Regularityes and irregularities of the Stark broadening parameters for singly ionized noble gases

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Abstract. In the last years, different trends and regularities of Stark broadening parameters (halfwidths and shifts of spectral lines) have been analyzed. Conditions related to atomic structure of the element, as well as plasma conditions are responsible for regular or irregular behavior of the Stark broadening parameters. The absence of very close perturbing levels makes Ne II a good candidate for the analysis of the Stark broadening parameters regularities. The other two elements considered in this work, Kr II and Xe II, have complex spectra and present strong perturbations, leading to the appearance of Stark broadening parameters irregularities in some cases. In this work, we analyze the influence of perturbations on Stark broadening parameters within the multiplets.

1. Introduction

Spectroscopy of ionized noble gases has a great importance for both laboratory and astrophysical plasmas. Generally, spectra of inert gases are important for many physics areas, like laser physics, fusion diagnostics, photoelectron spectroscopy, collision physics, astrophysics etc. Stark halfwidths and shifts of spectral lines are frequently employed for plasma diagnostic purposes. For example, atomic data of argon, krypton and xenon will be useful for the spectral diagnostics of ITER [1]. In addition, the software used for stellar atmosphere simulation, like TMAP [2] and SMART [3], require a large amount of atomic and spectroscopic data. Availability of these parameters will be useful for a further development of stellar atmosphere and evolution models [4].

Stark broadening parameters data can be useful for verification of theoretical calculations, as well as for investigation of regularities and systematic trends of these parameters within a multiplet, supermultiplet or transition array [5,6]. This regular or nearly regular behavior has been experimentally found in many different works, for ionized atoms see Ref. [7-11]. The existence of Stark broadening parameters regularities within a multiplet, supermultiplet or transition array may be useful in order to make data interpolation. In this work we analyze these similarities of Stark broadening parameters of Ne II, Kr II and Xe II spectral lines within the chosen multiplets. According to Ref. [5,6], differences in the Stark halfwidth and shift values of the lines belonging to the same multiplet should be within a few percents and possibly lower than 1% and 10%, respectively.
2. Plasma Stark broadening parameters measurements and data treatment

Stark broadening parameters analyzed in this work have been measured in the laboratory of plasma spectroscopy of the University of Valladolid. The experimental set-up is described in detail in previous work [12]. Here, only short description is given.

Measurements were performed in a pulsed plasma. Pulses were created by discharging a capacitor bank, charged up to 9 kV, through a cylindrical Pyrex tube. A mixture of helium, as carrying gas, and several percents of the investigated gas was continuously flowing through the tube at a pressure of 3 kPa. The percentage of the noble gas and the flow of the gas mixture was adjusted in order to obtain minimal self-absorption, which was checked for every line in the recorded spectrum. Self-absorption was negligible for all lines considered in this work.

Electron density was determined by a two wavelength interferometric method and the highest density was about \(2 \times 10^{23} \text{ m}^{-3}\) with the estimated experimental error lower than 10%. Electron temperature was determined by a Boltzmann-plot and it was in the range \(15000 \text{ to } 27000 \text{ K}\) for Kr II and Xe II, and \(25000 \text{ to } 45000 \text{ K}\) for Ne II. The error of temperature measurements was estimated to be lower than 15%. An example of the typical evolution of electron density and temperature along the plasma life is shown in figure 1. Line spectra were recorded during the first 200 \(\mu\text{s}\) of the plasma life and the typical exposure time was 5 \(\mu\text{s}\).

In order to obtain the Stark halfwidth from the total halfwidth other broadening mechanisms, like Doppler or instrumental broadening, have been taken into account. On the other hand, van der Waals and resonance broadening were negligible for the plasma conditions in this experiment. Stark halfwidths were plotted as a function of the electron density and linear trends were obtained. The value of the slope at \(10^{23} \text{ m}^{-3}\) corresponds to the Stark halfwidth of the line. The Stark shift was obtained by plotting the relative position of the line centre as a function of electron density. The procedure is described in detail in Ref. [13].

![Figure 1](image-url)

**Figure 1.** Typical evolution of electron density, \(N_e\), obtained by two wavelength interferometry, and temperature \(T_e\), obtained from Boltzmann-plot.

