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On the Stark Broadening of Ga II Spectral Lines - 4d–nf Spectral Series

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Abstract. Using the Semiclassical perturbation method, Stark broadening parameters, widths and shifts, have been calculated for six Ga II multiplets, belonging to the 4d–nf (n=4,5,6) spectral series. The calculations have been performed for temperatures from 5 000 K to 100 000 K and an electron density of 10^{16} cm^{-3}. The obtained results have been used to investigate regularities within spectral series. The obtained data are especially useful in astrophysics, for analyzis and synthezis of stellar spectra and modelling of atmospheres, but also for laboratory and laser produced plasmas.

Key words: Stark broadening – Ga II – line profiles – atomic data – atomic processes – line formation – stellar atmospheres

1. Introduction

Broadening of spectral lines in a medium where emitting or absorbing atoms or ions are surrounded by electrons and ions, and under the influence of their microfields, or Stark broadening, is the most important pressure broadening mechanism when we have higher electron densities in high temperature plasmas. Such conditions, convenient for Stark broadening, can often be found in stellar plasma. In such a case we need Stark broadening data for various spectral lines, in order to perform an adequate investigation (Beauchamp *et al.*, 1997; Adelman, 1989; Dimitrijević, 2003; Dimitrijević, Sahal-Bréchot, 2014). Stark broadening data are needed and for investigation, modelling and diagnostics of laboratory plasma (Konjević, 1999; Capelli, Measures, 1987; Torres *et al.*, 2006) as well as for diagnostics, optimisation and modelling of inertial fusion plasma (Griem, 1992; Iglesias *et al.*, 1998). Such data are also of interest for designing and optimisation of lasers (see e.g. Griem *et al.*, 1992; Deng *et al.*, 2006; Dimitrijević, Sahal-Bréchot, 2014) and for diagnostics and research of laser produced plasma (Gornushkin *et al.*, 1999; Nicolosi *et al.*, 1978; Sorge *et al.*, 2000).

Another research field where Stark broadening data might be very useful are various plasmas which can be found in technology (Yilbas *et al.*, 2015), as e.g. in the case of welding, melting or piercing of various metals by laser radiation, or for example if one needs to design or optimise plasma light sources (see for example Dimitrijević, Sahal-Bréchot, 2014). According to our analysis (Dimitrijević, Sahal-Bréchot, 2014; Dimitrijević, 2020), the principal research field where Stark broadening data is used is astronomy. There, these data are needed for abundance determinations, stellar spectra analysis and synthesis, stellar atmosphere modelling, opacity and radiative transfer calculations, stellar spectral type determination, modelling of subphotospheric layers, monitoring of thermonuclear reactions in stellar interiors and for other topics. Stark broadening data for spectral lines are particularly significant for investigation of different types of white dwarfs. The importance of Stark broadening for various spectral lines of different atoms and ions has been demonstrated for a number of white dwarfs of various spectral types as for example DB (Thejll *et al.*, 1991) and DA white dwarfs (Vennes, 1992; Bergeron *et al.*, 1994), as well as OB subdwarfs (Michaud *et al.*, 1989). This line broadening mechanism may be of interest and for A and late B stars (Musielok, Madej, 1988; Smith *et al.*, 1994; Israelian *et al.*, 1996; Zakharova, Ryabchikova, 1996; Leone *et al.*, 1997; Bonifacio *et al.*, 1995).

Gallium spectral lines are usually observed in stellar spectra (Smith, 1995; Dworetsky *et al.*, 1998; Vauclair, Vauclair, 1982; Smith, 1996; Castelli, Hubrig, 2004; Hubrig *et al.*, 2014; Sadakane, Nishimura, 2018; Monier, 2023). It is often overabundant in chemically peculiar (CP) stars, which are mostly of A and late B spectral type where Stark broadening is of interest, since hydrogen is mainly ionized, so that it is the principal pressure broadening mechanism. In the case of CP stars observations indicate that gallium spectral lines are prominent, strong and a proper tool for abundance determination. Consequently, Stark broadening data are needed for analysis and synthesis of such stellar spectra, as well as for modelling of stellar atmospheres, opacity and radiative transfer calculations etc.

