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# Stark broadening of Zr IV spectral lines in the atmospheres of chemically peculiar stars

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## ABSTRACT

Stark widths for 18 Zr IV spectral lines have been calculated by using the modified semi-empirical method. The obtained results have been used to investigate the influence of Stark broadening on the spectra of atmospheres of chemically peculiar stars of A spectral type and hydrogen-rich DA and helium-rich DB white dwarfs. Our results have been used also to test possibility to predict new data using some approximate methods developed on the basis on regularities and systematic trends.

**Key words:** atomic data – atomic processes – line: formation.

## 1 INTRODUCTION

Stark broadening parameters of neutral atom and ion lines are of interest for a number of problems in astrophysical, laboratory, laser produced, fusion or technological plasma investigations. Theory and calculation of Stark line broadening in the impact approximation showed a great expansion from the second half of the last century, and are considered now as mature for many applications. Therefore, Stark broadening data could be important for laboratory plasma diagnostics, laser produced plasma investigation and modelling, the design of laser devices, inertial fusion plasma and for analysis and modelling of various plasmas in technology, such as laser welding and piercing and for plasmas in light sources (Hoffman, Szymanski & Azharonok 2006; Shaikh et al. 2016).

As an example, zirconium is a very important metal in the mining industry. The cubic structure of ZrO<sub>2</sub> is a concurrent industrial substitute for a diamond. Recent investigations into the spectrum of zirconium ions in laboratory plasma conditions have already been completed, but without Stark width included (Gaft, Nagli & Gornushkin 2013).

In comparison with laboratory plasmas, conditions in astrophysical plasmas, where the Stark broadening mechanism is important, are incomparably more varied. When Stark broadening is of interest, the corresponding line broadening parameters (line widths and shifts) are significant, for example, for interpretation, synthesis and analysis of stellar spectral lines, determination of chemical abundances of elements from equivalent widths of absorption lines, estimation of the radiative transfer through the stellar atmospheres and subphotospheric layers, opacity calculations, radiative acceleration

considerations, nucleosynthesis research and other astrophysical topics.

Zirconium is often found overabundant in HgMn star spectrum. As a member of Sr–Y–Zr triad, zirconium appeared very important in the studying s- and r-processes of nucleosynthesis in HgMn type stars, providing us with useful information about their evolution. The Sr–Y–Zr abundance pattern in chemically peculiar (CP) stars is mostly of two kinds. In the first scenario, Sr is overabundant among the other two elements, which is as a result of the s-process of nucleosynthesis in the deep interior of the star. In the second, Zr or both Zr and Sr, are overabundant, which is a possible consequence of the r-process. However, there is still no strong evidence that abundance of Sr, Y and Zr has some non-nuclear pattern (Allen 1977).

The typical representative member of a non-magnetic subclass of HgMn CP stars is a spectroscopic binary  $\chi$  Lupi, where Zr is also overabundant, but its spectrum (Leckrone et al. 1993; Sikström et al. 1999) shows very strange behaviour – the zirconium abundance determination from weak Zr II optical and from strong Zr III UV spectral lines gives significantly different results, differing in order of magnitude. This so-called ‘zirconium conflict’ can probably be justified by not taking into account non-local thermodynamic equilibrium effects or diffusion. However, there can be more solutions – in spite of the binary nature of  $\chi$  Lupi, zirconium conflict could also be explained by the interaction process between two stellar components. The second component, which is classified as an Ap star, has a longitudinal magnetic field of  $\sim 274$  G and therefore could represent a possible answer to this question (Mathis & Hubrig 1995). The small radial velocity of the first stellar component can also be a possible reason for the strange behaviour of this HgMn star. Slow rotation that is evident for many HgMn stars could also favour diffusive separation of elements and suppress the meridional circulation (Allen 1977).

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The more recent explanations include so-called light induced drift theory, which describes the additional effect of radiative acceleration due to the selective transfer of photon momentum to an atomic particle in the line absorption process, see for example Aret & Sapar (1999). This theory offers a good explanation for a line asymmetry that occurs in almost every spectrum of HgMn stars and has already been discussed by Michaud (1978) with the classic radiative diffusion theory.

In any case, the importance of precise abundance estimation is evident from this example. Determination of abundances can depend on including or neglecting a more or less exact descriptions of the processes of spectral line broadening. Stark broadening is usually the main pressure broadening mechanism for spectral lines from hot star atmospheres, and therefore should not be neglected. It is already mentioned elsewhere (Popović, Milovanović & Dimitrijević 2001) that neglecting the Stark broadening influence on line width calculations can cause errors in abundance determination.

Another type of celestial bodies where it is interesting to consider the influence of Stark broadening on stellar spectra are white dwarfs. White dwarfs are traditionally divided into hydrogen-rich (DA) and helium-rich (DB), where D denotes degenerate objects. In the atmosphere of such an object, the concentration of charged particles is very high and the influence of collisions with charged particles on the broadening of a white dwarf's spectrum lines can be important. White dwarfs have a strong gravitational field intensity on their surface, causing the change of particle density to be more rapid with optical depth than in some other stellar objects. Since Stark width increases with electron density, and Doppler width depends on temperature only, the difference between the Stark width and Doppler width will be more significant in white dwarf spectra, which is already shown in some recent investigations (Simić et al. 2006).

