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Theoretical study of the Stark width and shift parameters of Pb III lines: predictions and regularities

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ABSTRACT

Semiclassical approximate values of the Stark parameters for several lines of Pb III are reported in this paper. The parameters were calculated using a set of wavefunctions obtained from Hartree–Fock relativistic calculations. Stark widths for 122 lines of Pb III arising from $5d^{10}\,6s\,np$ ($n = 6,7,8$), $5d^{10}\,6s\,ns$ ($n = 7,8,9$) and $5d^{10}\,6s\,nd$ ($n = 6,7$) configurations have been calculated in this way. Stark widths and shifts are presented as a function of temperature for an electron density of 10^{17} cm^{-3}. Our results are compared with available experimental data. These atomic data are relevant to the analysis of isotopic abundances of Pb III found in the atmospheres of the star χ Lupy and several subdwarf B and OB stars.

Key words: atomic data – atomic processes.

1 INTRODUCTION

Stark broadening parameters for a large number of transitions in many atomic and ionic spectra are needed to model a stellar plasma and to investigate its physical properties and abundances. When calculating the opacities of large-scale plasmas in stellar atmospheres, the Stark-broadened line profiles of resonance transitions are of the utmost importance because these transitions provide a relatively large contribution to the radiative energy transport.

In astrophysics, a number of problems depend on an extensive list of elements and line-broadening parameters. Recent observations with the *Hubble Space Telescope* have created a need for accurate radiative parameters for heavy atoms in different ionization states. As an example, Pb II spectral lines have been observed in ς Oph (Cardelli et al. 1993; Welty et al. 1995), Pb III and Pb IV resonance lines have been detected in Far Ultraviolet Spectroscopic Explorer (FUSE) spectra of hot subdwarf B (sdB) stars (Chayer et al. 2006), and Pb IV has been detected in several sdB and sdOB stars (O'Toole 2004). Furthermore, Pb III has been detected in the star χ Lupy (Leckrone & Proffitt 1999; Wahlgren 2004).

Using data from the new generation of telescopes, such as NASA's *Next Generation Space Telescope* (*NGST*), the spectral lines of doubly ionized lead can be analysed, providing information on the physical conditions of hot stars. Knowledge of the Stark broadening of the spectral lines will enable the modelling of various physical processes in the plasmas of hot stars, where this effect is the principal mechanism of spectral line broadening.

For these reasons, the determination of the Stark broadening parameters of Pb III is timely in order to meet the needs of astrophysicists interested in the determination of the density of electrons in stellar atmospheres.

Published works on the atomic parameters of Pb III are scarce (see, for example, Andersen, Kirkegard Nielsen & Sorensen 1972; Migdalek & Baylis 1985; Ansbacher, Pinnington & Kernahan 1987; Pinnington et al. 1988; Colón et al. 1999; Curtis et al. 2001). In a recent work (Alonso-Medina & Colón 2007), we measured experimental Stark widths for 10 spectral lines of Pb III using a laser-induced plasma at 25 200 K and an electron density of 10^{17} cm^{-3}.

A reasonable number of articles have been published that use various 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 – see, for example, Roberts (1970), Dimitrijevic & Konjevic (1980), Dimitrijevic & Krsljanin (1986), Popovic & Dimitrijevic (1996) and Dimitrijevic & Sahal-Bréchot (1996).

In this paper we present semi-empirical approximate values of the Stark broadening parameters for 122 spectral lines of Pb III arising from $5d^{10}\,6s\,np$ ($n = 6,7,8$), $5d^{10}\,6s\,ns$ ($n = 7,8,9$) and $5d^{10}\,6s\,nd$ ($n = 6,7$) configurations. The results were 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^{17} cm^{-3}.

