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RESEARCH ARTICLE

CORE-POLARIZATION EFFECTS FOR THE STARK BROADENING OF PB III SPECTRAL LINES: PREDICTIONS AND REGULARITIES

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Abstract: Using a semi-classical approach, we have calculated values of the Stark broadening parameters for several lines of Pb III. Stark widths and shifts are presented for an electron density of 10^{17} cm^{-3} and temperatures T = 11000-100000 K. In this work, we have carried out a study of the influence of the introduction of the terms that allow us to take into account the Core Polarization (CP) effects in the calculation of the Stark broadening parameters. Our results are compared with available experimental and theoretical data. Common trends for the several lines have been found and are discussed.

Keywords: Atomic data–atomic processes.

1. INTRODUCTION

The Stark broadening parameters of Pb III spectral lines are of interest not only for the astrophysical purposes but for the plasma diagnosis, for the research of regularities and systematic trends and theoretical considerations as well.

The previous works, published in literature, about the atomic parameters of the Pb III are scarce (see e.g. Andersen et al. (1972), Migdalek and Baylis (1985), Ansbacher et al. (1987), Pinnington et al. (1988), Colón et al. (1999), Curtis et al.(2001)). In 2007 experimental Stark widths for 10 spectral lines of Pb III by using a Laser Induced Plasma at 25 200 K and a electron density of 10^{17} cm^{-3} were measured by Alonso-Medina and Colón.

Quite a large number of articles have been published that use different theoretical approximations to calculate these parameters, and to study their dependence on the nuclear charge number, effective ionization potential, atomic polarizability or principal quantum number, Roberts (1970), Dimitrijevic and Konjevic (1980), Dimitrijevic and Krsljanin (1986), Popovic and Dimitrijevic (1996) and Dimitrijevic and Sahal-Brechot 1996). In a recent work (Alonso-Medina et al. 2008), we calculated Stark width and shift parameters for 122 lines of Pb III using a semi-classical approach.

In this paper, we present semi-empirical approximate values of the Stark broadening parameters for 30 spectral lines of Pb III arising from $5d^{10}6snp$ (n = 6, 7, 8), $5d^{10}6s5f$ and $5d^{10}6$ sng (n = 5, 6) configurations. The results have been obtained using Griem´s (1968) semi-classical calculations. Stark widths and shifts are presented as functions of temperature and for an electron density of 10^{23} m^{-3}.

Dimitrijevic and Konjevic (1980), Dimitrijevic and Krsljanin (1986), Popovic and Dimitrijevic (1996) have carried out calculations for multiply ionized ions by using the semi-empirical approach (the so-called "MSE-Modified Semi-Empirical-" method). This approach has numeric advantages: it uses a limited number of matrix elements, it includes an improved effective Gaunt factor and it supposes an LS coupling approximation. This model doesn't work well in the case of the Pb III. In the Pb III is remarkable the multiplet inversion indicating a strong presence of mixed configurations. They also exists

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transitions of great relevance astrophysics that would be forbidden according to this coupling model.

We compare the theoretical values obtained in this work with the experimental and theoretical data published. Except for the exceptions that will be studied in the Section 3, a relatively good agreement between experimental and theoretical data is found. We have studied the dependence of the Stark width, ω (s^{-1}), on principal quantum number, *n*, of the Pb III for several series of the Pb III. Also we present the regularity of the Stark broadening parameters versus the temperature.

2. THEORETICAL CALCULATIONS

In 1968 Griem formulated a simple semi-empirical impact approximation, based on Baranger´s original formulation (1958) and the use of an effective Gaunt factor, proposed by Seaton (1962) and Van Regemorter (1962). In this approach the Stark line width and Stark line shifts can be calculated from the followings semi-empirical formulas:

$$\varpi_{se} \approx 8\left(\frac{\pi}{3}\right)^{3/2}\frac{\hbar}{ma_0}N_e\left(\frac{E_H}{kT}\right)^{1/2}\left[\sum_{i'}\left|\langle i'|\vec{r}|i\rangle\right|^2 g_{se}\left(\frac{E}{\Delta E_{i'i}}\right)\right.$$

$$\left.+\sum_{f'}\left|\langle f'|\vec{r}|f\rangle\right|^2 g_{se}\left(\frac{E}{\Delta E_{f'f}}\right)\right] \quad \ldots (1)$$