The Stark broadening of spectral lines in stellar plasma has already been studied theoretically in the case of singly (Zr II) and doubly (Zr III) charged zirconium ions (Popović & Dimitrijević 1996; Popović et al. 2001). In addition to the Stark broadening data for Zr II and Zr III, it is also of interest to provide Stark broadening data for triply charged zirconium ion (Zr IV), which opens the possibility for a different estimation of Zr abundance in order to contribute to the clarification of the zirconium conflict.

Using the modified semi-empirical theory (Dimitrijević & Konjević 1980), Stark widths of 18 Zr IV spectral lines have been calculated in this work. These data, useful for astrophysical, laboratory and technological plasma investigations, are missing in the existing literature and are used in this work for the investigation of the influence of Stark broadening on Zr IV spectral lines in atmospheres of CP stars of A type and DA and DB white dwarfs. Our results have also been used to test the possibility of predicting new data on the basis of the approximative method of Purić & Šćepanović (1999) based on regularities and systematic trends.

## 2 CALCULATIONS

The most sophisticated theoretical method for the calculation of a Stark broadened line profile is the quantum mechanical strong coupling approach (Baranger 1958; Barnes & Peach 1970; Bely & Griem 1970; Dimitrijević, Feautrier & Sahal-Bréchet 1980; Elabidi et al. 2008; Elabidi, Ben Nessib & Sahal-Bréchet 2009; Duan et al. 2012, 2014), but due to its complexity and numerical difficulties, it is not adequate for large-scale determination of Stark broadening parameters. For example, complex spectra, heavy elements or transitions between highly excited energy levels.

Whenever large numbers of theoretical data of the Stark line widths are required (e.g. for opacity evaluations), and only a good average accuracy is sufficient, tedious calculations can be avoided if one uses simple, approximate formulas. For this purpose, simple formulas with good average accuracy for a larger number of lines are especially convenient.

One of these approximative theories is the modified semi-empirical method (MSE; Dimitrijević & Konjević 1980; Dimitrijević & Kršljanin 1986) for the Stark broadening of isolated, non-hydrogenic ion lines which is used here for evaluation of Stark widths of Zr IV spectral lines. Compared to some other approaches for Stark width and shift calculations, such as the semi-empirical method of Griem (1968) or the semi-classical perturbation method of Sahal-Bréchet (1969a,b), it needs less atomic data.

The required matrix elements are obtained with the Coulomb approximation formalism of Bates & Damgaard (1949), while the line and multiplet factors are taken from Shore & Menzel (1968) whenever they are necessary. The energy levels used to calculate electron-impact full widths at half-intensity maximum (FWHM) of spectral lines have been taken from Reader & Acquista (1997). The calculations have been performed under the assumption that all conditions for the validity of the MSE approach are satisfied, for example plasma ideality, impact approximation, non-overlapping spectral lines, etc. (Milovanović et al. 2004; Milovanović 2005).

MSE formula for the FWHM has the following form:

$$W_{\text{MSE}} = C \frac{\lambda^2 N}{\sqrt{T}} \sum_{j=i,f} \left[ \mathbf{R}_{l_j, l_{j+1}}^2 \tilde{g}(x_{l_j, l_{j+1}}) + \mathbf{R}_{l_j, l_{j-1}}^2 \tilde{g}(x_{l_j, l_{j-1}}) + \sum_{j'} (\mathbf{R}_{jj'}^2)_{\Delta n \neq 0} g(x_{jj'}) \right], \quad (1)$$

where  $C$  is the numerical constant ( $C = 2.2155 \times 10^{-30} \text{ m}^3 \text{ \AA}^{-1} \text{ K}^{1/2}$ ),  $W_{\text{MSE}}$  is the Stark width in  $\text{\AA}$ ,  $\lambda$  is the wavelength in  $\text{\AA}$ ,  $N$  – perturber density in  $\text{m}^{-3}$ ,  $E$  – average perturber energy,  $T$  is the temperature in  $\text{K}$ ,  $g$  is the semi-empirical Gaunt factor,  $\tilde{g}$  is the modified Gaunt factor,  $\mathbf{R}_{l_j, l_{j+1}}$ ,  $\mathbf{R}_{jj'}$  are coordinate operator matrix elements. Letters  $i$  and  $f$  stand for initial and final state, respectively. The quadratic matrix elements are calculated as follows:

$$\mathbf{R}_{l_j, l_{j\pm 1}}^2 \approx \left( \frac{3n_j^*}{2Z} \right)^2 \frac{l_{\text{max}}}{2l_j + 1} \left[ n_{l_j}^{*2} - l_{\text{max}}^2 \right] \Phi^2(n_{l-1}^*, n_l^*, l), \quad (2)$$

$$\sum_{j'} (\mathbf{R}_{jj'}^2)_{\Delta n \neq 0} \approx \left( \frac{3n_{l_j}^*}{2Z} \right)^2 \frac{1}{9} \left[ n_{l_j}^{*2} + 3l_j^2 + 3l_j + 11 \right], \quad (3)$$

where  $n$  is principal and  $l$  orbital quantum numbers. The other values used in formula are defined as

