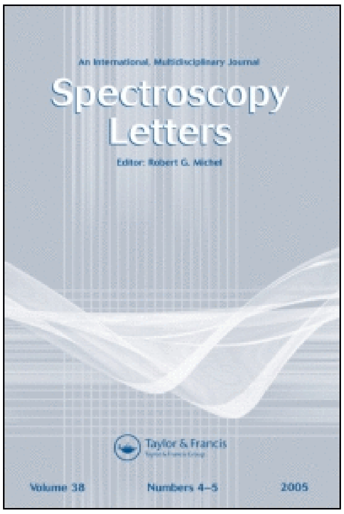

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Systematic Trends and Relevant Atomic Parameters for Stark Line Shifts and Widths

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SYSTEMATIC TRENDS AND RELEVANT ATOMIC PARAMETERS FOR STARK LINE SHIFTS AND WIDTHS

Key words: Spectroscopy - Atoms - Line shifts and widths - Stark effect.

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ABSTRACT: After an extensive study of line shifts and widths of one and two times ionized noble gases, we found simple empirical relations betweens such quantities (when multiplied by the respective atomic number, Z) and the inverse of the upper level ionization potential, I. In the adjustment process, a high value for the correlation coefficient is obtained. Thus, Z and I^{-1} are relevant atomic parameters for Stark line shifts and widths.

INTRODUCTION

The systematic trends and regularities of line broadening phenomena are of interest for the treatment of experimental data and applications.

The connection between Stark line shifts and widths and plasma parameters (electron density and temperature) is well established; however atomic parameters are involved in a complicated manner.

From the semiempirical approach a knowledge of transition probabilities A_{ij} is necessary for line shifts and widths calculations but data about A_{ij}'s are in many cases scarce or null. Then, it is important to know what atomic parameters describe the Stark line shifts and widths.

In a previous work /1/ a statistical linear correlation between the shifts (d) and the inverse for the upper level ionization potential (I) was showed for more than 900 Xe II transitions with a correlation coefficient r = 0.93.

In this paper, as a consequence of an extensive analysis of nearly three hundred spectral lines belonging to Kr III and Xe III spectra, whose shifts (d) were published elsewhere /2/ and, in addition of line widths (w) for Ne II /3/ and Xe II /4/ we present a series of general expressions relating Zw and Zd (Z: atomic number) with the inverse of the upper level ionization potential, I.

PLASMA CONDITIONS AND ATOMIC STRUCTURE ANALYSIS

The shifts and widths are originated through collisions with electrons (in our conditions, ions collisions are negligible). Plasma parameters are as follows: electron density (N) of the order of 5 - 10 x 10^{15} m^{-3}; electron temperature (T) in the range 1.5 - 3.5 eV, estimated with Saha relations and compared with experimental values of N and T /5/. The microscopic electric field is of the order of 1 - 5 x 10 V/m.

In the impact approximation /6/, when w and d are measured in cm^{-1}:

$$w + id = 2.88 \times 10^{-22} \, N T^{-1/2} \, Y_D$$

where Y_D is the thermally averaged collision strength.

For establish the dependence between (Zd, Zw) with I, a certain care must be taken when defining the last quantity.

Each atom or ion has several ionization potentials, corresponding to the levels of the fundamental configuration of the parent ion. For each level, the ionization limit must be calculated taking into account the corresponding parent.

The analysis for Ne II /7/, Kr II /8/ and Xe II /9/ indicates that the levels appear in distinct groups according to parentage and jK coupling scheme is the best for these ions. Furthermore, the new theoretical analysis of Kr III /10/ and Xe III /11/ shows that, in several cases, the level composition indicates strong mixing parents and an average value for I must be taken.

LINE WIDTHS AND REGULARITIES

For an ion, the functional dependence of Stark line widths (w) on I is of the form /3/

$$w = AI^{-B} \tag{1}$$

In the above quoted reference, the authors claims that the widths for np-nd transitions for the homologous sequence Ne II, Ar II, Kr II and Xe II satisfy

$$Z\, w\, I^{4.90} = \text{cte.} \tag{2}$$

within 20%.

In the same work, for eighteen experiments concerning to seven 3s-3p transitions, the full widths at half maximun (FWHM) in cm^{-1} satisfy, when normalized to $N = 10^{22}\ m^{-3}$, $T = 10^4$ K

$$W_{Ne} = (3.05 \pm 0.15) \times 10^3\ I^{-3.25} \tag{3}$$

where I is in eV; the correlation coefficient is r = 0.80.

