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Stark Width Regularities within Neutral Calcium Spectral Series

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Abstract: Dependences of electron and proton impact Stark width on the upper level ionization potential within different series of the neutral calcium spectral lines have been evaluated and discussed. The similar dependences previously found for the electron impact contribution were also obtained for the proton impact contribution to the Stark broadening. The emphasis is on the term structure influence on the studied Stark width dependences. The influence of the lower transition level and transition term is higher at low temperatures. After establishing these dependences, predictions were made for Stark widths of neutral calcium spectral lines not measured experimentally or calculated theoretically until now.

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

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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 the number of Stark width data of astrophysical interest. Such data are also used to analyze element abundance, to estimate radiative transfer through stellar plasmas for some classes of hot stars and to investigate other astrophysical problems (Leckrone 1971; Lanz & Artru 1985; Seaton 1987; Iglesias et al. 1990; Reyna et al. 2009). For example, calcium spectral lines can be used in calculating low-temperature opacities as described in Jason et al. (2005) or for other astrophysical calculations (see Grevesse 1984, Holweger 1972, Adelman & Davis Philip 1992). Therefore, it is of interest to exploit any possible theoretical approach that might provide simple relations, such as investigation of possible regularities and systematic trends of Stark broadening parameters.

The main task 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 spectral series of Ca I spectral lines which can be used for the prediction of Stark widths for missing spectral lines from these series.

The approach based on the systematic trends found in Stark broadening parameters has been developed in a series of articles devoted to the Stark parameter dependences on the upper-level ionization potential and rest core charge of the emitter (Purić et al. 2008 and references

therein). Such an approach differs from earlier Stark broadening trend analyses primarily in the choice of the variable conveying atomic structure information to the Stark broadening parameters (Purić, Miller & Lesage 1993). It is of interest to note that the work of several authors presented in papers (Wiese & Konjević 1982, 1992) was based on the hydrogenic model, which uses integer principal quantum numbers instead of the upperstate ionization potential χ chosen here. Both variables take into account the density of states perturbing the emitting state. However, some advantages of the present method are: (i) χ -based trend analyses achieve better fits (compared to those obtained when integer quantum number is used instead (Purić et al. 1987)); (ii) in χ-values, the lowering of the ionization potential (Inglis & Teller 1939) can be taken into account, predicting merging with continuum when the plasma environment causes a line's upper state ionization potential to approach zero; and (iii) the Stark width (w) dependence on χ is theoretically expected (Purić et al. 1993; Purić et al. 2008). In fact it is the bounding energy of the electron on the upper level of the corresponding transition. In order to avoid misunderstanding the positive value of this quantity (χ) , it is called the upper level ionization potential.

This paper is in continuation with already published papers devoted to the regularities within spectral series of Mg I (Tapalaga, Dojčinović & Purić 2011), Be I (Dojčinović, Tapalaga & Purić 2011a) and He I (Dojčinović, Tapalaga & Purić 2011b).

For these purposes the theoretical Stark broadening data of neutral calcium spectral lines were taken from Griem (1974) and Dimitrijević & Sahal-Bréchot (1999, 2000) which can be found in the Stark-B data base

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(Sahal-Bréchot, Dimitrijević & Moreau 2011). Valuable experimental data has been taken from Kusch & Pritschow (1970) and Hühn & Kusch (1973). Experimental data are summarised in Konjevic & Roberts (1976). The energy levels of spectral lines are taken from the NIST database (Ralchenko et al. 2011). A total of 151 Ca 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 the lines originating from the following spectral series: 4d-np (1), 4d-np (3), 4p-nd (1), 4p-nd (3), 4p-ns (1), 4p-ns (3), 4s-np (1), 5d-np (1), 5d-np (3), 5p-nd (1), 5p-nd (3), 5p-ns (1), 5p-ns (3), 5s-np (1), 5s-np (3), 6d-np (1), 6d-np (3), 6p-nd (1), 6p-nd (3), 6p-ns (1), 6p-ns (3), 6s-np (1), 6s-np (3), 7d-np (1), 7d-np (3), 7p-nd (1), 7p-nd (3), 7p-ns (1), 7p-ns (3), 7s-np (1), 7s-np (3). Next to the series notation there is a number in parentheses, 1 or 3, indicating a singlet or triplet series, respectively.

