atoms

MDPI

Article

Semiclassical Stark Broadening Parameters of Ar VII Spectral Lines

Milan S. Dimitrijević [1,2,†], Aleksandar Valjarević [3,†] and Sylvie Sahal-Bréchot [2,*,†]

1 Astronomical Observatory, Volgina 7, 11060 Belgrade 38, Serbia; mdimitrijevic@aob.rs
2 LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, UPMC (Univ. Pierre & Marie Curie) Paris 06, 5 Place Jules Janssen, 92190 Meudon, France
3 Department of Geography, Faculty of Natural Sciences and Mathematics, University of Kosovska Mitrovica, Ive Lole Ribara 29, 38220 Kosovska Mitrovica, Serbia; aleksandar.valjarevic@pr.ac.rs
* Correspondence: sylvie.sahal-brechot@obspm.fr; Tel.: +381-64-297-8021
† These authors contributed equally to this work.

Academic Editor: Robert C. Forrey
Received: 16 August 2017; Accepted: 6 September 2017; Published: 8 September 2017

Abstract: Using the semi-classical perturbation approach in the impact approximation, full width at half maximum and shift have been determined for eight spectral lines of Ar VII, for broadening by electron-, proton-, and He III-impacts. The results are provided for temperatures from 20,000 K to 500,000 K, and for an electron density of 10^{18} cm^{-3}. The obtained results will be included in the STARK-B database, which is also in the virtual atomic and molecular data center (VAMDC).

Keywords: stark broadening; atomic data; atomic processes; line profiles; Ar VII

1. Introduction

With the development of space astronomy and satellite-born spectroscopy, trace elements—which have been without importance for astrophysics—now become increasingly important, and the corresponding data of interest for the analysis of stellar spectra. For example, spectral lines of Ar VII have been observed in the spectrum of extremely hot and massive galactic O3 If supergiant HD 93129A [1]. Additionally, Werner et al. [2] have found Ar VII lines in some of the hottest known central stars of planetary nebulae, with the effective temperatures of 95,000–110,000 K, and in (pre-) white dwarfs by analyzing high-resolution spectra from the Far Ultraviolet Spectroscopic Explorer (FUSE). We note that Stark broadening is the principal pressure broadening mechanism in such hot stars, and without the corresponding Stark broadening data, reliable analysis and modelling of high-resolution spectra are not possible.

Concerning Stark broadening parameters for Ar VII spectral lines, there is only one article where Stark broadening parameters are provided for three transitions [3]. Here, full widths at half intensity maximum (FWHM) W and shifts d for eight additional transitions have been calculated by using semiclassical perturbation method (SCP, [4,5]) for collisions of Ar VII ions with electrons, protons, and He III ions, since hydrogen and helium are the main constituents of stellar atmospheres.

2. The Impact Semiclassical Perturbation Method

The semiclassical perturbation formalism (SCP) applied here for the calculations of Stark broadening parameters, full width at half intensity maximum (FWHM-W), and shift of spectral line (d) has been formulated in [4,5], and later updates, optimisations, and innovations are presented in Sahal-Bréchot [6], Sahal-Bréchot [7], Dimitrijević et al. [8], Dimitrijević and Sahal-Bréchot [9], and Sahal-Bréchot et al. [10]. Within the frame of this method, FWHM (W) and shift (d) may be expressed by the following relation:

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

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

Here, N is electron density, $f(v)$ the Maxwellian velocity distribution function for electrons, ρ is the impact parameter of the incoming electron, and with i', f' are denoted the perturbing levels of the initial (i) and final (f) state. The inelastic cross-section $\sigma_{jj'}(v)$, $j = i, f$ is expressed as:

$$\sum_{i' \neq i} \sigma_{ii'}(v) = \frac{1}{2} \pi R_1^2 + \int_{R_1}^{R_D} 2\pi \rho d\rho \sum_{i' \neq i} P_{ii'}(\rho, v), \quad (2)$$

where $P_{jj'}(\rho, v), j = i, f; j' = i', f'$ is the transition probability. The elastic cross-section is

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

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

The phase shift due to the polarization potential is φ_p (r^{-4}), and due to the quadrupolar potential φ_q (r^{-3}) (see Section 3 of Chapter 2 in Sahal-Bréchot [4]). R_1, R_2, R_3, and R_D are cut-offs, defined and described in Section 1 of Chapter 3 in Sahal-Bréchot [5]. σ_r denotes the contribution of Feshbach resonances, explained in detail in [11].