In reference 4 fourteen 6s-6p Xe II spectral lines were studied, both theoretically and experimentally. When the results are reduced to $N = 10^{22}\ m^{-3}$ and $T = 10^4$, the adjustment gives

$$w_{Xe} = 5.42 \times 10^2\ I^{-3.35} \tag{4}$$

with r = 0.81.

From Eqs. (3) and (4), a general trend for Ne II and Xe II widths is established; we have

$$Zw = (3.00 \pm 0.15) \times 10^4\ I^{-3.30} \tag{5}$$

for ns-np transitions, where $n = n_0 + 1$ and n_0 is the principal quantum number of the ground level of the emitter.

In Table 1, we have the data for Ne II /3/ where now the widths are FWHM in cm^{-1} and normalized to $N = 10^{22}$ and $T = 10^4$. The spectroscopic information about I^{-1} is from Ref.7. In Table 2 the same information is for Xe II. The experimental widths are from Ref.4 and the I's values from Ref.9. In Fig.1 we plotted Zw vs I^{-1} for these lines.

Table 1: Ne II 3s-3p line widths (w) normalized to $N = 10^{22}$ m^{-3}, T = 10 K (from Ref.3).

λ (Å)	w(cm^{-1})	I^{-1} $(eV)^{-1}$
3694	1.737	0.0958
	1.619	"
	1.739	"
3709	1.505	0.0963
	1.886	"
	1.701	"
3334	1.828	0.0992
	1.829	"
	2.402	"
3355	1.805	0.0996
	1.829	"
	2.430	"
3713	2.035	0.1016
	1.961	"
3323	2.045	0.1058
	2.667	"
3658	1.744	0.0986
	2.066	"

LINE SHIFTS REGULARITIES

The wave numbers measured with our source were published elsewhere /2,10,11/ and compared with the values obtained by others.

For each transition, the inverse of the ionization potential was calculated, using in all cases the limit of the corresponding parent, according to line classification /7,8/.

Table 2: Xe II 6s–6p line widths (w) normalized to $N = 10^{22}$ m^{-3}, $T = 10^4$ K (from Ref.4).

λ (Å)	w(cm^{-1})	I^{-1} $(eV)^{-1}$
5976.46	0.74	0.1405
5751.03	0.86	0.1475
5438.96	0.74	0.1396
5372.39	0.77	0.1453
5261.95	0.76	0.1484
5191.37	0.74	0.1418
4972.71	0.69	0.1425
4921.48	0.87	0.1444
4890.09	0.74	0.1449
4887.30	0.71	0.1448
4883.53	0.77	0.1449
4524.21	0.84	0.1448
4215.60	0.86	0.1539

When the shifts in cm^{-1} (d) with their proper sign (in our convention, positive shifts are to the violet) are plotted vs I^{-1}, a linear trend

(6) $$d = b + aI^{-1}$$

is noticeable.

The analysis of the data indicates that for $N = 7.5 \times 10^{21}$ m^{-3} and $T = 10^4$ K we have, respectively for Kr III and Xe III