$$d \approx -8\left(\frac{\pi}{3}\right)^{3/2}\frac{\hbar}{ma_0}N_e\left(\frac{E_H}{kT}\right)^{1/2}$$

$$\left[\sum_{i'}\left(\frac{\Delta E_{i'i}}{|\Delta E_{i'i}|}\right)\left|\langle i'|\vec{r}|i\rangle\right|^2 g_{sh}\left(\frac{E}{\Delta E_{i'i}}\right)\right.$$

$$\left.-\sum_{f'}\left(\frac{\Delta E_{f'f}}{|\Delta E_{f'f}|}\right)\left|\langle f'|\vec{r}|f\rangle\right|^2 g_{sh}\left(\frac{E}{\Delta E_{f'f}}\right)\right] \ldots (2)$$

In these formulas, ω_{se} and *d* are the Stark line width and shifts respectively in angular frequency units, E_H is the hydrogen ionization energy, N_e is the free electron perturber density, *T* the electron temperature, $E = (3/2)\,kT$ the mean energy of the perturbing electron and g_{se}, and g_{sh} are the effective Gaunt factors suggested by Niemann et al (2003). These factors are slowly varying functions of $x_{i'i} = E/\Delta E_{i'i}$, where $\Delta E_{i'i}$ is the energy difference between a perturbing level *i´* and the perturbed level *i*. The indices *i* and *f* denote the initial (upper) and final (lower) levels of the transitions, respectively.

The atomic matrix elements were obtained using relativistic Hartree-Fock calculations and configuration interaction in an intermediate coupling (IC) scheme. The Cowan code (1981), in which we have incorporated the CP effects by means of a potential model and a correction to the electric dipole operator, was selected for this purpose.

The C-P effects are included following the suggestions of Migdalek and Baylis (1978): The core polarization effects can be written as the one-particle, V_{P1}, and two-particle, V_{P2}, potential models:

$$V_{P1} = -\frac{1}{2}\alpha_d\sum_{i=1}^{n}\frac{r_i^2}{\left(r_i^2+r_c^2\right)^3} \quad \ldots (3)$$

$$V_{P2} = -\alpha_d\sum_{i>j}^{n}\frac{\vec{r}_i\cdot\vec{r}_j}{\left[\left(r_i^2+r_c^2\right)\left(r_j^2+r_c^2\right)\right]^{3/2}} \quad \ldots (4)$$

where α_d is the dipole polarizability of the core and r_c is the cut-off radius chosen as a measure of the size of the ionic core.

A modification in the radial matrix element can be made in order to take into account the potential change. The $<P_{nl}\,|\,r\,|\,P_{n'l'}>$ is replaced by:

$$\int_0^\infty P_{nl}\,r\left(1-\frac{\alpha_d}{\left(r^2+r_c^2\right)^{3/2}}\right)P_{n'l'}\,dr$$

$$-\frac{\alpha_d}{r_c^3}\int_0^{r_c}P_{nl}(r)\,rP_{n'l'}(r)\,dr \quad \ldots (5)$$

where the core penetration term suggested by Hameed (1972) has been also included.

For the dipole polarizability and the cut-off radius we use the values, $\alpha_d = 3.986$ (in au) and $r_c = 1.268$ (in au), computed by Fraga, Karwowski & Saxena, (1976).

In order to calculate the matrix elements, we have used a basis set consisting of 6 configurations of even parity, namely, $5d^{10}6s^2$, $5d^{10}6p^2$, $5d^{10}6s6d$, $5d^{10}6s7d$, $5d^{10}6s8d$ and $5d^{10}6s9d$ and 8 configurations of odd parity, namely, $5d^{10}6s6p$, $5d^{10}6s7p$, $5d^{10}6s8p$, $5d^{10}6s5f$, $5d^{10}6s6f$, $5d^{9}6s^2$ 6p, $5d^{10}6p7s$, and $5d^{10}6p6d$. To provide level energies for our calculations, the table of Moore (1958) has been used. A more detailed discussion can be seen in Alonso-Medina et al. (2009).

