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Data Descriptor

Data on Stark Broadening of N VI Spectral Lines

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Abstract: Data on Stark broadening parameters, spectral line widths, and shifts for 15 multiplets of N VI, whose spectral lines are broadened by collisions with electrons, protons, alpha particles (He III) and B III, B IV, B V and B VI ions, are presented. They have been calculated using the semiclassical perturbation theory, for temperatures from 50,000 K to 2,000,000 K, and perturber densities from 10^{16} cm^{-3} up to 10^{24} cm^{-3}. The data for e, p and He III are of particular interest for the analysis and modelling of atmospheres of hot and dense stars, as, e.g., white dwarfs, and for investigation of their spectra, and data for boron ions are used for analysis and modelling of laser-driven plasma in proton–boron fusion research.

Dataset: The dataset is submitted as a Supplementary File.

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Keywords: atomic data; Stark broadening; N VI; proton–boron fusion; line profiles; atomic processes; stellar atmospheres

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1. Introduction

The data for spectral lines, broadened by collisions with surrounding charged particles (Stark broadening), are useful for the analysis, modelling and diagnostics of various plasmas in astrophysics, laboratories, fusion experiments and technology, as well as for laser-produced plasma. Such data, and their corresponding databases, are especially needed in astronomy and astrophysics for stellar spectroscopy, radiative transfer calculations, abundance determination, stellar atmosphere modelling, etc.

Spectral lines of N VI are present in cosmic plasma (see, e.g., [1–3]), so the corresponding Stark broadening data are needed for their analysis and synthesis. Such data are particularly needed for hot and dense stars such as, for example, white dwarfs, since, in the conditions in their atmospheres, Stark broadening is often the dominant broadening mechanism. Since Stark broadening data enter into the calculation of the absorption coefficients, in addition to abundance determination and atmosphere modelling, they are needed for the calculation of a number of quantities and equations where the absorption coefficient enters.

Another interesting topic for the application of Stark broadening data for N VI is the proton–boron fusion [4], producing energy by aneutronic fusion reactions without radioactive species. We note that, in some experimental devices [5], two boron nitride (BN) targets are used. A laser beam is focused on the first BN target, which generates protons that collide with the other BN target, triggering nuclear reactions. In order to optimize the fusion yield, a plasma diagnostic is needed [6], and Stark broadening data for N VI may be useful for such a purpose. Also, the presence of the multiply charged boron ions B IV, B V and B VI is clearly identified [7], so that broadening of N VI by collisions with multiply charged boron ions is also of interest.

By employing the semiclassical perturbation theory (see, for example, [8] and references therein), we calculated the Stark widths and shifts for 15 multiplets of N VI broadened by collisions with the most important charged constituents of stellar plasma: electrons, protons, and alpha particles (He III), and for proton–boron fusion plasma: B III, B IV, B V and B VI ions, for a grid of temperatures and perturber densities. The behaviour of the N VI Stark widths and shifts within a spectral series has been discussed in [9], where the linewidths and shifts due to different perturbers have been compared and discussed in detail. The data for a perturber density of 10^{16} cm^{-3}, together with the applications to white dwarf atmospheres, have been presented in [10]. Here, all data for a grid of temperatures and perturber densities are presented as an online data set in computer readable form.

Except for the present calculations, the Stark widths for four N VI spectral lines exist in Ref. [11], where a modified semiempirical method [12] has been used, and for the same four lines in Ref. [13], were calculations have been performed using Griem's simplified semiclassical method ([14] Equation (526)). These results, and the comparison with present calculations, have been discussed in [10].

2. The Semiclassical Perturbation Method

For calculations of the Stark broadening parameters, the semiclassical perturbation theory [8,15,16] has been used. Within the frame of this theory, the full width at half intensity maximum (FWHM-W) and shift (d) of an isolated spectral line of a non-hydrogenic ion, which is broadened by collisions with charged particles, are given with the following expression:

$$W = N \int v f(v) dv \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el} \right)$$

$$d = N \int v f(v) dv \int_{R_3}^{R_D} 2\pi\rho d\rho \sin(2\varphi_p). \tag{1}$$

where i and f are the initial and final level of the corresponding transition, i' and f' are their perturbing levels, N is the perturber density, v velocity of the perturber, $f(v)$ the Maxwellian velocity distribution, and ρ is the impact parameter of the perturbing particle.