(7) $$d_{Kr} = -1.75 + 24.15\ I^{-1}$$

and

(8) $$d_{Xe} = -1.35 \times 15.95\ I^{-1}$$

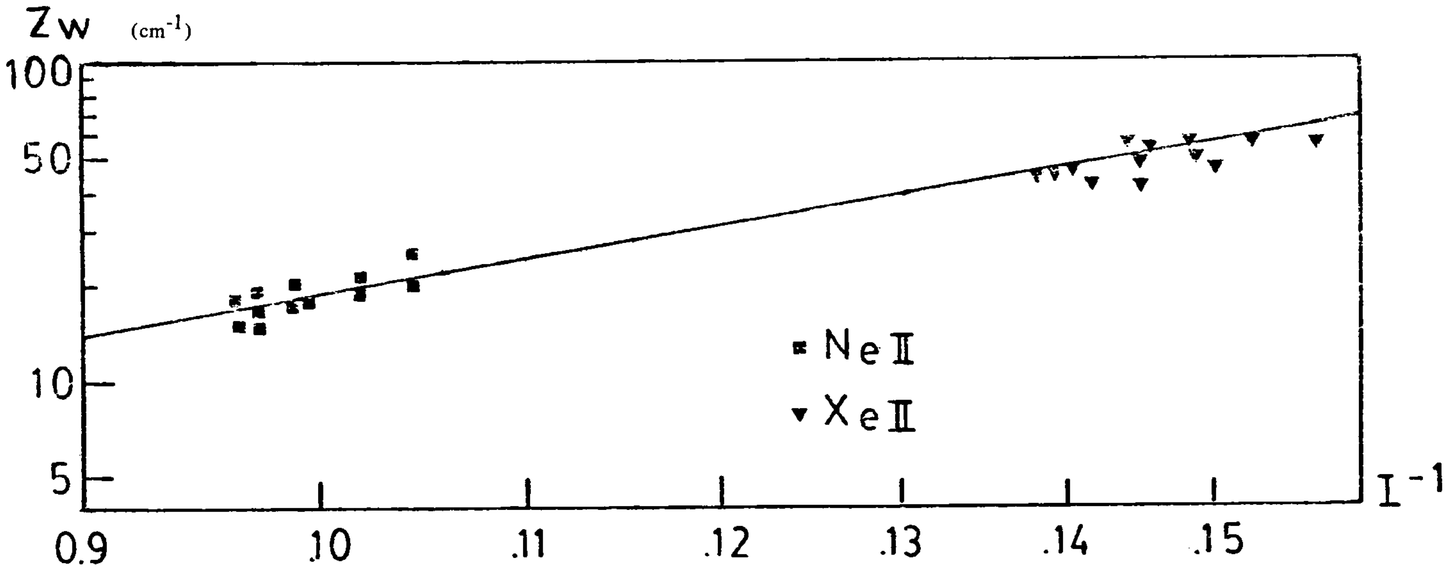

Fig. 1: Line widths (FWHM) times atomic number Z vs. the inverse of the upper level ionization potential.

TABLE 3

Wavelengths, shifts and the inverse of the Ionization Potential for Xe III lines.

λ (Å)	d(cm⁻¹)	I⁻¹(eV)⁻¹	λ (Å)	d(cm⁻¹)	I⁻¹(eV)⁻¹	λ (Å)	d(cm⁻¹)	I⁻¹(eV)⁻¹
3196.51	0.03	.0805	5223.61	0.06	.0794	4109.08	-0.03	.0755
3236.84	0.03	.0826	5367.03	0.06	.0764	4145.74	-0.07	.0774
3242.86	0.03	.0820	6238.18	0.18	.0794	4176.52	0.03	.0780
3256.25	-0.16	.0815	3268.98	-0.16	.0820	4226.97	-0.03	.0811
3295.94	-0.07	.0811	3338.99	-0.07	.0820	4308.00	-0.03	.0794
3306.80	0.03	.0764	3349.76	0.02	.0794	4434.17	-0.03	.0764
3314.87	0.03	.0764	3357.99	-0.06	.0794	4657.78	0.02	.0794
3340.06	0.02	.0745	3454.27	-0.14	.0857	4673.67	-0.06	.0794
3340.67	0.12	.0857	3519.11	-0.05	.0815	4683.54	-0.06	.0780
3467.22	-0.14	.0857	3565.19	-0.06	.0811	4723.59	-0.11	.0780
3539.94	0.18	.0794	3579.70	-0.05	.0780	4794.49	-0.05	.0755
3544.86	0.11	.0815	3583.65	-0.06	.0811	5748.67	0.09	.0820
3552.12	0.11	.0794	3596.59	0.10	.0805	3169.75	0.72	.1148
3561.37	0.10	.0794	3623.13	0.02	.0774	3177.11	0.82	.1148
3601.87	0.18	.0780	3624.06	-0.05	.0794	3222.99	0.51	.1205
3615.86	0.18	.0820	3632.14	0.03	.0764	3244.13	0.50	.1274
3636.02	0.10	.0794	3649.57	-0.05	.0832	3278.44	0.40	.1186
3640.99	0.10	.0794	3676.63	0.02	.0826	3301.54	0.57	.1186
3644.14	0.02	.0745	3708.15	0.03	.0826	3350.35	0.83	.1153
3654.61	0.17	.0820	3711.91	-0.05	.0832	3381.64	0.90	.1153
3745.71	0.10	.0857	3762.28	-0.12	.0764	3386.23	0.64	.1247
3841.87	0.09	.0820	3765.85	0.02	.0764	3472.35	0.60	.1161
3854.28	0.16	.0820	3772.53	0.03	.0826	3488.13	0.60	.1230
3861.04	0.09	.0774	3776.32	-0.12	.0764	3890.98	0.82	.1262
3880.46	0.02	.0755	3781.00	-0.12	.0820	4528.24	0.66	.1262
3884.99	0.09	.0780	3791.67	0.02	.0794	6283.74	0.47	.1196
4078.70	0.20	.0832	3841.53	-0.04	.0764	3184.27	0.82	.1148
4110.04	0.10	.0764	3877.82	-0.11	.0794	3227.16	0.79	.1211
4132.40	0.14	.0857	3895.05	-0.11	.0815	3285.82	0.68	.1186
4141.99	0.10	.0764	3922.55	-0.10	.0780	3336.24	0.65	.1148
4240.24	0.03	.0857	3950.59	-0.16	.0780	3501.65	1.00	.1230
4272.58	0.13	.0811	3985.96	0.02	.0811	3593.38	0.57	.1148
4748.93	-0.02	.0811	3992.85	0.02	.0820	4528.24	0.66	.1216
5008.52	0.11	.0764	4043.23	-0.10	.0745	4644.17	0.40	.1211
5107.33	0.18	.0826	4050.07	-0.10	.0805	6484.78	0.57	.1186