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3. RESULTS AND CONCLUSIONS

Our results for the Stark line width (FWHM) and line shift at an electron density of 10^{23} m^{-3} and several temperatures T = 11000-100000 K are displayed in Tables 1-2. The first three columns denote the corresponding transition array, the multiplet and the wavelengths (in nm, Moore 1958) for each studied transition. Temperatures are shown in column four.

In Table 1, we present results for transitions arising from $5d^{10}6snp$ (n = 6, 7, 8). Stark broadening line-widths (in Å) and line-shift (in Å) are displayed in columns 5 and 6 respectively. The remaining column displays the experimental and theoretical values found in the bibliography.

As can be seen our results are in agreement with our previous experimental results, except for the values corresponding of intercombination lines. This situation is similar to the found in our previous work (Alonso-Medina et al. 2008) in which they were not take into account the Core Polarization effects. In our previous

Table 1
Pb III $5d^{10}6snp$ line-widths (FWHM) and shifts normalized to Ne = 10^{23} m^{-3}. Line widths are compared with theoretical published values of Alonso-Medina et al. 2008 (A-MCZ) and with experimental published values of Alonso-Medina and Colón 2007 (A-MC)

Transition Array	*Multiplet*	*λ (nm)*[a]	*T (10^3 K)*	*Present Results*		*A-MC*	*A-MCZ*	
				ω (Å)	*d (Å)*	*ω (Å)*	*ω (Å)*	*d (Å)*
$6s^2$-6p	$^1S_0 - {}^1P_1$	104.89	11	0.018	0.012		0.043	0.030
			16	0.014	0.0096		0.033	0.023
			20	0.012	0.0082		0.028	0.020
			25.2	0.010	0.0070		0.024	0.017
			33	0.0087	0.0059		0.020	0.014
			75	0.0052	0.0035			
			100	0.0043	0.0030			
$6s^2$-6p	$^1S_0 - {}^3P_1$	155.30	11	0.029	0.028		0.068	0.066
			16	0.022	0.021		0.053	0.051
			20	0.019	0.018		0.045	0.043
			25.2	0.016	0.015		0.038	0.037
			33	0.013	0.013		0.032	0.031
			75	0.0079	0.0076			
			100	0.0067	0.0064			
$6s^2$-7p	$^1S_0 - {}^3P_1$	58.45	11	0.016	0.0029		0.021	0.006
			16	0.013	0.0022		0.016	0.004
			20	0.011	0.0019		0.014	0.004
			25.2	0.0099	0.0016		0.012	0.003
			33	0.0084	0.0013		0.010	0.003
			75	0.0054	0.0007			
			100	0.0046	0.0006			
$6s^2$-8p	$^1S_0 - {}^3P_1$	48.31	11	0.033	−0.0004		0.035	0.001
			16	0.026	−0.0006		0.028	0.001
			20	0.023	−0.0007		0.025	0.001

Table Contd.

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Table 1 Contd.

			25.2	0.020	−0.0007		0.022	0.000
			33	0.018	−0.0007		0.019	0.000
			75	0.012	−0.0006			
			100	0.010	−0.0006			
7s-7p	$^3S_1 - {}^1P_1$	369.03	20	0.59	0.35			
			25.2	0.51	0.30			
			33	0.43	0.26			
7s-7p	$^3S_1 - {}^3P_2$	385.52	11	0.93	0.079		1.72	0.65
			16	0.74	0.060		1.35	0.51
			20	0.64	0.051		1.17	0.44
			25.2	0.56	0.043	0.75 ± 0.16	1.02	0.38
			33	0.47	0.036		0.87	0.32
6d-7p	$^1D_2 - {}^3P_2$	414.28	11	1.48	0.47			
			16	1.16	0.36			
			20	1.01	0.31		1.15	0.37
			25.2	0.88	0.27	2.7 ± 0.6	0.99	0.32
			33	0.74	0.22		0.84	0.27
7s-7p	$^1S_0 - {}^1P_1$	427.39	20	0.45	0.20		0.51	0.23
			25.2	0.39	0.17		0.44	0.20
			33	0.33	0.15		0.38	0.17
7s-7p	$^3S_1 - {}^3P_1$	476.11	11	1.99	0.88		2.28	1.07
			16	1.57	0.69		1.79	0.83
			20	1.36	0.60		1.55	0.72
			25.2	1.18	0.51	1.0 ± 0.2	1.35	0.62
			33	1.01	0.44		1.15	0.53
7s-7p	$^3S_1 - {}^3P_0$	479.99	11	1.31	0.74		1.56	0.95
			16	1.03	0.58		1.22	0.74
			20	0.89	0.51		1.06	0.64
			25.2	0.77	0.44	1.0 ± 0.2	0.92	0.56
			33	0.66	0.37		0.78	0.47
6d-7p	$^1D_2 - {}^3P_1$	520.92	20	1.33	0.55		1.53	0.66
			25.2	1.15	0.47	2.2 ± 0.6	1.32	0.56
			33	0.98	0.39		1.12	0.47
6d-7p	$^3D_1 - {}^3P_2$	538.25	20	1.88	0.59		2.15	0.71
			25.2	1.63	0.51	2.7 ± 0.7	1.87	0.61
			33	1.39	0.43		1.59	0.52
6d-7p	$^3D_2 - {}^3P_2$	552 55	20	2.41	0.96		2.85	1.19

