Bull. Astr. Soc. India (2012) **40**, in press

Stark width regularities of neutral potassium lines within different spectral series

D. Jevtić, I. P. Dojčinović, I. Tapalaga* and J. Purić
University of Belgrade, Faculty of Physics, P. O. Box 44, 11000 Belgrade, Serbia

Received 2012 March 06; accepted 2012 May 14

Abstract. The effects of upper level ionization potential on Stark widths of different spectral series of neutral potassium have been studied and discussed in this paper. Proton impact contribution to the Stark broadening show similar dependences as that of electron impact contribution. It is also shown that the term structure influences the Stark widths. Higher correlation between the empirical parameters were found when the temperature was increased. The deviation of the lowest transition from 4p-*n*d series trend can be explained by absence of close perturbing states to the emitting state. After establishing these dependences, the relations found were used for prediction of Stark widths for the missed lines, thus avoiding complicated calculation procedures.

Keywords : atomic data – line: profiles – opacity – plasmas – radiative transfer

1. Introduction

There has been an increase in the experimental and theoretical values of Stark braodening data in the last forty years (Purić et al. 2008; Elabidi & Sahal-Bréchot 2011). Nevertheless, there is still a lack of data for many of the observed spectral lines and lines used in modelling different objects of astrophysical interest. Such data are used in analyses of relative abundances of chemical elements, opacity calculations, radiative transfer through stellar atmospheres and effects of line profiles on synthetic spectra (Zhang et al. 2006; Thomas 1996; Burrows & Volobuyev 2003; Chaffee & White 1982; Takeda et al. 2012). Therefore, it is of interest to exploit any possible theoretical approach which can provide simple relations for the acquisition of new data and for the evaluation of available theoretical and experimental results.

*email: irinel@ff.bg.ac.rs

For these purposes the regularities of Stark parameters have been analysed using different approaches. All approaches tend to use the least number of parameters and variables due to the unavailability of essential data required for evaluating complicated dependences. The primary difference was in the choice of a parameter that describes atomic structure influence and consequently affects spectral line broadening. For instance, some papers were devoted to investigate the Stark parameters' dependence on the principal quantum number (Colón & Alonso-Medina 2002; Dimitrijević & Sahal-Brechot 1984), the others on effective quantum number (Sarandaev & Salakhov 1996) or on atomic number and the ionization potential from the ground level (Purić, Ćuk & Lakićević 1985). A series of papers were devoted to the study of the Stark parameter dependences on the upper level ionization potential (Purić, Lakićević & Glavonjić 1980; Purić et al. 1985; Purić & Ščepanović 1999; Purić et al. 2008, 1988; Puric, Miller & Lesage 1993; Šćepanović & Purić 2003). It is very convenient for studying Stark broadening parameters regularities by defining the binding energy of the electron undergoing transition. The upper level ionization potential (χ) used in those papers reflects the exposure of electron undergoing transition to plasma electric micro-field. The Stark broadening effect is dependent on electric field and therefore it is expected for χ to convey that influence on the Stark broadening parameters.

This dependence was successfully used recently in a series of papers devoted to the study of regularities within spectral series of Mgı (Tapalaga, Dojčinović & Purić 2011), Beı (Dojčinović, Tapalaga & Purić 2011), Heı (Dojčinović, Tapalaga & Purić 2012) and Caı (Tapalaga et al. 2012) where coefficients obtained suggested that the upper level ionization potential χ is an appropriate parameter for studying the Stark broadening dependence within similar spectra.

The aim of this paper is to analyse functional dependence of Stark widths of spectral lines (FWHM) on the upper level ionization potential, χ, of the corresponding transition within spectral series of Kı. Using the proposed simple model, one can provide Stark broadening data for transitions that have not yet been calculated due to the lack of parameters needed in more complicated models.

