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Stark Widths Regularities Within: *ns*-*np*, *np*-*ns*, *np*-*nd*, *nd*-*np* and *nd*-*nf* Spectral Series of Potassium Isoelectronic Sequence

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Abstract: Results presented in this paper show a regular behaviour of Stark widths within the studied spectral series of potassium isoelectronic sequence. These regularities have been found and verified on the basis of the existing theoretical and experimental data being normalized for the same plasma conditions (chosen electron density and temperature). Using the available set of data the corresponding formulas expressing the Stark widths of the lines originated from the spectral series studied here as a function of the upper-level ionization potential and the rest core charge of the emitter seeing by the electron undergoing transition, are obtained here. Well established and verified dependence is used to calculate Stark width data needed but not available so far. For the purposes of the operation with a large number of data, algorithms for the analysis of Stark width dependence on temperature and electron density and for the investigation of the assumed correlation between Stark width and ionization potential of the upper level of analyzed transition, have been made. Developed algorithms enable fast data processing.

Keywords: atomic data; atomic and molecular databases; stellar spectra; stars

1. Introduction

Effects of electric fields from electrons on spectral line shapes are important over a wide range of plasma parameters. The knowledge of Stark widths data is of great importance for analysis and calculations in the field of plasma physics. Our results may be applied in the field of astronomy and astrophysics, as well as in fusion research. There is a need for computing values of Stark widths and for analysis and comparing of Stark widths calculated using different approaches [1,2]. It is the researcher's aim in this field to complete the existing Stark databases and provide data that cover the astrophysical relevant temperature and density space [3,4]. Stark broadening regularities which have been examined inside spectral series of one atom or ion, as well as inside one isoelectronic sequence, can give us large amount of Stark width data by applying the obtained simple formulas as the results of the performed study of the existing regularities. This can be very important: (i) for transitions with no calculated or measured values for Stark widths, because of the lack of required parameters or (ii) for experimental purposes where it can be used, as a test of the accuracy of the Stark widths measured or calculated data published so far. A number of recently published papers were devoted to the study of different kinds of existing Stark widths regularities being used for such purposes. The present paper is concentrated on the investigation of Stark broadening within spectral series of potassium isoelectronic sequence: K I, Ca II, Sc III, Ti IV, V V, Cr VI, Mn VII, Fe VIII, Co IX, Zn X, Ga XI, Ge XII ... For example, values of K I line widths are important for precise abundance calculation related to the very popular topic of globular clusters. Recent spectroscopic and photometric observations have included potassium between elements of interest for the investigation of correlated star-to-star inhomogeneities within

globular clusters which had been considered, for years, as very simple populations with all stars having the same year and chemical population [5]. Knowledge of Ca II Stark widths is useful for analyzing spectra of special class of calcium-rich supernovae. Scandium widths are of interest for the investigation of spectra of Am Fm stars, where diffusion of atoms and structure evolution of stellar object are main problems needed to solve. Titanium and vanadium alloys are of interest for fusion application as low activation structural materials for the first wall construction. If these alloys are present under fusion conditions, presence of Ti and V ions can be expected, too. It is useful to have a wide range of Stark widths data for transitions within spectral series of Ti and V ions for application in spectral analysis during fusion related experiments. Stark widths of Fe, Cr and Mn ions are of interest for investigations related with first wall materials for fusion reactors, too [6].

2. Theoretical Background

All members of one isoelectronic sequence have the same number of electrons and it is expected that they have similar characteristics. Potassium has 19 electrons and one is in the outermost shell, a valence electron. If we analyze the first few elements of potassium isoelectronic sequence, we can conclude that K I and Ca II have [Ar]4s electronic configuration of ground state with term ^2S. Sc III, Ti IV, V V, Cr VI, Mn VII, Fe VIII, Co IX, Zn X, Ga XI, Ge XII... have [Ar]3d configuration, with term ^2D, but they all have similar excited states. In the present study, we are concentrated just in one-electron transition processes and in the electron impact contribution to the Stark broadening of spectral lines. The theory used in present research project is based on analyzing the dependence of Stark width, w, expressed in angular frequency units, rad/s, on the value of the ionization potential of the upper level of analyzed transition, χ, expressed in eV. The general formula used for regularity analysis is based on Purić et al. [7]:

$$\frac{w}{Z_e^c} = w^*[rad/s] = a \cdot log((\chi)^{-b}) \quad (1)$$

where w^* is the reduced value of the Stark width of the spectral line in angular frequency units, Z_e is the rest core charge of the emitter, $a = a_1 \cdot N_e \cdot f(T_e)$ and a_1, b and c are coefficients independent on N_e and χ. Influence of electron density and temperature on Stark broadening of spectral lines, within spectral series of potassium isoelectronic sequence, have been studied before Equation (1) has been applied in regularity analyzing procedure. Regularity approach used in present paper has been successfully applied previous articles of our group [8–15], where other emitters were analyzed.