In spite of the need for various topics in stellar physics, data on broadening of Ga II spectral lines are scarce. In order to provide new reliable Stark broadenig data for Ga II lines, we calculated here Stark broadening parameters, full widths at half intensity maximum (FWHM) - W, and shifts -d, for Ga II lines within six multiplets from 4d–nf (n=4,5,6) transitions. The calculations have been performed using the semiclassical perturbation theory (Sahal–Bréchot, 1969 a, 1969 b; Sahal–Bréchot *et al.*, 2014), and obtained results are used to consider Stark broadening regularities within the 4d–nf (n=4,5,6) spectral series.

2. The impact semiclassical perturbation method

An outline of the semiclassical perturbation method (Sahal–Bréchot, 1969 a, 1969 b), for calculations of Stark broadening parameters, FWHM - W and shift

- d, is given in Sahal–Bréchot *et al.* (2014). Collisional line broadening in the impact approximation considers a neutral (ionized) atom surrounded by a bath of perturbers. The interactions between atom/ion and perturbers do not perturb bath's distribution. Within impact approximation the interactions are separated in time. The atom/ion interacts with one perturber only for a given time which means that the mean duration of the collision is much smaller than the time interval between two interactions (collisions). In addition, atom/ion–radiation process and atom/ion–perturber interactions are decoupled: the emission of a photon arises when the interaction process is completed. The atom/ion–perturber interaction is treated by the time–dependent perturbation theory in long range approximation. Neutral atom follows straight line trajectory and ionized atom – a hyperbola. The full width at half maximum (FWHM) and shift of the line profile of an isolated non-hydrogenic spectral line are expressed by the equations (Sahal–Bréchot, 1969 a, 1969 b):

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

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

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 notices the electron density; v is a perturber velocity, and v represents the Maxwellian distribution of electron velocities, and ρ is the perturber's impact parameter.

The cross sections $\sigma_{kk'}(v)$, $k=i,f$, express cross sections for inelastic interactions of emitters in initial atomic energy level with charged particles. It could be written by an integration of the transition probability $P_{kk'}(\rho,v)$, over the impact parameter ρ :

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

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

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

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

where δ denotes the phase shift due to polarization $(\varphi_p \quad (r^{-4}))$ and quadrupole $(\varphi_q \quad (r^{-3}))$ 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. Stark broadening parameter calculations

With the semiclassical perturbation theoretical method (Sahal–Bréchot, 1969 a, 1969 b; Sahal–Bréchot *et al.*, 2014), here are calculated electron-impact broadening parameters, full width at half maximum of intensity (FWHM - W) and shift (d) for Ga II 4d–*n*f (n=4,5,6) transitions. The calculations are performed for temperatures of 5 000 K, 10 000 K, 30 000 K, 50 000 K and 100 000 K for a perturber density of 10^{16} cm^{-3}.

The needed atomic energy levels for Ga II, have been taken from Shirai *et al.* (2007). The needed oscillator strengths have been calculated in the Coulomb approximation. For details see for example Dimitrijević *et al.* (2022). The obtained results for six Ga II multiplets, are given in Table 1, for a perturber density of 10^{16} cm^{-3} and temperatures within the interval from 5 000 K up to 100 000 K.

It should be noted that the wavelengths in the Table 1 are calculated using atomic energy levels of terms making a multiplet.

From the beginning of spectroscopy, regularities and similarities are observed in wavelengths, energy levels, oscillator strengths, collision cross sections also, etc. Two factors determine principally the broadening of a spectral line in plasma, the environment around the emitting/absorbing particle as well as the atomic structure of the radiating particle. Atomic structures involve many regularities and similarities which consequence are regularities and similarities that could be found among the width and shift parameters of plasma broadened spectral lines. Generally, these regularities come from the atomic structure. In the case of pressure broadening of spectral lines in a plasma, regularities are expected in the cross sections for elastic and inelastic interactions between radiating (absorbing) particles and perturbers, which enter in the calculation of Stark broadening parameters. Consequently, sveral kinds of regularities and similarities can be found among the Stark broadening parameters (see e.g. Wiese, Konjević, 1982). (*i*) Regularities within a given spectrum for spectral lines within a multiplet, supermultiplet and transition array. For example, it is usually assumed in theoretical calculations that all lines exhibit the same width within a multiplet. (*ii*) Regularities exist and within a spectral series. (*iii*) Similarities can be found also in the case of analogous transitions which are in homologous atoms; (iv) Systematic behavior for given transitions along an isoelectronic sequence.