A review of the theory, all approximations and details of applications is given in Sahal-Bréchot et al. [10].

3. Stark Broadening Parameter Calculations

By using Equations (1)–(3) we have calculated widths (FWHM) and shifts for eight transitions (triplets) in Ar VII spectrum. The necessary atomic energy levels have been taken from Saloman [12]. The oscillator strengths—needed for calculations—have been obtained by using the method of Bates and Damgaard [13] and the tables of Oertel and Shomo [14]. When there was no corresponding data in Oertel and Shomo [14] (for some higher levels), the needed oscillator strengths have been calculated using the method of Van Regemorter et al. [15].

In Table 1 are shown widths (FWHM) and shifts of Ar VII spectral lines broadened by electron-, proton-, and He III-impacts, for a perturber density of 10^{18} cm^{-3} and for a set of temperatures from 20,000 K to 500,000 K. The temperature range is of interest for astrophysics, laboratory plasmas, fusion research, various plasmas in technology and laser-produced plasmas. If we want to use these data for higher perturber densities, the influence of Debye screening should be checked and taken into account if needed (e.g., [16]).

The accuracy of the semiclassical perturbation method is estimated by comparison with numerous experimental data for different elements and spectral lines, and is estimated to be 20–30% (see discussion in [10]). Since Ar VII is a member of the magnesium isoelectronic sequence with relatively simple spectrum, we suppose that the error of results shown in Table 1 is not much higher than 20%.

Table 1. Electron-, proton-, and doubly charged helium-impact broadening parameters for Ar VII spectral lines, for a perturber density of 10^{18} cm^{-3} and temperatures from 20,000 to 500,000 K. The calculated wavelength of the transitions (in Å) and parameter *C* are also given. When divided by the corresponding Stark width, this parameter gives an estimate for the maximal perturber density for which the line may be treated as isolated. W_e: electron-impact full width at half maximum of intensity; d_e: electron-impact shift; W_p: proton-impact full width at half maximum of intensity; d_p: proton-impact shift; $W_{He^{++}}$: doubly charged helium ion-impact full width at half maximum of intensity; $d_{He^{++}}$: doubly charged helium ion-impact shift.