Stark broadening data used for the analysis presented in this paper was taken from Griem (1974) and Dimitrijević & Sahal-Bréchot (1987, 1990). Most of this data are available on-line (Sahal-Bréchot, Dimitrijević & Moreau 2012). The experimental data of Kı were found in the works of Hohimer (1985) and Purić et al. (1976) and are used for verification of theoretical results. Data for ionization potential of Kı spectral lines were taken from NIST database (Ralchenko et al. 2011). A total of 50 spectral lines of Kı have been collected and analysed. Within these data the following series have been investigated: 3d-*n*p (2), 4d-*n*p (2), 4p-*n*d (2), 4p-*n*s (2), 4s-*n*p (2), 5d-*n*p (2), 5p-*n*s (2), 5s-*n*p (2). Next to the series notation there is a number in parentheses (2) indicating doublet spectral lines.

2. Theory

Similar behaviour of Stark broadening data and χ have been found by Purić, Lakićević & Glavonjić (1979). This discovery was followed by investigation of analytic relation between Stark widths

Table 1: The appropriate fitting parameters a and b are given for T= 5 000 K together with corresponding coefficient of determination R^2 for the electron and proton impact contributions to the Stark widths for all studied series (N_e=10^{22} m^{-3}).

Spectral	Electron impact broadening			Proton impact broadening		
series	*a*	*b*	R^2	*a*	*b*	R^2
3d-*n*p (2)	2.199E+11	2.289	1.0000	7.143E+10	2.190	0.9994
4d-*n*p (2)	2.458E+11	2.201	0.9999	5.634E+10	2.392	0.9991
4p-*n*d (2)	2.966E+11	2.334	0.9997	7.598E+10	2.275	0.9996
4p-*n*s (2)	2.539E+11	2.146	0.9999	5.543E+10	2.275	0.9996
4s-*n*p (2)	2.019E+11	2.388	0.9987	7.689E+10	2.137	0.9998
5p-*n*d (2)	2.931E+11	2.344	0.9996	6.855E+10	2.344	0.9989
5p-*n*s (2)	2.558E+11	2.145	0.9999	5.683E+10	2.056	0.9998
5s-*n*p (2)	2.061E+11	2.354	0.9997	7.609E+10	2.139	0.9998

Table 2: The appropriate fitting parameters a and b are given for T= 25 000 K together with corresponding coefficient of determination R^2 for the electron and proton impact contributions to the Stark widths for all studied series (N_e=10^{22} m^{-3}).

Spectral	Electron impact broadening			Proton impact broadening		
series	*a*	*b*	R^2	*a*	*b*	R^2
3d-*n*p (2)	3.283E+11	2.271	1.0000	7.758E+10	2.207	0.9995
4d-*n*p (2)	4.704E+11	1.969	0.9987	5.514E+10	2.513	0.9983
4p-*n*d (2)	3.672E+11	2.337	0.9997	9.230E+10	2.288	0.9996
4p-*n*s (2)	3.296E+11	2.183	0.9994	7.143E+10	2.074	0.9998
4s-*n*p (2)	3.062E+11	2.339	0.9999	8.336E+10	2.153	0.9998
5p-*n*d (2)	4.171E+11	2.251	1.0000	8.351E+10	2.357	0.9988
5p-*n*s (2)	3.701E+11	2.112	0.9987	7.013E+10	2.098	1.0000
5s-*n*p (2)	3.513E+11	2.214	0.9997	7.971E+10	2.188	0.9996

and χ in paper of Purić et al. (1980). The quantum theoretical basics for this relation are given by Griem (1968). The final form of Stark width dependence is given by:

$$w(rad/s) = a \cdot (\chi(eV))^{-b} \tag{1}$$

In this equationi, w is Stark width in rad/s, χ is the upper level ionization potential taken in eV; and a, b are the fitting coefficients independent of χ.

Explicit dependence of Stark width on the upper level ionization potential, as presented by equation (1), has the form that is unsuitable for analyses due to wide range of available data.