An appropriate computer program has been designed in order to be able to get firstly the Stark width dependence on the temperature of any particular spectral line originating from the abovementioned series of neutral calcium.

2 Theory

Theoretical relations for Stark width as a function of the upper level ionisation potential and the rest core charge of the emitter were evaluated by Purić et al. (1993) starting from equation 77 of Griem (1974). The proposed method is based on the fact that the Stark widths in angular frequency units exhibit a certain functional dependence on the upper level ionization potential of the corresponding transition. These relations were successfully fitted to a number of spectral lines and confirmed in a series of articles (see e.g. Purić & Šćepanović 1999; Šćepanović & Purić 2003; Purić et al. 2008; Tapalaga, Dojčinović & Purić 2011; Dojčinović, Tapalaga & Purić 2011a; Dojčinović, Tapalaga & Purić 2011b) and found to be of the form:

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

where w is the line width, χ is the corresponding upper level ionization potential, and a and b are coefficients corresponding to the chosen temperature and electron density, independent of ionization potential for particular transition. Upper level ionization potential (χ) is a function of upper level principal quantum number (n) so they can be used equally. In cases where understanding of physical processes is required n will be used, and in cases in which regularities are investigated χ will be used. Although Equation 1 is a popular form of Stark broadening connection to upper level ionization potential, we have used the form

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

as it is easier to analyse the data in linear form.

In order to investigate different Stark parameter regularities, an accurate set of theoretical and experimental data, normalised to the particular electron density and temperature, is necessary. The normalisation to the same N_e can be done by linear scaling due to the linear dependence of Stark widths on N_e . However, Stark width dependence on the electron temperature is different from one spectral line to another for all spectra. Therefore, the correction to temperature dependence must be done with great care for every spectral line separately. For instance, instead of the commonly adopted temperature dependence of $T^{-1/2}$ for ion lines, one has to use, from line to line (Purić & Šćepanović 1999; Purić et al. 2008), the whole spectrum of functions given by:

$$f(T) = A + BT^{-C}, (3)$$

where the coefficients A, B and C are independent of electron temperature. This equation was used for a large temperature range between $10^{-2}\chi_0$ and χ_0 (Griem 1974), where χ_0 is the ionisation potential of a given emitter whose spectrum is used for plasma diagnostic purposes. It was found that the same type of function can be used in the case of neutral spectral lines, and consequently in the case of Ca I spectral lines. For all the studied series it was found that the relation given by Equation 3 is appropriate for any particular temperature in both cases (the electron impact and proton impact contributions to the Stark widths). During these analyses one has to use Stark width data in angular frequency units and ionization potential in electron volts. In order to be able to obtain these data for any missed line from the series one has to use the obtained functional dependence expected according to Equation 1 knowing only the upper level ionization potential, and to substitute it in the same equation. Using this procedure and the temperature dependence of the Stark widths given by Equation 3, it is possible to obtain Stark broadening data by extrapolation or interpolation for any temperature of interest within the range given above. As an example, the following function

$$w = 2.77 \cdot 10^{11} \chi^{-2.11},\tag{4}$$

where χ has to be taken in eV in order to get w in angular frequency units, can be used at a temperature of $10\,000\,\mathrm{K}$ for the electron impact contribution to Stark broadening of the 4p-ns triplet series. For n=4,5,6,7,8,9,10, Stark widths are already calculated, so Equation 4 can be used for prediction of 4p-11s (3) and higher spectral transitions. In the same manner, predictions can be made for any series given in Table 1.

