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► **To cite this version:**

Milan Dimitrijevic, Sylvie Sahal-Bréchet. On the stark broadening of Ar VII spectral lines. The University Thought - Publication in Natural Sciences, 2017, 7 (1), pp.46-50. 10.5937/univtho7-13884 . obspm-03988869

HAL Id: obspm-03988869

<https://hal-obspm.ccsd.cnrs.fr/obspm-03988869>

Submitted on 16 Feb 2023

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ON THE STARK BROADENING OF Ar VII SPECTRAL LINES

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ABSTRACT

Stark broadening parameters, full width at half maximum of spectral line and shift, have been calculated for 3 spectral lines of Ar VII, for broadening by electron, proton, and He III impacts. For calculations, the semiclassical perturbation approach in the impact approximation has been used. The results are provided for temperatures from 20 000 K to 500 000 K and for an electron density of 10^{17} cm^{-3} . Obtained results will be included in the STARK-B database which is also included in Virtual atomic and molecular data center (VAMDC).

Keywords: Stark broadening, atomic data, atomic processes, line profiles.

INTRODUCTION

Data on the Stark broadening of spectral lines are important for diagnostics, modeling and investigation of laboratory plasmas (Konjević, 1999; Torres et al., 2006), inertial fusion plasma research (Griem, 1992), laser produced plasma analysis and diagnostics (Gornushkin et al., 1999; Sorge et al., 2000), as well as for different plasmas in technology, like for example for welding and piercing with laser produced plasma (Hoffman et al., 2006), or for design and development of light sources based on plasmas (Dimitrijević & Sahal-Bréchet, 2014a), and lasers (Csillag & Dimitrijević, 2004). An important topic where Stark broadening data are needed are astrophysical plasmas (Beauchamp et al., 1997; Dimitrijević & Sahal-Bréchet, 2014b), in particular atmospheres of white dwarfs, pre white dwarf stars, and post AGB (Asymptotic Giant Branch) stars (Tankosić et al., 2003; Milovanović et al., 2004; Simić et al., 2006; Dufour et al., 2011).

Additionally, since for temperatures higher than around 10 000 K hydrogen is mainly ionized, Stark broadening is, in such a case, the principal pressure broadening mechanism (Griem, 1974). Consequently, in some atmospheric layers of A and late B stars, where such plasma conditions are typical, it should be taken into account. Such cases have been analysed for example in Simić et al. (2005b,a) and Simić et al. (2009).

Due to development of satellite-born spectroscopy, data on trace elements, which have been without significance for astrophysics, become more and more important for analysis of stellar spectra. It is also worth to notice that Rauch et al. (2007) accentuated that accurate Stark broadening data for as much as possible large number of atoms and ions and the corresponding spectral lines “are of crucial importance for sophisticated analysis of stellar spectra by means of NLTE model atmospheres”.

Spectral lines of Ar VII have been found by Taresch et al. (1997) in the spectrum of extremely hot and massive galactic O3 If supergiant HD 93129A. Also Werner et al. (2007), by analyzing high-resolution spectra taken with the Far Ultraviolet Spectroscopic Explorer (FUSE), have identified Ar VII lines in some of the hottest known central stars of planetary nebulae, with the effective temperatures of 95000 - 110000 K, and in (pre-) white dwarfs, where Stark broadening is very important and the corresponding Stark broadening data are needed for a reliable analysis and modelling.

In order to provide the needed Stark broadening parameters for Ar VII spectral lines, completely missing in the existing literature, Stark Full Widths at Half intensity Maximum (FWHM) W and shifts d for three transitions have been calculated by using semiclassical perturbation method (SCP, Sahal-Bréchet (1969a,b)) for collisions of Ar VII ions with electrons, protons and He III ions, which are the main constituents of stellar atmospheres.

THE IMPACT SEMICLASSICAL PERTURBATION METHOD

For the calculations of Stark broadening parameters, full width at half intensity maximum (FWHM - W) and shift of spectral line (d) here is used the semiclassical perturbation formalism (SCP), developed in Sahal-Bréchet (1969a,b). Further innovations and modernisations are presented in Sahal-Bréchet (1974, 1991); Dimitrijević et al. (1991); Dimitrijević & Sahal-Bréchet (1996); Sahal-Bréchet et al. (2014).