Stark widths in a single series can differ up to 10 000 times. Due to this fact we have used the form that displays the data linearly:

$$log(w) = log(a) + b \cdot log(\chi^{-1}) \tag{2}$$

The available Stark broadening data is given for different plasma conditions and cannot be used in this analysis and compared directly without normalisation to the same plasma conditions. The data can be normalized to the same N_e by linear scaling due to the linear dependence of Stark widths for non-hydrogenic atoms on N_e. In this paper the data were normalized to $N_e = 10^{16}$ cm^{-3}. Temperature of plasma also influences Stark broadening. It was commonly expected for Stark width broadening to be a weak function of temperature. For ion spectral lines dependence was found to be of the form $w \sim T^{1/2}$. However, the whole spectrum of different temperature dependences has to be used in this case instead in order to match the data more precisely (Purić & Ščepanović 1999; Purić et al. 2008). Temperature dependence in the case of neutrals has to be of the form:

$$f(T) = A + B \cdot T^{-c} \tag{3}$$

In a series of articles (Tapalaga et al. 2011, 2012; Dojčinović et al. 2011, 2012) it was shown that this dependence was appropriate for every spectral line. Coefficients A, B and C are independent of temperature. Temperature range, in which equation (3) is suitable for application, is defined by Griem (1974) and it lies between $10^{-2} \cdot \chi_0$ and χ_0.

3. Results and discussion

Normalization of source data was done by custom made software according to the above equations. This software enables the normalization to any electron density or temperature and provides coefficient of determination that is used to evaluate the credibility of proposed theoretical models. By definition, the coefficient of determination is a measure of how well a regression line approximates the real data points. $R^2 = 1$ indicates that the regression line perfectly fits the data. Additionally the software analyses Stark broadening dependence on the upper level ionization potential and compares the data with theoretical model given by equation (2).

For all the studied series it was found that the relation given by equation (2) is appropriate for temperature 5 000 K and 25 000 K in the case of electron and proton impact contributions to the Stark widths. The dependences of the Stark width on the upper level ionization potential were verified for 46 out of 50 K I spectral lines belonging to 8 from 10 spectral series studied here. In Table 1 and Table 2 the appropriate best-fitting coefficients a and b are given for 5 000 K and 25 000 K temperature together with corresponding coefficient of determination R^2 for the electron and proton impact contributions to the Stark widths for 8 studied series. The best fit coefficients (a) and (b), given in Tables 1 and 2, are obtained using data taken from Dimitrijević & Sahal-Bréchot (1987, 1990). The appropriate dependences expressed by equation (2) for all studied series are given graphically by straight lines in all corresponding four figures. It was found that deviation of the used data from these dependences are less then 56.2% in all studied cases.

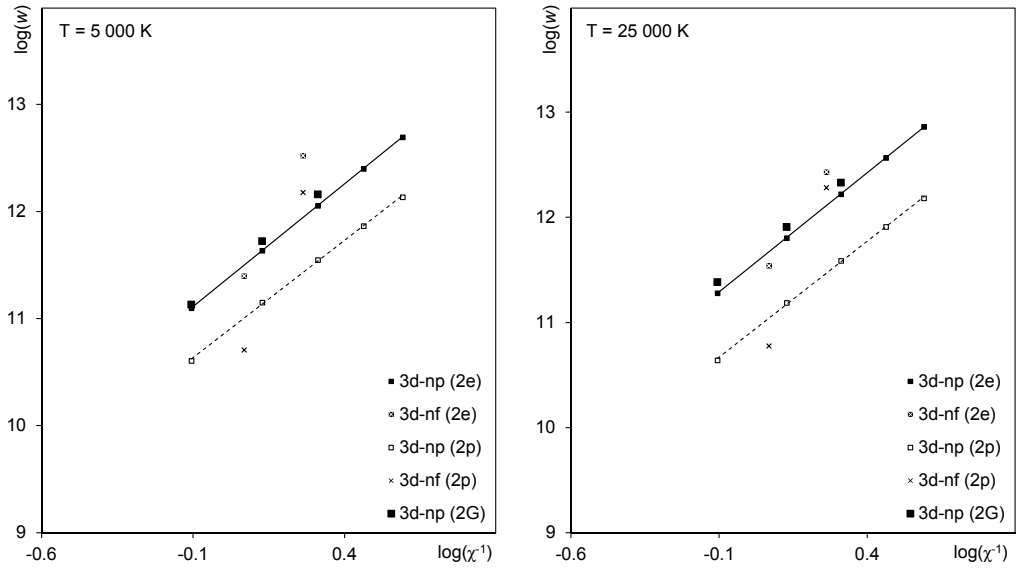

Figure 1: The electron (solid line) and proton impact (dash line) contributions to Stark widths (in rad/s) and Griem´s data versus inverse upper level ionization potential (in eV) presented in log-log scale for different Kı spectral series with principal quantum number of lower level equal to n=3 at temperatures 5 000 K and 25 000 K. The number 2 in brackets indicates doublets, letters e, p and G indicate electron, proton and theoretical Griem´s data, respectively.