3. Results and Discussion

Dependence of Stark widths on environmental conditions has been investigated according to the data in the Stark B database which contains data of widths at different temperatures and electron densities [16].

Stark width dependence on electron density has been analyzed and linearity has been found as a good approximation. All available data are normalized at the same value of electron density $N_e = 10^{22}$ m^{-3}. Temperature dependence used in present investigation has been used and confirmed in our previous research projects related with Stark broadening [7]. For each analyzed transition, dependence of line width on temperature is fitted according to formula:

$$w(T) = A + B \cdot T^{-c} \quad (2)$$

Parameters A, B and C are temperature independent. Algorithm for this fitting process has been made and it gives parameters A, B and C for all transitions within one chosen emitter for which there are adequate input data. This procedure has been done for all analyzed members of potassium isoelectronic sequence. Each spectral line (transition) has its own values of A, B and C parameters, and they have been used for temperature normalization. In this paper results of Stark width regularity investigation have been represented at temperature T = 100,000 K. At Figures 1 and 2

two examples of above explained fitting procedure are represented where transitions 4s-4p and 3d-6p have been analyzed. The values of parameters are $A = 6.26 \times 10^7, B = 1.89 \times 10^5, C = -0.47$ for 4s-4p transition and $A = -4 \times 10^7, B = 8.53 \times 10^7, C = -0.22$ for 3d-6p transition, respectively. Stark widths data at temperature T = 100,000 K are calculated before the start of regularity investigation for all analyzed transitions.

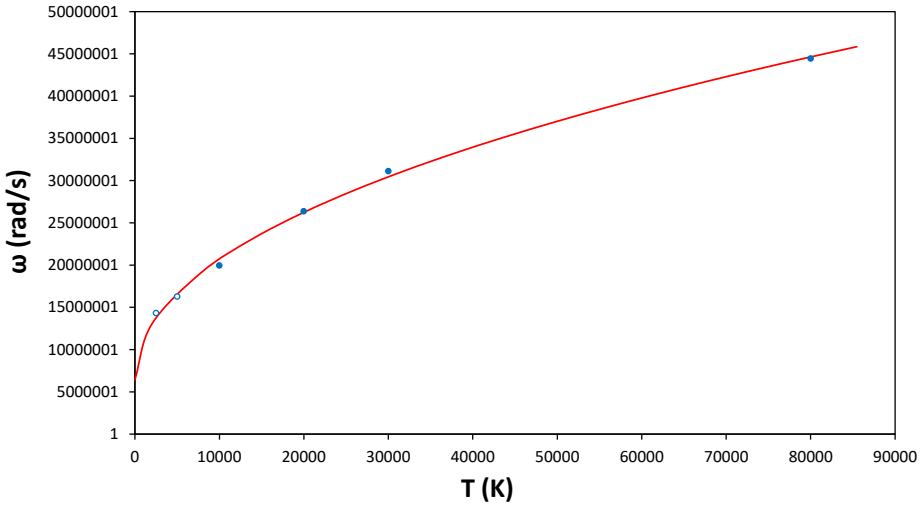

Figure 1. Stark widths functional dependence on temperature for transition 4s-4p (767.62 nm) within emitter K I ($N_e = 10^{22}$ m^{-3}).