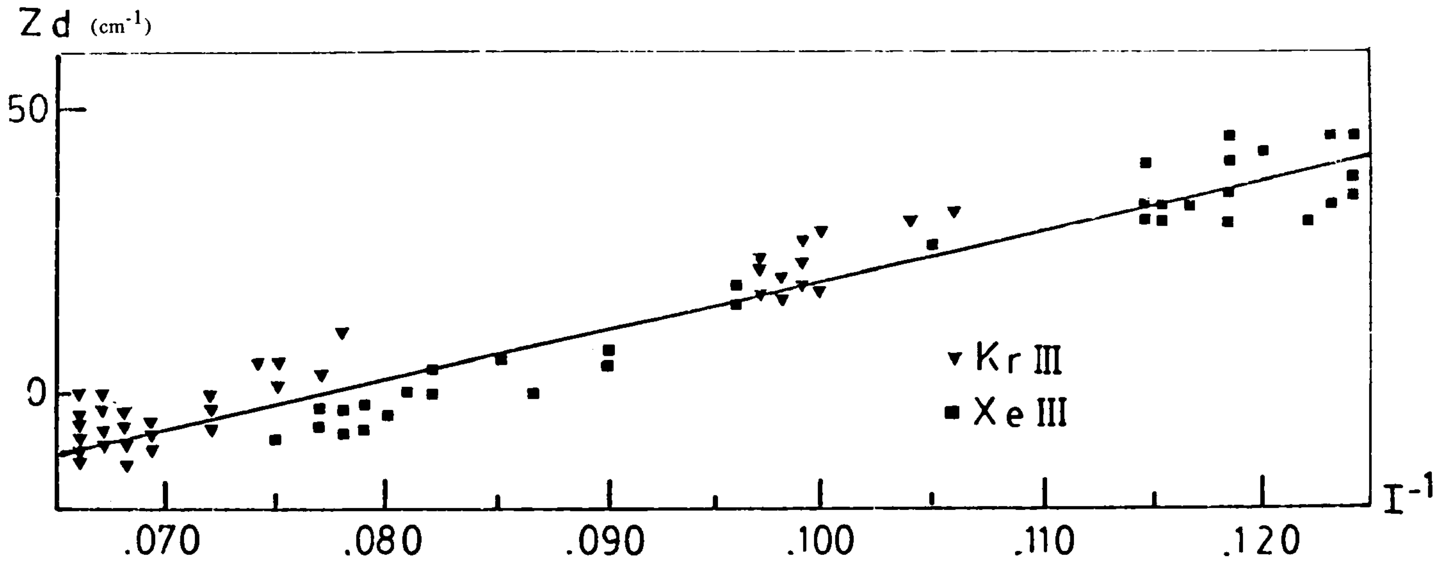

Fig. 2: Line shifts times atomic number Z vs. the inverse of the upper level ionization potential.

In order to test the validity of the statistical procedure the correlation coefficient r was calculated, being $r = 0.93$ for Kr III and $r = 0.96$ for Xe III.

From Eqs. (7) and (8), we obtained the following trend for Kr III and Xe III line shifts:

$$Zd = -66.80 + 865.35\ I^{-1} \tag{9}$$

In Table 3 are indicated, for 105 Xe III strong lines, the wavelenght λ , the shifts d and I^{-1}. Furthermore, the 4f - 6d transitions whose I^{-1}'s, values are between 0.118 and 0.125 $(eV)^{-1}$ have shifts between 0.50 and 0.90 cm^{-1}. Graphically, the results given by Eq.(9) are in Fig.2.

CONCLUSIONS

In this work, data from several experiments were considered. It was found that for homologous ions, the line shifts and widths, when they are multiplied by the corresponding atomic numbers, are simple functions of I^{-1}. The functional dependences are linear for the line shifts (when all type of transitions are considered) whereas is exponential for the line widths; in this case, the exponent depends on the type of transitions.

The foremost conclusion is that Z and I^{-1} are relevant atomic parameters for the description of Stark line shifts and widths.

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