The inelastic cross sections $\sigma_{kk'}(v)$, $k = i, f$, in the equation above, are included as an integral of the transition probability $P_{kk'}(\rho, v)$, over the impact parameter ρ:

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

The elastic collisions and resonances are taken into account with the formula:

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

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

Here, σ_{el} is the elastic cross section, and φ_p (r^{-4}) and φ_q (r^{-3}) are phase shifts due to the polarization and quadrupolar potential (for more details, see [15]). The symmetrization procedure and cut-offs R_1, R_2, R_3, and R_D, are described in [16]. The term σ_r, which gives the contribution of Feshbach resonances, σ_r is described in detail in [17].

For positively charged perturbers, i.e., protons and ions, since the Coulomb force is not attractive but repulsive, the trajectories are different. Moreover, there is no contribution of Feshbach resonances.

3. Data Description

Within the frame of the semiclassical perturbation theory [8,15,16], the Stark broadening parameters, widths (FWHM) and shifts of spectral lines for the 15 N VI multiplets have been calculated. The obtained data set is for collisions of N VI ions with electrons, protons, He III (alpha particles) and boron ions B III, B IV, B V and B VI, which are charged perturbers of particular importance for white dwarfs and the proton–boron fusion. The data for the full width at half maximum of intensity (W) and shift (d) are given in Tables within the data set in the Supplementary Materials for temperature values of 50,000 K, 100,000 K, 300,000 K, 500,000 K, 1,000,000 K and 2,000,000 K, and perturber densities from 10^{16} cm^{-3} up to 10^{24} cm^{-3}, in the case of N VI collisions with electrons, protons and alpha particles (He III), and up to 10^{21} cm^{-3} for boron ions because, for higher densities, the impact approximation is not valid.

The needed atomic energy levels for N VI are from [18], and they are also in the NIST database [19]. All details of calculations are described in [10].

In the Tables in the Supplementary Materials is given and the quantity C [20]. When it is divided by the corresponding FWHM (W), one obtains the maximal perturber density for the validity of the isolated line approximation.

Dependence of the Stark width of N VI $1s^2\ ^1S–2p^1P^o$ spectral line on the electron density, for T = 2,000,000 K, is shown in Figure 1, and the dependence of the shift for T = 50,000 K and 2,000,000 K in Figure 2. One can see that the deviation from linear dependence due to Debye screening starts for lower temperature on lower densities, and that the deviation is more pronounced for the shift.

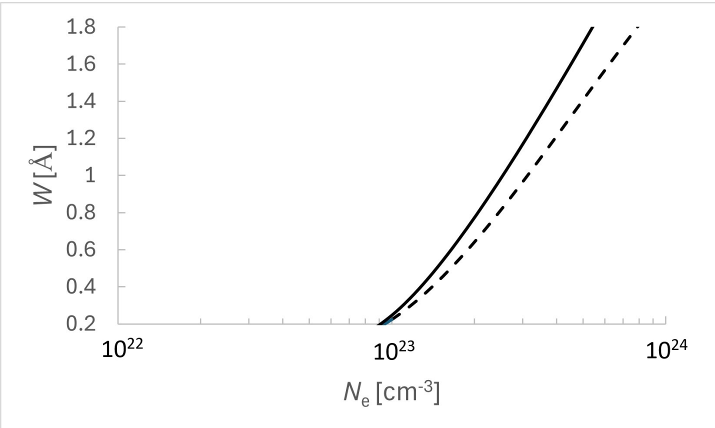

Figure 1. Dependence of Stark full widths at half intensity maximum of N VI $1s^2\ ^1S-2p^1P^o$, spectral line (T = 2,000,000 K), on the electron density (dashes). Solid line for linear dependence.

