On the Stark broadening of N VI spectral lines

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Abstract. Results for the Stark broadening parameters for spectral lines within one spectral series of N VI 2s-np (n = 2 – 4) triplet transitions are included. Plasma conditions of interest cover temperatures from 50 000 K to 2 000 000 K, perturber density is 10^{17} cm⁻³, and electrons, and boron ions (B III, B IV, B V and B VI) are perturbers. These conditions correspond to those in laser driven plasma for proton boron fusion reaction. The contribution in Stark width and shift of different types of perturbers is analyzed. The width versus principal quantum number is presented.

Key words: Stark broadening – spectral line shapes – atomic data – N $\rm VI$ – proton-boron fusion

1. Introduction

Stark broadening data, or data for broadening by collisions with charged particles, are of interest in many research topics. They are particularly needed for astrophysical plasma research, but also for laboratory plasma diagnostics, for fusion plasma, laser research and for various plasmas in technology.

Data for Stark broadening of five times charged nitrogen ion (N VI) spectral lines are important particularly for investigation of white dwarfs where N VI lines are present (see e.g. Rauch 2007) and Stark broadening is the dominant pressure broadening mechanism. Reliable data for Stark broadening of N VI are also of interest for proton-boron fusion plasma since in a number of investigations (see e,g, Margarone *et al.*, 2015; Giuffrida *et al.*, 2020; Istokskaia *et al.*, 2023) the target is boron nitride (BN).

Fusion reaction is known in the universe as the dominant energy source that occurs in the stellar interiors. Several international and national projects as the International Thermonuclear Energy Reactor (ITER), and the National Ignition Facility (NIF) perform continuous efforts to obtain controlled fusion reaction device in laboratory. Using the semiclassical perturbation theory (see for example Sahal-Bréchot *et al.*, 2014 and references therein), we calculated Stark widths and shifts, determining line profile, for 15 multiplets containing 33 spectral lines of N VI broadened by collisions with the most important charged constituents of stellar and proton-boron fusion plasma: electrons, protons, alpha particles, B III, B IV, B V and B VI ions. Calculations have been performed for a grid of temperatures and perturber densities. The obtained results will be also prepared in VO (Virtual Observatory) and XSAMS (XML Schema for Atomic, Molecular and Solid Data) format for the implementation of results in the international, on-line database STARK-B (Sahal-Bréchot *et al.* 2015 - https://stark-b.obspm.fr/) a part of VAMDC (Virtual Atomic and Molecular Data Center, Dubernet *et al.*, 2010), after the publication of the main article.

In this contribution we will present and discuss a part of the results which will be published in entirety elsewhere (Dimitrijević, Christova and Sahal-Bréchot, 2023).

2. The impact semiclassical perturbation method

Spectral line profiles of detected emitted or absorbed spectral lines ensure important data for the interactions between emitters and surrounding particles. As a result of these interactions in the plasma environment, the profiles are broadened and shifted. The degree of profile's change depends on temperature and density. This plasma phenomenon is known in the theory as pressure broadening mechanism. Pressure broadening can be provoked by interactions with charged particles and due to interactions with neutral atoms. In the case of interactions between emitters and charged particles (electrons, protons, ions), pressure broadening is named Stark broadening. In this work, we investigate Stark broadening parameters of several spectral lines belonging to N VI transitions. This study is first of all oriented for application in laser driven proton boron plasma, but also and for astrophysical purposes. The semiclassical perturbation theory (Sahal-Bréchot, 1969 a,b) is applied. This theory is developed for the case of an isolated, non-hydrogenic spectral line which full width at half maximum (FWHM) and shift are expressed as:

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

where the indexes i and f concern the initial and final level of a given transition; i' and f' are the corresponding perturbing levels, respectively. N is electron density, v perturber velocity, f(v) represents the Maxwellian distribution of electron velocities, and ρ is the perturber's impact parameter. The cross sections for inelastic collisions $\sigma_{kk'}(v)$, k = i, f, could be written by an integration of the transition probability $P_{kk'}(\rho, v)$, over the impact parameter ρ :