Dimitrijevic & Konjevic (1980), Dimitrijevic & Krsljanin (1986) and Popovic & Dimitrijevic (1996) carried out calculations for multiply-ionized ions using a semi-empirical approach (the so-called MSE (modified semi-empirical) method). This approach has a number of numerical advantages: it uses a limited number of matrix elements; it includes an improved effective Gaunt factor; and it supposes a LS coupling approximation. This model does not, however, work well in the case of Pb III: the Pb III is remarkable the multiplet inversion, indicating a strong presence of mixed

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Table 1. Oscillator strengths of a number of Pb III lines. Oscillator strengths are compared with the theoretical (Colón & Alonso-Medina 2000) and the experimental (Colón et al. 1999) published values.

Transition	Wavelength (Å)	Oscillator strength		
		This work	Others works	
			Theoretical	Experimental
$7s^3S_1 - 7p^3P_0$	4799.9	0.165	0.161	0.197
$- 7p^3P_1$	4762.4	0.384	0.391	0.404
$- 7p^3P_2$	3855.2	0.746	1.02	0.783

configurations. Moreover, transitions of great relevance to astrophysics exist that would be forbidden according to this simple LS coupling model.

We compare the theoretical values obtained in this work with published experimental data. With a few exceptions, which will be studied in 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 the principal quantum number, n, of Pb III for several series of Pb III. We also present the systematic trends of the Stark broadening parametersversus 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 linewidth and Stark lineshifts can be calculated from the following semi-empirical formulae:

$$\varpi_{se} \approx 8 \left(\frac{\pi}{3}\right)^{3/2} \frac{\hbar}{m a_0} N_e \left(\frac{E_H}{kT}\right)^{1/2} \left[\sum_{i'} |\langle i'|\boldsymbol{r}|i\rangle|^2 g_{se}\left(\frac{E}{\Delta E_{i'i}}\right) + \sum_{f'} |\langle f'|\boldsymbol{r}|f\rangle|^2 g_{se}\left(\frac{E}{\Delta E_{f'f}}\right)\right], \quad (1)$$

$$d \approx -8 \left(\frac{\pi}{3}\right)^{3/2} \frac{\hbar}{m a_0} N_e \left(\frac{E_H}{kT}\right)^{1/2} \left[\sum_{i'} \left(\frac{\Delta E_{i'i}}{|\Delta E_{i'i}|}\right) |\langle i'|\boldsymbol{r}|i\rangle|^2 g_{sh}\left(\frac{E}{\Delta E_{i'i}}\right) - \sum_{f'} \left(\frac{\Delta E_{f'f}}{|\Delta E_{f'f}|}\right) |\langle f'|\boldsymbol{r}|f\rangle|^2 g_{sh}\left(\frac{E}{\Delta E_{f'f}}\right)\right]. \quad (2)$$

In these formulae, ω_{se} and d are the Stark linewidth and lineshift, respectively, in angular frequency units, E_H is the hydrogen ionization energy, N_e is the free electron perturber density, T is the electron temperature, $E = (3/2)kT$ is 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 $x_{ii'} = E/\Delta E_{ii'}$, where $\Delta E_{ii'}$ 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. ω_{se} is the half width at half-maximum (HWHM) of the Lorentz profile in frequency units. ω_{se} is proportional to the full width at half-maximum (FWHM) line ω in wavelength units, through the expression $\omega = \omega_{se}\lambda^2/(\pi c)$.