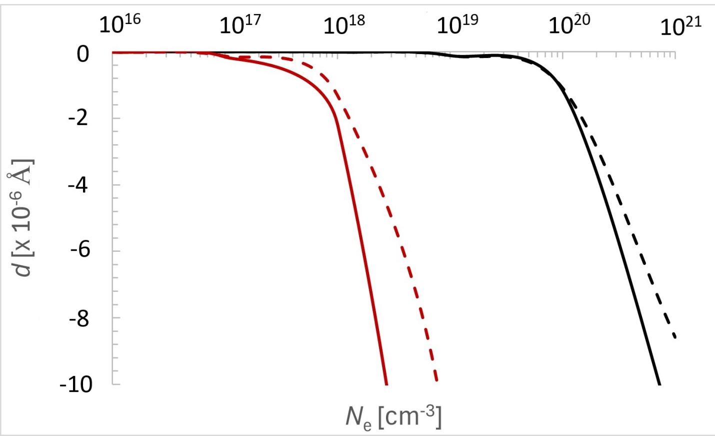

Figure 2. Dependence of Stark shift of N VI $1s^2\ ^1S-2p^1P^o$, spectral line on the electron density (dashes) for T = 50,000 K (red) and 2,000,000 K. Solid line for linear dependence.

4. User Notes

It should be noted that the wavelengths given in the Tables in the Supplementary Materials are calculated using the atomic energy levels, which are used for the Stark broadening parameter calculations, and may be different from wavelengths present in the NIST database. If we want to change wavelength for the wavelength of a line within the considered multiplet, to the wavelength from NIST or for the experimental one, we can perform this for the width using the expression:

$$W_{cor} = \left(\frac{\lambda_{new}}{\lambda}\right)^2 W. \tag{4}$$

and the same scaling law applies to the shift. Here, W_{cor} is the corrected width, λ_{new} is the NIST, or experimental, or observed value, or the value for a line within a multiplet, λ is the calculated wavelength, or the value for a multiplet as a whole, and W is the corresponding width from Tables in the Supplementary Materials.

If we want to obtain the line profile $F(\omega)$, where ω is angular frequency, we can use the following relation for a Lorentzian:

$$F(\omega) = \frac{W/(2\pi)}{(\omega - \omega_{if} - d)^2 + (W/2)^2}. \tag{5}$$

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.

5. Conclusions

The computer readable data set presented here, and available online in the Supplementary Materials, contains the Stark broadening parameters, widths and shifts for 15 N VI multiplets, obtained with the help of the semiclassical perturbation theory [8,15,16]. The data for the N VI spectral lines broadened by collisions with electrons, protons, He III, B III, B IV, B V and B VI ions, are given for a grid of temperatures and perturber densities.

The presented data set is, first of all, of interest for hot and dense stars like white dwarfs, where they can be used for abundance determination, analysis and synthesis of stellar spectra, stellar atmosphere modelling and opacity, and radiative transfer calculations. This data set is also important for proton–boron fusion experiments, particularly when the boron nitride (BN) is used as a target for laser radiation.

Supplementary Materials: The following supporting information are available online at: https://www.mdpi.com/article/10.3390/data9060077/s1, Tables S1–S16 and S9–S24 present the Stark widths and shifts in Å units of the N VI spectral lines broadened by collisions with electrons, protons and alpha particles (He III), from a perturber density of 10^{16} cm^{-3} (S1–S16) up to 10^{24} cm^{-3} (S9–S24). Tables S10–S16 and S15–S21 present the Stark widths and shifts of N VI spectral lines broadened by collisions with B III, B IV, B V and B VI ions, from a perturber density of 10^{16} cm^{-3} (S10–S16) up to 10^{21} cm^{-3} (S15–S21). For values presented in the tables, we 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. We excluded the cases when $NV > 0.5$ from the tables, since than 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 to the fact that this value is on the limit of validity of impact approximation.

