition the impact approximation is not valid at an electron density of \(10^{17}\) cm\(^{-3}\) within the whole interval of the considered temperatures and they are not included in the figures.

The dependence of the broadening parameters of spectral lines due to impacts with charged particles versus principal quantum number within a spectral series is an important information. If we know the trend of Stark broadening parameters within a spectral series, it is possible to interpolate or extrapolate the eventually missing values within the considered series. The regular behavior of Stark broadening widths and shifts versus principal quantum number within spectral series is presented in Fig. 5 and Fig. 6. The both parameters increase with principal quantum number which reflects the decrease of the distance to the nearest perturbing levels with the increase of the principal quantum number.
Table 1: Stark broadening parameters for singlet B IV multiplets for a perturber density of $10^{17}$ cm$^{-3}$ and temperatures from 20 000 to 500 000 K. The width (FWHM) $W$ and shift $d$ (a positive shift is towards the red) values from different perturbers are given in (Å) for 36 multiplets. The ratio of the included parameter $C$ versus the corresponding Stark width gives an estimate of the maximal perturber density for which the line may be treated as isolated. The asterisks indicate that the impact approximation reaches the limit of validity.

| Transition | T(K)  | $W_e$(Å) | $d_e$(Å) | $W_p$(Å) | $d_p$(Å) | $W_{He^+}$(Å) | $d_{He^+}$(Å) |
|-----------|------|---------|---------|---------|---------|-------------|-------------|
| B IV 2p-3d | 20000 | 0.044E-02 | 0.11E-03 | 0.246E-02 | 0.345E-02 | 0.199E-02 | 0.245E-02 |
|           | 50000 | 0.108E-02 | 0.11E-03 | 0.492E-02 | 0.579E-02 | 0.304E-02 | 0.424E-02 |
| C= 0.24E+18 | 100000 | 0.212E-02 | 0.11E-03 | 0.785E-02 | 0.859E-02 | 0.428E-02 | 0.506E-02 |
|           | 200000 | 0.706E-02 | 0.11E-03 | 0.318E-02 | 0.393E-02 | 0.189E-02 | 0.227E-02 |
| B IV 2p-4d | 20000 | 0.581E-02 | 0.221E-03 | 0.309E-02 | 0.385E-02 | 0.208E-02 | 0.239E-02 |
|           | 50000 | 0.451E-02 | 0.308E-03 | 0.275E-02 | 0.349E-02 | 0.208E-02 | 0.239E-02 |
| C= 0.17E+16 | 100000 | 0.369E-02 | 0.288E-03 | 0.349E-02 | 0.421E-02 | 0.297E-02 | 0.328E-02 |
|           | 200000 | 0.298E-02 | 0.365E-03 | 0.349E-02 | 0.421E-02 | 0.297E-02 | 0.328E-02 |

