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Stark width regularities within homologous spectral series of alkaline earth metals

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Abstract. Stark width regularities within homologous spectral series of neutral atoms of alkaline earth metals were found and discussed. The emphasis is on: (i) the Stark width dependence on the upper level ionization potential (χ); and (ii) term structure influence on the found Stark parameter dependences. The relations found for particular electron temperature and density were of the form $\omega = a\chi^{-b}$, where a, b are constants, for particular homologous spectral series. Published Stark widths data are used to demonstrate the existence of these kinds of regularities for the electron impact contributions to the Stark widths. The obtained functions were used to predict the electron impact Stark widths data for 37 lines of strontium and 29 for barium neither calculated nor measured so far.

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

1. Introduction

Recently published papers devoted to the study of Stark parameter regularities of multiply charged ion spectral lines originating from the same transition array (Purić et al. 2008) and checking the dependence on the upper level ionization potential of electron impact widths using quantum mechanical calculations (Elabidi & Sahal-Bréchot 2011) have shown that these dependences can be used for enlarging number of Stark widths data of astrophysical interest. In addition, a number of papers have been published dealing with regularities within spectral series of Mg I (Tapalaga, Dojčinović & Purić 2011), Be I (Dojčinović, Tapalaga & Purić 2011), He I (Dojčinović, Tapalaga & Purić 2012) and Ca I (Tapalaga et al. 2012). It is known that Stark widths data of neutral spectral lines of various elements are useful for studying radiative transfer through stellar plasmas for some classes of hot stars and to investigate other astrophysical problems (Leckrone 1971; Artru

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& Lanz 1987; Seaton 1987; Iglesias, Rogers & Wilson 1990; Almandos et al. 2009). Spectral lines of alkaline earth metals can be, for example, used in abundance calculations as described in Lambert & Warner (1968). For example Sr I and Ba I spectral lines are of interest for studying nuclear reactions in stellar interiors since they are thermonuclear s-processes products. Their overabundances are observed in CH sub-giants, characterized by Sr and Ba lines and in metal deficient Ba stars (Dimitrijević & Sahal-Bréchot 1997).

The main aim of this paper is to investigate the relationship between Stark widths of spectral lines (FWHM) and the upper level ionization potential of the corresponding transition within homologous spectral series of alkaline earth metals neutral emitters (Be I, Mg I, Ca I, Sr I and Ba I). The Stark widths dependencies on the upper level ionisation potential found within several groups of homologous spectral series (resonant, off-resonant, etc.) of all these elements (Be I, Mg I, Ca I, Sr I and Ba I) were established using all the existing data published so far. For these purposes the theoretical Stark broadening data of neutral atoms of alkaline earth metals spectral lines were taken from Dimitrijević & Sahal-Bréchot (1992, 1993, 1994a,b,c, 1996a,b,c,d, 1997, 1998, 1999, 2000) which can be found in Stark-B data base (Sahal-Bréchot, Dimitrijević& Moreau 2012). The energy levels of spectral lines are taken from NIST database (Ralchenko et al. 2011). A total number of 404 spectral lines, of which 28 Be I, 150 Mg I, 185 Ca I, 27 St I and 14 Ba I spectral lines with their corresponding Stark widths were used in further study of the Stark width dependences on the upper level ionization potential at different temperatures for particular electron density.

For example, a homologous group of resonant spectral series originating from the different alkaline earth metals e.g.: 2s-np (Be singlets), 3s-np (Mg singlets), 4s-np (Ca singlets), 5s-np (Sr singlets) and 6s-np (Ba singlets) were used for the studying regularities within these series. Similarly, the Stark width data belonging to the following homologous group of off-resonant spectral series: 3s-np (Be singlets), 4s-np (Mg singlets), 5s-np (Ca singlets), 6s-np (Sr singlets) and 7s-np (Ba singlets) were used to validate regularities in other homologous groups. Namely, the predictions of the electron impact Stark widths data were done for missed 37 Sr and 29 Ba spectral lines from the studied series not being calculated or measured so far. An appropriate computer program has been designed in order to get firstly as large as possible Stark widths data at particular temperature and electron density of any chosen spectral line originating from the above mentioned series of neutral atoms of alkaline earth metals.