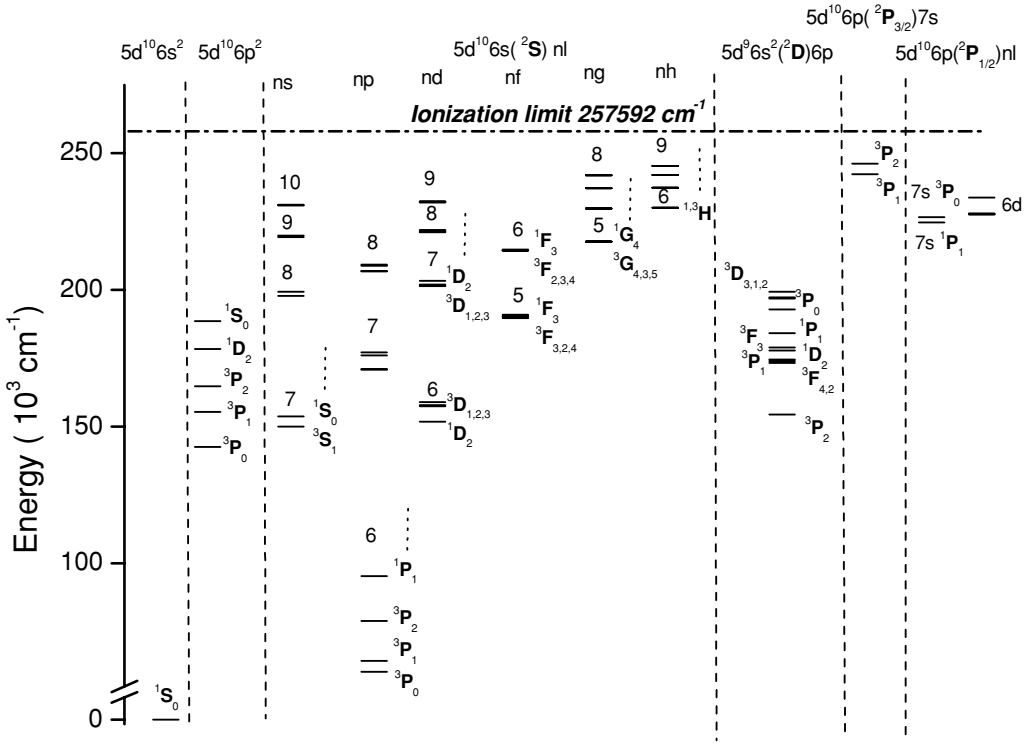

Figure 1. Energy level diagram of Pb III (Moore 1958).

Table 2. Pb III $5d^{10}\,6s\,nl$, $5d^{10}\,6p^2$ and $5d^{10}\,6s^2 - 5d^{10}6s\,mp$ linewidths (FWHM) and shifts normalized to $N_e = 10^{17}$ cm^{-3}. Linewidths are compared with the experimental published values (Alonso-Medina & Colón 2007).

Transition array	Multiplet	λ (Å)[a]	T ($\times 10^3$ K)	ω (Å) This work	ω (Å) Experiments	d (Å)
$6s^2$-6p	$^1S_0$–$^3P_1$	1553.0	11	0.068		0.066
			16	0.053		0.051
			20	0.045		0.043
			25.2	0.038		0.037
			33	0.032		0.031
	$^1S_0$–$^1P_1$	1048.9	11	0.043		0.030
			16	0.033		0.023
			20	0.028		0.020
			25.2	0.024		0.017
			33	0.020		0.014
$6s^2$-7p	$^1S_0$–$^3P_1$	584.5	11	0.021		0.006
			16	0.016		0.004
			20	0.014		0.004
			25.2	0.012		0.003
			33	0.010		0.003
$6s^2$-8p	$^1S_0$–$^3P_1$	483.1	11	0.035		0.001
			16	0.028		0.001
			20	0.025		0.001
			25.2	0.022		0.000
			33	0.019		0.000
7s-7p	$^3S_1$–$^3P_0$	4799.9	11	1.56		0.948
			16	1.22		0.741
			20	1.06		0.642
			25.2	0.92	1.0 ± 0.2	0.556
			33	0.78		0.472
	$^3S_1$–$^3P_1$	4761.1	11	2.28		1.07
			16	1.79		0.835
			20	1.55		0.722
			25.2	1.35	1.0 ± 0.2	0.623
			33	1.15		0.527
	$^3S_1$–$^3P_2$	3855.2	11	1.72		0.646
			16	1.35		0.505
			20	1.17		0.438
			25.2	1.02	0.75 ± 0.16	0.379
			33	0.87		0.321
	$^1S_0$–$^3P_1$	5781.0	20	1.53		0.437
			25.2	1.33	2.9 ± 0.7[b]	0.375
			33	1.13		0.314
7s-7p	$^1S_0$–$^1P_1$	4273.9	20	0.509		0.234
			25.2	0.442		0.203
			33	0.376		0.173
6d-7p	$^3D_1$–$^3P_0$	7422.1	20	2.27		1.26
			25.2	1.97		1.09
			33	1.67		0.93
	$^1D_2$–$^3P_1$	5209.2	20	1.53		0.656
			25.2	1.32	2.2 ± 0.6	0.561
			33	1.12		0.469
	$^1D_2$–$^3P_2$	4142.8	20	1.15		0.373
			25.2	0.99	2.7±0.6	0.320
			33	0.84		0.268
	$^3D_1$–$^3P_1$	7332.8	20	3.43		1.45
			25.2	2.98		1.25
			33	2.53		1.05
	$^3D_1$–$^3P_2$	5382.5	20	2.15		0.709
			25.2	1.87	2.7±0.7	0.613
			33	1.59		0.519
	$^3D_2$–$^3P_2$	5525.5	20	2.85		1.19
			25.2	2.47	2.4±0.6	1.03
			33	2.10		0.87