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Table 1 Contd.

			25.2	2.09	0.83	2.4 ± 0.6	2.47	1.03
			33	1.78	0.71		2.10	0.87
7s-7p	$^1S_0 - {}^3P_1$	578.10	20	1.39	0.39		1.53	0.44
			25.2	1.21	0.33	2.9 ± 0.7	1.33	0.38
			33	1.03	0.28		1.13	0.31
7s-7p	$^3D_3 - {}^3P_2$	585.97	20	3.22	1.48		3.86	1.86
			25.2	2.79	1.28	1.1 ± 0.3	3.34	1.61
			33	2.37	1.09		2.84	1.36
6d-7p	$^1D_2 - {}^1P_1$	395.30	20	0.50	0.31			
			25.2	0.43	0.26			
			33	0.37	0.22			
$6p^2$-7p	$^3P_1 - {}^3P_2$	485.51	20	1.30	0.28		1.51	0.28
			25.2	1.13	0.24	1.4 ± 0.4	1.31	0.24
			33	0.96	0.20		1.11	0.20

* Moore (1958). *A positive shift is solid.*

work, we supposed that without the effects of Core Polarization in the Cowan calculations we will obtain an overestimated set of matrix elements. We also indicated that the fitting process of the theoretical levels to the experimental ones account partially the Core Polarization effects and therefore our results would be overestimated but they would not be very far from the experimental values.

In the present calculations, due to the introduction of the Core Polarization effects, a set of theoretical matrix elements not overestimated has been used in the Stark broadening estimations. Our results are now lower than obtained in the previous work. In Fig. 1, measured and calculated Stark widths FWHM (ω (Å)) versus temperature for 385.52 nm, 476.11 Å and 479.99 nm Pb III lines are displayed. As can be seen, the present values are systematically lower than those obtained with calculations that don't include CP effects. Also, it can be appreciated an improvement in the approach between the experimental values and the present calculated data. Our values are now in agreement with the experimental data shown -within the experimental error.

Figures 2 and 3, display Stark line-widths FWHM (ω) for resonant transitions $6s^2\ {}^1S_0$ — 6s np $^3P_1$ (155.30, 58.45 and 48.31Å lines) versus the principal quantum number of the upper state. In Fig. 2 the present results are compared with the previously calculated data (CP effects not included). As it has been said above, the present values are systematically lower than those obtained with calculations that don't include CP effects. In Fig. 3, data are displayed at several temperatures.

For comparison reasons, in the Fig 4, for those spectral lines with accessible experimental values, calculated and experimental Stark line-widths FWHM (ω) is presented. As it can be appreciated we have not been able to correct the discrepancies in the intercombinación lines. But this problem has its origin in the previous calculations of the matrix elements and not in the Griem model. In our work, (Alonso-Medina et al. 2009) it can be observed that the calculations of Cowan provide for the lines of 414.28 nm, 520,92 nm and 578.10 nm some transition probabilities until an order of magnitude below their experimental values. The introduction in the Griem model of the experimental values of the matrix elements of these lines instead of the theoretical ones (calculated by Cowan code) would solve the discrepancies.

Therefore, these discrepancies are due to the configurations mix with other excited no experimental configurations not included in this work. As we pointed in our previous work attempts to carry out a least-square fitting including many no experimental configurations, in order to correct the discrepancies, resulted in no reasonable improvement while presenting difficulties due to the increase in the numbers of parameters above the number of experimentally observed energy levels.