$$x_{l_j, l_{j\pm 1}} = \frac{E}{\Delta E_{l_j l_{j\pm 1}}}, \quad (4)$$

$$E = \frac{3}{2} kT \quad (5)$$

$$\Delta E_{l_j l_{j\pm 1}} = |E_{l_j} - E_{l_{j\pm 1}}| \quad (6)$$

$$|\Delta E_{n_j, n_{j+1}}| \approx \frac{2Z^2 E_{\text{H}}}{n_j^{*3}}, \quad (7)$$

$$n_j^{*2} = Z^2 [E_{\text{H}} / (E_{\text{ion}} - E_j)], \quad (8)$$

$$j = i, f, \quad (9)$$

**Table 1.** Stark line full widths ( $W_{\text{MSE}}$ ) at half intensity maximum (FWHM) for spectral lines of Zr IV as a function of temperature.

Perturber density = $10^{23} \text{ m}^{-3}$					
transition	$T$ (K)	Width ( $\text{\AA}$ )	Transition	$T$ (K)	Width ( $\text{\AA}$ )
Zr IV 2287.38 $\text{\AA}$ $5s^2S_{1/2}-5p^2P_{1/2}^{\circ}$	10000.	0.0844	Zr IV 1846.37 $\text{\AA}$ $5d^2D_{5/2}-5f^2F_{7/2}^{\circ}$	10000.	0.0825
	20000.	0.0596		20000.	0.0583
	50000.	0.0377		50000.	0.0369
	100000.	0.0270		100000.	0.0294
	200000.	0.0215		200000.	0.0290
	300000.	0.0199		300000.	0.0300
Zr IV 2164.36 $\text{\AA}$ $5s^2S_{1/2}-5p^2P_{3/2}^{\circ}$	500000.	0.0105	Zr IV 5781.45 $\text{\AA}$ $6s^2S_{1/2}-6p^2P_{1/2}^{\circ}$	500000.	0.0305
	10000.	0.0768		10000.	1.97
	20000.	0.0543		20000.	1.39
	50000.	0.0344		50000.	0.917
	100000.	0.0246		100000.	0.765
	200000.	0.0196		200000.	0.693
Zr IV 760.16 $\text{\AA}$ $5s^2S_{1/2}-6p^2P_{1/2}^{\circ}$	300000.	0.0181	Zr IV 5463.85 $\text{\AA}$ $6s^2S_{1/2}-6p^2P_{3/2}^{\circ}$	300000.	0.66
	500000.	0.0170		500000.	0.616
	10000.	0.0099		10000.	1.78
	20000.	0.0070		20000.	1.26
	50000.	0.0044		50000.	0.828
	100000.	0.0034		100000.	0.69
Zr IV 754.39 $\text{\AA}$ $5s^2S_{1/2}-6p^2P_{3/2}^{\circ}$	200000.	0.0030	Zr IV 3577.13 $\text{\AA}$ $6p^2P_{1/2}-6d^2D_{3/2}^{\circ}$	200000.	0.626
	300000.	0.0030		300000.	0.596
	500000.	0.0030		500000.	0.557
	10000.	0.0102		10000.	0.702
	20000.	0.0073		10000.	0.497
	50000.	0.0046		50000.	0.319
Zr IV 1546.17 $\text{\AA}$ $5p^2P_{1/2}-5d^2D_{3/2}^{\circ}$	100000.	0.0036	Zr IV 3795.07 $\text{\AA}$ $6p^2P_{3/2}-6d^2D_{3/2}^{\circ}$	100000.	0.262
	200000.	0.0032		200000.	0.245
	300000.	0.0031		300000.	0.239
	500000.	0.0030		500000.	0.229
	10000.	0.0422		10000.	0.811
	20000.	0.0298		20000.	0.573
Zr IV 1607.95 $\text{\AA}$ $5p^2P_{3/2}-5d^2D_{3/2}^{\circ}$	50000.	0.0189	Zr IV 3687.95 $\text{\AA}$ $6p^2P_{3/2}-6d^2D_{5/2}^{\circ}$	50000.	0.367
	100000.	0.0134		100000.	0.302
	200000.	0.0106		200000.	0.283
	300000.	0.0101		300000.	0.275
	500000.	0.0101		500000.	0.264
	10000.	0.0469		10000.	0.756
Zr IV 1598.95 $\text{\AA}$ $5p^2P_{3/2}-5d^2D_{5/2}^{\circ}$	20000.	0.0332	Zr IV 3751.67 $\text{\AA}$ $6d^2D_{3/2}-6f^2F_{5/2}^{\circ}$	20000.	0.535
	50000.	0.0201		50000.	0.342
	100000.	0.0149		100000.	0.281
	200000.	0.0118		200000.	0.264
	300000.	0.0112		300000.	0.256
	500000.	0.0112		500000.	0.246
Zr IV 1598.95 $\text{\AA}$ $5p^2P_{3/2}-5d^2D_{5/2}^{\circ}$	10000.	0.0463	Zr IV 3751.67 $\text{\AA}$ $6d^2D_{3/2}-6f^2F_{5/2}^{\circ}$	10000.	0.747
	20000.	0.0327		20000.	0.528
	50000.	0.0207		50000.	0.353
	100000.	0.0147		100000.	0.330
	200000.	0.0117		200000.	0.342
	300000.	0.0112		300000.	0.343
500000.	0.0110	500000.	0.335		

where  $Z - 1$  is ionic charge,  $n^*$  – effective principal quantum number,  $l_{\text{max}} = \max(l, l')$ ,  $E_{\text{H}}$  – hydrogen atom ionization energy,  $E_{\text{ion}}$  – ionization energy,  $E_j$  – energy of upper(lower) level,  $\Phi$  – factor of Bates & Damgaard (1949) and  $k$  – Boltzmann constant.