Table 1. This table gives Stark broadening parameters, W - full widths at half intensity maximum (FWHM) and shifts, for Ga II lines broadened by collisions with electrons in angstroms and in 10^{12} s^{-1} . Calculated wavelength of the transitions (in Å) are also given. Results are for a perturber density of 10^{16} cm^{-3} and temperatures are from 5 000 to 100 000 K. A positive shift is towards the red part of the spectrum.

Transition	**T [K]**	**W [Å]**	**d [Å]**	**W [10^{12} s^{-1}]**	**d [10^{12} s^{-1}]**
$4d^1D-4f^1F^o$	5000.	0.630	0.127	0.148	0.0297
λ = 8964.6 Å	10000.	0.523	0.103	0.123	0.0241
	30000.	0.457	0.0769	0.107	0.0180
	50000.	0.454	0.0653	0.106	0.0153
	100000.	0.451	0.0550	0.106	0.0129
$4d^1D-5f^1F^o$	5000.	0.640	0.280	0.548	0.239
λ = 4693.6 Å	10000.	0.577	0.229	0.494	0.196
	30000.	0.520	0.168	0.445	0.144
	50000.	0.500	0.139	0.427	0.119
	100000.	0.464	0.107	0.397	0.0912
$4d^1D-6f^1F^o$	5000.	0.957	0.494	1.30	0.670
λ = 3728.3 Å	10000.	0.900	0.412	1.22	0.559
	30000.	0.852	0.303	1.16	0.411
	50000.	0.818	0.247	1.11	0.335
	100000.	0.754	0.189	1.02	0.257
$4d^3D-4f^3F^o$	5000.	0.293	-0.00771	0.305	-0.00801
λ = 4259.0 Å	10000.	0.232	-0.0138	0.241	-0.0143
	30000.	0.169	-0.0127	0.176	-0.0132
	50000.	0.150	-0.0106	0.156	-0.0110
	100000.	0.129	-0.00864	0.134	-0.00898
$4d^3D-5f^3F^o$	5000.	0.492	0.0939	1.05	0.200
λ = 2973.4 Å	10000.	0.433	0.0864	0.924	0.184
	30000.	0.350	0.0812	0.745	0.173
	50000.	0.314	0.0651	0.668	0.139
	100000.	0.267	0.0482	0.570	0.103
$4d^3D-6f^3F^o$	5000.	0.687	0.217	1.99	0.626
λ = 2554.5 Å	10000.	0.645	0.192	1.86	0.555
	30000.	0.567	0.158	1.64	0.455
	50000.	0.522	0.129	1.51	0.374
	100000.	0.455	0.0960	1.31	0.277

With the obtained results, we will discuss here the regularities within spectral series, in order to see if the behavior in the examined spectal series of Al IV is regular in such a manner that interpolations and extrapolations within these spectral series can provide good estimates of new data and checks of con-

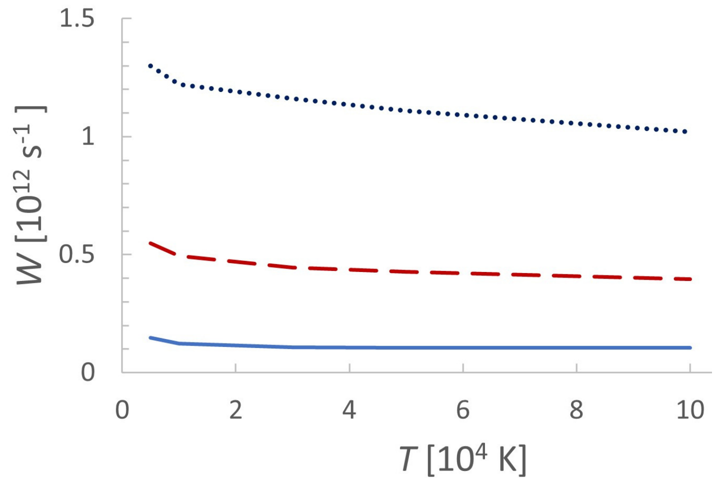

Figure 1. Behavior of Stark widths – W, in angular frequency units, with temperature, for the three members of 4d–nf spectral series (singlets). Full blue line – $4d^1D$ – $4f^1F^o$, λ = 8964.6 Å. Dashed red line – $4d^1D$ – $5f^1F^o$, λ = 4693.6 Å. Dotted dark blue line – $4d^1D$ – $6f^1F^o$, λ = 3728.3 Å. Electron density is 10^{16} cm^{-3}.