3 Results

All spectral lines used in this paper are normalised to an electron density of $N_e=10^{16}\,\mathrm{cm}^{-3}$ and to a temperature of $T=10\,000\,\mathrm{K}$ for Figure 1, $T=50\,000\,\mathrm{K}$ for Figure 2, $T=10\,000\,\mathrm{K}$ for Figure 3 and $T=50\,000\,\mathrm{K}$ for Figure 4.

Table 1. The appropriate fitting parameters a and b are given for $10\,000\,\mathrm{K}$ and $50\,000\,\mathrm{K}$, together with corresponding correlation factor R^2 for the electron and proton impact contributions to the Stark widths for all studied series ($N_e = 10^{22}\,\mathrm{m}^{-3}$)

Spectral	Electron impact broadening						Proton impact broadening					
series	$T = 10000\mathrm{K}$			$T = 50000\mathrm{K}$			$T = 10000\mathrm{K}$			$T = 50000\mathrm{K}$		
	а	b	R^2	a	b	R^2	а	b	R^2	а	b	R^2
4d- <i>n</i> p (1)	5.53E+11	1.7209	0.9717	7.10E+11	1.7785	0.9880	1.16E+11	1.7995	0.9649	1.35E+11	1.7451	0.9382
4d- <i>n</i> p (3)	7.90E+11	2.0742	0.9332	8.72E + 11	1.9837	0.9747	1.98E + 11	2.1783	0.8849	2.53E+11	2.2094	0.8606
4p-nd (1)	4.10E+11	2.2521	0.9342	4.63E+11	2.3125	0.9775	1.04E+11	2.1329	0.8438	1.35E+11	2.0899	0.7957
4p-nd (3)	4.70E+11	2.2651	0.9128	5.07E+11	2.3151	0.9658	1.16E+11	2.1396	0.8478	1.48E + 11	2.1420	0.8059
4p-ns (1)	2.74E+11	2.0682	0.9654	3.65E+11	2.1912	0.9730	5.15E+10	1.6856	0.8609	6.63E + 10	1.7033	0.8618
4p-ns (3)	2.77E+11	2.1103	0.9995	3.59E+11	2.1936	0.9987	6.09E+10	2.0107	0.9996	7.94E+10	2.0150	0.9997
4s-np (1)	2.93E+11	2.2681	0.9781	4.09E+11	2.2531	0.9864	8.55E+10	2.0704	0.9855	9.40E + 10	2.0678	0.9739
5d- <i>n</i> p (1)	5.84E+11	1.7408	0.9720	8.93E + 11	1.6598	0.9836	1.13E+11	1.8602	0.9634	1.20E + 11	1.8850	0.9393
5d- <i>n</i> p (3)	1.67E + 12	1.4914	0.8498	1.57E + 12	1.5522	0.9529	3.96E+11	1.5837	0.7200	5.52E+11	1.5421	0.6564
5p-nd (1)	5.72E+11	2.0329	0.8874	6.16E + 11	2.1278	0.9657	1.49E + 11	1.8791	0.7053	2.04E+11	1.7941	0.6216
5p-nd (3)	9.17E+11	1.7702	0.8561	8.41E+11	1.9486	0.9564	2.63E+11	1.5240	0.7280	3.80E + 11	1.4327	0.6373
5p-ns (1)	4.51E+11	1.6470	0.9291	5.83E+11	1.8203	0.9328	6.22E+10	1.4850	0.8154	8.11E+10	1.4917	0.8195