Table 2 – *continued*

Transition array	Multiplet	λ (Å)	T ($\times 10^3$ K)	ω (Å) This work	ω (Å) Experiments	d (Å)
	$^3D_3$–$^3P_2$	5859.7	20	3.86		1.86
			25.2	3.34	1.1±0.3	1.61
			33	2.84		1.36
$6p^2$-7p	$^3P_1$–$^3P_2$	4855.1	20	1.51		0.285
			25.2	1.31	1.4±0.4	0.243
			33	1.11		0.203

A positive shift is red; [a]Moore (1958).

Table 3. Pb III $5d^{10}6s$ *n*p and $5d^96s^2$ 6p – $5d^{10}6s$ *m*s linewidths (FWHM) and shifts normalized to $N_e = 10^{17}$ cm^{-3}.

Transition array	Multiplet	λ (Å)[a]	T ($\times 10^3$ K)	ω (Å) This work	d (Å) This work
6p-7s	$^3P_0$–$^3S_1$	1115.0	20	0.046	0.039
			25.2	0.040	0.033
			33	0.034	0.028
	$^3P_1$–$^3S_1$	1167.0	20	0.063	0.053
			25.2	0.054	0.046
			33	0.046	0.039
	$^3P_2$–$^3S_1$	1406.5	20	0.105	0.092
			25.2	0.090	0.079
			33	0.076	0.067
	$^1P_1$–$^3S_1$	1826.7	20	0.178	0.130
			25.2	0.153	0.112
			33	0.129	0.095
	$^3P_1$–$^1S_0$	1118.7	20	0.029	0.025
			25.2	0.025	0.022
			33	0.021	0.018
	$^1P_1$–$^1S_0$	1711.1	20	0.089	0.059
			25.2	0.077	0.051
			33	0.064	0.043
6p-8s	$^3P_0$–$^3S_1$	727.3	20	0.042	0.027
			25.2	0.037	0.024
			33	0.031	0.021
	$^3P_1$–$^3S_1$	749.0	20	0.049	0.033
			25.2	0.043	0.029
			33	0.037	0.025
	$^3P_2$–$^3S_1$	841.0	20	0.067	0.047
			25.2	0.058	0.041
			33	0.050	0.035
	$^1P_1$–$^3S_1$	975.1	20	0.019	0.011
			25.2	0.016	0.010
			33	0.014	0.008
	$^3P_1$–$^1S_0$	740.7	20	0.022	0.016
			25.2	0.019	0.014
			33	0.016	0.012
	$^1P_1$–$^1S_0$	961.0	20	0.043	0.027
			25.2	0.038	0.024
			33	0.032	0.020
6p-9s	$^3P_0$–$^3S_1$	629.1	20	0.017	−0.014
			25.2	0.015	−0.012
			33	0.013	−0.010
	$^3P_1$–$^3S_1$	645.3	20	0.022	−0.011
			25.2	0.019	−0.010
			33	0.016	−0.009
	$^3P_2$–$^3S_1$	712.5	20	0.030	−0.010
			25.2	0.026	−0.009
			33	0.022	−0.008
	$^1P_1$–$^3S_1$	806.4	20	0.038	−0.017
			25.2	0.033	−0.015
			33	0.028	−0.014
	$^3P_1$–$^1S_0$	643.0	20	0.010	0.000
			25.2	0.009	0.000
			33	0.008	0.000
	$^1P_1$–$^1S_0$	802.8	20	0.021	0.000
			25.2	0.018	0.000
			33	0.015	0.000
7p-8s	$^3P_0$–$^3S_1$	3707.1	20	1.20	0.65
			25.2	1.05	0.58
			33	0.91	0.50
	$^3P_1$–$^3S_1$	3729.7	20	1.53	0.72
			25.2	1.34	0.63
			33	1.15	0.55
	$^3P_2$–$^3S_1$	4572.5	20	2.52	1.03
			25.2	2.20	0.91
			33	1.89	0.79
	$^1P_1$–$^3S_1$	4828.2	20	2.14	1.20
			25.2	1.88	1.06
			33	1.62	0.92
	$^3P_1$–$^1S_0$	3531.2	20	0.78	0.28
			25.2	0.68	0.25
			33	0.58	0.21
	$^1P_1$–$^1S_0$	4500.6	20	0.90	0.45
			25.2	0.78	0.40
			33	0.68	0.34
7p-9s	$^3P_0$–$^3S_1$	2065.0	20	0.22	−0.16
			25.2	0.19	−0.14
			33	0.17	−0.12
	$^3P_1$–$^3S_1$	2072.0	20	0.32	−0.14
			25.2	0.28	−0.13
			33	0.24	−0.11
	$^3P_2$–$^3S_1$	2308.3	20	0.45	−0.19
			25.2	0.39	−0.17
			33	0.34	−0.15
	$^1P_1$–$^3S_1$	2371.8	20	0.32	−0.19
			25.2	0.28	−0.17
			33	0.24	−0.15
	$^3P_1$–$^1S_0$	2048.0	20	0.20	−0.028
			25.2	0.17	−0.025
			33	0.15	−0.023
	$^1P_1$–$^1S_0$	2340.3	20	0.16	−0.038
			25.2	0.14	−0.033
			33	0.12	−0.029
8p-9s	$^3P_0$–$^3S_1$	7977.7	20	4.62	−2.53
			25.2	4.07	−2.24
			33	3.52	−1.94
	$^3P_1$–$^3S_1$	8087.4	20	9.15	−2.76
			25.2	8.06	−2.46
			33	6.98	−2.16