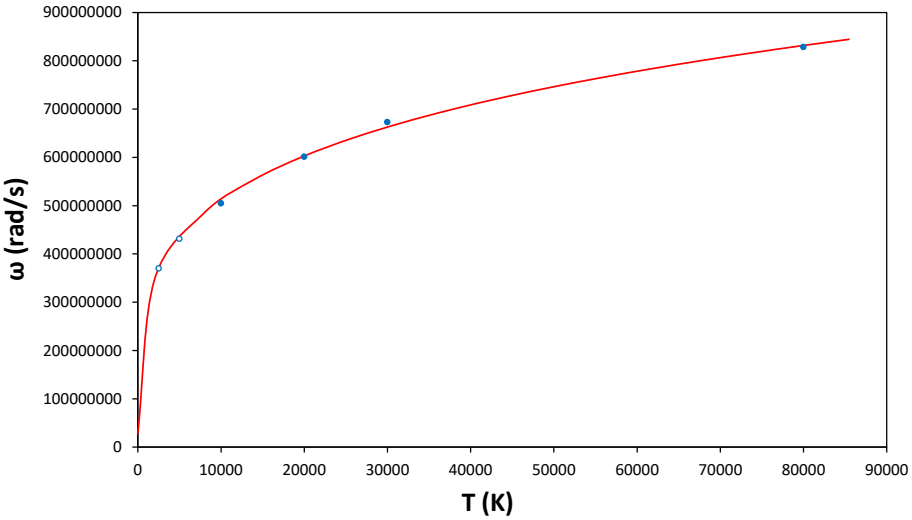

Figure 2. Stark widths functional dependence on temperature for transition 3d-6p (1338.4 nm) within emitter K I ($N_e = 10^{22}$ m^{-3}) .

The next step is to determine the value of the parameter c in Equation (1). χ values are taken from the NIST atomic database [17]. This has been done automatically by analyzing fit quality for different values of parameter c. As it can be seen from the Figure 3 fit has the best quality (the biggest value of R^2) for 2.8 value of parameter c.

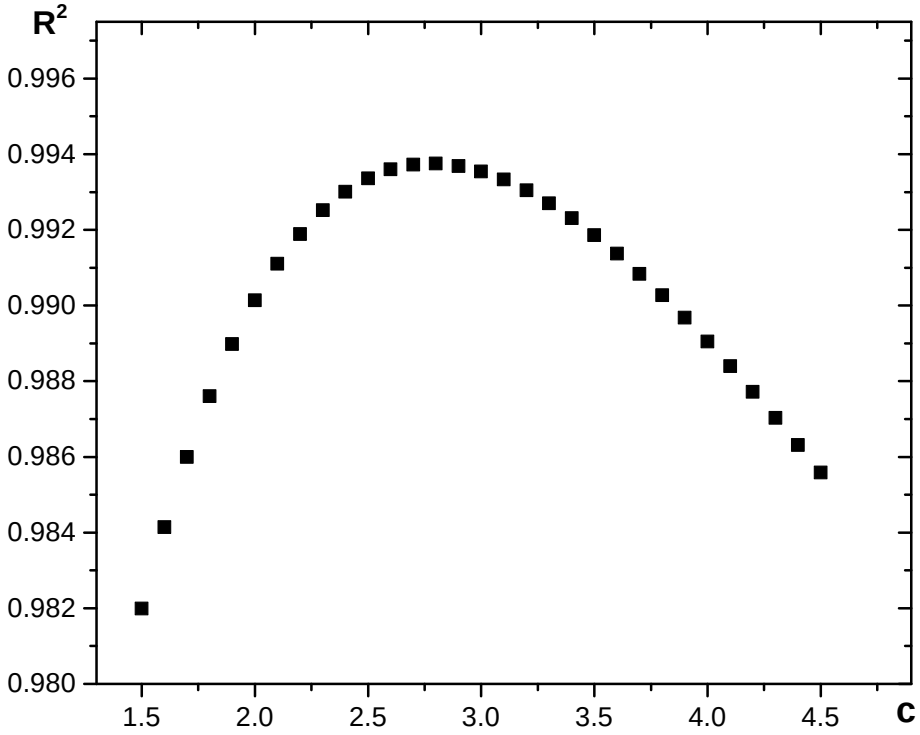

Figure 3. Determination of the best value of parameter c in Equation (1) (T = 100,000 K, $N_e = 10^{22}$ m^{-3}).

In Table 1 one can find the number of spectral lines used in final process of regularity analysis.

Table 1. Number of spectral lines used in the regularity investigation.

Element	Number of Lines
K I	46
Ca II	56
Sc III	10
Ti IV	10
V V	26

Within analysed data the following series have been investigated: 4s-*n*p, 5s-*n*p, 6s-*n*p, 4p-*n*s, 5p-*n*s, 4p-*n*d, 5p-*n*d, 3d-*n*d, 4d-*n*p, 3d-*n*f, 4d-*n*f, 5d-*n*f, 4f-*n*p, 4f-*n*d, 4f-*n*g, 5f-*n*g, 5g-*n*h, 6g-*n*h, 7g-*n*h.