5p-ns (3)	3.13E+11	2.0297	0.9981	4.65E+11	2.0199	0.9972	4.88E+10	2.2039	0.9993	5.96E+10	2.2667	0.9980
5s-np (1)	4.27E+11	1.9053	0.9800	6.29E+11	1.8659	0.9908	9.15E+10	1.9885	0.9837	1.03E+11	1.9604	0.9655
5s-np (3)	6.30E + 11	2.2664	0.9279	7.37E+11	2.1223	0.9708	1.70E + 11	2.3161	0.8836	2.16E+11	2.3525	0.8598
6d- <i>n</i> p (1)	7.59E+11	1.6963	0.9562	1.30E + 12	1.5150	0.9631	9.13E+10	2.0772	0.9567	9.24E+10	2.1564	0.9278
6d-np(3)	1.48E + 13	-0.0538	0.0782	6.20E + 12	0.6184	0.9777	1.00E+13	-0.8280	0.9638	2.07E + 13	-1.1589	0.9876
6p-nd (1)	1.11E+12	1.5897	0.8200	9.98E + 11	1.8171	0.9602	3.63E+11	1.2820	0.4581	5.72E+11	1.1016	0.3226
6p-nd (3)	2.41E+12	1.1548	0.7202	1.60E + 12	1.5541	0.9349	7.17E+11	0.8477	0.4272	1.19E+12	0.6622	0.2477
6p-ns (1)	2.64E+11	2.1479	0.9994	4.07E+11	2.2077	0.9926	3.83E+10	1.9695	0.8763	4.42E+10	2.0597	0.8841
6p-ns (3)	6.66E + 11	1.5544	0.9872	8.88E + 11	1.6253	0.9905	7.19E+10	1.7060	0.7629	9.06E+10	1.7335	0.7462
6s-np (1)	4.87E + 11	1.8602	0.9784	8.21E+11	1.7175	0.9869	8.33E+10	2.0840	0.9824	9.00E+10	2.0955	0.9623
6s-np(3)	1.04E+12	1.8091	0.8505	1.10E + 12	1.7991	0.9438	2.87E + 11	1.8331	0.7337	3.96E+11	1.7950	0.6783
7d-np (1)	3.55E+12	1.0376	0.9261	3.38E+12	1.1117	0.9178	1.64E+12	0.6361	0.6684	2.86E + 12	0.5077	0.6356
7d-np(3)	1.98E + 13	-0.0181	N/A	1.65E + 13	0.1460	N/A	3.69E+09	4.5885	N/A	1.26E+10	4.0146	N/A
7p-nd (1)	4.16E+12	0.8076	0.9315	2.44E+12	1.3165	0.9849	3.24E+12	-0.0729	0.0602	7.01E+12	-0.4531	0.6605
7p-nd (3)	7.53E+12	0.5023	0.4344	3.87E+12	1.0694	0.8735	2.76E+12	0.0234	0.0005	5.78E+12	-0.3169	0.0561
7p-ns (1)	7.02E+11	1.5627	0.9856	1.32E+12	1.4674	0.9920	8.61E+10	1.5371	0.8967	6.79E + 10	1.8712	0.9256
7p-ns (3)	1.60E + 12	1.1340	0.9854	1.75E+12	1.3124	0.9929	1.13E+12	-0.5278	0.6351	1.61E+12	-0.5822	0.7496
7s- <i>n</i> p (1)	3.13E+11	2.2117	0.9845	7.05E+11	1.8507	0.9741	5.14E+10	2.4658	0.9911	4.33E+10	2.6754	0.9871
7s-np (3)	2.26E+12	1.2027	0.6349	2.00E+12	1.3641	0.8842	7.41E+11	1.0640	0.3668	1.15E+12	0.9348	0.2616