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

The following two equations estimate the cross section of elastic collisions between emitters and charged particles:

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi \rho d\rho \sin^2 \delta + \sigma_r,$$

$$\delta = (\varphi_p^2 + \varphi_q^2)^{\frac{1}{2}}.$$
 (3)

where δ denotes the phase shift due to polarization (φ_p (r^{-4})) and quadrupole (φ_q (r^{-3})) potentials for atom-perturber elastic interactions. The details for cut-off parameters R_1 , R_2 , R_3 , the Debye cut-off R_D and the symmetrization are explained in Sahal–Bréchot (1969 b) (Section 1 of Chapter 3). The term σ_r gives the contribution of Feshbach resonances (Sahal–Bréchot, 2021).

3. Results and Discussion

Two main research fields where Stark broadening data for N VI spectral lines are needed are first of all white dwarfs, where Stark broadening is the dominant pressure broadening mechanism and N VI lines are present in their spectra. The other research field is the proton-boron fusion experiments, where nitrogen is an important target. In order to satisfy the needs of both fields, we have calculated, using the semiclassical perturation method (Sahal-Bréchot, 1969 a, b; Sahal-Bréchot et al., 2014). Stark broadening of spectral lines within 15 multiplets of N VI. The temperature values are in a wide interval from 50 000 K to 2 000 000 K and perturber densities from 10^{17} cm⁻³ to 10^{24} cm⁻³. Broadening due to collisions with electrons, protons, alpha particles and boron ions in different degrees of ionization (B III, B IV, B V and B VI), charged particles of interest for white dwarfs and proton-boron fusion, are examined. The complete results will be published in entirety elsewhere (Dimitrijević, Christova and Sahal-Bréchot, 2023). Here, in Tables 1-2 are presented line widths and in Tables 3-4 shifts of three lines within one spectral series, for all examined temperatures and for perturber density 10^{17} cm⁻³. These lines belong to triplets N VI 2s-2p, 1901.5 Å; N VI 2s-3p, 161.2 Å; N VI 2s-4p, 122.4 Å. These results are used for discussion of systematic trend of Stark widths within a spectral series and for comparison and analysis of the influence of different perturbers. The parameter C (Dimitrijević, Sahal-Bréchot, 1984), provided in Tables 1-4, when divided by the corresponding width (W), gives the maximal perturber density for which the line may be considered as isolated.

Transition	T[K]	We	WBIII	WBIV
N VI 2s-2p	50000.	0.730E-02	0.205E-04	0.206E-04
1901.5 A	100000.	0.523E-02	0.729E-04	0.780 E-04
C = 0.19E + 21	300000.	0.321E-02	0.365E-03	0.483 E-03
	500000.	0.259E-02	0.549E-03	0.790 E- 03
	1000000.	0.198E-02	0.852E-03	0.136E-02
	2000000.	0.155E-02	0.111E-02	0.178E-02
N VI 2s-3p	50000.	0.199E-03	0.500E-05	0.552E-05
161.2 A	100000.	0.147 E-03	0.113E-04	0.140 E-04
C = 0.19E + 18	300000.	0.959E-04	0.241E-04	0.352 E-04
	500000.	0.800E-04	0.289E-04	0.442 E-04
	1000000.	0.634E-04	0.350E-04	0.560 E-04
	2000000.	0.511E-04	0.405E-04	0.679 E-04
N VI 2s-4p	50000.	0.337E-03	0.295E-04	0.394E-04
122.4 A	100000.	0.258E-03	0.480 E-04	0.694 E-04
C = 0.48E + 17	300000.	0.177 E-03	0.743E-04	0.120E-03
	500000.	0.150E-03	0.854 E-04	0.141E-03
	1000000.	0.121E-03	0.105E-03	0.174 E-03
	2000000.	0.979E-04	0.124 E-03	0.193E-03

Table 1. Stark full widths (Å) at half intensity maximum of N VI spectral lines due to interactions with electrons, B III and B IV ions. The presented lines belong to triplets within one spectral series. The perturber density is 10^{17} cm⁻³.