The electron and proton impact contributions to the Stark widths dependences versus inverse value of the upper level ionization potential given for all investigated spectral series for different Kı spectral series with principal quantum number of lower level equal to n=3 is presented in Fig. 1, with principal quantum number of lower level equal to n=4 in Fig. 2 and with n=5 in Fig. 3, all of them at electron temperature of 5 000 K and 25 000 K. Values taken from Griem (1974) are also included in figures for the sake of comparison. Agreement was found to be within 20% at temperature 5 000 K and 25% at 25 000 K. One can mention that the proton impact contribution to Stark widths is significantly smaller than the electron impact contribution, but nevertheless it cannot be neglected. The average relative contribution of proton impact is 26% of electron contribution at 5 000 K, and 23% at temperature of 25 000 K. It is interesting to note that dispersion of Stark widths data is decreasing with increasing temperature. It has been found that temperature increment reduces differences in Stark broadening data of investigated spectral series by 8%. The effect can be noticed if charts belonging to the same figure are compared. Similar behaviour was noticed in preceding papers (Tapalaga et al. 2011; Dojčinović et al. 2011, 2012; Tapalaga et al. 2012).

When the studied spectral series were treated separately, the majority of the corresponding coefficients of determinations R^2 were better than 0.99, except for series 4p-nd. The reason for low R^2 value for this series lies in low Stark width for transition 4p-3d because 3d state has no

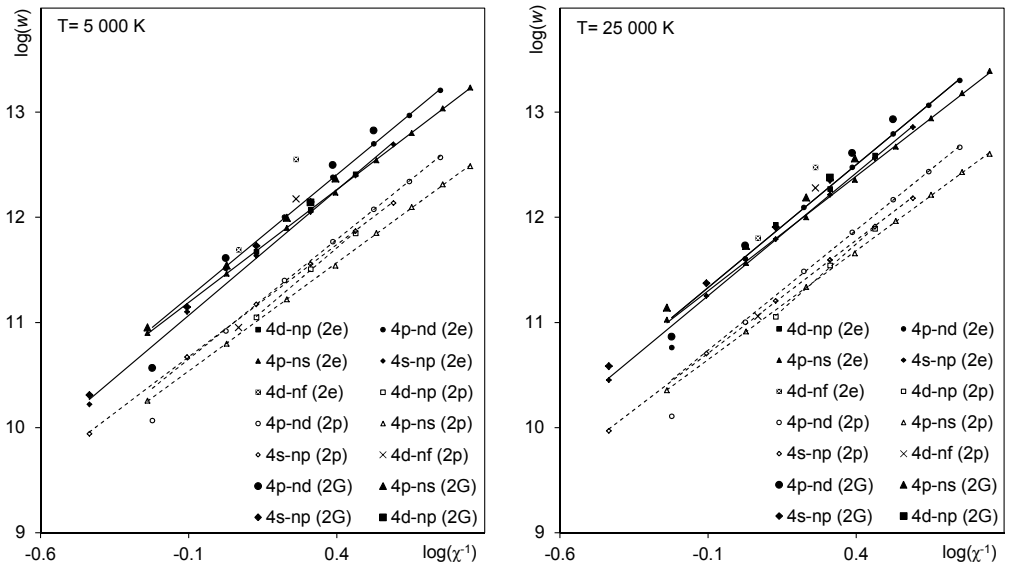

Figure 2: The electron and proton impact contributions to Stark widths (in rad/s) and Griem´s data versus inverse upper level ionization potential (in eV) presented in log-log scale for different KI spectral series with principal quantum number of lower level equal to n=4 at temperatures 5 000 K and 25 000 K. The number 2 in brackets indicates doublets, letters e, p and G indicate electron, proton and theoretical Griem´s data, respectively.