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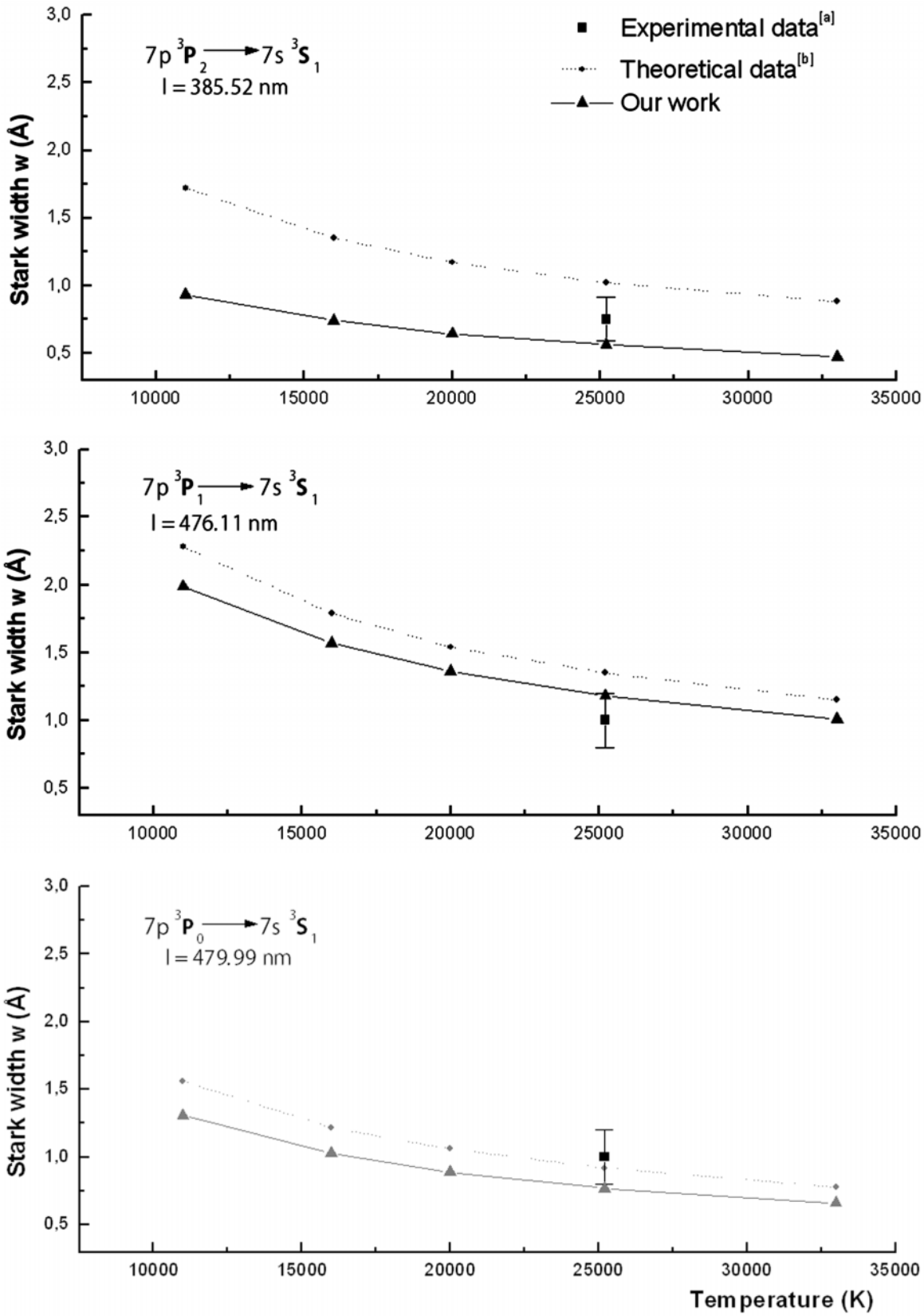

Fig. 1: Stark width (FWHM) versus temperature for 385.52 nm, 476.11 nm and 479.99 nm Pb III lines. Measured ([a] Alonso-Medina and Colón 2007), theoretical ([b]Alonso-Medina et al. 2008) and calculated stark line-width (including core-polarization effects)