MSE is tested and confirmed many times on many spectral lines of ions calculating their Stark widths and comparing them with experiments. Despite the theoretically predicted accuracy, which is around  $\pm 50$  per cent (Dimitrijević & Konjević 1980; Popović et al. 2001), it is found that even in the cases of emitters with a

very complex spectra, such as Xe II and Kr II, this method can give relatively good agreement with experiments, with accuracy better than  $\pm 30$  per cent (see for example Kochukhov et al. 2006).

The Stark width calculations for 18 Zr IV transitions, permitted by the LS coupling selection rules for dipole allowed transitions, have been performed using MSE formalism. The Stark widths are calculated for the standard electron density of  $10^{23} \text{ m}^{-3}$  and for temperatures from 10 000 K to 500 000 K in unequal steps, and tabulated in Table 1.

**Table 1** – *continued*

Perturber density = $10^{23} \text{ m}^{-3}$					
transition	$T$ (K)	Width (Å)	Transition	$T$ (K)	Width (Å)
	10000.	0.0816		10000.	0.757
	20000.	0.0577		20000.	0.535
Zr IV	50000.	0.0365	Zr IV	50000.	0.358
1836.15 Å	100000.	0.0291	3775.08 Å	100000.	0.335
5d $^2D_{3/2}$ –5f $^2F_{5/2}^{\circ}$	200000.	0.0287	6d $^2D_{5/2}$ –6f $^2F_{5/2}^{\circ}$	200000.	0.346
	300000.	0.0296		300000.	0.347
	500000.	0.0302		500000.	0.339
	10000.	0.0827		10000.	0.750
	20000.	0.0585		20000.	0.530
Zr IV	50000.	0.0370	Zr IV	50000.	0.355
1848.03 Å	100000.	0.0295	3765.39 Å	100000.	0.332
5d $^2D_{5/2}$ –5f $^2F_{5/2}^{\circ}$	200000.	0.0291	6d $^2D_{5/2}$ –6f $^2F_{7/2}^{\circ}$	200000.	0.344
	300000.	0.0300		300000.	0.345
	500000.	0.0306		500000.	0.337

### 3 COMPARISON WITH APPROXIMATE FORMULAE

Sometimes, when the conditions for using MSE or similar approximate method are not satisfied, it is convenient to apply some approximate relations for a quick estimation of Stark width. We choose some of our results at random to test the possibility of using the statistical estimates of Purić & Šćepanović (1999), in the rest of this text, for quick prediction of unknown Stark widths. Comparing the great amount of Stark width data from the STARK-B data base (Sahal-Bréchet et al. 2014), Purić & Šćepanović found the correlation between Stark width and the difference between ionization energy and energy of the upper state. The equation for Stark width, obtained from regression analysis of existing sets of Stark broadening data in Pur99, was adopted for our purpose. After conversion of width from angular frequency units to Angstroms (see for example Hamdi et al. 2013, eq. 7), the formula (4) of Pur99 for the estimate of Stark widths becomes

$$W_{\text{Pur}} = aZ^c \lambda^2 N f(T) (E_{\text{ion}} - E_{\text{upper}})^{-b}, \quad (10)$$

where  $W_{\text{Pur}}$  is the estimated width in Å,  $\lambda$  is the spectral line wavelength in Å,  $E_{\text{ion}}$  and  $E_{\text{upper}}$  are the energies of ionization and of the upper level of transition in eV, respectively,  $T$  is the temperature in K,  $Z$  is the rest core charge (e.g.  $Z - 1$  is ionic charge) and  $N$  is the electron density in  $\text{m}^{-3}$ . Here,  $f(T)$  is a function of temperature:

$$f(T) = A + BT^C, \quad (11)$$

where  $A$ ,  $B$  and  $C$  in equation (3) are coefficients independent of temperature. The parameters  $A = 0$ ,  $B = 1$  and  $C = -0.5$  are chosen here in agreement with results about the temperature dependence of Stark width near the threshold of regularities and systematic trends (Elabidi et al. 2009; Sahal-Bréchet, Dimitrijević & Ben Nessib 2011). Coefficients  $a$ ,  $b$  and  $c$  in equation (10) are independent of temperature, ionization potential and electron density for a given transition. Coefficient values are  $a = 3.27 \times 10^{28}$ ,  $b = 3.1$  and  $c = 5.2$  (recalculated from Pur99, where these coefficients are given for Stark widths measured in  $\text{rad s}^{-1}$ ).