B IV 2p-5d

B IV 2p-6d

B IV 2p-7d

B IV 3p-4d

B IV 3p-5d

B IV 3p-6d

B IV 3p-7d

B IV 4p-5d

B IV 4p-6d

B IV 4p-7d

B IV 5p-6d

B IV 5p-7d

B IV 6p-7d

B IV 7p-8d

B IV 8p-9d
| Transition | T(K) | W_e (˚A) | d_e (˚A) | W_p (˚A) | d_p (˚A) | W_{He}+ (˚A) | d_{He}+ (˚A) |
|------------|------|----------|----------|----------|----------|--------------|--------------|
| B IV 3d-4p | 20000 | 0.105 | -0.806E-02 | 0.122E-01 | -0.128E-01 | *0.115E-01 | *-0.104E-01 |
| 1163.5 Å | 50000 | 0.768E-01 | -0.843E-02 | 0.193E-01 | -0.181E-01 | *0.163E-01 | *-0.151E-01 |
| C= 0.76E+18 | | | | | | | |
| | 100000 | 0.615E-01 | -0.783E-02 | 0.255E-01 | -0.222E-01 | *0.209E-01 | *-0.184E-01 |
| | 200000 | 0.496E-01 | -0.691E-02 | 0.324E-01 | -0.252E-01 | 0.251E-01 | -0.210E-01 |
| | 300000 | 0.438E-01 | -0.613E-02 | 0.377E-01 | -0.271E-01 | 0.281E-01 | -0.226E-01 |
| | 500000 | 0.375E-01 | -0.506E-02 | 0.448E-01 | -0.300E-01 | 0.330E-01 | -0.254E-01 |
| B IV 3d-5p | 20000 | 0.121 | -0.988E-02 | | | | |
| 798.8 Å | 50000 | 0.911E-01 | -0.103E-01 | *0.302E-01 | -0.265E-01 | | |
| C= 0.18E+18 | 100000 | 0.737E-01 | -0.921E-02 | *0.391E-01 | -0.314E-01 | | |
| | 200000 | 0.596E-01 | -0.881E-02 | *0.474E-01 | -0.357E-01 | *0.367E-01 | -0.305E-01 |
| | 300000 | 0.526E-01 | -0.749E-02 | *0.524E-01 | -0.394E-01 | *0.404E-01 | -0.315E-01 |
| | 500000 | 0.448E-01 | -0.601E-02 | *0.662E-01 | -0.429E-01 | *0.466E-01 | -0.361E-01 |
| B IV 3d-6p | 20000 | 0.174 | -0.139E-01 | | | | |
| 682.5 Å | 50000 | 0.210 | -0.197E-01 | | | | |
| C= 0.77E+17 | 100000 | 0.113 | -0.133E-01 | | | | |
| | 200000 | 0.925E-01 | -0.140E-01 | | | | |
| | 300000 | 0.817E-01 | -0.118E-01 | | | | |
| | 500000 | 0.697E-01 | -0.923E-02 | | | | |
| B IV 3d-7p | 20000 | 0.257 | -0.183E-01 | | | | |
| 627.3 Å | 50000 | 0.210 | -0.197E-01 | | | | |
| C= 0.40E+17 | 100000 | 0.113 | -0.133E-01 | | | | |
| | 200000 | 0.925E-01 | -0.140E-01 | | | | |
| | 300000 | 0.817E-01 | -0.118E-01 | | | | |
| | 500000 | 0.697E-01 | -0.923E-02 | | | | |
| B IV 3d-6p | 20000 | 0.111 | -0.843E-01 | | | | |
| 1350.9 Å | 50000 | 0.877 | -0.907E-01 | | | | |
| C= 0.32E+17 | 100000 | 0.727 | -0.829E-01 | | | | |
| | 200000 | 0.594 | -0.893E-01 | | | | |
| | 300000 | 0.524 | -0.749E-01 | | | | |
| | 500000 | 0.446 | -0.586E-01 | | | | |
| B IV 3d-7p | 20000 | 1.11 | -0.881E-01 | | | | |
| 1350.9 Å | 50000 | 0.113 | -0.923E-01 | | | | |
| C= 0.32E+17 | 100000 | 0.727 | -0.829E-01 | | | | |
| | 200000 | 0.594 | -0.893E-01 | | | | |
| | 300000 | 0.524 | -0.749E-01 | | | | |
| | 500000 | 0.446 | -0.586E-01 | | | | |
| B IV 3d-6p | 20000 | 0.111 | -0.749 | | | | |
| 4623.3 Å | 50000 | 0.594 | -0.893E-01 | | | | |
| C= 0.27E+18 | 100000 | 0.727 | -0.829E-01 | | | | |
| | 200000 | 0.594 | -0.893E-01 | | | | |
| | 300000 | 0.524 | -0.749E-01 | | | | |
| | 500000 | 0.446 | -0.586E-01 | | | | |
| B IV 3d-7p | 20000 | 0.68 | -0.436 | | | | |
| 2697.7 Å | 50000 | 0.594 | -0.893E-01 | | | | |
| C= 0.11E+18 | 100000 | 0.409E-01 | -0.373E-03 | | | | |
| | 200000 | 0.347 | 0.817E-01 | -0.691E-03 | | | |
| | 300000 | 0.220 | 0.170E-02 | -0.170E-02 | | | |
| 627.3 Å | 50000 | 0.190 | 0.148E-02 | | | | |
| C= 0.67E+15 | 100000 | 0.162 | 0.133E-02 | | | | |
| | 200000 | 0.133 | 0.301E-03 | | | | |
| | 300000 | 0.118 | 0.872E-03 | | | | |
| 500000 | 0.998E-01 | 0.103E-02 | | | | |
| Transition | T(K)     | $W_e$(Å) | d_e(Å) | $W_p$(Å) | d_p(Å) | $W_{He}^+(A)$ | d_{He}^+(Å) |
|------------|----------|----------|--------|----------|--------|--------------|------------|
| B IV 4d-5f| 200000   | 1.08     | -0.50E-02 |          |        |              |            |
| 2530.1 Å  | 500000   | 0.900    | -0.156E-01 |          |        |              |            |
| C= 0.21E+17 | 1000000  | 0.753    | -0.134E-01 |          |        |              |            |
|           | 2000000  | 0.615    | -0.304E-01 |          |        |              |            |
|           | 3000000  | 0.542    | -0.225E-01 |          |        |              |            |
|           | 5000000  | 0.469    | -0.116E-01 |          |        |              |            |
| B IV 4d-6f| 200000   | 0.920    | 0.264E+02  |          |        |              |            |
| 1639.7 Å  | 500000   | 0.775    | -0.399E-02 |          |        |              |            |
| C= 0.59E+16 | 1000000  | 0.651    | -0.334E-02 |          |        |              |            |
|           | 2000000  | 0.532    | -0.173E-01 |          |        |              |            |
|           | 3000000  | 0.468    | -0.107E-01 |          |        |              |            |
|           | 5000000  | 0.396    | -0.358E+02 |          |        |              |            |
| B IV 4d-7f| 200000   | 1.100    | 0.394E+02  |          |        |              |            |
| 1352.8 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.31E+16 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 5d-6f| 200000   | 0.950    | 0.137     |          |        |              |            |
| 4657.0 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.48E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 5d-7f| 200000   | 1.100    | 0.394E+02  |          |        |              |            |
| 1906.0 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.14E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 4f-5d| 200000   | 1.230    | 0.315E-01  |          |        |              |            |
| 2532.0 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.82E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 4f-6d| 200000   | 1.050    | 0.262E+01  |          |        |              |            |
| 1640.5 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.95E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 4f-7d| 200000   | 0.300    | 0.276E+01  |          |        |              |            |
| 1353.1 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.57E+16 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 5f-6d| 200000   | 1.103    | 0.189     |          |        |              |            |
| 3461.8 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.72E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
| B IV 5f-7d| 200000   | 0.530    | 0.328E-01  |          |        |              |            |
| 2907.4 Å  | 500000   | 0.943    | 0.187E-02  |          |        |              |            |
| C= 0.26E+17 | 1000000  | 0.802    | 0.170E-02  |          |        |              |            |
|           | 2000000  | 0.661    | -0.457E-02 |          |        |              |            |
|           | 3000000  | 0.583    | -0.760E-03 |          |        |              |            |
|           | 5000000  | 0.495    | 0.137E-02  |          |        |              |            |
4. Conclusion