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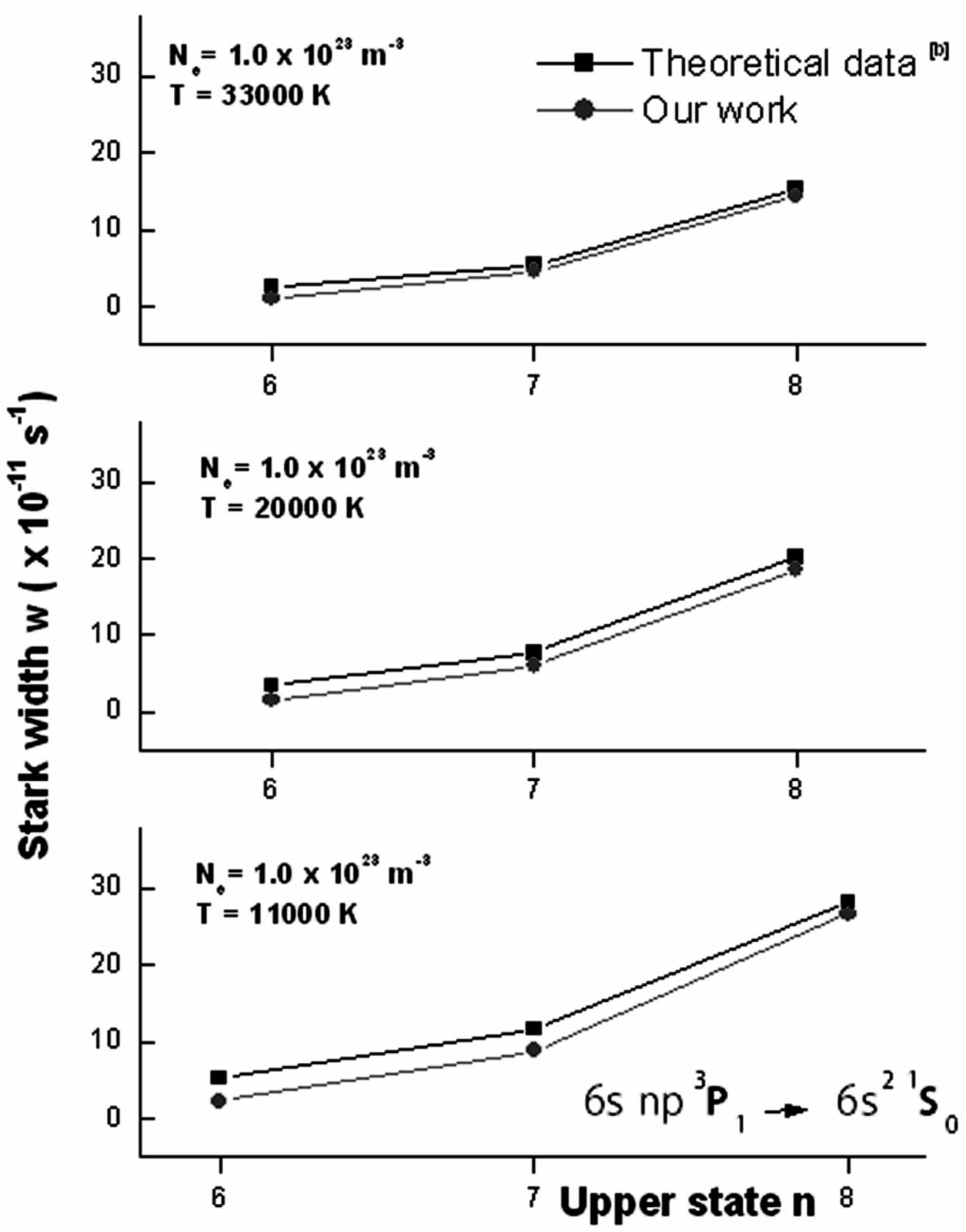

Fig. 2: Stark width (FWHM) calculated taking into account core polarization effects and calculated without core polarization effects ([b] Alonso-Medina et al., 2008) versus the principal quantum number of the upper state