2. Theory

The theoretical model that has been used is described in previous paper (Jevtić et al. 2012). Only the most important equation will be given here:

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

In this equation w is Stark width expressed in rad/s, χ is the upper level ionization potential taken in eV; and a, b are the fitting coefficients independent on χ. As an example, the following function

Table 1. Comparison of coefficient of determination for different groups of spectral lines. The best value is marked with bold

Fig.	Group of spectral lines	R^2
-	Be I 2s-2p(1), Mg I 3s-3p(1), Ca I 4s-4p(1) , Sr I 5s-5p(1), Ba I 6s-6p(1)	0.773
1(a)	Be I 2s-np(1), Mg I 3s-np(1), Ca I 4s-np(1) , Sr I 5s-np(1), Ba I 6s-np(1)	**0.982**
-	Be I ms-np(1), Mg I ms-np(1), Ca I ms-np(1) , Sr I ms-np(1), Ba I ms-np(1)	0.980
-	Mg I 3p-3d(1), Ca I 4p-4d(1) , Sr I 5p-5d(1), Ba I 6p-6d(1)	0.835
1(b)	Be I 2p-nd(1), Mg I 3p-nd(1), Ca I 4p-nd(1) , Sr I 5p-nd(1), Ba I 6p-nd(1)	**0.954**
-	Be I mp-nd(1), Mg I mp-nd(1), Ca I mp-nd(1) , Sr I mp-nd(1), Ba I mp-nd(1)	0.928
-	Be I 2p-3s(3), Mg I 3p-4s(3), Ca I 4p-5s(3)	0.899
1(c)	Be I 2p-ns(3), Mg I 3p-ns(3), Ca I 4p-ns(3)	**0.999**
-	Be I mp-ns(3), Mg I mp-ns(3), Ca I mp-ns(3) , Sr I mp-ns(3)	0.961
-	Mg I 3p-4d(3), Ca I 4p-5d(3) , Sr I 5p-6d(3)	0.508
1(d)	Mg I 3p-nd(3), Ca I 4p-nd(3) , Sr I 5p-nd(3)	**0.929**
-	Be I mp-nd(3), Mg I mp-nd(3), Ca I mp-nd(3) , Sr I mp-nd(3)	0.898
-	Be I 3s-3p(1), Mg I 4s-4p(1), Ca I 5s-np(1) , Sr I 6s-np(1), Ba I 7s-np(1)	0.101
2(a)	Be I 3s-np(1), Mg I 4s-np(1), Ca I 5s-np(1) , Sr I 6s-np(1), Ba I 7s-np(1)	**0.959**
-	Be I ms-np(1), Mg I ms-np(1), Ca I ms-np(1) , Sr I ms-np(1), Ba I ms-np(1)	0.980
-	Be I 3p-3d(1), Mg I 4p-4d(1), Ca I 5p-5d(1) , Sr I 6p-6d(1), Ba I 7p-7d(1)	0.383
2(b)	Be I 3p-nd(1), Mg I 4p-nd(1), Ca I 5p-nd(1) , Sr I 6p-nd(1), Ba I 7p-nd(1)	0.895
-	Be I mp-nd(1), Mg I mp-nd(1), Ca I mp-nd(1) , Sr I mp-nd(1), Ba I mp-nd(1)	**0.928**
-	Ca I 5p-6s(3)	trivial
2(c)	Mg I 4p-ns(3), Ca I 5p-ns(3)	**0.993**
-	Be I mp-ns(3), Mg I mp-ns(3), Ca I mp-ns(3) , Sr I mp-ns(3)	0.961
-	Mg I 4p-4d(3), Ca I 5p-5d(3)	trivial
2(d)	Mg I 4p-nd(3), Ca I 5p-nd(3) , Sr I 6p-nd(3)	**0.907**
-	Be I mp-nd(3), Mg I mp-nd(3), Ca I mp-nd(3) , Sr I mp-nd(3)	0.898

(were χ has to be taken in eV in order to get ω in angular frequency units)

$$\omega = 2.655 \cdot 10^{11} \chi^{-2.327} \tag{2}$$

can be used at 10000 K temperature for calculation of electron impact contribution to Stark broadening of 2s-np (Be singlets), 3s-np (Mg singlets), 4s-np (Ca singlets), 5s-np (Sr singlets) and 6s-np (Ba singlets). For low values of n Stark widths are already calculated so equation (2) can be used for prediction of Stark widths of the spectral lines of higher spectral transitions.