Table 3 – *continued*

Transition array	Multiplet	λ (Å)[a]	T (× 10^3 K)	ω (Å) This work	d (Å) This work
	$^3P_2$–$^3S_1$	9595.1	20	19.12	−4.22
			25.2	16.84	−3.76
			33	14.59	−3.29
	$^1P_1$–$^3S_1$	9974.1	20	13.74	−4.29
			25.2	12.10	−3.81
			33	10.48	−3.32
	$^3P_1$–$^1S_0$	7733.5	20	6.77	−0.90
			25.2	5.97	−0.83
			33	5.17	−0.74
	$^1P_1$–$^1S_0$	9441.1	20	11.01	−1.58
			25.2	9.70	−1.42
			33	8.40	−1.26
$6s^2$6p-8s	$^3P_2$–$^3S_1$	2304.2	20	0.40	0.25
			25.2	0.35	0.22
			33	0.30	0.19
	$^3P_1$–$^3S_1$	4293.3	20	1.65	0.98
			25.2	1.45	0.86
			33	1.25	0.75
	$^1D_2$–$^3S_1$	5003.4	20	2.11	1.18
			25.2	1.85	1.05
			33	1.60	0.91
	$^1P_1$–$^3S_1$	7339.6	20	4.54	2.63
			25.2	3.98	2.32
			33	3.44	2.03
	$^3P_1$–$^1S_0$	4032.3	20	0.68	0.39
			25.2	0.60	0.34
			33	0.51	0.30
	$^1P_1$–$^1S_0$	6608.3	20	1.60	0.86
			25.2	1.40	0.76
			33	1.21	0.66
$6s^2$6p-9s	$^3P_2$–$^3S_1$	1542.0	20	0.093	−0.091
			25.2	0.082	−0.080
			33	0.071	−0.070
	$^3F_2$–$^3S_1$	2204.7	20	0.23	−0.18
			25.2	0.20	−0.16
			33	0.17	−0.14
	$^3P_1$–$^3S_1$	2235.0	20	0.27	−0.16
			25.2	0.23	−0.14
			33	0.20	−0.12
	$^1D_2$–$^3S_1$	2413.3	20	0.28	−0.22
			25.2	0.25	−0.19
			33	0.21	−0.17
	$^1P_1$–$^3S_1$	2851.0	20	0.39	−0.30
			25.2	0.35	−0.26
			33	0.30	−0.23
	$^3P_1$–$^1S_0$	2207.1	20	0.13	−0.026
			25.2	0.12	−0.023
			33	0.10	−0.020
	$^1P_1$–$^1S_0$	2805.7	20	0.17	−0.075
			25.2	0.15	−0.066
			33	0.13	−0.056
	$^3D_1$–$^1S_0$	4426.5	20	0.25	−0.23
			25.2	0.22	−0.20
			33	0.19	−0.17

A positive shift is red [a]Moore (1958).

The atomic matrix elements were obtained using relativistic Hartree–Fock (HFR) calculations and configuration interaction in an intermediate coupling (IC) scheme. The Cowan code (1981) was selected for this purpose. Level energies for our calculations are from the table in Moore (1958).