close perturbing f or any other state. For series 3d-nf and 4d-nf coefficients of determination R^2 were not available for only two lines per series existing. It was found, as well, that for 3d-3f and 4d-3f there are no close perturbing states for 3f transition and so lines obtained were narrower than expected. Therefore those two series were excluded from further analysis but they are presented along with other series studied in Figs. 1 and 2 for sake of comparison. If 4p-3d transition is excluded from trend analysis, obtained R^2 values for electron contribution are much better, namely, 0.9997 instead of 0.9879 for temperature of 5 000 K. Average relative error for all spectral transitions is 3.10% at T=5 000 K and 2.86% at T=25 000 K. Maximum relative error was 56.2% obtained for 4p-3d transition at T=5 000 K. Analysing electron and proton contribution, as well as the Griem'values for transition 4p-3d the same behaviour was noticed. Lowering of Stark widths for the lowest transition in one of the series was previously observed in works devoted to MgI by Tapalaga et al. (2011) (3p-nd triplet), HeI by Dojčinović et al. (2011) (2s-np singlet and triplet) and CaI by Tapalaga et al. (2012) (4p-nd singlet and triplet).

The total Stark width (sum of electron and proton impact contributions) dependences on the upper level ionization potential together with the corresponding experimental values are graphically presented in Fig. 4 at 5 000 K and 25 000 K. By comparing theoretical values of total line width with experimental ones, we found good agreement for both investigated temperatures,

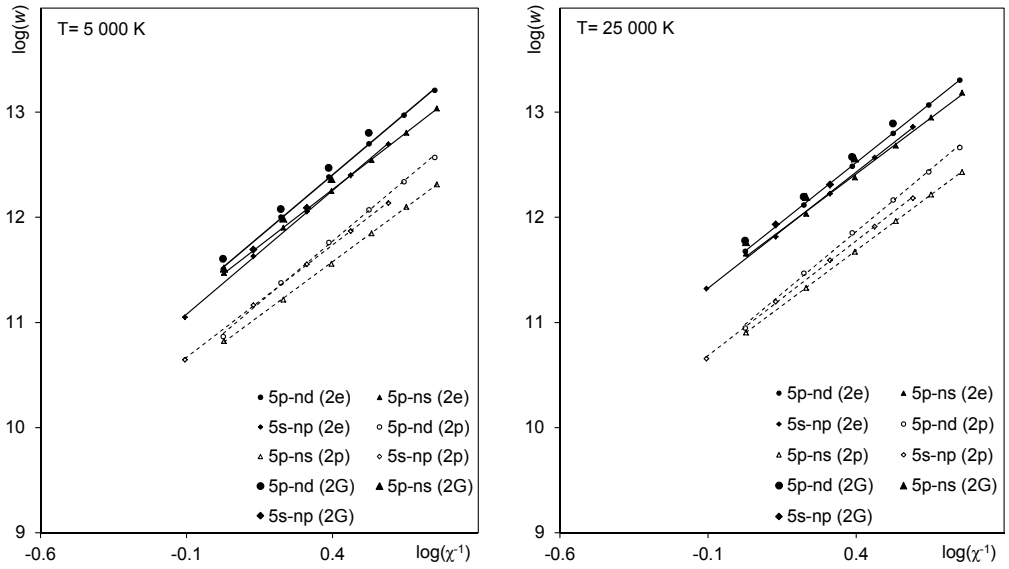

Figure 3: The electron and proton impact contributions to Stark widths (in rad/s) and Griem´s data versus inverse upper level ionization potential (in eV) presented in log-log scale for different Kı spectral series with principal quantum number of lower level equal to n=5 at temperatures 5 000 K and 25 000 K. The number 2 in brackets indicates doublets, letters e, p and G indicate electron, proton and theoretical Griem´s data, respectively.

namely, 20% (Hohimer 1985) for temperature 5 000 K and 55% (Purić et al. 1976) for temperature 25 000 K.

In addition to trend analysis, the obtained Stark width dependences on the upper level ionization potential can be used for prediction of Stark widths data for the lines of interest in astrophysics as well as in atomic physics not investigated until now. Stark widths data for 18 lines missing so far from 8 spectral series studied here are predicted and given in Table 3. Based on the above described analysis it is possible to predict Stark widths at any temperature but the results in this paper are given only for T = 5 000 K and T = 25 000 K.