3. Results and discussion

As there is an extremely small amount of data for Sr I and Ba I, the regularities of spectral line broadening could not be found just by analysing data within those elements, although regularities were found for other alkaline earth metals. Stark broadening within spectral series exhibits well established regularities, thus precise predictions can be made for high transitions within spectral

Table 2. The calculated values for the total impact contribution to i the Stark widths (FWHM) w (nm) of Sr ı and Ba ı spectral lines; at T = 10000 K and T = 50000 K normalized to an electron density of $N_e = 10^{22}$ m^{-3} are given.

Sr ı transitions				Ba ı transitions			
λ(Å)	Transition	w(nm) T=10000K	w(nm) T=50000K	λ(Å)	Transition	w(nm) T=10000K	w(nm) T=50000K
2570.2	5s-7p (1)	0.013	0.018	3072.5	6s-7p (1)	0.009	0.013
2354.3	5s-8p (1)	0.056	0.079	2785.3	6s-8p (1)	0.021	0.029
2307.3	5s-9p (1)	0.104	0.149	2646.5	6s-9p (1)	0.044	0.062
2275.9	5s-10p (1)	0.189	0.270	2543.8	6s-10p (1)	0.114	0.163
12026.3	6s-7p (1)	0.330	0.504	23165.3	7s-7p (1)	0.655	1.020
8424.4	6s-8p (1)	0.710	1.036	13051.0	7s-8p (1)	0.516	0.782
7851.6	6s-9p (1)	1.124	1.610	10476.6	7s-9p (1)	0.715	1.058
7492.7	6s-10p (1)	1.789	2.518	9023.9	7s-10p (1)	1.352	1.943
6792.9	5p-6s (3)	0.014	0.017	4995.6	6p-7s (3)	0.032	0.041
4327.7	5p-7s (3)	0.024	0.031	4619.9	6p-8s (3)	0.030	0.039
3781.6	5p-8s (3)	0.053	0.070	4121.0	6p-9s (3)	0.063	0.085
3554.5	5p-9s (3)	0.107	0.147	31626.9	7p-8s (3)	1.759	2.411
3435.3	5p-10s (3)	0.200	0.282	16235.9	7p-9s (3)	1.155	1.616
28001.9	6p-7s (3)	1.260	1.723	5161.4	6p-7d (1)	0.072	0.094
14476.2	6p-8s (3)	0.905	1.265	5161.3	6p-8d (1)	0.151	0.198
11631.1	6p-9s (3)	1.281	1.823	4700.4	6p-9d (1)	0.448	0.594
10445.0	6p-10s (3)	1.986	2.867	4558.3	6p-10d (1)	0.826	1.102
4967.0	5p-7d (1)	0.184	0.242	3565.3	6p-7d (3)	2.578	2.758
4689.9	5p-8d (1)	0.372	0.493	3948.6	6p-8d (3)	0.233	0.236
4533.6	5p-9d (1)	0.697	0.929	3766.6	6p-9d (3)	0.493	0.509
4436.4	5p-10d (1)	1.218	1.630	3664.9	6p-10d (3)	0.946	0.991
4833.4	5p-5d (3)	0.034	0.033	20458.8	7p-7d (1)	1.408	1.963
3941.9	5p-6d (3)	0.084	0.084	20457.7	7p-8d (1)	2.801	3.851
3630.2	5p-7d (3)	0.197	0.200	14731.9	7p-9d (1)	4.730	5.570
3477.9	5p-8d (3)	0.416	0.429	13420.4	7p-10d (1)	7.333	9.730
3391.3	5p-9d (3)	0.797	0.834	10132.8	7p-7d (3)	18.715	19.027
3336.7	5p-10d (3)	1.416	1.501	13993.1	7p-8d (3)	3.606	3.613
12931.5	6p-7d (1)	1.443	1.975	11947.2	7p-9d (3)	5.520	5.558
11207.4	6p-8d (1)	2.317	3.122	10981.0	7p-10d (3)	8.678	8.771
10354.8	6p-9d (1)	3.768	5.014				
9860.9	6p-10d (1)	5.965	7.850				
87827.8	6p-5d (3)	18.305	18.107				
17189.5	6p-6d (3)	2.239	2.231				
12506.2	6p-7d (3)	2.888	2.894				
10867.3	6p-8d (3)	4.525	4.556				
10063.8	6p-9d (3)	7.186	7.262				
9598.2	6p-10d (3)	11.144	11.300				

series that have data for low transitions. Since this is not the case for Sr I and Ba I, an alternate approach was found. Spectral series of different elements that have similar behaviour were grouped together, thus allowing predictions to be made for strontium and barium spectral series with insufficient data. Similar behaviour was found for series that have similar physical properties. As 6s is the ground level for Ba I its behaviour is different from 6s in Be I where it is an