We also calculated some of Stark widths with the simple formula of Cowley (1971), which was a very popular approximation in the past century and is still in use, to do quick Stark width calculations (Killian, Montenbruck & Nissen 1991; Suleimanov et al. 2014; Przybilla et al. 2016; Rauch et al. 2016a,b, 2017) and compared the

**Table 2.** Comparison of calculated and estimated Stark widths for spectral lines of Zr IV for a temperature of  $T = 10000$  K. With  $W_{\text{MSE}}$  are denoted present results obtained by MSE, with  $W_{\text{Pur}}$  our estimations according to Purić & Šćepanović (1999) and with  $W_{\text{Cow}}$  our calculations according to Cowley (1971) using equation (4). Electron density is  $10^{23} \text{ m}^{-3}$ .

Transition	Wavelength (Å)	$W_{\text{MSE}}$ (Å)	$W_{\text{Pur}}$ (Å)	$W_{\text{Cow}}$ (Å)
5s $^2S_{1/2}$ –5p $^2P_{1/2}^{\circ}$	2287.38	0.0844	0.118	0.0486
5s $^2S_{1/2}$ –5p $^2P_{3/2}^{\circ}$	2164.36	0.0768	0.110	0.0442
5s $^2S_{1/2}$ –6p $^2P_{1/2}^{\circ}$	760.16	0.0099	0.0826	0.0128
5s $^2S_{1/2}$ –6p $^2P_{3/2}^{\circ}$	754.39	0.0102	0.0837	0.0128
5p $^2P_{1/2}$ –5d $^2D_{3/2}^{\circ}$	1546.17	0.0422	0.1870	0.0430
5p $^2P_{3/2}$ –5d $^2D_{3/2}^{\circ}$	1607.95	0.0469	0.2020	0.0469
5p $^2P_{3/2}$ –5d $^2D_{5/2}^{\circ}$	1598.95	0.0463	0.2010	0.0466
5d $^2D_{3/2}$ –5f $^2F_{5/2}^{\circ}$	1836.15	0.0816	1.390	0.1650
5d $^2D_{5/2}$ –5f $^2F_{5/2}^{\circ}$	1848.03	0.0827	1.410	0.167
5d $^2D_{5/2}$ –5f $^2F_{7/2}^{\circ}$	1846.37	0.0825	1.410	0.167
6s $^2S_{1/2}$ –6p $^2P_{1/2}^{\circ}$	5781.45	1.97	4.77	1.07
6s $^2S_{1/2}$ –6p $^2P_{3/2}^{\circ}$	5463.85	1.78	4.39	0.965
6p $^2P_{1/2}$ –6d $^2D_{3/2}^{\circ}$	3577.13	0.702	4.64	0.663
6p $^2P_{3/2}$ –6d $^2D_{3/2}^{\circ}$	3795.07	0.811	5.22	0.751
6p $^2P_{3/2}$ –6d $^2D_{5/2}^{\circ}$	3687.95	0.756	4.96	0.711
6d $^2D_{3/2}$ –6f $^2F_{5/2}^{\circ}$	3751.67	0.747	18	1.53
6d $^2D_{5/2}$ –6f $^2F_{5/2}^{\circ}$	3775.08	0.757	18.2	1.55
6d $^2D_{5/2}$ –6f $^2F_{7/2}^{\circ}$	3765.39	0.750	18.2	1.55

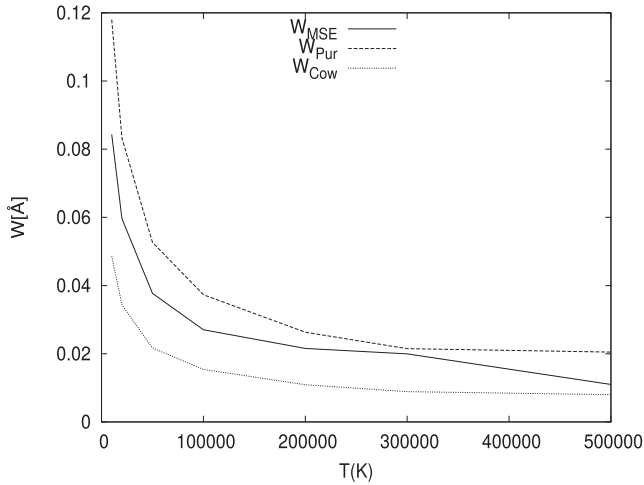
obtained results with our MSE values. Cowley’s estimation for the Stark width ( $W_{\text{Cow}}$ ) obtained in Å has a form:

$$W_{\text{Cow}} = 1.1075 \times 10^{30} \frac{\lambda^2 N}{Z^2 \sqrt{T}} \left( n_i^{*4} + n_f^{*4} \right), \quad (12)$$

where  $n_i^*$  and  $n_f^*$  are the effective principal quantum numbers of initial and final transition level, respectively. Values of  $T$ ,  $\lambda$ ,  $Z$  and  $N$  have the same meaning and the same units as in (10).