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References

1. Fleig, J.; Rauch, T.; Werner, K.; Kruk, J.W. FUSE spectroscopy of the sdOB primary of the post common-envelope binary LB3459 (AADoradus). *Astron. Astrophys.* **2008**, *492*, 565–573. [CrossRef]
2. Newman, J.; Tsuruta, S.; Liebmann, A.C.; Kunieda, H.; Haba, Y. Combined Analysis of X-ray Spectra of NGC 3227. *Astrophys. J.* **2021**, *907*, 45. [CrossRef]
3. Ness, J.-U.; Beardmore, A.P.; Bode, M.F.; Darnley, M.J.; Dobrotka, A.; Drake, J.J.; Magdolen, J.; Munari, U.; Osborne, J.P.; Orio, M.; et al. High-resolution X-ray spectra of RS Ophiuchi (2006 and 2021): Revealing the cause of SSS variability. *Astron. Astrophys.* **2023**, *670*, A131. [CrossRef]
4. Batani, K. Perspectives on research on laser driven proton-boron fusion and applications. *J. Instrum.* **2023**, *18*, C09012. [CrossRef]
5. Schollmeier, M.S. Investigation of Proton Beam-Driven Fusion Reactions Generated by an Ultra-Short Petawatt-Scale Laser Pulse. *Laser Part. Beams* **2022**, 2404263. [CrossRef]
6. Hegelich, B.M.; Labun, L.O.; Labun, Z.; Mehlhorn, T.A. Photon and Neutron Production as In Situ Diagnostics of Proton-Boron Fusion. *Laser Part. Beams* **2023**, *2023*, 6924841. [CrossRef]
7. Kong, D.; Xu, S.; Shou, Y.; Gao, Y.; Mei, Z.; Pan, Z.; Liu, Z.; Cao, Z.; Liang, Y.; Peng, Z.; et al. Alpha-Particle Generation from H-^{11}B Fusion Initiated by Laser-Accelerated Boron Ions. *Laser Part. Beams* **2022**, *2022*, 5733475. [CrossRef]
8. Sahal-Bréchot, S.; Dimitrijević, M.S.; Ben Nessib, N. Widths and Shifts of Isolated Lines of Neutral and Ionized Atoms Perturbed by Collisions with Electrons and Ions: An Outline of the Semiclassical Perturbation (SCP) Method and of the Approximations Used for the Calculations. *Atoms* **2014**, *2*, 225–252. [CrossRef]
9. Dimitrijević, M.S.; Christova, M.D.; Sahal-Bréchot, S. On the Stark broadening of N VI spectral lines. *Contrib. Astron. Obs. Skalnaté Pleso* **2023**, *53*, 84–93. [CrossRef]
10. Dimitrijević, M.S.; Christova, M.D.; Sahal-Bréchot, S. Stark broadening of N VI spectral lines. *Universe* **2023**, *9*, 511. [CrossRef]
11. Dimitrijević, M.S. Electron-impact widths of four- and five-times charged ion lines of astrophysical importance. *A&AS* **1993**, *100*, 237–241.
12. Dimitrijević, M.S.; Konjević, N. Stark widths of doubly- and triply-ionized atom lines. *J. Quant. Spectrosc. Radiat. Transf.* **1980**, *24*, 451–459. [CrossRef]
13. Dimitrijević, M.S. Stark widths of fourthly and fifthly charged ion lines. *Astrophys. Lett. Commun.* **1993**, *28*, 385–388.
14. Griem, H.R. *Spectral Line Broadening by Plasmas*; McGraw-Hill: New York, NY, USA, 1974.
15. Sahal-Bréchot, S. Impact Theory of the Broadening and Shift of Spectral Lines due to Electrons and Ions in a Plasma. *Astron. Astrophys.* **1969**, *1*, 91–123.
16. Sahal-Bréchot, S. Impact Theory of the Broadening and Shift of Spectral Lines due to Electrons and Ions in a Plasma (Continued). *Astron. Astrophys.* **1969**, *2*, 322–354.
17. Sahal-Bréchot, S. The Semiclassical Limit of the Gailitis Formula Applied to Electron Impact Broadening of Spectral Lines of Ionized Atoms. *Atoms* **2021**, *9*, 29. [CrossRef]
18. Kelly, R.L. Atomic and Ionic Spectrum Lines below 2000 Angstroms: Hydrogen through Krypton. *J. Phys. Chem. Ref. Data* **1987**, *16* (Suppl. S1), 1–1698; Erratum in *J. Phys. Chem. Ref. Data* **1998**, *17*, 953.

19. Kramida, A.; Ralchenko, Y.; Reader, J.; NIST ASD Team. *NIST Atomic Spectra Database (Ver. 5.10)*; National Institute of Standards and Technology: Gaithersburg, MD, USA, 2022. Available online: https://physics.nist.gov/asd (accessed on 30 October 2023).
20. Dimitrijević, M.S.; Sahal-Bréchot, S. Stark broadening of neutral helium lines. *J. Quant. Spectrosc. Radiat. Transf.* **1984**, *31*, 301–313. [CrossRef]