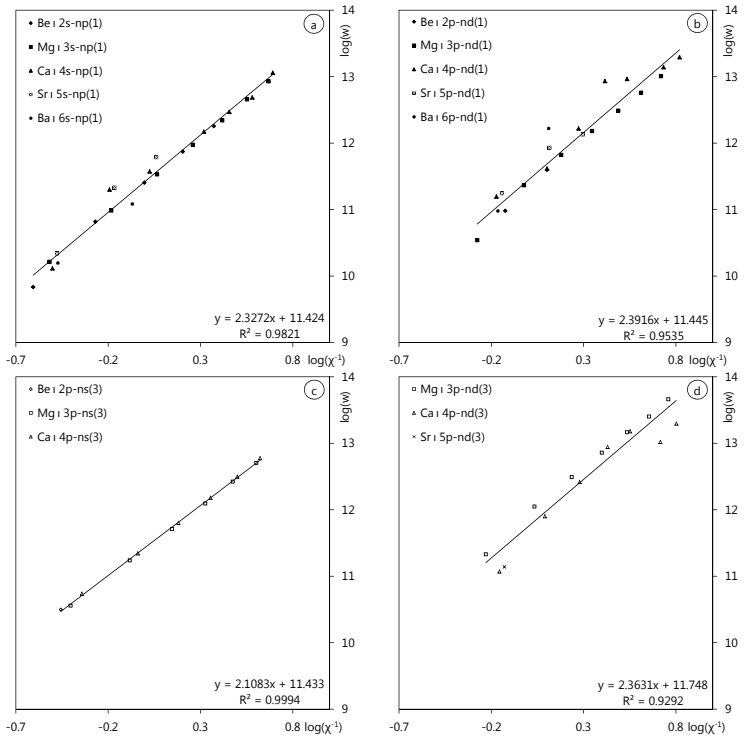

Figure 1. Stark widths dependence on the upper level ionization potential (expressed in eV) at the 10000K temperature for singlet spectral transitions: a) from p levels to first s level, b) from d levels to first p level; triplet spectral transitions: c) from s levels to first p level and d) triplet spectral transitions from d levels to first p level. The numbers 1 and 3 in brackets indicate singlets and triplets respectively.

highly excited state, consequently the 6s-np(1) series behaves different in Be I and Ba I. Rather than grouping spectral series with the same name, it is better to compare series originating from ground states in one case and in other to compare spectral series that originate from first excited state etc. Although both methods have been evaluated, only results that exhibit a better regularity are presented here. The summary of coefficients of determination for some groups of spectral lines are given in Table 1. Based on this data we conclude that groups of homologous spectral series have the best regularity and are the most suitable for prediction of missed data.

In Fig. 1(a) Be I 2s-np(1) spectral series was grouped with Mg I 3s-np(1), Ca I 4s-np(1) , Sr I 5s-np(1) and Ba I 6s-np(1) which are basically singlet transitions from a p level to the lowest s level. As expected this group of spectral series has a well-noticed regularity. Similarly, Fig. 1(b) shows singlet transitions from d levels to the lowest p level, e.g. Be I 2p-nd(1), Mg I 3p-nd(1), Ca I 4p-nd(1) , Sr I 5p-nd(1) and Ba I 6p-nd(1). Triplet series are shown in Fig. 1(c) Be I 2p-ns(3), Mg I 3p-ns(3), Ca I 4p-ns(3) , Sr I 5p-ns(3), Ba I 6p-ns(3) and in 1(b) Be I 2p-nd(3), Mg I 3p-nd(3), Ca I 4p-nd(3) , Sr I 5p-nd(3) and Ba I 6p-nd(3). In this group of spectral series the