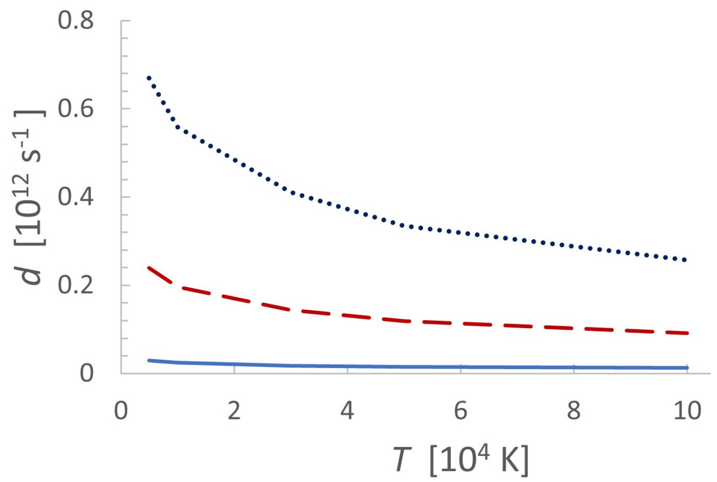

Figure 2. The same as in Fig. 1 but for the shift – d.

sistency for data existing in the literature. In order to do this, in the Table 1 are included Stark broadening parameters not only in angstroms but also in angular frequency units, obtained by the expression:

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

where c is the speed of light.

4. Discussion

We used the obtained results to study behavior of Stark broadening parameters (widths (FWHM) W, and shift d) with temperature, and with principal quantum number of the upper state, within spectral series. Fig. 1 and Fig. 2 present Stark width and shift of Ga II singlet multiplets $3d^{10}4d$ – $3d^{10}nf$ (n = 4–6) with the corresponding wavelengths 8964.6 Å, 4693.6 Å, and 3728.3 Å, belonging to the same spectral series. These results are obtained for perturber density of 10^{16} cm^{-3}. Both parameters decrease in the whole temperature interval for three spectral lines. The decrease is almost constant for higher temperatures. For λ = 8964.6 Å the Stark width varies 28 % within the 5 000 K – 100 000 K interval and Stark shift 57 %; for λ = 4693.6 Å: 28 % and 62 %, respectively, and for λ = 3728.3 Å: 21 % and 62 % for the shift. Based on these results, we can conclude that the width variations decrease with increasing of principal quantum number of the upper state. Additionally, the widths vary weakly for $T > 20\ 000$ K. The shift changes increase with the principal quantum number, and these changes are particularly distinguishable in the first part of the temperature interval for given line. In the first part of the curve, where variation with temperature is more pronounced, elastic collisions as well as strong collisions are more important while for higher temperatures, where variation with temperature is much smaller, the inelastic collisions become dominant. We can see that for higher temperatures, due to week variation of Stark width with temperature, the exact value of temperature is not so critical and we can use value obtained experimentally or theoretically for a specific temperature in a wider temperature range if higher accuracy is not needed.

Both parameters notably increase with n: from 8.9 times for T = 5 000 K to 9.6 times for T = 100 000 K, at the end of T-interval, for the width, and, 22.6 and 19.9 times, respectively, for the shift. If we look at these parameters in angstroms, we can see from Table 1 that these values for the widths are 1.5 and 1.7, while for the shifts they are 3.9 and 3.4 respectively. This is because in the case of Stark broadening in angstrems we have the influence of wavelength, which decreases with the increase of the principal quantum number n, while, on the other hand, due to the fact that perturbing atomic energy levels became closer to the upper level of the considered transition, values of Stark broadening parameters increase with the increase of n. Since there is no the influence of wavelength for Stark widths and shifts in angular frequency units, the increase with n is much larger.