Dependence of the reduced values of Stark widths on the values of ionization potential for *n*s-*n*p, *n*p-*n*s, *n*p-*n*d, *n*d-*n*p and *n*d-*n*f series of potassium isoelectronic sequence are represented at Figures 4–8, respectively. For *n*f-*n*g and *n*g-*n*f series, there is no enough data for regularity behavior analysis.

In Figure 4 significant deviations of experimental data for 4s-4p transition within Ca II ion are present (line 394.6 nm). The highest value of width for 4s-4p transition is measured by Kusch and Pritschow [18] and listed by Konjević and Wiese [19]. The smallest width value for 4s-4p transition is measured by Goldbach et al. [20]. A disagreement between theoretical and experimental data for 4s-4p transition is a well-known problem and it is pointed out by Konjević and Wiese [19], too. At this example, special quality of regularity approach can be concluded because it can be used for quality control of available data.

In Figure 5 one can see very regular change of reduced Stark widths values. There is an excellent agreement between theoretical and experimental values of K I lines: 4p-7s (578.24 nm), 4p-8s (532.33 nm), 4p-9s (508.42 nm), 4p-10s (494.20 nm), as well as big dispersal of Ca II line 4p-5s (373.62 nm). Within *n*p-*n*d spectral series (Figure 6) there is very good theory-experiment agreement for K I lines: 4p-5d (583.19 nm), 4p-6d (535.96 nm), 4p-7d (511.22 nm), 4p-8d (496.50 nm) and dispersal

of Ca II line 4p-4d (315.89 nm). *n*d-*n*p spectral series have the best quality of linear fit, ie. the biggest value of R^2: 0.9978 (Figure 7). Expected regularity behavior are present within *n*d-*n*f spectral series, too (Figure 8).

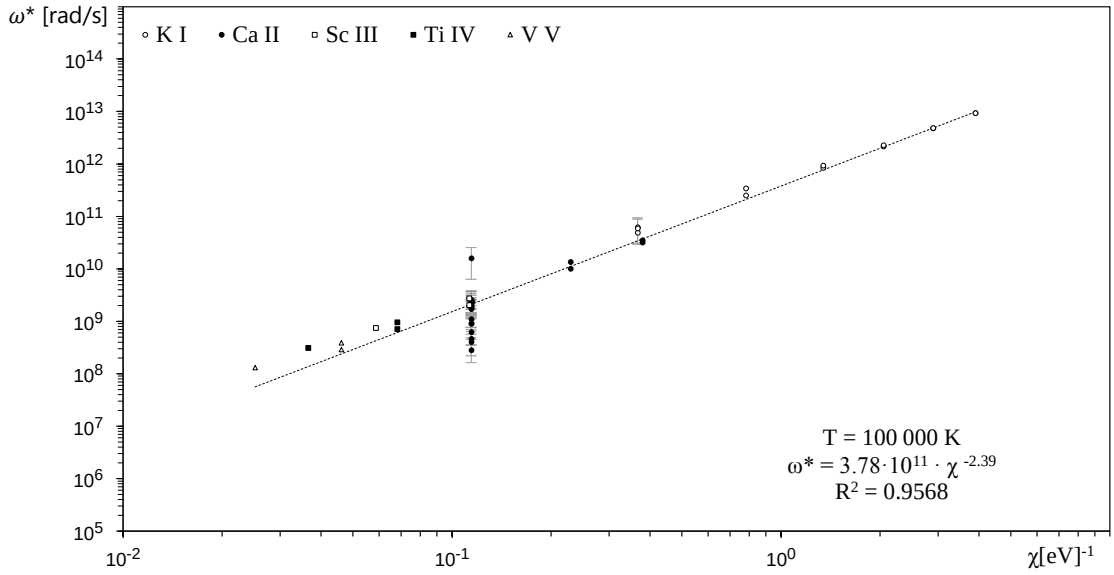

Figure 4. Stark width regularities within *n*s-*n*p spectral series of the potassium isoelectronic sequence – the electron impact contribution (T = 100,000 K, $N_e = 10^{22}$ m^{-3}). Experimental data are represented with appropriate errors.