New Stark broadening parameters for 36 multiplets of B IV have been determined within the frame of the semi-classical perturbation formalism. The results for Stark broadening parameters of boron lines could be applicable for the adequate interpretation of the observed spectra in astrophysics, astrochemistry, and cosmology, in technological plasma research, for thermonuclear reaction devices, and for laser produced plasma investigation. We also note that the Stark broadening data obtained in the present research, will be inserted in the STARK-B database (Sahal-Bréchot et al., 2012; Sahal-Bréchot et al., 2013), which is a part of Virtual Atomic and Molecular Data Center (VAMDC - (Dubernet et al., 2010; Rixon et al., 2010)). Additionally, it has been confirmed that the behaviour of Stark broadening parameters within B IV spectral series is regular, enabling the interpolation and extrapolation of new data.

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Figure 1: Temperature dependence of the electron impact width for B IV 1s2p1P0 - 1s3s1S, 1s2p1P0 - 1s3d2D, 1s3p1P0 - 1s4s1S and 1s3p1P0 - 1s4d1D transitions at an electron density of 1.10^{17} \text{ cm}^{-3}.

Figure 2: Temperature dependence of the electron impact shift for 1s2p1P0 - 1s3s1S, 1s2p1P0 - 1s3d2D, 1s3p1P0 - 1s4s1S and 1s3p1P0 - 1s4d1D transitions at an electron density of 1.10^{17} \text{ cm}^{-3}.

Figure 3: Temperature dependence of the proton impact width for 1s2p1P0 - 1s3s1S, 1s2p1P0 - 1s3d2D, 1s3p1P0 - 1s4s1S and 1s3p1P0 - 1s4d1D transitions at an electron density of 1.10^{17} \text{ cm}^{-3}.

Figure 4: Temperature dependence of the proton impact shift for 1s2p1P0 - 1s3s1S, 1s2p1P0 - 1s3d2D, 1s3p1P0 - 1s4s1S and 1s3p1P0 - 1s4d1D transitions at an electron density of 1.10^{17} \text{ cm}^{-3}. 
Figure 5: Principal quantum number dependence of the electron-impact width for transitions within $1s2p^1P^o - \text{1sns}^1S, 1s2p^1P^o - \text{1snd}^3D, 1s3p^1P^o - \text{1sns}^1S$ and $1s3p^1P^o - \text{1snd}^3D$ spectral series at an electron density of $1.10^{17}$ cm$^{-3}$ and $T=200000$ K.

Figure 6: Principal quantum number dependence of the electron-impact width for transitions within $1s2p^1P^o - \text{1sns}^1S, 1s2p^1P^o - \text{1snd}^3D, 1s3p^1P^o - \text{1sns}^1S$ and $1s3p^1P^o - \text{1snd}^3D$ spectral series at an electron density of $1.10^{17}$ cm$^{-3}$ and $T=200000$ K.