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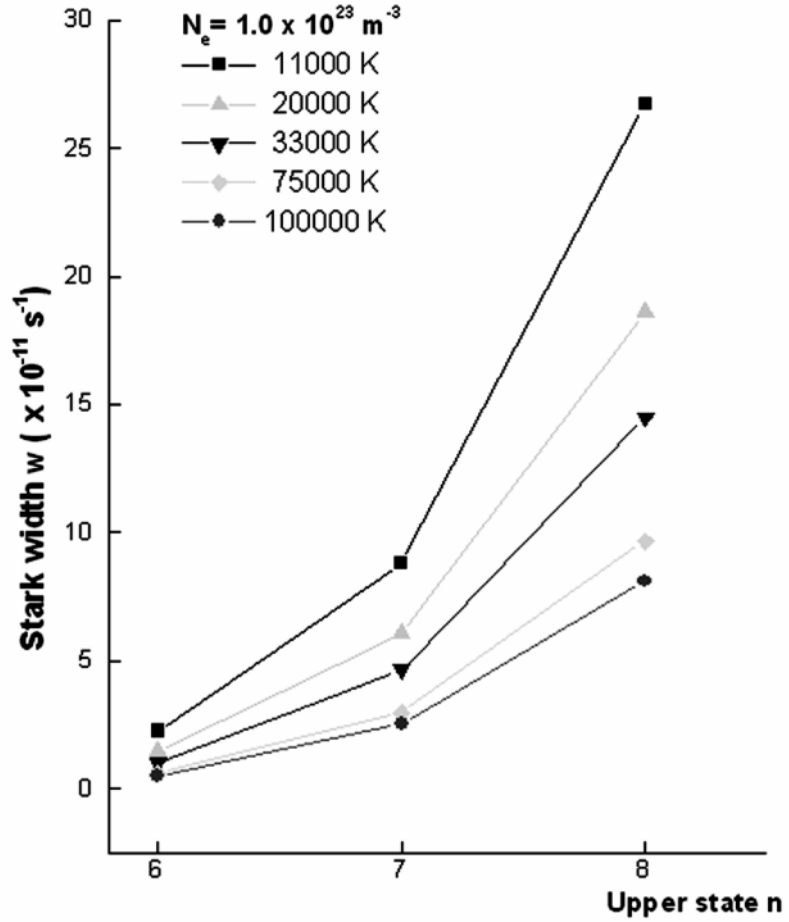

Fig. 3: Stark FWHM (ω (s^{-1})) for the $6s^2\ ^1S_0$ – 6snp $^3P_1$ lines of Pb III versus the principal quantum number of the upper state

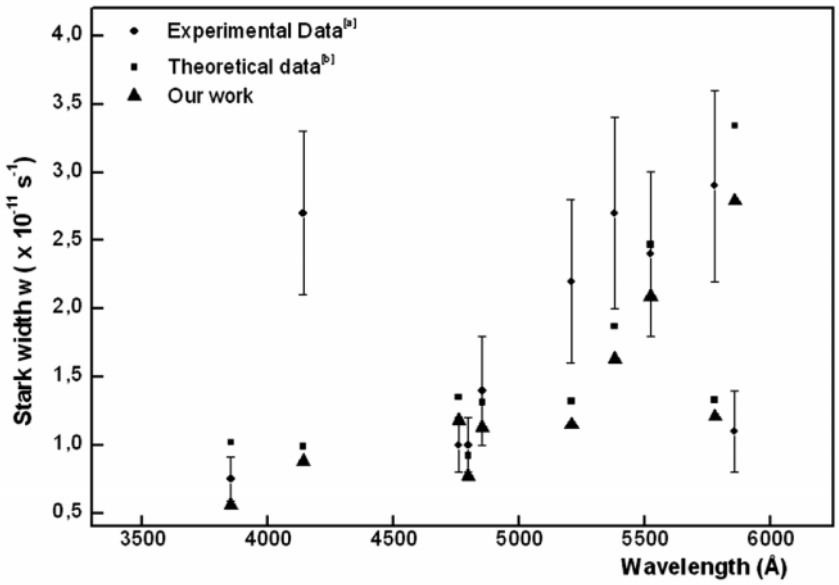

Fig. 4: Stark width (FWHM), at 25200 K and 10^{23} m^{-3}, for several lines of Pb III versus wavelength. Measured ([a]Alonso-Medina and Colón 2007), theoretical ([b] Alonso-Medina et al. 2008) and calculated stark line-width (including core-polarization effects)

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Table 2, include results for transitions arising from $5d^{10}6s5f$ and $5d^{10}6sng$ configurations. Stark broadening line- widths (in Å) are displayed in column 5. The remaining column displays the theoretical Stark line-shift. We have not found any experimental results in the literature about these transitions.