Table 4. Pb III $5d^{10}$ 6s *n*p and $5d^9$ $6s^2$ 6p – $5d^{10}$ 6s *m*d linewidths (FWHM) and shifts normalized to $N_e = 10^{17}$ cm^{-3}.

Transition array	Multiplet	λ (Å)[a]	T (× 10^3 K)	ω (Å) This work	d (Å) This work
6p-6d	$^3P_1$–$^1D_2$	1142.9	20	0.044	0.041
			25.2	0.038	0.035
			33	0.032	0.029
	$^3P_2$–$^1D_2$	1371.7	20	0.077	0.073
			25.2	0.066	0.063
			33	0.055	0.053
	$^1P_1$–$^1D_2$	1768.5	20	0.13	0.098
			25.2	0.11	0.084
			33	0.092	0.070
	$^3P_0$–$^3D_1$	1030.4	20	0.035	0.028
			25.2	0.030	0.024
			33	0.025	0.020
	$^3P_1$–$^3D_1$	1074.6	20	0.048	0.039
			25.2	0.041	0.034
			33	0.035	0.029
	$^3P_2$–$^3D_1$	1274.5	20	0.078	0.068
			25.2	0.067	0.058
			33	0.057	0.049
	$^1P_1$–$^3D_1$	1610.2	20	0.13	0.088
			25.2	0.11	0.076
			33	0.091	0.064
	$^3P_1$–$^3D_2$	1069.1	20	0.069	0.056
			25.2	0.059	0.048
			33	0.050	0.041
	$^3P_2$–$^3D_2$	1266.8	20	0.11	0.090
			25.2	0.093	0.078
			33	0.078	0.066
	$^1P_1$–$^3D_2$	1597.8	20	0.17	0.12
			25.2	0.15	0.11
			33	0.12	0.091
	$^3P_2$–$^3D_3$	1250.4	20	0.13	0.11
			25.2	0.12	0.096
			33	0.098	0.081
6p-7d	$^3P_0$–$^3D_1$	709.2	20	0.037	0.023
			25.2	0.033	0.020
			33	0.028	0.018
	$^3P_1$–$^3D_1$	729.9	20	0.044	0.029
			25.2	0.039	0.025
			33	0.033	0.022
	$^3P_2$–$^3D_1$	816.9	20	0.060	0.041
			25.2	0.052	0.036
			33	0.045	0.031
	$^1P_1$–$^3D_1$	942.9	20	0.080	0.048
			25.2	0.070	0.042
			33	0.060	0.036
	$^3P_1$–$^3D_2$	728.8	20	0.069	0.043
			25.2	0.061	0.038
			33	0.052	0.033
	$^3P_2$–$^3D_2$	815.6	20	0.091	0.059
			25.2	0.080	0.052
			33	0.069	0.045
	$^1P_1$–$^3D_2$	941.1	20	0.12	0.072
			25.2	0.11	0.064
			33	0.092	0.055
	$^3P_2$–$^3D_3$	812.6	20	0.12	0.078
			25.2	0.11	0.069
			33	0.091	0.059
	$^3P_1$–$^1D_2$	720.0	20	0.070	0.036
			25.2	0.061	0.031
			33	0.053	0.027