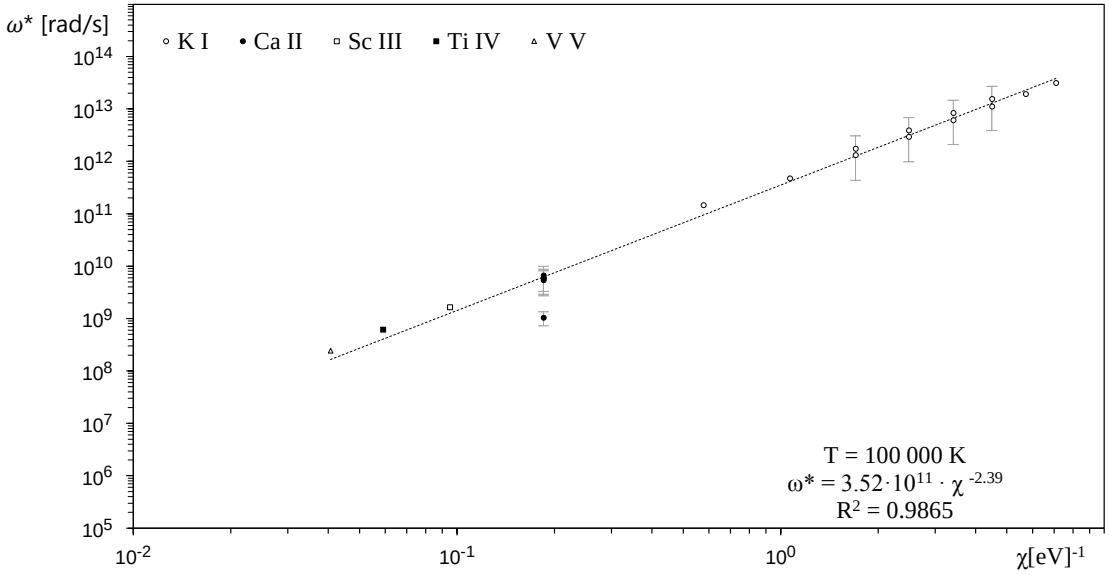

Figure 5. Stark width regularities within *n*p-*n*s spectral series of the potassium isoelectronic sequence – the electron impact contribution (T = 100,000 K, $N_e = 10^{22}$ m^{-3}). Experimental data are represented with appropriate errors.

Stark widths of spectral lines can be calculated according to the Equation (3) for *n*s-*n*p, *n*p-*n*s, *n*p-*n*d, *n*d-*n*p and *n*d-*n*f spectral series within potassium isoelectronic sequence.

$$\Delta\lambda = p \cdot 10^{-20} \cdot \frac{Z_e^{2.8} \cdot N_e}{\chi^q} \cdot \lambda^2 \quad (3)$$

where $\Delta\lambda$ is expressed in [m], N_e is expressed in [m^{-3}] and χ is expressed in [eV]. p and q are parameters given in Table 2 for each analyzed spectral series within isoelectronic sequence.

If the required atomic parameters for transitions within potassium isoelectronic sequence are known, Stark widths can be calculated using known theoretically derived formulas, but if there is a lack of required parameters, regularities derived in present paper enable determination of Stark broadening data.

Equation (3) enables calculation of Stark broadening data for investigated spectral series (Table 2) within isoelectronic sequence of potassium in temperature range $10^{-2} \cdot \chi_0$ and χ_0 (defined by Griem [21]). It can be used for prediction of widths, as well as for quality control of experimental results. Stark widths calculated according to the Equation (3) and Table 2, for some spectral lines of potassium isoelectronic sequence are given in Table 3.