Stark broadening parameters are normalized to the temperature of 35000 K in case of Ne II, 21000 K in case of Kr II and 22000 K in case of Xe II using \(T^{-1/2}\) dependence. Detailed description of experimental data treatment is given in Ref. [12]

3. Results and discussion

Measured Stark halfwidths and shifts of ionized noble gases Ne II, Kr II and Xe II are given in Tables 1, 2 and 3, respectively. In the first four columns Tables contain transitions, terms, degenerations and
wavelengths of the observed spectral lines. In the next two columns the measured parameters Stark halfwidths, \( w_m \), and Stark shifts, \( d_m \), are shown. Data are expressed in frequency units in order to avoid the influence of the wavelength, for the comparison purpose. The obtained results are compared with available results of other authors.

Experimental errors of the measured Stark halfwidths of Ne II lines are estimated to be lower than ±20%, while in case of shifts these errors can be even higher due to very small values of the measured shifts [13].

Two multiplets of the transition array 3p – 3d have been selected in case of Ne II. As can be seen in Table 1, Stark broadening parameters of the spectral lines belonging to the same multiplet have very similar values. The measured halfwidths of the lines belonging to the multiplet \(^1D^o – ^4F\) vary ±7% from the average value, while in case of multiplet \(^4P^o – ^4D\) the variation is ±3%, corresponding to differences lower than 2 pm. This value is close to the experimental precision. All the lines of the 3p – 3d transition array show similar red shifts. Differences between the measured shifts are within ±7% for multiplet \(^1D^o – ^4F\) and ±11% for multiplet \(^4P^o – ^4D\), corresponding to less than 1 pm. In order to illustrate these agreements, experimental profiles of seven Ne II lines belonging to the multiplet \((^3P)3p^4P^o – (^3P)3d^4D\) are shown in figure 2. The lines have been normalized in area and a clear overlapping can be observed.

Table 1. Experimental Stark broadening parameters of Ne II spectral lines normalized to electron density \(N_e = 1 \times 10^{23} \text{ m}^{-3}\) and electron temperature \(T_e = 35000 \text{ K}\). Results from this work [14] are marked as TW, from Platiša et al. [15] as PL, from Konjević and Pittman [16] as KP, from Purić et al. [17] as PU, from Milosavljević et al. [18] as MI and from Djeniže et al. [19] as DJE.

| Transition Term. | \(J\) | \(\lambda\) (nm) | \(w_m\) (10\(^{11}\)s\(^{-1}\)) | \(d_m\) (10\(^{11}\)s\(^{-1}\)) |
|-----------------|-----|-----------------|-----------------|-----------------|
| \((^3P)3p – (^3P)3d\) | \(^1D^o – ^4F\) | 5/2-5/2 | 318.874 | 3.10 TW | -0.63 TW |
| | 319.859 | 3.13 TW | -0.62 TW |
| | 3/2-7/2 | 3.08 KP | |
| | 1/2-3/2 | 321.374 | 3.43 TW | -0.68 TW |
| | 3/2-5/2 | 321.433 | 3.25 TW | -0.60 TW |
| | 7/2-9/2 | 321.819 | 3.03 TW | -0.65 TW |
| | 5/2-3/2 | 301.731 | 3.01 TW | -0.60 TW |
| | 3/2-3/2 | 303.772 | 3.02 TW | -0.62 TW |
| | 5/2-5/2 | 302.702 | 3.07 TW | -0.65 TW |
| | 3/2-7/2 | 303.446 | 3.13 TW | -0.72 TW |
| | 3/2-3/2 | 303.772 | 2.99 TW | -0.75 TW |
| | 1/2-1/2 | 304.556 | 3.02 TW | -0.61 TW |
| | 3/2-5/2 | 304.756 | 3.00 TW | -0.76 TW |
| | 1/2-3/2 | 305.467 | 3.02 TW | -0.62 TW |

Finally, a reasonable explanation for the Stark broadening parameters regularities observed in this work may come from the analysis of the Ne II energy levels scheme. Ne II energy levels are well described by LS coupling scheme and all perturbing levels are too far from the transition levels to be able to produce significant perturbations of the latter ones. Under these conditions, the predicted regularities of Stark broadening parameters within the same multiplet have been obtained experimentally.
Comparison between the present halfwidth results and the results of other authors (Table 1) shows a satisfactory agreement and supports the above conclusions. There is some disagreement between the present results and the results from Ref. [19] in case of measured shifts, for example, for the 303.446 nm and 303.772 nm line. Still, one should keep in mind that the difference is only about 3 pm.

The ratio of experimental and theoretical halfwidth values, \( w_m/w_{\text{MSE}} \), is about 1.5 for all considered spectral lines. For the theoretical calculations modified semiempirical formula MSE [20] was used. In case of shifts, the ratio \( d_m/d_{\text{MSE}} \) was between 2 and 2.5. Here, modified semiempirical formula [21] was used for theoretical calculations. It is well known that line shifts are less accurate than the line halfwidths, both measured and calculated.