Figure 1 shows the electron impact contribution to Stark widths of Ca I spectral lines at 10 000 K as a function of the inverse values of the upper level ionization potential. Three sources of data were available for these spectral lines and all three are presented in the figure for the sake of comparison and verification. Data taken from the Stark B database is compared to data calculated by Griem and experimentally measured data. The total number of spectral lines is too large for a single chart, so there are four charts in this figure. Therefore, the Stark widths of spectral line series with different quantum numbers of lower transition level are presented in this figure, as follows: (a) n = 4; (b) n = 5; (c) n = 6, and (d) n = 7. As Griem's calculations were done only for n = 3, 4, these data are given in Figure 1(a). Experimental measurements of Ca I spectral lines are also presented in Figure 1(a).

Analysing the results presented in this figure, one can conclude that spectral lines with greater χ^{-1} have higher Stark broadening values as predicted by Equation 1 and Equation 2. Spectral series have been successfully fitted according to Equation 2, and the results are presented in Table 1. From this figure one can conclude that the

connection between w and χ exists, and is of the form presented in Equation 2, although the discrepancy between the predicted line and the data is bigger in the case of Ca I than in the cases of He I (Dojčinović, Tapalaga & Purić 2011b), Be I (Dojčinović, Tapalaga & Purić 2011a) and Mg I (Tapalaga, Dojčinović & Purić 2011). This can be explained by the higher density of Ca I energy levels as compared with those of He I, Be I and Mg I. For some series, correlation factors R^2 are not available (N/A) because there were only two values in those series, so R^2 would have trivial values.

Figure 2 shows the electron impact contribution to Stark widths of Ca I spectral lines at 50 000 K. At this temperature no experimental measurements of Ca I spectral lines were made. The same conclusions apply for Stark broadening at 50 000 K as for Stark broadening at 10 000 K. Comparing these two temperatures, it is clear that the Stark width dependences of the spectral lines originating from different spectral series tend to merge to the same functional dependences at high temperatures and the scatter of data is smaller. Spectral series differ with the structure of their terms and with different lower level.

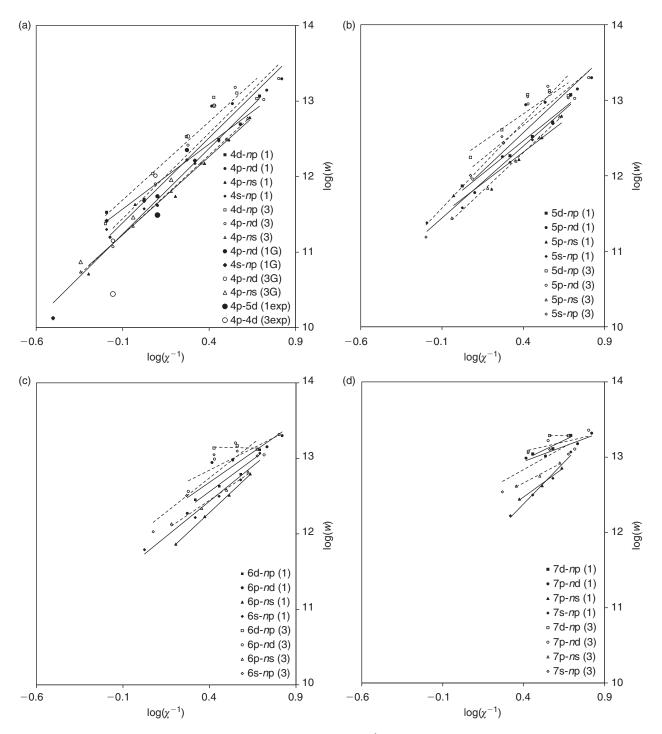


Figure 1 The electron impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse upper level ionisation potential (expressed in eV) at 10 000 K for different Ca I spectral series with principal quantum number of lower level equal to (a) n = 4; (b) n = 5; (c) n = 6; (d) n = 7. The numbers (1) and (3) indicate singlets and triplets, respectively. Values taken from Griem (1974) are specified with 3G for triplets and 1G for singlets. The corresponding experimental values (Kusch & Pritschow 1970; Hühn & Kusch 1973) are included.

The conclusion that can be drawn is that the influence of lower level and term structure is lower for high temperatures. This effect is more pronounced in He I (Dojčinović et al. 2011b), where high ionization potential allows a broad temperature range.

Figure 3 is similar to Figure 1, with one major difference: the proton impact contribution to Stark broadening is presented, instead of the electron impact contribution.

Similar functional behaviour for the proton impact and the electron impact contribution is observed, although the proton contribution is significantly smaller then the electron contribution. Both the electron and proton impact contributions need to be taken in account when predicting Stark broadening.