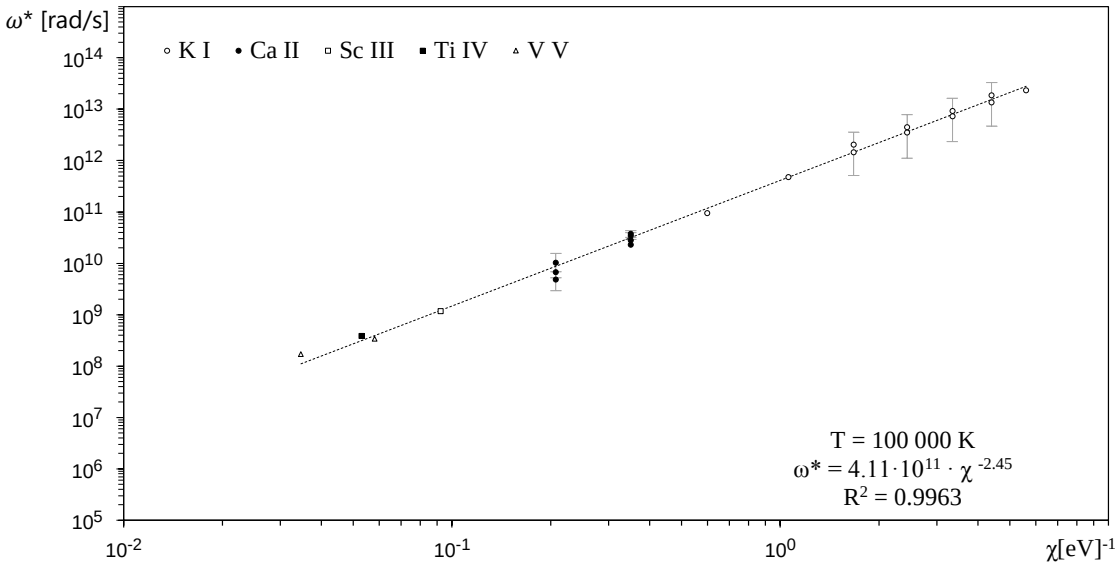

Figure 6. Stark width regularities within *n*p-*n*d spectral series of the potassium isoelectronic sequence – the electron impact contribution (T = 100,000 K, N_e=10^{22} m^{-3}). Experimental data are represented with appropriate errors.

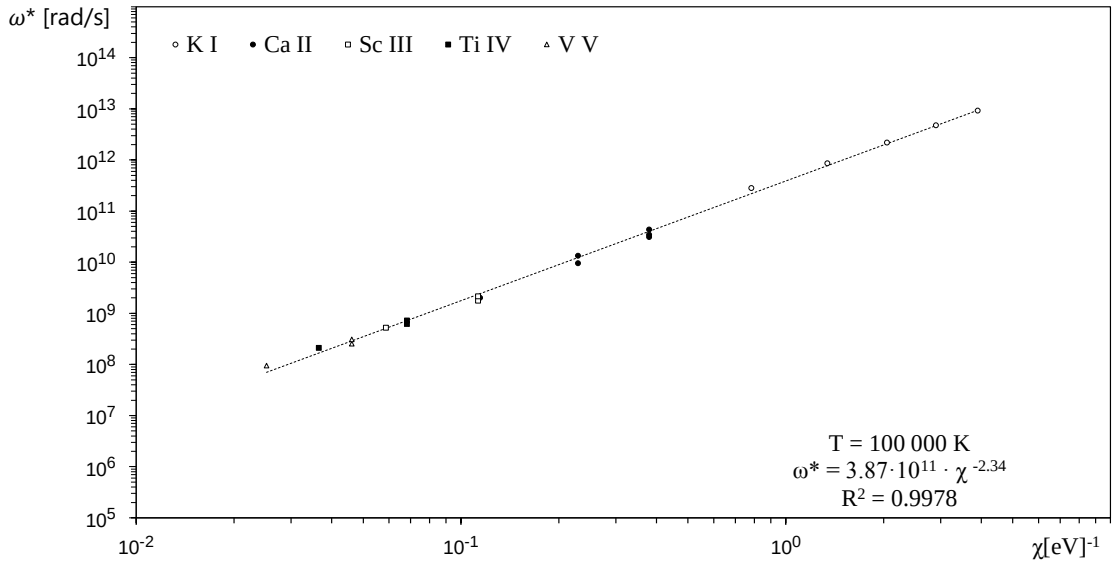

Figure 7. Stark width regularities within *n*d-*n*p spectral series of the potassium isoelectronic sequence – the electron impact contribution (T = 100,000 K, N_e = 10^{22} m^{-3}).