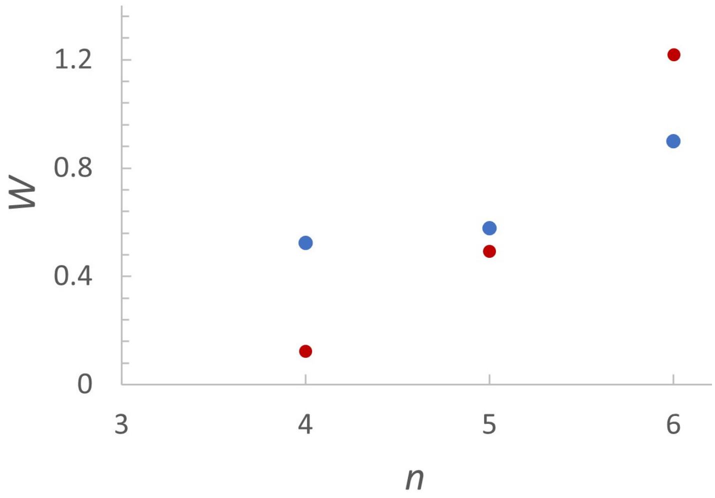

Figure 3. Behavior of Stark widths - W with principal quantum number - n of the upper atomic energy levels for $4d^1D$ - nf^1F^o (n = 4,5,6 - singlets) spectral series, in angstroms (blue dots) and in angular frequency units: 10^{12} s^{-1} (red dots). On ordinate are arbitrary units which are angstroms for blue dots and angular frequency units for red dots. Temperature is 10 000 K and electron density 10^{16} cm^{-3}.

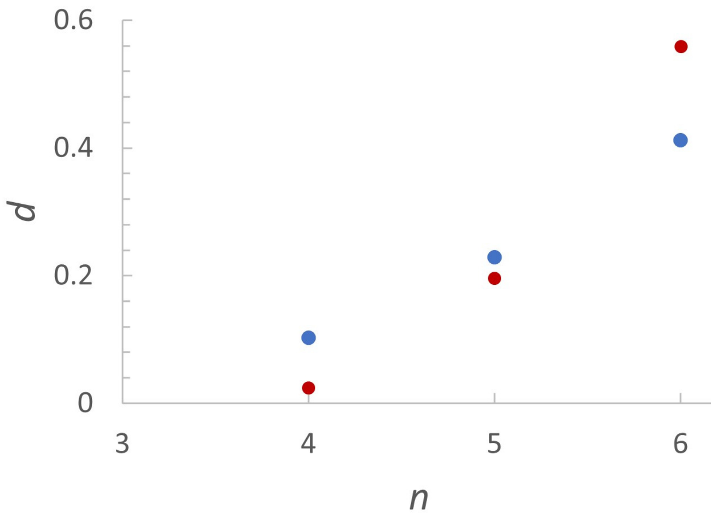

Figure 4. Same as in Fig. 3 but for the shift - d.

In the next two figures (Fig. 3 and Fig. 4) the dependence of Stark width and shift versus principal quantum number of the upper state for the same spectral series is given. The regularity of behavior of Stark broadening parameters within a spectral series provides possibility to interpolate or extrapolate new data and to check the consistency of experimental results or calculations. To illustrate this behavior, the values of electron density and temperature are fixed to 10^{16} cm^{-3} and 10 000 K. To see the difference of behavior with principal quantum number, we include both parameters in 10^{12} s^{-1} and in Å units. There is a significant increase of width and shift values versus n in the case of 10^{12} s^{-1} units, since in this case there is no the influence of wavelengths, as explained above. The difference between maximal and minimal width values in Å units is 72 %. The maximal shift in Å is three times larger than the minimal one. The same differences in 10^{12} s^{-1} units are 10 times for the width and 23 times for the shift. This means that broadening parameters in angular frequency units, liberated from the influence of wavelength, are more sensitive to the variation of principal quantum number. Both figures demonstrate a trend of broadening parameters within the series that could be useful for an estimation of line broadening for other members of the series and for checking the reliability of future experimental data.