Figure 4 shows the proton impact contribution to Stark widths of Ca I spectral lines at 50 000 K as a function of the

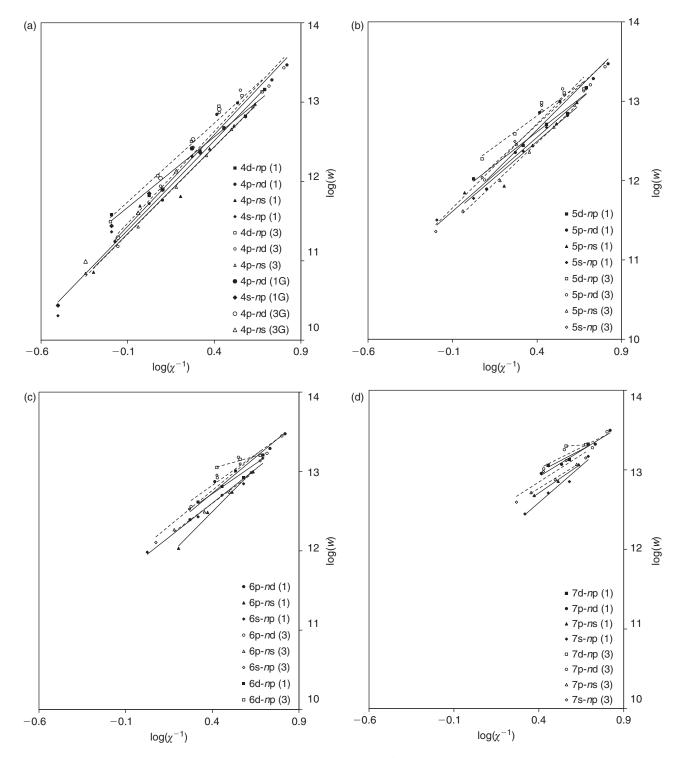


Figure 2 The electron impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse upper level ionisation potential (expressed in eV) at 50 000 K for different Ca₁ spectral series with principal quantum number of lower level equal to (a) n = 4; (b) n = 5; (c) n = 6; (d) n = 7. The numbers (1) and (3) indicate singlets and triplets, respectively. Values taken from Griem (1974) are specified with 3G for triplets and 1G for singlets.

inverse value of the upper level ionization potential. The scatter is greater in this case but the general Stark width dependence on the upper level ionization potential is still evident.

In addition to these, Figure 5 shows the influence of the principal quantum number of lower transition level (n) for

Ca I spectral lines originating from 4p-ns (3), 5p-ns (3), 6p-ns (3), 7p-ns (3) is demonstrated. From this figure one can see that for a higher principal quantum number of lower transition level, larger values of Stark broadening are obtained. A big increase in Stark widths is noticeable in the 4p-8s (3), 5p-8s (3), 6p-8s (3) and 7p-8s (3) spectral