To investigate the width's behavior in the spectral series we give Stark widths *versus* principal quantum number. To eliminate the influence of the wavelength, the broadening is given in angular frequency units in Fig. 1 for 300 000 K and electron density 10^{20} cm⁻³. This dependence is in accordance with the theory that spectral lines originated from higher transitions are more broadened. This systematic trend could be useful to roughly estimate by extrapolation, Stark width due to interactions with electrons for other spectral lines from the same series.

In the next two figures we present Stark broadening parameters due to different perturbers for spectral line with wavelength 9624.6 Å – transition (singlet) N VI 3s-3p. The perturber density is 10^{16} cm⁻³. The case of Stark width is illustrated in Fig. 2. The width due to collisions with electrons decreases with temperature and dominates for temperatures up to 200 000 K, while those due to protons, alpha particles, and boron ions with different degrees of ionization increase with T. The broadening is larger with the increasing of the electric charge of the perturber. The lowest values are obtained for protons and highest for boron ions B VI. All curves are well separated and distinguishable. The corresponding Stark shift values are shown in Fig. 3. They are all negative (towards the blue). The smallest shifts of the spectral line are obtained for N VI-electron

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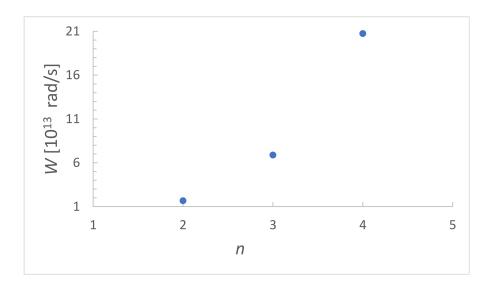


Figure 1. Stark widths due to interactions with electrons versus principal quantum number for spectral lines within one spectral series corresponding to N VI 2s-np (n = 2 - 4) triplets. The temperature is 300 000 K and the perturber density 10^{20} cm⁻³.

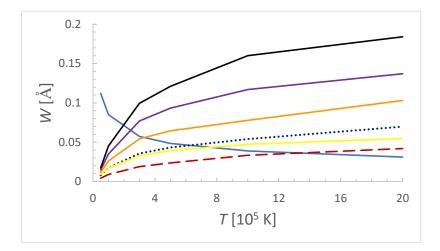


Figure 2. Stark width due to interactions with electrons (blue solid line), protons (red dashes), alpha particles (dark blue dots) and ions: B III (yellow solid line), B IV (orange solid line), B V (purple solid line), and B VI (black solid line) ions versus temperature. Spectral line corresponds to N VI 3s-3p singlet transition with $\lambda = 9624.6$ Å. The perturber density is 10^{16} cm⁻³.

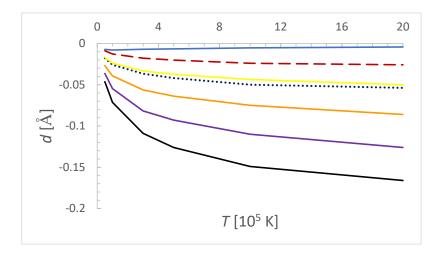


Figure 3. Stark shift due to interactions with electrons (blue solid line), protons (red dashes), alpha particles (dark blue dots) and ions: B III (yellow solid line), B IV (orange solid line), B V (purple solid line), and B VI (black solid line) ions versus temperature. Spectral line corresponds to N VI 3s-3p singlet transition with $\lambda = 9624.6$ Å. The perturber density is 10^{16} cm⁻³.