We can see from Table 2, where our calculations of Stark FWHM obtained with the MSE method (Dimitrijević & Konjević 1980) are compared with our results using equations (10) and (12) obtained





**Figure 1.** Dependence of calculated Stark width  $W_{\text{MSE}}$  – full line, estimated Stark width  $W_{\text{Pur}}$  – dashed line and estimated Stark width  $W_{\text{Cow}}$  – dotted line, for Zr iv  $5s^2 5p^2 S_{1/2} - 5p^2 P_{1/2}^o$ ,  $\lambda = 2287.38 \text{ \AA}$  spectral line. The electron density  $N_e$  is  $10^{23} \text{ m}^{-3}$ .

according to Pur99 and Cowley (1971) respectively, that the widths of Purić are larger than our MSE values. All results presented in Table 2 are calculated for a temperature of 10 000 K and electron density of  $10^{23} \text{ m}^{-3}$ . Fig. 1 represents temperature dependence for the mentioned Stark widths.

Moreover, Purić et al. (1997) investigated different statistical models based on systematic trends and regularities in triply and quadruply charged ions putting  $A = 0, B = 1$  and  $C = -0.25$  in (11), and in this way predicted the Stark widths for several heavy elements at different temperatures. According to Purić et al. (1997) calculated values for Stark widths of spectral line  $\lambda = 2287.38 \text{ \AA}$  are also overestimated compared to our MSE results. For example, at a temperature of  $T = 50\,000 \text{ K}$ , Purić’s predicted width (Purić et al. 1997) is  $0.0685 \text{ \AA}$ , while our MSE result is  $0.0378 \text{ \AA}$ .

Concerning this discrepancy, we can offer several possible reasons, of interest for further discussion and research:

(i) Existing parameters in (10) are still not adjusted properly. Comparison of quantum mechanical calculations of Stark widths for multiply-ionized atoms for a  $3s-3p$  transition array with predictions by Purić according to a similar method (Purić et al. 2008) shows a high increase in discrepancy when  $Z$  increases (Elabidi & Sahal-Bréchet 2011). This could be caused by the improper adjustment of constant  $c$  in (10). After comparing Purić’s and Cowley’s estimating formulas, we see that  $W_{\text{Cow}} \sim n^{*4}/Z^2$ , while from Pur99, follows  $W_{\text{Pur}} \sim Z^{5.2}(E_{\text{ion}} - E_{\text{upper}})^{-3} n^{*6}/Z^{0.8}$ , or according to Purić et al. (2008),  $W_{\text{Pur}} \sim Z^{5.2}(E_{\text{ion}} - E_{\text{upper}})^{-3} n^{*7}/Z^{1.8}$ . If we suppose that Purić’s assumptions hold, and Stark widths are dependent on effective ionization potential, Purić’s and Cowley’s formulas should be scaled in approximately the same way. On the other hand,  $c$  and  $b$  should be near to 2, in (10), or in the case of  $b = 3$  or  $3.3$ ,  $c$  should be 3 or  $3.5$  respectively. Instead of 5.2, for example, there should stand  $b$  and  $c$ , as it is shown in Purić, Miller & Lessage (1993), where  $b = c = 2$ .

(ii) There are some important parameters that are neglected in (10) but significantly contribute to the result. If we look at fig. 1 in Pur99, although the authors say that corresponding correlation factor is almost equal to 1, and less than 17 per cent of data corresponds to values two times larger than predicted ones, we can see the great

dispersion of presenting points related to the correlation line. If the standard deviation is too large it could mean that some parameters, which can influence results, are missing in the estimating formula. This could be the reason why the coefficient  $a$  in (10) should be adjusted again after the collection of analysing data is changed.

Besides, from fig. 1 of Pur99, it is evident that a large discrepancy of data comes from the middle of the curve, while for the very high and for the very low effective potentials, the data fit better. When effective ionization potential is very high,  $E_{\text{ion}} \gg E_{\text{upper}}$ , whereas for very low values  $E_{\text{ion}} \simeq E_{\text{upper}}$ . In the first case,  $E_{\text{upper}}$  and energy of lower level  $E_{\text{lower}}$  become mutually comparable and in the second case, both are comparable to  $E_{\text{ion}}$ . Therefore, the replacement of  $E_{\text{upper}}$  with  $E_{\text{lower}}$  in (10) would not affect the result of estimation significantly. Effective ionization potentials for Zr iv spectral levels for which Stark widths are calculated stand in the interval 10–25 eV, which corresponds to a range between 0.04 and 0.1 of their inverse values in the abscissa of fig. 1 (Pur99), for example, in the middle of the correlation line, where still large dispersion is noted on the graph, so that the bad agreement between Pur99 estimations and our MSE results is not so surprising. In this case, the replacement of  $E_{\text{upper}}$  with  $E_{\text{lower}}$  in (10) could reflect more significantly on the agreement of estimations with our results, even improving them, if a systematic trends of this kind exist at all.

Moreover, we found better agreement between our results and results of estimation (10) with parameters from Pur99, where  $E_{\text{upper}}$  is replaced with  $E_{\text{lower}}$  for 7 Zr iv spectral lines (Majlinger, Simić & Dimitrijević 2016), but this agreement is not confirmed for the rest of our results.