This work provides theoretical Stark width and shift parameters for 30 spectral lines of the Pb III, of astrophysical interest, arising from $5d^{10}6snp$, $5d^{10}6s5f$ and $5d^{10}6sng$ configurations. There is experimental data about Stark width of ten lines.

Our data has been displayed for an electron density of 10^{23} m^{-3} and several temperatures. As can be seen, some clear trends in the Stark width appear in our results. Data about $5d^{10}6s5f$ and $5d^{10}6sng$ configurations are presented for the first time in the bibliography.

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Table 2
Pb III $5d^{10}6s$ {5f, ng} line-widths (FWHM) and shifts normalized to Ne = 10^{23} m^{-3}

Transition Array	*Multiplet*	*λ (nm)*[a]	*T (10^3 K)*	*Present Results*	
				ω (Å)	*d (Å)*
6d-5f	$^1D_2 - {}^1F_3$	256.30	16	0.60	0.41
			20	0.52	0.36
			25.2	0.46	0.31
			33	0.39	0.26
			75	0.24	0.17
			100	0.21	0.14
6d-5f	$^3D_1 - {}^3F_2$	304.47	16	0.71	0.39
			20	0.62	0.34
			25.2	0.54	0.29
			33	0.46	0.25
			75	0.29	0.16
			100	0.25	0.14
6d-5f	$^3D_2 - {}^3F_2$	309.00	16	0.89	0.52
			20	0.78	0.45
			25.2	0.67	0.39
			33	0.57	0.34
			75	0.36	0.21
			100	0.31	0.18
6d-5f	$^3D_2 - {}^3F_3$	313.87	16	1.11	0.62
			20	0.96	0.54
			25.2	0.83	0.47
			33	0.71	0.40
			75	0.45	0.25

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			100	0.38	0.23
6d-5f	$^3D_3 - {}^3F_4$	317.74	16	1.54	0.87
			20	1.34	0.76
			25.2	1.16	0.66
			33	0.99	0.56
			75	0.62	0.36
			100	0.53	0.31
5f-5g	$^3F_3 - {}^3G_4$	359.09	16	4.40	0.84
			20	3.87	0.73
			25.2	3.40	0.62
			33	2.93	0.53
			75	1.91	0.33
			100	1.66	0.29
5f-5g	$^3F_2 - {}^3G_3$	365.67	16	3.51	0.66
			20	3.09	0.57
			25.2	2.71	0.49
			33	2.34	0.41
			75	1.53	0.26
			100	1.32	0.23
5f-5g	$^3F_4 - {}^3G_5$	367.24	16	5.73	1.12
			20	5.04	0.97
			25.2	4.43	0.83
			33	3.82	0.70
			75	2.49	0.44
			100	2.16	0.39
5f-5g	$^1F_3 - {}^1G_4$	373.70	16	4.82	1.13
			20	4.24	0.97
			25.2	3.73	0.84
			33	3.22	0.71
			75	2.10	0.45
			100	1.82	0.39
5f-6g	$^3F_3 - {}^3G_4$	249.63	16	3.21	2.29
			20	2.84	2.13
			25.2	2.51	1.89
			33	2.18	1.64
			75	1.43	1.09
			100	1.24	0.95

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5f-6g	$^3F_2 - {}^3G_3$	252.79	16	2.57	1.87
			20	2.28	1.66
			25.2	2.01	1.48
			33	1.74	1.29
			75	1.15	0.86
			100	1.00	0.74
5f-6g	$^3F_4 - {}^3G_5$	253.55	16	4.12	3.02
			20	3.64	2.68
			25.2	3.22	2.38
			33	2.79	2.08
			75	1.84	1.38
			100	1.59	1.20
5f-6g	$^1F_3 - {}^1G_4$	256.61	16	3.43	2.62
			20	3.04	2.33
			25.2	2.68	2.07
			33	2.33	1.80
			75	1.54	1.20
			100	1.33	1.04

* Moore (1958). *A positive shift is red*.

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