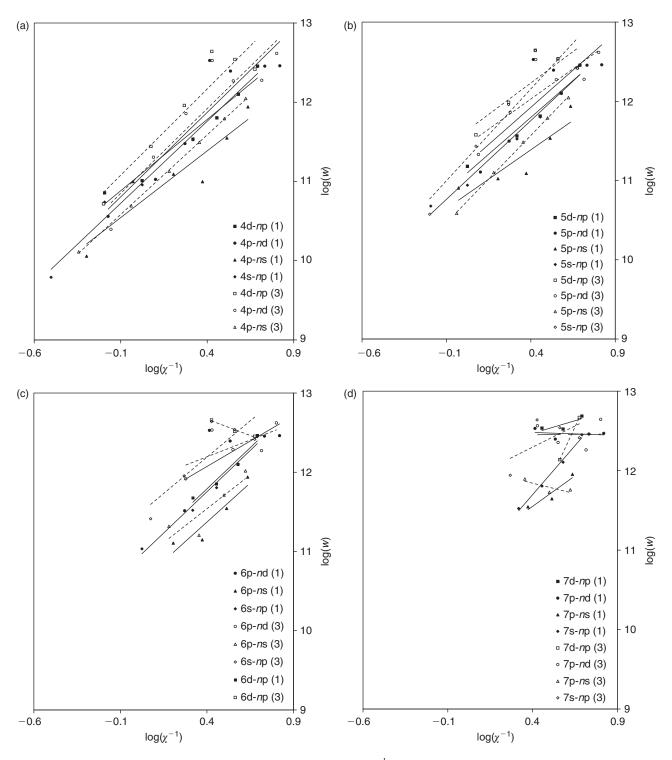


Figure 3 The proton impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse upper level ionisation potential (expressed in eV) at $10\,000\,\mathrm{K}$ temperature for different Ca I spectral series with principal quantum number of lower level equal to (a) n=4; (b) n=5; (c) n=6; (d) n=7. The numbers (1) and (3) indicate singlets and triplets, respectively.

lines, compared to the small increase in the 4p-10s (3), 5p-10s (3), 6p-10s (3) and 7p-10s (3) spectral lines.

As Ca I Stark broadening of spectral lines exhibits more expressed dependence on the lower transition level than other elements from the IIa group, an additional chart is presented in Figure 6. This chart explicitly shows the Stark width dependence of lower level ionization potential for *n*p-8s (3), *n*p-9s (3) and *n*p-10s (3) transitions. A small increase in Stark width is noticeable for *n*p-10s (3), while *n*p-9s (3) has a moderate increase and *n*p-8s (3) has a high increase. Comparing Figure 5 and Figure 6 one can see that Stark width dependence on upper level ionization

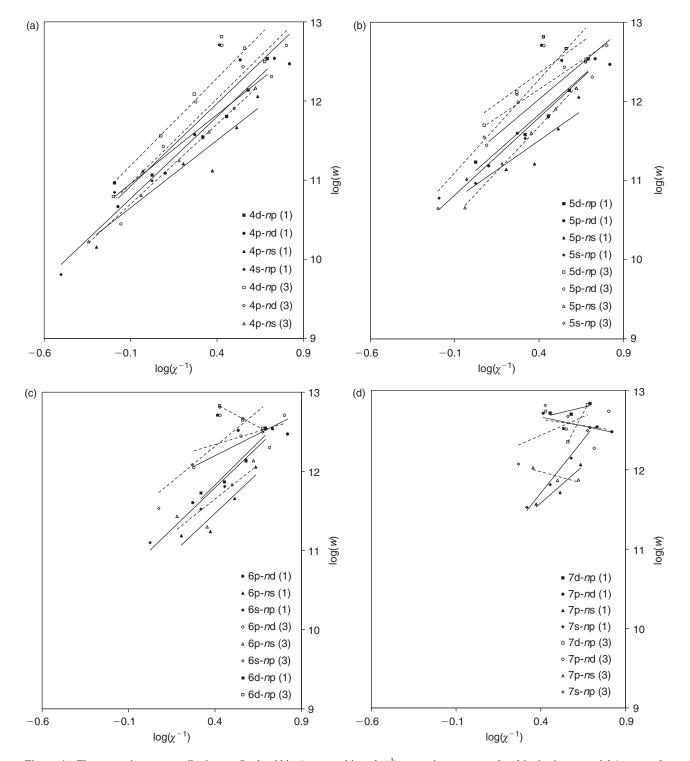


Figure 4 The proton impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse upper level ionisation potential (expressed in eV) at 50 000 K temperature for different Ca I spectral series with principal quantum number of lower level equal to (a) n = 4; (b) n = 5; (c) n = 6; (d) n = 7. The numbers (1) and (3) indicate singlets and triplets, respectively.

potential is much greater then on lower level ionization potential.