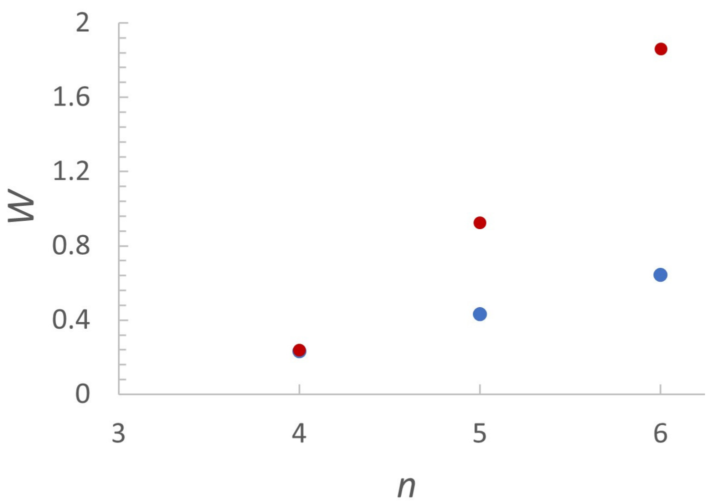

Figure 5. Behavior of Stark widths - W with principal quantum number - n of the upper atomic energy levels for $4d^3D$ – nf^3F^o (n = 4,5,6 - triplets) spectral series, in angstroms (blue dots) and in angular frequency units: 10^{12} s^{-1} (red dots). On ordinate are arbitrary units which are angstroms for blue dots and angular frequency units for red dots. Temperature is 10 000 K and electron density 10^{16} cm^{-3}.

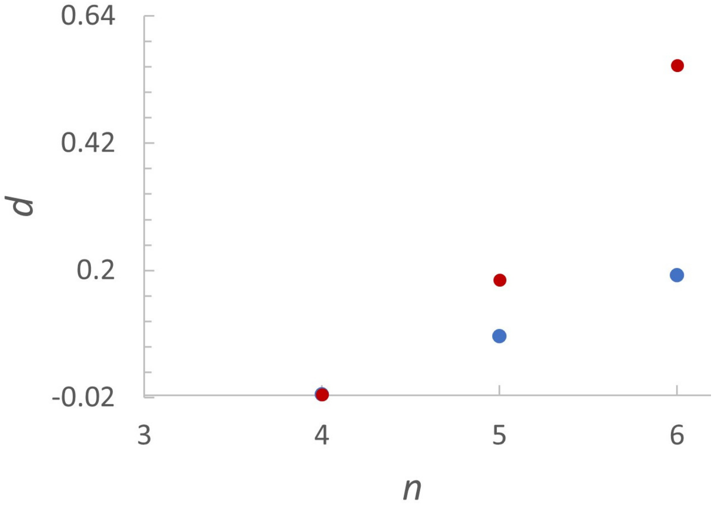

Figure 6. Same as in Fig. 5 but for the shift - *d*.

Figs. 5 and 6 show the same behavior for spectral lines of triplet transitions in Ga II $3d^{10}4d - 3d^{10}nf$ ($n = 4 - 6$) spectral series. To compare Stark broadening parameters from both series, the examined plasma conditions are the same: perturber density 10^{16} cm^{-3} and temperature 10 000 K. The symbols for width values in Å and in 10^{12} s^{-1} units coincide for principal quantum number of the upper state, four. The shift values (Å and 10^{12} s^{-1}) are negative and their symbols also coincide for $n = 4$. For $n = 5$ and $n = 6$ the shifts are positive. The width in Å varies 3 times and the shift – 15 times. The corresponding variations in 10^{12} s^{-1} units are 8 times and 40 times, respectively. The presentation of Stark broadening values in angular frequency units is more suitable, since then, the values are liberated from the influence of wavelength.

Stark widths and shifts for Ga II spectral lines calculated here will be implemented as well in the STARK-B database (Sahal–Bréchot *et al.*, 2015, 2023). This database is also a part of Virtual Atomic and Molecular Data Center (VAMDC - Albert *et al.*, 2020). It is worth to note as well, that a link to STARK-B exist also on the web site of the Serbian Virtual Observatory (SerVO, http:servo.aob.rs).

The obtained data could be useful for a number of problems in astrophysics, physics and technological plasmas, as for example for analysis and synthesis of stellar spectra, modelling of stellar atmospheres, opacity and radiative transfer calculations, determination of abundances of gallium, labortory plasma diagnostics etc.

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