Transition	T(K)	W_e (Å)	d_e (Å)	W_{H^+} (Å)	d_{H^+} (Å)	$W_{He^{++}}$ (Å)	$d_{He^{++}}$ (Å)
4s ^{3}S − 5p ^{3}P^o	20,000	0.510E−01	0.174E−03	0.298E−03	0.197E−04	0.492E−03	0.272E−04
443.2 Å	50,000	0.328E−01	0.217E−03	0.898E−03	0.636E−04	0.173E−02	0.117E−03
C = 0.47E+20	100,000	0.243E−01	0.158E−03	0.148E−02	0.129E−03	0.291E−02	0.249E−03
	200,000	0.186E−01	0.215E−03	0.203E−02	0.223E−03	0.403E−02	0.444E−03
	300,000	0.162E−01	0.211E−03	0.220E−02	0.275E−03	0.439E−02	0.550E−03
	500,000	0.139E−01	0.227E−03	0.242E−02	0.352E−03	0.482E−02	0.709E−03
3p ^{3}P^o − 4s ^{3}S	20,000	0.490E−02	−0.779E−03	0.744E−06	0.135E−04	0.129E−05	0.186E−04
250.4 Å	50,000	0.270E−02	0.615E−04	0.642E−05	0.432E−04	0.124E−04	0.792E−04
C = 0.32E+20	100,000	0.191E−02	0.113E−03	0.295E−04	0.835E−04	0.579E−04	0.161E−03
	200,000	0.142E−02	0.131E−03	0.819E−04	0.133E−03	0.163E−03	0.265E−03
	300,000	0.121E−02	0.143E−03	0.113E−03	0.162E−03	0.227E−03	0.323E−03
	500,000	0.101E−02	0.136E−03	0.173E−03	0.196E−03	0.347E−03	0.396E−03
3p ^{3}P^o − 3d ^{3}D	20,000	0.911E−02	−0.564E−03	0.361E−05	−0.107E−05	0.598E−05	−0.148E−05
477.5 Å	50,000	0.585E−02	−0.436E−04	0.148E−04	−0.348E−05	0.282E−04	−0.639E−05
C = 0.48E+21	100,000	0.417E−02	−0.288E−04	0.396E−04	−0.740E−05	0.767E−04	−0.143E−04
	200,000	0.297E−02	−0.165E−04	0.900E−04	−0.150E−04	0.176E−03	−0.298E−04
	300,000	0.245E−02	−0.134E−04	0.129E−03	−0.220E−04	0.253E−03	−0.438E−04
	500,000	0.195E−02	−0.237E−04	0.177E−03	−0.333E−04	0.349E−03	−0.669E−04
3p ^{3}P^o − 4d ^{3}D	20,000	0.421E−02	−0.445E−03	0.671E−05	0.621E−05	0.111E−04	0.858E−05
192.3 Å	50,000	0.249E−02	0.896E−05	0.263E−04	0.200E−04	0.506E−04	0.366E−04
C = 0.94E+19	100,000	0.181E−02	0.259E−04	0.589E−04	0.394E−04	0.115E−03	0.760E−04
	200,000	0.135E−02	0.428E−04	0.100E−03	0.646E−04	0.199E−03	0.128E−03
	300,000	0.115E−02	0.345E−04	0.127E−03	0.782E−04	0.252E−03	0.156E−03
	500,000	0.951E−03	0.379E−04	0.155E−03	0.971E−04	0.308E−03	0.196E−03
4p ^{3}P^o − 4d ^{3}D	20,000	0.309	−0.849E−02	0.811E−03	0.262E−03	0.134E−02	0.362E−03
1425.9 Å	50,000	0.199	0.324E−03	0.292E−02	0.845E−03	0.562E−02	0.155E−02
C = 0.52E+21	100,000	0.145	0.336E−03	0.577E−02	0.169E−02	0.113E−01	0.327E−02
	200,000	0.108	0.126E−02	0.877E−02	0.286E−02	0.173E−01	0.569E−02
	300,000	0.927E−01	0.595E−03	0.106E−01	0.346E−02	0.211E−01	0.691E−02
	500,000	0.777E−01	0.645E−03	0.120E−01	0.440E−02	0.237E−01	0.886E−02
3d ^{3}D − 4p ^{3}P^o	20,000	0.184E−01	−0.111E−02	0.352E−04	0.757E−05	0.584E−04	0.105E−04
416.0 Å	50,000	0.116E−01	0.474E−04	0.133E−03	0.245E−04	0.256E−03	0.450E−04
C = 0.87E+20	100,000	0.835E−02	0.115E−03	0.286E−03	0.513E−04	0.560E−03	0.991E−04
	200,000	0.612E−02	0.105E−03	0.469E−03	0.946E−04	0.926E−03	0.188E−03
	300,000	0.518E−02	0.121E−03	0.577E−03	0.126E−03	0.114E−02	0.251E−03
	500,000	0.427E−02	0.140E−03	0.679E−03	0.161E−03	0.135E−02	0.323E−03
3d ^{3}D − 5p ^{3}P^o	20,000	0.139E−01	−0.555E−03	0.900E−04	0.185E−04	0.148E−03	0.256E−04
240.6 Å	50,000	0.868E−02	0.137E−03	0.271E−03	0.587E−04	0.523E−03	0.108E−03
C = 0.14E+20	100,000	0.642E−02	0.162E−03	0.445E−03	0.109E−03	0.877E−03	0.211E−03
	200,000	0.490E−02	0.190E−03	0.616E−03	0.166E−03	0.122E−02	0.331E−03
	300,000	0.425E−02	0.199E−03	0.669E−03	0.204E−03	0.133E−02	0.406E−03
	500,000	0.362E−02	0.199E−03	0.739E−03	0.237E−03	0.147E−02	0.479E−03
4d ^{3}D − 5p ^{3}P^o	20000	0.243	−0.224E−03	0.163E−02	0.134E−03	0.269E−02	0.185E−03
952.0 Å	50,000	0.158	0.166E−02	0.477E−02	0.431E−03	0.923E−02	0.790E−03
C = 0.22E+21	100,000	0.118	0.174E−02	0.767E−02	0.856E−03	0.151E−01	0.165E−02
	200,000	0.902E−01	0.184E−02	0.104E−01	0.142E−02	0.207E−01	0.283E−02
	300,000	0.786E−01	0.221E−02	0.113E−01	0.172E−02	0.224E−01	0.343E−02
	500,000	0.672E−01	0.208E−02	0.124E−01	0.217E−02	0.246E−01	0.437E−02