The Stark broadened profile $F(\omega)$ of an isolated spectral line has Lorentzian form and can be represented as:

$$F(\omega) = \frac{W/2\pi}{(\omega - \omega_f - d)^2 + (W/2)^2}. \quad (1)$$

Here,

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$$\omega_{if} = \frac{E_i - E_f}{h}.$$

In the upper equation E_i and E_f are energies of the initial and final states, while (W) and (d) , in angular frequency units, are given by equation:

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

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

with N is here denoted the electron density and with $f(v)$ 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 and final state. The inelastic cross section $\sigma_{ij}(v), j=i, f$ is given with the formula:

$$\sum_{i'=i} \sigma_{ii'}(v) = \frac{1}{2} \pi R_1^2 + \int_{R_1}^{R_D} 2\pi \rho d \rho \sum_{i'=i} P_{ii'}(\rho, v). \quad (3)$$

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

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_1}^{R_D} 2\pi \rho d \rho \sin^2 \delta + \sigma_r,$$

$$\delta = (\varphi_p^2 + \varphi_q^2)^{\frac{1}{2}}. \quad (4)$$

The phase shifts due to the polarization potential is $\varphi_p(r^{-4})$ and due to the quadrupolar potential $\varphi_q(r^{-3})$. They are defined in Section 3 of Chapter 2 in Sahal-Br  chot (1969a). The cut-offs R_1, R_2, R_3 , and the Debye radius R_D are described in Section 1 of Chapter 3 in Sahal-Br  chot (1969b). The contribution of Feshbach resonances, σ_r is explained in details in (Fleurier et al., 1977).

All approximations and the details of the theory are discussed in detail in Sahal-Br  chot et al. (2014). The electrons are moving along hyperbolic paths while for ionic perturbers the paths are different because for them the Coulomb force is repulsive and for them, in Eqs. (2-4), there is no the contribution of Feshbach resonances.

STARK BROADENING PARAMETER CALCULATIONS

Within the frame of semiclassical perturbation theory (Sahal-Br  chot, 1969a,b; Sahal-Br  chot et al., 2014) we have calculated using Eqs. (2-4) widths (FWHM) and shifts for three multiplets of six time charged argon ion Ar VII. Energy levels necessary for present calculations have been taken from Saloman (2010). The needed oscillator strengths have been calculated within the Coulomb approximation by using the method of Bates & Damgaard (1949) and the tables of Oertel & Shomo (1968). For higher levels, when there is no the corresponding data in Oertel & Shomo (1968), the required oscillator strengths have been calculated according to the article of Van Regemortel et al. (1979).

In Table 1, the obtained results of our calculations of Stark widths (FWHM) and shifts for electron- proton- and doubly charged helium ion-impact broadening, for a perturber density of 10^{17} cm^{-3} and for a set of temperatures from 20 000 K to 500 000 K, are shown. The temperature range covers needs in astrophysics, laboratory plasma, fusion research, technology and the topic of lasers and laser produced plasma. Extrapolation to perturber densities lower than 10^{17} cm^{-3} is linear. For higher perturber densities the influence of Debye screening should be checked and eventually taken into account (see e.g. (Griem, 1974)). With known Stark broadening parameters, W and d it is easy to obtain the line profile using Eq. (1).

One can see from Table 1, that spectral line width due to collisions with electrons is always dominant in comparison with line widths produced by ionic collisions, since ions are much heavier than electrons and their velocities are much smaller. At low temperatures ion width is completely negligible but its influence increases with temperature and it should not be neglected at high temperatures. One can see as well that widths due to collisions with doubly charged helium ions are larger than widths produced by collisions with protons. Shifts are much smaller and they are of the same order of magnitude for collisions with electrons as well as with both species of ions. At higher temperatures ion shifts are larger than electron ones and proton shifts are smaller than He^{++} ones.