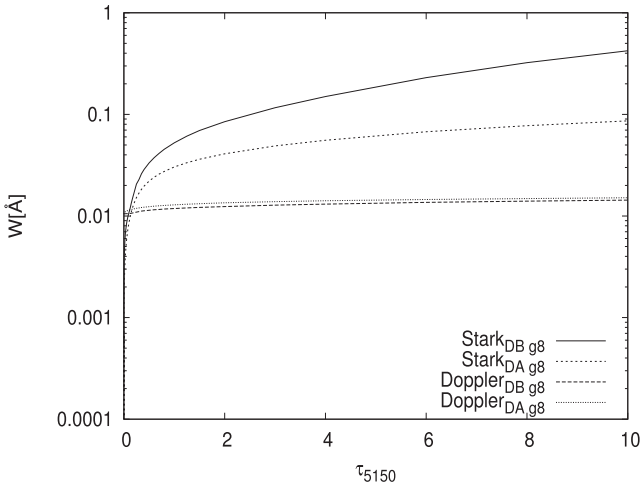
(iii) Temperature function (11) could be incorrect, or correct but with improper choice of coefficients  $A, B$  and  $C$ . It is already shown that temperature function (11), although it may be convenient for low temperature intervals, is not the most accurate one (Al-Towyan et al. 2016). According to Purić et al. (2008), constant  $C$  in (11) should be between  $-1.3$  and  $-0.7$ , instead of  $-0.5$  as for instance it is concluded in Elabidi et al. (2009) and Elabidi & Sahal-Bréchet (2011). However, if expression (11) is adequate for intermediate temperature, while for low temperature  $W \sim T^{-1/2}$  and for high temperature  $W \sim \ln T/T$  or  $W \sim \ln T/T^{-1/2}$  (Elabidi & Sahal-Bréchet 2011), very smooth interpolation between these mentioned functions is achieved by (2), if  $A \simeq 0, B \simeq 100$  and  $C \simeq -1$  in the temperature interval from 5000 to 15 000 K. But, for example, for  $T = 10\,000 \text{ K}$ , this choice of coefficients gives the same results as a choice of  $A = 0, B = 1$  and  $C = -0.5$ . However, it is very questionable if either of the estimation formulae (10) and (12) may be used above this temperature interval limit.

Although Purić’s works are shown to be useful in some analysis and comparisons and investigations of systematic trends and regularities, for example in cases of searching the regularities and trends *via* specific homologous sequences (Peláez et al. 2010), we did not find applicability of his general formula from Pur99 on our Zr iv Stark widths.

On the contrary, much better agreement is found between all of our results and results of estimation for multiply-charged heavy ions obtained by equation (8) from Purić et al. (1991), but only if dependence of estimation on residual charge  $Z$  is neglected (e.g. parameters should be adopted to be  $c = 0$  or  $Z = 1$ ). In that case, relative errors of this comparison are between 0.4 and 2.2.

Instead we found the polynomial dependence between Stark widths and the corresponding spectral line wavelengths in a form:

$$W_{\text{MSE}}(\lambda) = C_4 \lambda^4 + C_3 \lambda^3 + C_2 \lambda^2 + C_1 \lambda + C_0, \quad (13)$$



**Figure 2.** Dependence of electron-impact FWHM and thermal Doppler width on optical depth ( $\tau_{5150}$ ) in the DA and DB White Dwarf atmosphere for Zr IV  $5s^2S_{1/2}-5p^2P_{1/2}^o$   $\lambda = 2287.38$  Å spectral line. Models of DA and DB white dwarf atmospheres (Wickramasinghe 1972) are with parameters  $T_{\text{eff}} = 15\,000$  K and  $\log g = 8$ .

where  $C_4 = -0.6 \times 10^{-14}$ ,  $C_3 = 0.63 \times 10^{-10}$ ,  $C_2 = -0.12 \times 10^{-6}$ ,  $C_1 = 0.7 \times 10^{-4}$  and  $C_0 = 0.44 \times 10^{-2}$ . The correlation coefficient for this polynomial regression of the 4<sup>th</sup> degree is 99.9 per cent. In all of those estimations, parameters are obtained for condition of  $T = 10\,000$  K and  $N = 10^{23}$  m<sup>-3</sup>. This implies that a more complex relation between width and effective ionization potential (or effective principal quantum number) exists for a case of Zr IV spectral lines, and that both upper and lower level of transition should be somehow included in the estimation formula (10) to achieve better agreement with calculated MSE values. To test this, we investigated the dependence of Zr IV calculated widths on an average of upper and lower effective ionization potential, but a correlation coefficient of nearly 80 per cent is found also with large deviation of data, as in previous cases (e.g. ratios between the estimated widths and calculated widths are within the range of 0.5–1.5).