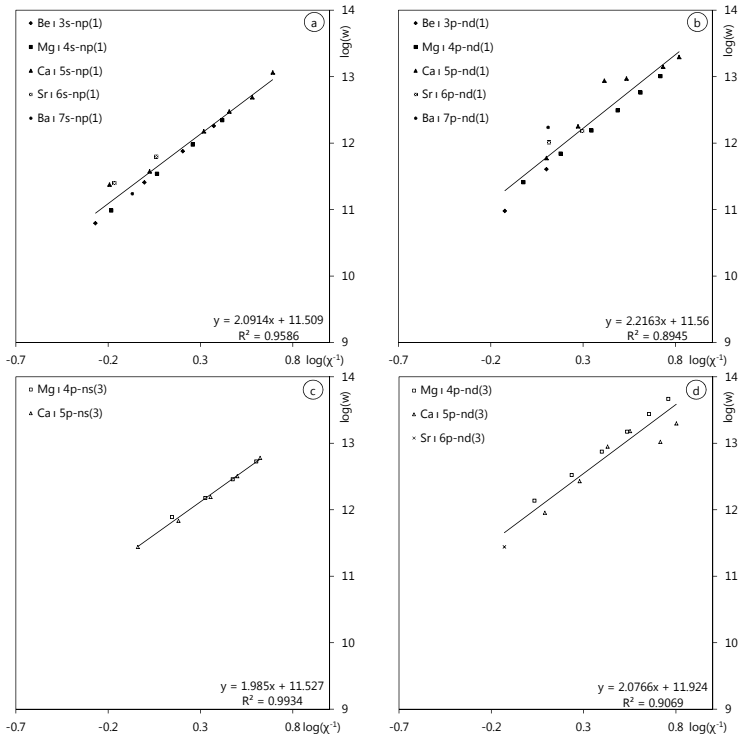

Figure 2. Stark widths dependence on the upper level ionization potential (expressed in eV) at the 10000K temperature for singlet spectral transitions: a) from p levels to second s level, b) from d levels to second p level; triplet spectral transitions: c) from s levels to second p level and d) triplet spectral transitions from d levels to second p level. The numbers 1 and 3 in brackets indicate singlets and triplets respectively.

deviation is exhibited by spectral lines of Sr I, which eventually lead to uncertainty of predictions up to 3 times.

Singlet and triplet spectral lines generally have different values of Stark broadening and must be treated separately. Nevertheless, the same patterns are observed in behaviour within triplet spectral lines as within singlet spectral lines. Namely, spectral series of alkaline earth are forming a line indicating regularity in Stark broadening and thus allowing us to predict the Stark broadening of higher transitions.

The ionization potential of alkaline earth neutrals is lowest for Ba I 5.21 eV and highest for Be I 9.3 eV. The temperature of 50000K is chosen as it is the highest temperature that allows the existence of these neutrals. At this temperature spectral lines have an increased regularity compared to 10000K. We call this effect the merging of Stark widths of these spectral lines.

Fig. 2 shows the behaviour of off-resonant spectral series and Figs. 3 and 4 have the same