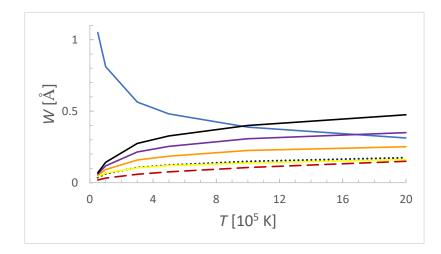


Figure 4. Stark width due to interactions with electrons (blue solid line), protons (red dashes), alpha particles (dark blue dots) and ions: B III (yellow solid line), B IV (orange solid line), B V (purple solid line), and B VI (black solid line) ions versus temperature. Spectral line corresponds to N VI 4s-4p singlet transition with $\lambda = 17182$ Å. The perturber density is 10^{16} cm⁻³.

Transition	T[K]	\mathbf{WBV}	WBVI
N VI 2s-2p	50000.	0.206E-04	0.206E-04
1901.5 A	100000.	0.808E-04	0.824 E-04
C = 0.19E + 21	300000.	0.574 E-03	$0.673 \text{E}{-}03$
	500000.	0.107 E-02	0.134E-02
	1000000.	0.185 E-02	0.232 E-02
	2000000.	0.251 E-02	0.328E-02
N VI 2s-3p	50000.	0.581E-05	0.598E-05
161.2 A	100000.	0.165 E-04	0.185 E-04
C = 0.19E + 18	300000.	0.451E-04	0.557 E-04
	500000.	0.616E-04	0.788 E-04
	1000000.	0.781E-04	0.101E-03
	2000000.	0.923E-04	0.127 E-03
N VI 2s-4p	50000.	0.465 E-04	0.531E-04
122.4 A	100000.	0.905 E-04	0.110E-03
C = 0.48E + 17	300000.	0.169E-03	0.220E-03
	500000.	0.169E-03	0.257 E-03
	1000000.	0.234E-03	0.326E-03
	2000000.	0.304E-03	0.383E-03

Table 2. Stark full widths (Å) at half intensity maximum of N VI spectral lines due to interactions with B V and B VI ions. The presented lines belong to triplets within one spectral series. The perturber density is 10^{17} cm⁻³.

interactions and the largest – for N VI-B VI ion interactions. All shifts increase with temperature and the T-gradient increases with electric charge of the perturbing particle.

The similar dependencies of Stark broadening parameters for N VI 4s-4p singlet transition are given in Fig. 4 and Fig. 5, respectively. The perturber density is 10^{16} cm⁻³. In the case of Stark width (Fig. 4), the electron width is largest for temperatures up to 1 000 000 K. Even that then it slowly decreases, it stays significant for the rest of the examined temperature interval. As for the previous line, the broadening due to other perturbers increases with their electric charge. Here, the separations between different curves are smaller, they increase with the electric charge, also. Concerning line shift (Fig. 5), all components are negative and increase with temperature. The different curves are well separated from each other. Perturbers with large electric charges are more effective in the case of shift of the considered spectral line. The presented results for all spectral lines in this study could be used for spectroscopic diagnostics of astrophysical objects, laser driven plasmas in proton-boron fusion experiments with nitrogen target, and other high temperature laboratory and industrial plasma environment.

Transition	T[K]	de	dBIII	dBIV
N VI 2s-2p	50000.	-0.518E-04	-0.110E-03	-0.161E-03
1901.5 A	100000.	-0.155E-03	-0.226E-03	-0.337E-03
C = 0.19E + 21	300000.	-0.176E-03	-0.522E-03	-0.839E-03
	500000.	-0.165E-03	-0.668E-03	-0.108E-02
	1000000.	-0.155E-03	-0.844E-03	-0.144E-02
	2000000.	-0.140E-03	-0.102E-02	-0.172E-02
N VI 2s-3p	50000.	0.114 E-05	0.669E-05	0.993E-05
161.2 A	100000.	0.194 E-05	0.119E-04	0.184E-04
C = 0.19E + 18	300000.	0.152 E- 05	0.206E-04	0.341E-04
	500000.	0.157 E-05	0.237 E-04	0.395E-04
	1000000.	0.114 E-05	0.281E-04	0.476E-04
	2000000.	0.892 E-06	0.329E-04	0.561E-04
N VI 2s-4p	50000.	0.949 E-05	0.325E-04	0.510E-04
122.4 A	100000.	0.908 E-05	0.473E-04	0.756E-04
C = 0.48E + 17	300000.	$0.805 \text{E}{-}05$	0.651E-04	0.110E-03
	500000.	0.685 E-05	0.740E-04	0.127 E-03
	1000000.	0.542 E-05	0.853E-04	0.143E-03
	2000000.	0.443E-05	0.991E-04	0.166E-03

Table 3. Stark shifts (Å) of the intensity maximum of N VI spectral lines due to interactions with electrons, B III and B IV ions. The presented lines belong to triplets within one spectral series. The perturber density is 10^{17} cm⁻³.