It should be noticed that wavelengths given in Table 1 are calculated ones, so that they are different from experimental ones. However, they are correct in angular frequency units since then, for the calculation of Stark broadening parameters, relative and not absolute positions of energy levels are significant. In order to transform the Stark widths in  ° -units to the width in angular frequency units the following formula can be used:

$$W(\text{ }^{\circ}) = \frac{\lambda^2}{2\pi c} w(\text{s}^{-1}). \quad (5)$$

where c is the speed of light. If the correction of widths and/or shifts for the difference between calculated and experimental wavelength is needed, this can be performed for the width as:

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

Here, with W_{cor} is denoted the corrected width, λ_{exp} is the experimental, λ the calculated wavelength and W the width from Table 1. Formulas for the shifts are analogous to Eqs. (5) and (6).

Parameter C (Dimitrijevi   & Sahal-Br  chot, 1984) in Table 1, enables to estimate the maximal perturber density for which the line may be treated as isolated, when it is divided by the corresponding full width at half maximum.

ON THE IMPLEMENTATION OF RESULTS IN THE STARK-B DATABASE

The presented in Table 1 Stark broadening parameters for Ar VII spectral lines, will be also implemented in the STARK-B

database (Sahal-Bréchet et al., 2015, 2017), intended for the investigations, modelling and diagnostics of the plasma of stellar atmospheres, diagnostics of laboratory plasmas, and investigation of laser produced, inertial fusion plasma and for plasma technologies.

The STARK-B database contains Stark widths and shifts calculated by authors of this article and their coauthors, by using the SCP computer code for spectral lines, and published in more than 150 publications. Actually, in this database are SCP data for the following elements and ionization degrees: Ag I, Al I, Al III, Al XI, Ar I, Ar II, Ar III, Ar VIII, Au I, B II, B III, Ba I, Ba II,

Be I, Be II, Be III, Br I, C II, C III, C IV, C V, Ca I, Ca II, Ca V, Ca IX, Ca X, Cd I, Cd II, Cl I, Cl VII, Cr I, Cr II, Cu I, F I, F II, F III, F IV, F V, F VI, F VII, Fe II, Ga I, Ge I, Ge IV, He I, Hg II, I I, In II, In III, K I, K VIII, K IX, Kr I, Kr II, Kr VIII, Li I, Li II, Mg I, Mg II, Mg XI, Mn II, N I, N II, N III, N IV, N V, Na I, Na X, Ne I, Ne II, Ne III, Ne IV, Ne V, Ne VIII, Ni II, O I, O III, O IV, O V, O VI, O VII, P IV, P V, Pb IV, Pd I, Rb I, S III, S IV, S V, S VI, Sc III, Sc X, Sc XI, Se I, Si I, Si II, Si IV, Si V, Si VI, Si XI, Si XII, Si XIII, Sr I, Te I, Ti IV, Ti XII, Ti XIII, Tl III, V V, V XIII, Y III, Xe VI, Xe VIII and Zn I.

Table 1. This table gives electron-, proton-, and doubly charged helium-impact broadening parameters for Ar VII spectral lines, for a perturber density of 10^{17} cm^{-3} and temperatures from 20 000 to 500 000 K. 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 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)
Ar VII $3s^2 \ ^1S - 3p \ ^1P^o$ 585.7 Å $C = 0.59E+20$	20000.	0.144E-02	0.504E-04	0.414E-06	-0.397E-06	0.789E-06	-0.716E-06
	50000.	0.919E-03	-0.130E-05	0.164E-05	-0.109E-05	0.316E-05	-0.210E-05
	100000.	0.653E-03	-0.449E-05	0.447E-05	-0.221E-05	0.865E-05	-0.438E-05
	200000.	0.465E-03	-0.587E-05	0.106E-04	-0.434E-05	0.206E-04	-0.869E-05
	300000.	0.386E-03	-0.496E-05	0.155E-04	-0.621E-05	0.304E-04	-0.124E-04
	500000.	0.309E-03	-0.637E-05	0.222E-04	-0.902E-05	0.438E-04	-0.181E-04
Ar VII $4s \ ^1S - 4p \ ^1P^o$ 2445.8 Å $C = 0.24E+21$	20000.	0.860E-01	0.166E-03	0.126E-03	-0.194E-03	0.241E-03	-0.349E-03
	50000.	0.546E-01	-0.106E-02	0.488E-03	-0.524E-03	0.948E-03	-0.101E-02
	100000.	0.396E-01	-0.903E-02	0.109E-02	-0.952E-03	0.215E-02	-0.189E-02
	200000.	0.297E-01	-0.126E-02	0.186E-02	-0.145E-02	0.369E-02	-0.292E-02
	300000.	0.255E-01	-0.121E-02	0.239E-02	-0.176E-02	0.474E-02	-0.355E-02
	500000.	0.213E-01	-0.113E-02	0.289E-02	-0.210E-02	0.578E-02	-0.425E-02
Ar VII $3s \ ^3S - 4p \ ^3P^o$ 1982.0 Å $C = 0.20E+21$	20000.	0.534E-01	0.172E-02	0.781E-04	-0.877E-04	0.149E-03	-0.158E-03
	50000.	0.333E-01	-0.387E-03	0.295E-03	-0.239E-03	0.571E-03	-0.460E-03
	100000.	0.240E-01	-0.512E-03	0.653E-03	-0.449E-03	0.128E-02	-0.892E-03
	200000.	0.179E-01	-0.607E-03	0.110E-02	-0.714E-03	0.219E-02	-0.144E-02
	300000.	0.153E-01	-0.649E-03	0.139E-02	-0.865E-03	0.277E-02	-0.174E-02
	500000.	0.128E-01	-0.572E-03	0.169E-02	-0.107E-02	0.338E-02	-0.216E-02