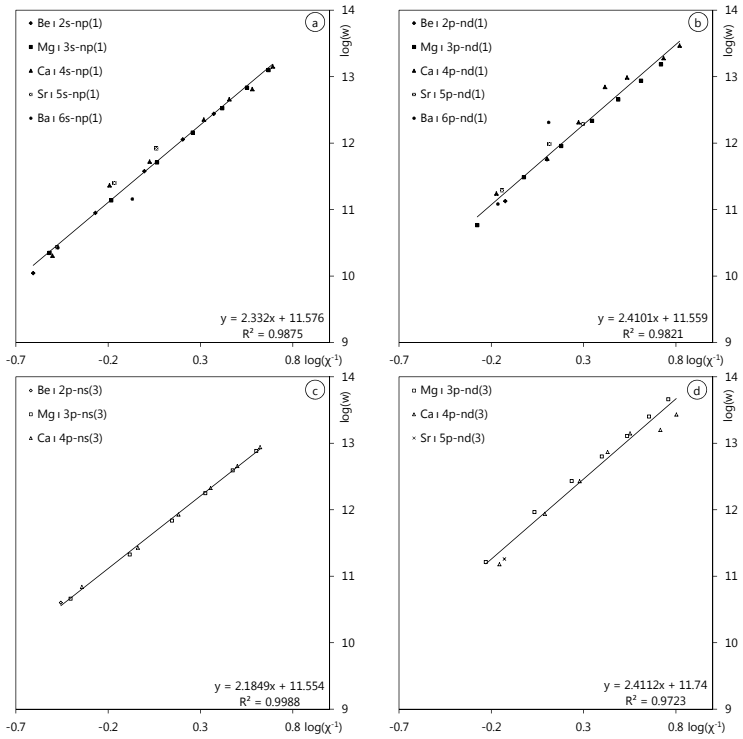

Figure 3. Stark widths dependence on the upper level ionization potential (expressed in eV) at the 50000K temperature for singlet spectral transitions: a) from p levels to first s level, b) from d levels to first p level; triplet spectral transitions: c) from s levels to first p level and d) triplet spectral transitions from d levels to first p level. The numbers 1 and 3 in brackets indicate singlets and triplets respectively.

series as 1 and 2 but are given for the temperature of 50000K. The effect of merging is evident for triplet lines too. This allows us to give more reliable predictions for triplet spectral lines at 50000K.

In Table 1 the predictions for Sr I and Ba I spectral lines are given. As there are no experimental data for these elements and only a few theoretically calculated widths, these predictions aim to complete the available data. These calculations are given for electron density of $N_e = 10^{22} m^{-3}$.

In calculation of these predictions only electron impact contribution to Stark broadening was taken into account while the proton impact contribution was neglected. For most elements the proton contribution is ten times smaller than electron contribution so this simplification is justified. By analysing the available data we come to conclusion that error of these predictions is within 30%.

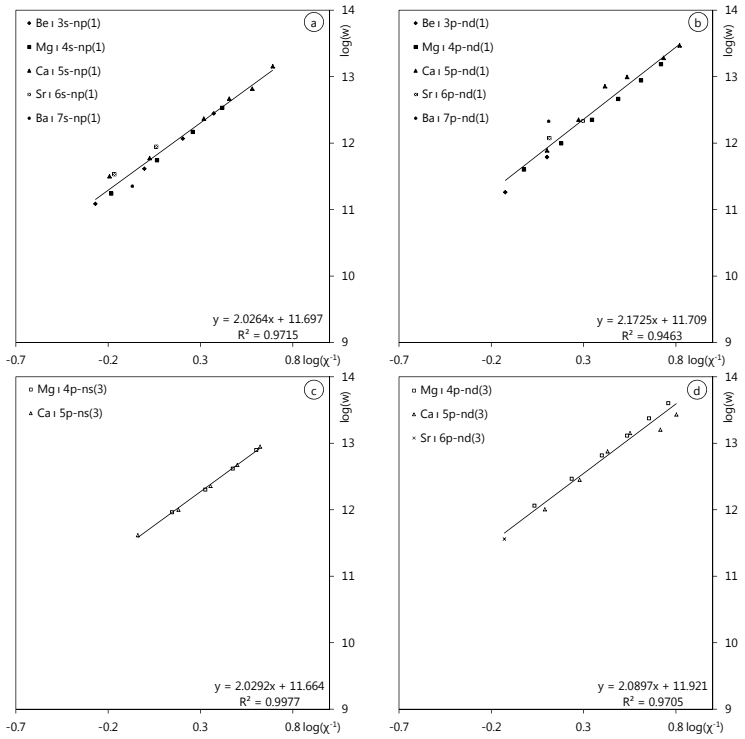

Figure 4. Stark widths dependence on the upper level ionization potential (expressed in eV) at the 50000K temperature for singlet spectral transitions: a) from p levels to second s level, b) from d levels to second p level; triplet spectral transitions: c) from s levels to second p level and d) triplet spectral transitions from d levels to second p level. The numbers 1 and 3 in brackets indicate singlets and triplets respectively.

4. Conclusions

A regularity of Stark broadening has been found within neutral alkaline earth metals which can be used in stellar environment investigation.

This work successfully proves the existence of the functional Stark widths dependences on the upper level ionization potential within homologous spectral series of alkaline earth metals. The relation between upper level ionisation potential and Stark broadening has been verified according to Equation (1). The homologous spectral series that were used are appropriate choices for prediction of unavailable broadening data.

Based on these dependences, predictions were made for Sr I and Ba I spectral lines. It is expected that the accuracy of the predicted data are of the order of the accuracy of the data used in the establishment of the studied regularities.

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