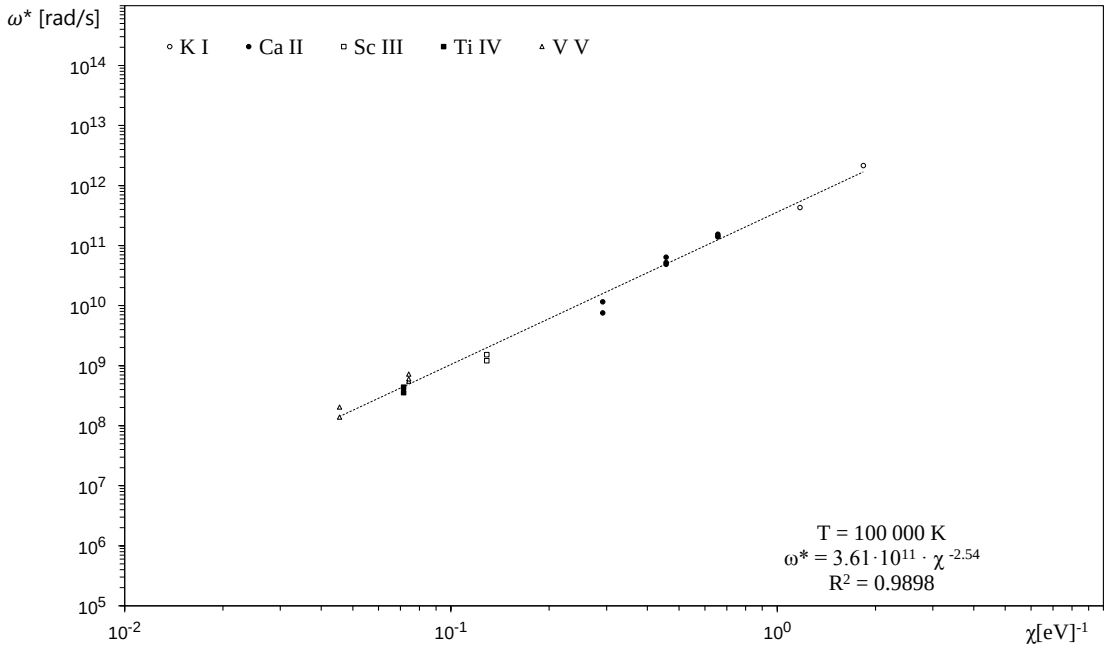

Figure 8. Stark width regularities within *n*d-*n*f spectral series of the potassium isoelectronic sequence – the electron impact contribution (T = 100,000 K, $N_e = 10^{22}$ m^{-3}).

Table 2. Values of parameters p and q in Equation (3) for analyzed spectral series.

Spectral Series	p	q
*n*s-*n*p	2.00	2.39
*n*p-*n*s	1.87	2.39
*n*p-*n*d	4.11	2.45
*n*d-*n*p	3.87	2.34
*n*d-*n*f	3.61	2.54

Table 3. The calculated values for the total electron impact contribution to the Stark widths (FWHM) $\Delta\lambda$ of spectral lines within K isoelectronic sequence; at T = 100,000 K normalized to an electron density of $N_e = 10^{22}$ m^{-3} are given.

Emitter	Transition	λ [nm]	$\Delta\lambda$ [nm]
Ti IV	4d-5f	126.51	1.04×10^{-3}
Ti IV	6p-7d	315.67	3.40×10^{-2}
Cr VI	4d-5p	116.72	2.77×10^{-4}
Cr VI	4d-4f	126.48	1.43×10^{-4}
Cr VI	5p-6s	134.27	3.54×10^{-4}
Cr VI	4s-4p	141.76	4.17×10^{-5}
Cr VI	5p-5d	217.66	1.18×10^{-3}
Fe VIII	3d-7f	14.98	3.23×10^{-7}
Fe VIII	3d-6f	15.76	3.57×10^{-7}
Fe VIII	3d-5f	17.28	4.30×10^{-7}
Fe VIII	3d-4p	19.47	1.38×10^{-6}
Fe VIII	3d-4f	20.98	6.33×10^{-7}

4. Conclusions

Regularities of Stark broadening within spectral series of potassium isoelectronic sequence have been investigated and approved. The aim of this paper was to establish as precisely as possible the

Stark parameters dependence on the rest core charge of emitters for any chosen transition within *n*s-*n*p, *n*p-*n*s, *n*p-*n*d, *n*d-*n*p and *n*d-*n*f series of potassium isoelectronic sequence. The simple model proposed in this investigation enables calculation of Stark widths for any chosen transition within investigated series of potassium isoelectronic sequence. Additionally, developed algorithms for fast data processing give a special quality to this work. Presented model is important for getting a new Stark line broadening data and as a referent point for experimental data. Regularity approach can simplify complicated theoretical calculations and it is of special interest for problems where it is not possible to calculate the value of Stark widths using other methods because of the lack of parameters needed for calculation.

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