4. Conclusions

New calculated results for Stark broadening parameters of N VI spectral lines are obtained. Conditions of interest include temperatures and densities corresponding to the white dwarfs and to the laser driven proton-boron plasma for fusion reaction. Stark width dependence versus principal quantum number is presented for spectral lines from triplet transitions within one spectral series N VI 2s - np (n = 2 - 4). The result is in accordance with the theory. The role of different perturbers in the Stark broadening of two spectral lines belonging to singlet transitions (N VI 3s-3p and N VI 4s-4p) is investigated. More effective in the broadening and shifting of spectral lines are perturbers with larger electric charge. The shifts are negative, the spectral lines are shifted towards high frequencies (towards blue). Obtained new results for Stark broadening parameters of N VI spectral lines will be included in the Stark-B database (Sahal-Bréchot et al. 2015 - https://stark-b.obspm.fr/), part of Virtual Atomic and Molecular Data Center (VAMDC - Dubernet et al., 2010). Additionally, there is a link to Stark-B on the website of Serbian Virtual Observatory (SerVO, http://servo.aob.rs).

The results obtained in this work will be of interest for example for investigation of white dwarfs, stellar subphotospheric layers, laser driven plasma in

Transition	T[K]	dBV	dBVI
N VI 2s-2p	50000.	-0.209E-03	-0.254E-03
1901.5 A	100000.	-0.448E-03	-0.556E-03
C = 0.19E + 21	300000.	-0.116E-02	-0.148E-02
	500000.	-0.153E-02	-0.201E-02
	1000000.	-0.209E-02	-0.277E-02
	2000000.	-0.250E-02	-0.333E-02
N VI 2s-3p	50000.	0.0.130E-04	0.159E-04
161.2 A	100000.	0.252 E-04	0.320E-04
C = 0.19E + 18	300000.	0.482 E-04	0.635 E-04
	500000.	0.576E-04	0.772 E-04
	1000000.	0.691E-04	0.921E-04
	2000000.	0.819E-04	0.111E-03
N VI 2s-4p	50000.	0.848E-04	0.681E-04
122.4 A	100000.	0.136E-03	0.106E-03
C = 0.48E + 17	300000.	0.214E-03	0.161E-03
	500000.	0.243E-03	0.182 E- 03
	1000000.	0.288E-03	0.213E-03
	2000000.	0.331E-03	0.247 E-03

Table 4. Stark shifts (Å) of N VI spectral lines due to interactions with B V and B VI ions. The presented lines belong to triplets within one spectral series. The perturber density is 10^{17} cm⁻³.

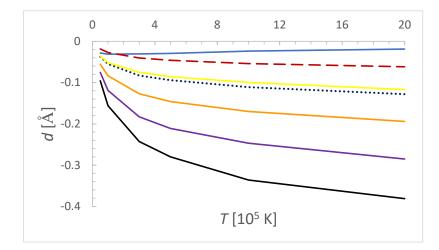


Figure 5. Stark shift due to interactions with electrons (blue solid line), protons (red dashes), alpha particles (dark blue dots) and ions: B III (yellow solid line), B IV (orange solid line), B V (purple solid line), and B VI (black solid line) ions versus temperature. Spectral line corresponds to N VI 4s-4p singlet transition with $\lambda = 17182$ Å. The perturber density is 10^{16} cm⁻³.

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proton-boron fusion experiments, laboratory plasmas and other topics in astrophysics and plasma physics.

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