The electron and proton contributions to Stark broadening combined together give the total Stark broadening, and using Equation 1 predictions are made for spectral lines not studied experimentally or theoretically in the literature so far. These predictions are listed in Table 2, both for $T = 10\,000\,\mathrm{K}$ and for $T = 50\,000\,\mathrm{K}$.

4 Conclusion

Searching for different types of regularities and systematic trends which can simplify complicated theoretical

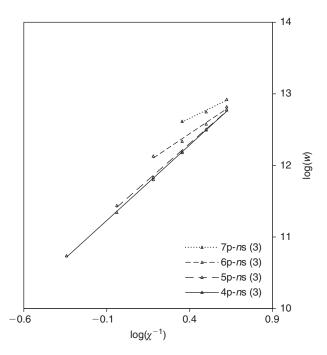


Figure 5 The electron impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse upper level ionisation potential (expressed in eV) at 10 000 K temperature for the Ca I np-ns (3) spectral series. The influence of principal quantum number of lower transition level is evident.

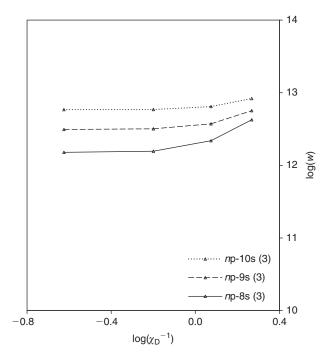


Figure 6 The electron impact contributions to Stark widths (expressed in rad s⁻¹) versus inverse lower level ionisation potential (expressed in eV) at 10 000 K temperature for the np-8s (3), np-9s (3) and np-10s (3) transitions. The number (3) indicate triplet transitions.

calculations used in astrophysics is of great interest. This work successfully proves the existence of the strong functional Stark width dependence on the upper level ionisation potential for lines originating from the same

Table 2. The calculated values for Stark widths (FWHM) w (nm) of 12 Ca | spectral lines at $T_e=10\,000\,\mathrm{K}$ and $T_e=50\,000\,\mathrm{K}$, normalized to an electron density of $N_e=10^{21}\,\mathrm{m}^{-3}$, are given

Ion	λ(Å)	Transition	Terms	w (nm) T = 10000 K	w (nm) T = 50 000 K
Ca	4134.2	4p-11s	¹ Po- ¹ S	0.097	0.157
Ca	9000.3	5p-11s	¹ Po- ¹ S	0.367	0.625
Ca	16 223.3	6p-11s	¹ Po- ¹ S	1.660	2.779
Ca	3063.3	4p-11s	³ Po- ³ S	0.059	0.087
Ca	8883.3	5p-11s	³ Po- ³ S	0.499	0.721
Ca	18 901.2	6p-11s	³ Po- ³ S	2.020	2.993
Ca	2083.7	4s-11p	¹ S- ¹ Po	0.053	0.069
Ca	6812.8	5s-11p	¹ S- ¹ Po	0.437	0.572
Ca	13 687.1	6s-11p	¹ S- ¹ Po	1.862	2.341
Ca	9347.7	4d-11p	¹ D- ¹ Po	0.754	1.020
Ca	19 693.6	5d-11p	¹ D- ¹ Po	3.661	4.679
Ca	33 252.7	6d-11p	¹ D- ¹ Po	12.519	15.213

series. Equation 1 has been confirmed for Ca I spectral lines, although the dissipation is greater than in He I, Be I and Mg I. Based on available data for Ca I, we can conclude that the temperature dependence of Stark broadening is as Equation 3 suggests. The electron and proton impact contributions to Stark broadening have the same type of behaviour, but the proton contribution is significantly smaller. These results can also be used to verify the results of Stark broadening data that is already measured or calculated, although the main intention of authors is to obtain new data that is used in astrophysical calculations.

In the case of Ca I, the influence of the lower transition level is not negligible. This influence is especially visible for 10 000 K, while for 50 000 K the influence is smaller. As in the cases of He I, Be I and Mg I, high temperatures tend to eliminate differences in Stark broadening for all other parameters except upper level ionization potential.

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