Behavior of the Ne II lines is not a typical situation. Kr II has more complex spectra and its energy levels are not well described by the LS coupling scheme, especially the levels having high \( l \). In addition, the average distance between the transition and perturbing levels is lower. Therefore, in some situations, there are strong perturbations that break the regularities in transition arrays and multiplets. Stark broadening parameters of Kr II lines from 6 multipletes in 2 transition arrays are shown in Table 2 [22].

Experimental errors for the measured halfwidths are estimated to be lower than ±6%, while in case of shifts are within ±12%.

It is obvious that, in case of 516.680 nm and 520.022 nm line, halfwidths similarity within the multiplet \( ^2D - ^2D^0 \) is broken. \( ^2D_{5/2} \), the upper level of 516.680 nm line, has no close perturbing levels and the halfwidth of the line is 4.45-10^{11} s^{-1}. On the other hand, \( ^2D_{3/2}^0 \), the upper level of 520.022 nm line, has a very close perturbing level \( ^3P_{1/2} \), so the line has a twice larger halfwidth. One part of the
energy levels diagram, containing the considered levels, is shown in figure 3 [23]. Positions of the perturbing levels can also explain the difference between the shifts of the 520.022 nm and 616.880 nm line. The halfwidth of the 516.680 nm line and the halfwidths of other two spectral lines, 616.880 nm and 660.501 nm, from the multiplets belonging to the 4d – 5p transition array, show a reasonable regularity (differences < 15% from the average value of 3.9·10\(^{-11}\) s\(^{-1}\)).

Perturbations of the upper energy levels of the transitions are more evident. But, if the lower level has a very close perturbing level, perturbation in the broadening can also be detected. In the 5p – 6s transition array we can distinguish two lines (459.280 nm and 503.385 nm) whose lower levels \(^2\)P\(^{3/2}\) and \(^2\)D\(^{5/2}\) are perturbed, as shown in figure 3. In this case, the upper and lower levels approach each other; hence there is an additional red shift which is in good agreement with the measurements. In this particular case, the energy differences between the lower transition level and the perturbing level are only 23.6 cm\(^{-1}\) for \(^2\)P\(^{3/2}\) and 5.1 cm\(^{-1}\) for \(^2\)D\(^{3/2}\). This is the reason why these perturbing effects cause a bit higher shifts than the shifts of the other two lines in 5p – 6s transition array.

\[
\begin{align*}
\text{({}'D'\text{) 5p}) & \quad \text{({}'D'\text{) 4d}} \\
\end{align*}
\]

**Figure 3.** Energy scheme of some (\(^1\)D)5p Kr II levels (continuous lines), and the nearest perturbing 4d and (\(^1\)D)4d levels (dashed lines).

In case of Kr II there are no available experimental data of other authors for the comparison. Similar situation is with the theoretical MSE calculations [20, 21]. There are no available data for the complete sets of perturbing levels necessary for the calculations of halfwidths and shifts of considered spectral lines [24].

**Table 3.** Experimental Stark broadening parameters of Xe II spectral lines normalized to electron density \(N_e = 1 \times 10^{23}\) m\(^{-3}\) and electron temperature \(T_e = 22000\) K. Results from this work [25] are marked as TW, from Nick and Helbig [26] as NH, from Di Rocco [27] as DR, from Bertucelli et al. BE1 for Ref. [28] and BE2 for Ref. [29], and from Djurović et al.[12] as DJU and from Ćirišan et al.[30] as CI.

| Transition  | Term.   | \(J\) | \(\bar{\lambda}\) (nm) | \(w_\text{m}(10^{11}\text{s}^{-1})\) | \(d_\text{m}(10^{11}\text{s}^{-1})\) |
|-------------|---------|-------|-------------------------|-------------------------------|----------------------------------|
| \((^3\text{P}_1)_{6\text{s}} – (^3\text{P}_1)_{6\text{p}}\) | [1]-[1] \(^a\) | 3/2-3/2 | 465.194 | 5.64 TW | -0.82 TW |
|             |         |       |                         | 5.77 BE1                      |                                  |
|             |         |       |                         | 2.78 NH                       |                                  |
|             |         |       |                         | 3.93 DJU                      |                                  |
|             |         | 1/2-1/2 | 565.938 | 4.20 TW | 0.24 TW |
|             |         |       |                         | 3.47 BE2                      |                                  |
|             |         | 1/2-3/2 | 575.103 | 6.14 TW | -1.32 TW |
|             |         |       |                         | 3.80 DJU                      | 0.56 CI |
| \((^3\text{P}_1)_{6\text{s}} – (^3\text{P}_1)_{6\text{p}}\) | [0]-[1] \(^a\) | 1/2-1/2 | 426.984 | 3.89 TW | 0.42 TW |
|             |         |       |                         | 3.80 DJU                      | 0.56 CI |
|             |         | 1/2-3/2 | 432.182 | 7.43 TW | -0.75 TW |

\(^a\) Results from this work [25].