Since the wavelengths in Table 1 are calculated ones, they are different from experimental wavelengths. However, we notice that they are correct in angular frequency units, because in such

a case, relative and not absolute positions of energy levels are important for calculations. For the transformation of the Stark widths from Å-units to angular frequency units, the following formula can be used:

$$W(\mathring{A}) = \frac{\lambda^2}{2\pi c} W(s^{-1}) \tag{4}$$

where c is the speed of light. For the correction of widths and/or shifts for the difference between calculated and experimental wavelength, one can use the expression:

$$W_{cor} = \left(\frac{\lambda_{\exp}}{\lambda}\right)^2 W. \tag{5}$$

The corresponding expressions for the shifts are analogous to Equations (4) and (5). Here, W_{cor} denotes the corrected width, while λ_{exp} is the experimental wavelength, λ the calculated wavelength, and W the width from Table 1.

Dividing the parameter C [17] from Table 1 by the corresponding full width at half maximum, one obtains the maximal perturber density for which the line may be treated as isolated.

The obtained Ar VII Stark broadening parameters shown in Table 1 will be implemented in the STARK-B database [18,19]. This database contains Stark widths and shifts needed first of all for the investigations, modelling, and diagnostics of the plasma of stellar atmospheres, but also for diagnostics of laboratory plasmas and investigation of laser produced, inertial fusion plasma, and for plasma technologies.

The STARK-B database is one of the databases included in the virtual atomic and molecular data center—VAMDC [20,21], created in order to enable more effective search and mining of atomic and molecular data which are in different databases. Databases with atomic and molecular data which are in VAMDC—including STARK-B—can be accessed and searched through the VAMDC portal: http://portal.vamdc.org/.

4. Conclusions

The semiclassical perturbation calculation of Stark broadening parameters, widths, and shifts for spectral lines broadened by collisions of Ar VII ions with electrons, protons, and doubly charged helium ions have been performed for eight multiplets of Ar VII. The obtained values of Stark broadening parameters will be implemented in the STARK-B database—one of the databases included in the virtual atomic and molecular data center (VAMDC). Since Stark broadening data for Ar VII spectral lines considered here do not exist in the literature, we hope that they will be of interest for the relevant problems in astrophysical, laboratory, laser-produced, inertial fusion, and technological plasmas.

Acknowledgments: The support of the Ministry of Education, Science and Technological Development of the Republic of Serbia through project 176002 is gratefully acknowledged. This work has also been supported by the Paris Observatory, the PADC (Paris Data Center_OV), and the CNRS which are greatly acknowledged. We also acknowledge financial support from "Programme National de Physique Stellaire" (PNPS) of CNRS/INSU, CEA and CNES, France. This work has also been supported by the VAMDC (Virtual Atomic and Molecular Data Centre). VAMDC is funded under the Combination of Collaborative Projects and Coordination and Support Actions Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure, Grant Agreement number: 239108. A part of this work has also been supported by the LABEX Plas@par project and received financial state aid managed by the Agence Nationale de la Recherche, as part of the programme "Investissements d'Avenir" under the reference, ANR11IDEX000402.