STARK-B contains also our Stark broadening data obtained by using the Modified SemiEmpirical method (MSE) (Dimitrijević & Konjević, 1980; Dimitrijević & Kršljanin, 1986; Dimitrijević & Popović, 2001). These data are of lower accuracy

than SCP data but this approach is convenient for the cases where atomic data are not sufficiently complete for an adequate SCP calculation. MSE Stark line widths, in some cases together with line shifts, of the following emitters are in STARK-B

database: Ag II, Al III, Al V, Ar II, Ar III, Ar IV, As II, Au II, B III, B IV, Be III, Bi II, Bi III, Br II, C III, C IV, C V, Cd II, Cd III, Cl III, Cl IV, Cl VI, Co II, Co III, Cu III, Cu IV, Eu II, Eu III, F III, F V, F VI, Fe II, Ga III, Ge III, Ge IV, I II, Kr II, Kr III, La II, La III, Lu III, Mg III, Mg IV, Mn II, Mn III, N II, N III, Na III, Na VI, Nb III, Ne III, Ne IV, Ne V, Ne VI, Ne VII, Ne VIII, O III, O IV, P III, P IV, P VI, Pt II, Ra II, S IV, Sb II, Sc II, Se II, Se III, Si IV, Si V, Si VI, Si XI, Sn III, Sr III, Ti II, Ti III, V II, V III, V IV, Xe II, Y II, Zn II, Zn III, Zr II and Zr III.

We note as well that STARK-B database is one of the databases which are in the Virtual Atomic and Molecular Data Center - VAMDC (Dubernet et al., 2010; Rixon et al., 2011; Dubernet et al., 2016). VAMDC is created in order to enable an efficacious search and mining of atomic and molecular data scattered in different databases and to make more convenient their adequate use. It has been the principal aim of a FP7 founded project of the same name (Dubernet et al., 2010), which started on July 1 2009 and lasted 42 months. During this project an interoperable e-infrastructure for atomic and molecular data upgrading and integrating European (and wider) A&M database services has been build, and a forum of data producers, data users and databases developers has been created. Currently in VAMDC are 30 databases with atomic and molecular data, including STARK-B, and can be accessed and searched through VAMDC portal: <http://portal.vamdc.org/>. The web site of VAMDC Consortium is: <http://www.vamdc.org/>.

CONCLUSION

We have performed a SCP calculation of Stark broadening parameters for three multiplets of Ar VII. Stark broadening parameters - widths and shifts, have been calculated for collisions of Ar VII ions with electrons, protons and doubly charged helium ions. The obtained data will be implemented in STARK-B database. There is no neither theoretical, nor experimental data for Stark broadening of Ar VII spectral lines and we hope that the obtained results will be of interest. for a number of problems in astrophysical, laboratory, laser produced, inertial fusion and technological plasmas.

ACKNOWLEDGMENTS

This work is a part of the project 176002 "Influence of collisional processes on astrophysical plasma line shapes" supported by the Ministry of Education, Science and Technological Development of Serbia.

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