4. Conclusions

Searching for different types of regularities and systematic trends which can simplify complicated theoretical calculations is of great interest. Therefore the aim of this paper was to establish as precisely as possible the Stark parameters dependence on the upper level ionization potential for Kı spectral series and to demonstrate capabilities of described method.

In this work the existence of the functional dependences of Stark widths on the upper level

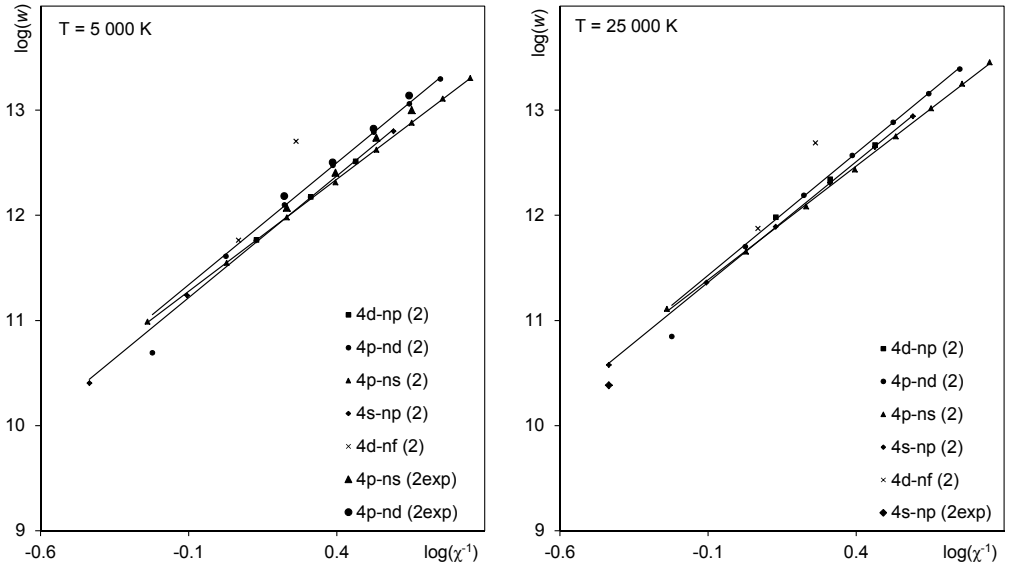

Figure 4: The total Stark widths (expressed in rad/s) versus inverse upper level ionization potential (expressed in eV) for different KI spectral series with principal quantum number of lower level equal to n=4 are presented at temperatures 5 000 K and 25 000 K. The number 2 in brackets indicates doublets. The corresponding experimental values are included at 5 000 K (Hohimer 1985) and 25 000 K (Purić et al. 1976).

ionization potential was shown for the lines originating from the 8 studied series. These dependences were obtained and found to be of the form given by equation (2). Electron and proton impact contribution to Stark width broadening have the same type of behaviour, but the proton contribution is significantly smaller. They can be used to evaluate the results of Stark broadening data that is already measured or calculated or for prediction of the Stark widths values not measured or theoretically calculated until now.

Temperature dependence is very important in Stark parameters regularities studies and therefore we have used theoretical values obtained by different authors for 50 KI spectral lines originating from 10 different series through the introduced coefficients A, B and C (equation 3). It was found that high temperatures tend to eliminate differences in Stark broadening for all other parameters except for upper level ionization potential.

The best precision can be obtained using the same equation for any particular series separately. In order to achieve better linear fitting for 3p-*n*d series, transition 3p-3d has to be neglected in the further analysis.

Table 3: The calculated values for the total impact contribution to i the Stark widths (FWHM) w (nm) of Kı spectral lines; at T = 5 000 K and T = 25 000 K normalized to an electron density of $N_e = 10^{22}$ m^{-3} are given.