Author Contributions: These authors contributed equally to this work.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Taresch, G.; Kudritzki, R.P.; Hurwitz, M.; Bowyer, S.; Pauldrach, A.W.A.; Puls, J.; Butler, K.; Lennon, D.J.; Haser, S.M. Quantitative analysis of the FUV, UV and optical spectrum of the O3 star HD 93129A. *Astron. Astrophys.* **1997**, *321*, 531–548.
2. Werner, K.; Rauch, T.; Kruk, J.W. Discovery of photospheric argon in very hot central stars of planetary nebulae and white dwarfs. *Astron. Astrophys.* **2007**, *466*, 317–322.
3. Dimitrijević, M.S.; Sahal-Bréchot, S. On the Stark broadening of Ar VII spectral lines. *Univ. Thought* **2017**, *7*, 46–50.
4. 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.
5. 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.
6. Sahal-Bréchot, S. Stark broadening of isolated lines in the impact approximation. *Astron. Astrophys.* **1974**, *35*, 319–321.
7. Sahal-Bréchot, S. Broadening of ionic isolated lines by interactions with positively charged perturbers in the quasistatic limit. *Astron. Astrophys.* **1991**, *245*, 322–330.
8. Dimitrijević, M.S.; Sahal-Bréchot, S.; Bommier, V. Stark broadening of spectral lines of multicharged ions of astrophysical interest. I-C IV lines. *Astron. Astrophys.* **1991**, *89*, 581–590.
9. Dimitrijević, M.S.; Sahal-Bréchot, S. Stark broadening of Li II spectral lines. *Phys. Scr.* **1996**, *54*, 50–55.
10. 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.
11. Fleurier, C.; Sahal-Bréchot, S.; Chapelle, J. Stark profiles of some ion lines of alkaline earth elements. *J. Quant. Spectrosc. Radiat. Transf.* **1977**, *17*, 595–603.
12. Saloman, E.B. Energy Levels and Observed Spectral Lines of Ionized Argon, Ar II through Ar XVIII. *J. Phys. Chem. Ref. Data* **2010**, *39*, 033101.
13. Bates, D.R.; Damgaard, A. The Calculation of the Absolute Strengths of Spectral Lines. *Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Sci.* **1949**, *242*, 101–122.
14. Oertel, G.K.; Shomo, L.P. Tables for the Calculation of Radial Multipole Matrix Elements by the Coulomb Approximation. *Astrophys. J. Suppl. Ser.* **1968**, *16*, 175–218.
15. Van Regemorter, H.; Hoang Binh, D.; Prud'homme, M. Radial transition integrals involving low or high effective quantum numbers in the Coulomb approximation. *J. Phys. B* **1979**, *12*, 1053–1061.
16. Griem, H.R. *Spectral Line Broadening by Plasmas*; Academic Press, Inc.: New York, NY, USA, 1974.
17. Dimitrijević, M.S.; Sahal-Bréchot, S. Stark broadening of neutral helium lines. *J. Quant. Spectrosc. Radiat. Transf.* **1984**, *31*, 301–313.
18. Sahal-Bréchot, S.; Dimitrijević, M.S.; Moreau, N. STARK-B Database, Observatory of Paris, LERMA and Astronomical Observatory of Belgrade, 2017. Available online: http://stark-b.obspm.fr (accessed on 24 August 2017).
19. Sahal-Bréchot, S.; Dimitrijević, M.S.; Moreau, N.; Ben Nessib, N. The STARK-B database VAMDC node: A repository for spectral line broadening and shifts due to collisions with charged particles. *Phys. Scr.* **2015**, *50*, 054008.
20. Dubernet, M.L.; Boudon, V.; Culhane, J.L.; Dimitrijevic, M.S.; Fazliev, A.Z.; Joblin, C.; Kupka, F.; Leto, G.; Le Sidaner, P.; Loboda, P.A.; et al. Virtual atomic and molecular data centre. *J. Quant. Spectrosc. Radiat. Transf.* **2010**, *111*, 2151–2159.
21. Dubernet, M.L.; Antony, B.K.; Ba, Y.A.; Babikov, Y.L.; Bartschat, K.; Boudon, V.; Braams, B.J.; Chung, H.K.; Daniel, F.; Delahaye, F.; et al. The virtual atomic and molecular data centre (VAMDC) consortium. *J. Phys. B* **2016**, *49*, 074003.