\(^\text{CI}\) Results from Ćirišan et al.[30].
Xe II is a multielectronic and heavy ion with a very complex energy structure, where $LS$ is not an appropriate coupling scheme. The coupling conditions in the Xe II configuration are intermediate, according to the strength of the spin-orbit interaction compared to the electrostatic interaction. In this case, the $JK$ coupling scheme is more appropriate and, in most cases, compositions of the energy levels configurations show more purity [31,32]. In Table 3, 5 Xe II lines from 2 multiplets are shown [14]. Experimental errors for halfwidths are estimated to be lower than ±15%, while in case of shifts these errors vary from ±15% for the highest value to ±70% for the lowest value, which is normal since the shift values are very low. It can be seen that there are large differences between the halfwidths, as well as between the shift values of the lines within the same multiplets. Measured values of the Stark broadening parameters of the lines in the multiplet $(^3P_i)_6s[1] - (^3P_i)_6p[1]^o$ are shown in the figure 4.

![Figure 4. Measured Stark halfwidths and shifts of the lines from the multiplet $(^3P_i)_6s[1] - (^3P_i)_6p[1]^o$.](image)

Energy scheme of Xe II around 124500 cm$^{-1}$ is shown in figure 5. The proximity of the levels $(^3P_i)_6p[1]_3/2^o$ and $(^3D_2)_5d[2]_3/2^o$ could explain the extra-broadening and extra-red shift of the lines 465.194 nm and 575.103 nm in the first multiplet and of the 432.182 nm line in the second one [14].

In case of halfwidths, results of other authors [12, 28] support the present results. There are some exceptions for 465.194 nm and 575.103 nm line. Results of Ref. [24,27] are in disagreement with our
and other results. In case of shifts, comparison with the results from other works [27,30] show satisfactory agreement.

Agreement of the present measured Stark halfwidth values and the MSE calculated values is reasonably good. For the $w_m$ values lower than $5 \cdot 10^{11}$s$^{-1}$, the ratio $w_m/w_{MSE}$ is about 1.15, while for higher $w_m$ values the ratio is about 1.65. The ratios between the measured and calculated shifts show a relatively large variation and in some cases there are opposite directions of the measured and calculated shift. There are many difficulties in the calculations of Stark broadening parameters, particularly in shift calculations. This is even more pronounced in cases of complex energy levels structure, such as in case of Xe II, where mixing of energy levels of different multiplets occurs. For detailed explanation see Ref. [14].

4. Conclusions

In this work we analyze regular and irregular behaviour of the Stark broadening parameters of spectral lines of ionized noble gases, neon, krypton and xenon, within certain multiplets and supermultiplets.

The spectral lines were observed from the pulsed discharge plasma. Apart from taking care of experimental conditions and plasma diagnostics, attention was also paid to proper fitting and deconvolution procedure.

Clear regular behaviour of both Stark halfwidths and shifts, in agreement with Ref. [5, 6] has been observed within Ne II multiplets. In case of Kr II and Xe II, which have more complex spectra and energy levels structure, intramultiplet irregularities occur. All presented irregularities of Stark broadening parameters can be explained by the presence of perturbing energy levels close to the upper level of the observed transition. The present cases show that a careful analysis of energy levels should be always performed when trying to estimate or predict Stark broadening parameters, particularly in atoms or ions with complex energy levels structure. In the future, it would be useful to analyze these and similar irregularities both experimentally and theoretically.

Acknowledgements

We thank S. González for his work on the experimental device, the Spanish Ministerio de Ciencia y Tecnología and the Consejería de Educación y Cultura de la Junta de Castilla y León for their financial support under contracts no FIS2005-03155 and VA015A05 respectively. Dr J. A. Aparicio wants to express his personal acknowledgement to the ONCE for help. S. Djurović thanks to Ministry of Science and Development of Republic of Serbia for support in Project 141024.

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