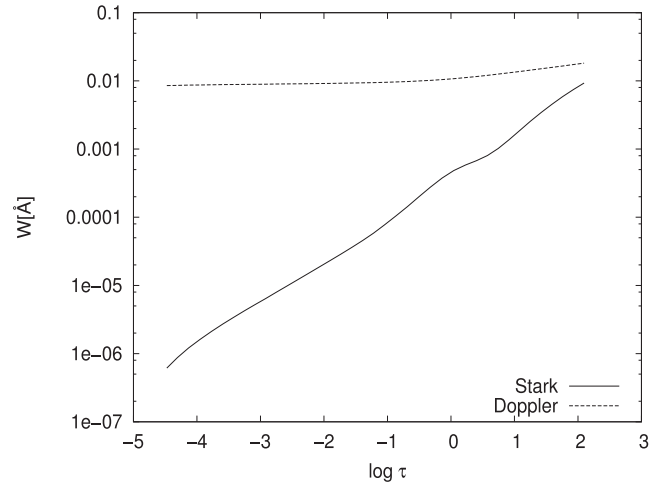
#### 4 ASTROPHYSICAL IMPLICATIONS

Finally, we investigated how Stark and Doppler width for one of the strongest lines of Zr IV ( $\lambda = 2287.38$  Å) change with the optical depth for several types of stellar atmospheres (Figs 2 and 3). The numerical simulation is done as a function of the optical depth corresponding to opacity at the wavelength of 5150 Å. To show this line width comparison, the existing stellar model atmospheres for DA and DB types of white dwarfs are used with parameters  $\log g = 8$  and  $T_{\text{eff}} = 15\,000$  K (Wickramasinghe 1972), with results presented in Fig. 2. The same procedure is carried out for A stars, where the Kurucz model (Kurucz 1979) is used, with parameters  $\log g = 4.5$  and  $T_{\text{eff}} = 10\,000$  K (Fig. 3), except that here the Rosseland opacity is in abscissa instead.

For the purpose of easier calculation of Stark width distribution within the atmosphere, here is the equation used to obtain the fitted data (Sahal-Bréchet et al. 2011):

$$\log W_{\text{MSE}}(T) = a + b \times \log T + c \times \log^2 T \quad (14)$$

from MSE calculated widths in Table 1, where  $W(T)$  is Stark width in Å,  $T$  is the temperature in Kelvin and  $a$ ,  $b$  and  $c$  are fitting param-



**Figure 3.** Dependence of Stark (solid) and Doppler (dashed) widths of Zr IV spectral line  $\lambda = 2287.38$  Å on optical depth in the atmosphere of an A type star. Model of stellar atmosphere (Kurucz, 1979) is with parameters  $= 10\,000$  K and  $\log g = 4.5$ .

eters. Parameters  $a$ ,  $b$  and  $c$  are calculated for electron density of  $10^{23}$  m<sup>-3</sup> and tabulated in Table 3 for all calculated lines. Unequal steps of temperatures are used in order to achieve better accuracy of interpolation. The comparisons show that Stark broadening becomes more important in the deeper layers of the stellar atmosphere. For example, electron-impact broadening is shown to be more significant than the thermal broadening even in the surface atmosphere layers of DA and DB white dwarfs (Fig. 2). We can see from Fig. 2 that Stark broadening of this particular line is larger in the atmosphere of helium-rich DB white dwarfs than in the hydrogen-rich ones, and this difference increases with the optical depth. On the contrary, in the model of an A star, Stark width of a given Zr IV spectral line cannot reach the Doppler width, even in the deeper parts of the atmosphere (Fig. 3). But, even when Stark widths are less than Doppler widths, the influence of Stark width still could be of significance on the shape of spectral line wings (Dimitrijević et al. 2011).

#### 5 CONCLUSION

The Zr IV Stark widths obtained here, will be also implemented in computer readable form, in the STARK-B data base (<http://stark-b.obspm.fr/>, Sahal-Bréchet et al. 2014, 2015; Sahal-Bréchet, Dimitrijević & Moreau 2017), which is a part of the Virtual Atomic and Molecular Data Center – VAMDC (<http://www.vamdc.org/>, Dubernet et al. 2010, 2016; Rixon et al. 2011).

The STARK-B data base is devoted to diagnostics, modelling and investigations of stellar atmospheres, diagnostics of laboratory plasmas, and investigation, analysis and modelling of laser produce, inertial fusion plasma and plasma technologies. There is a link to STARK-B in the Serbian Virtual Observatory’s website (SerVO, <http://servo.aob.rs>, Jevremović et al. 2009, 2012).

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**Table 3.** Fitting parameters for approximate formula (5).

Wavelength (Å)	a	b	c	Correlation coefficient( per cent)
2287.38	-0.2464	-0.0206	-0.0476	98.62
2164.36	3.6247	-1.7303	0.1372	99.86
760.16	4.1439	-2.3884	0.2137	99.82
754.39	3.5942	-2.1480	0.1885	99.87
1546.17	4.2920	-2.1123	0.1779	99.75
1607.95	4.0089	-2.0106	0.1673	99.67
1598.95	3.9991	-1.9900	0.1652	99.72
1836.15	5.8267	-2.7557	0.2575	99.64
1848.03	5.8267	-2.7531	0.2572	99.64
1846.37	5.8323	-2.7561	0.2575	99.63
5781.45	5.2387	-1.8993	0.1658	99.88
5463.85	5.2397	-1.9173	0.1676	99.88
3577.13	5.5021	-2.2054	0.1982	99.82
3795.07	5.5862	-2.2139	0.1989	99.82
3687.95	5.5711	-2.2203	0.1996	99.82
3751.67	5.8091	-2.3952	0.2275	98.81
3775.08	5.8136	-2.3948	0.2275	98.81
3765.39	5.8062	-2.3938	0.2275	98.79

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