Ion	λ(Å)	Transition	w (nm) T=5 000K	w (nm) T=25 000K
Kı	8421.47	3d-10p	0.429	0.591
Kı	8419.83	3d-11p	0.430	0.592
Kı	8041.68	3d-12p	1.045	1.434
Kı	7867.34	5s-11p	0.653	0.837
Kı	7724.60	5s-12p	1.009	1.267
Kı	18034.76	4d-9p	1.102	1.476
Kı	16633.17	4d-10p	1.669	2.143
Kı	15776.97	4d-11p	2.507	3.109
Kı	15209.89	4d-12p	3.698	4.453
Kı	11745.0	4p-3d	0.008	0.010
Kı	4805.67	4p-10d	0.414	0.516
Kı	4758.70	4p-11d	0.640	0.797
Kı	2992.99	4s-10p	0.057	0.077
Kı	2964.08	4s-11p	0.096	0.128
Kı	2943.53	4s-12p	0.153	0.202
Kı	10951.10	5p-10d	2.178	2.611
Kı	10710.23	5p-11d	3.291	3.892
Kı	10927.36	5p-12s	1.281	1.736

Acknowledgements

This work is financially supported by the Ministry of Education and Science of the Republic of Serbia within the project 171034. We thank the reviewer for his/her comments which helped improve the manuscript.

References

Burrows A., Volobuyev M., 2003, ApJ, 583, 985
Chaffee F. H., Jr., White R. E., 1982, ApJS, 50, 169
Colón C., Alonso-Medina A., 2002, JPhB, 35, 1143
Dimitrijević M. S., Sahal-Bréchot S., 1984, A&A, 136, 289
Dimitrijević M. S., Sahal-Bréchot S., 1987, JQSRT, 38, 37
Dimitrijević M. S., Sahal-Bréchot S., 1990, BOBeo, 142, 29
Dojčinović I. P., Tapalaga I., Purić J., 2011, PASA, 28, 281

Dojčinović I. P., Tapalaga I., Purić J., 2012, MNRAS, 419, 904
Elabidi H., Sahal-Bréchot S., 2011, EPJD, 61, 285
Griem H. R., 1968, PhRv, 165, 258
Griem H. R., 1974, Spectral Line Broadening by Plasmas, Academic Press, New York
Hohimer J. P., 1985, PhRvA, 32, 676
Purić J., Ščepanović M., 1999, ApJ, 521, 490
Purić J., Labat J., Djeniže S., Ćirković L., Lakićević I., 1976, PhLA, 56, 83
Purić J., Lakićević I., Glavonjić V., 1979, JPhys, 40, 795
Purić J., Lakićević I., Glavonjić V., 1980, PhLA, 76, 128
Purić J., Ćuk M., Lakićević I. S., 1985, PhRvA, 32, 1106
Purić J., Djeniže S., Srećković A., Ćuk M., Labat J., Platiša M., 1988, ZPhyD, 8, 343
Puric J., Miller M. H., Lesage A., 1993, ApJ, 416, 825
Purić J., Dojčinović I. P., Nikolić M., Šćepanović M., Obradović B. M., Kuraica M. M., 2008, ApJ, 680, 803
Ralchenko, Yu., Kramida, A.E., Reader, J., and NIST ASD Team (2011). NIST Atomic Spectra Database (ver. 4.1.0), [Online]. Available: http://physics.nist.gov/asd [2012, February 27]. National Institute of Standards and Technology, Gaithersburg, MD.
Sahal-Bréchot, S., Dimitrijević, M.S., Moreau N., 2012. Stark-B database, [online]. Available: http://stark-b.obspm.fr [Feb 27, 2012]. Observatory of Paris, LERMA and Astronomical Observatory of Belgrade
Sarandaev E. V., Salakhov M. K., 1996, JQSRT, 56, 399
Šćepanović M., Purić J., 2003, JQSRT, 78, 197
Takeda Y., Kang D.-I., Han I., Lee B.-C., Kim K.-M., Kawanomoto S., Ohishi N., 2012, PASJ, 64, 38
Tapalaga I., Dojčinović I. P., Purić J., 2011, MNRAS, 415, 503
Tapalaga I., Dojčinović I. P., Milosavljević M. K., Purić J., 2012, PASA, 29, 20
Thomas N., 1996, A&A, 313, 306
Zhang H. W., Butler K., Gehren T., Shi J. R., Zhao G., 2006, A&A, 453, 723