Table 4 – *continued*

Transition array	Multiplet	λ (Å)[a]	T (× 10^3 K)	ω (Å) This work	d (Å) This work
	$^3P_2$–$^1D_2$	804.4	20	0.091	0.049
			25.2	0.080	0.043
			33	0.069	0.037
	$^1P_1$–$^1D_2$	926.2	20	0.12	0.059
			25.2	0.11	0.052
			33	0.091	0.045
7p-7d	$^3P_0$–$^3D_1$	3280.7	20	0.89	0.46
			25.2	0.78	0.41
			33	0.67	0.35
	$^3P_1$–$^3D_1$	3298.4	20	1.15	0.51
			25.2	1.01	0.45
			33	0.87	0.39
	$^3P_2$–$^3D_1$	3940.8	20	1.80	0.69
			25.2	1.58	0.61
			33	1.36	0.53
	$^1P_1$–$^3D_1$	4129.3	20	1.49	0.80
			25.2	1.31	0.70
			33	1.13	0.61
	$^3P_1$–$^3D_2$	3277.0	20	1.64	0.80
			25.2	1.44	0.71
			33	1.24	0.61
	$^3P_2$–$^3D_2$	3910.2	20	2.49	1.10
			25.2	2.18	0.97
			33	1.88	0.85
	$^1P_1$–$^3D_2$	4095.7	20	2.26	1.25
			25.2	1.98	1.10
			33	1.71	0.96
	$^3P_2$–$^3D_3$	3842.6	20	3.09	1.49
			25.2	2.71	1.32
			33	2.34	1.14
	$^3P_1$–$^1D_2$	3103.6	20	1.51	0.59
			25.2	1.32	0.52
			33	1.14	0.45
	$^3P_2$–$^1D_2$	3665.9	20	2.24	0.79
			25.2	1.97	0.70
			33	1.69	0.61
	$^1P_1$–$^1D_2$	3828.4	20	2.03	0.90
			25.2	1.78	0.79
			33	1.54	0.69
$6s^2$6p-7d	$^3P_2$–$^3D_1$	2132.0	20	0.32	0.19
			25.2	0.28	0.17
			33	0.24	0.15
	$^3F_2$–$^3D_1$	3648.0	20	1.05	0.57
			25.2	0.92	0.50
			33	0.80	0.44
	$^3P_1$–$^3D_1$	3731.6	20	1.19	0.67
			25.2	1.04	0.59
			33	0.90	0.52
	$^1D_2$–$^3D_1$	4256.7	20	1.45	0.77
			25.2	1.27	0.68
			33	1.10	0.60
	$^1P_1$–$^3D_1$	5837.5	20	2.72	1.50
			25.2	2.39	1.33
			33	2.06	1.16
	$^3P_2$–$^3D_2$	2123.0	20	0.53	0.31
			25.2	0.47	0.28
			33	0.40	0.24
	$^3F_2$–$^3D_2$	3621.7	20	1.65	0.92
			25.2	1.45	0.81
			33	1.25	0.71
	$^3P_1$–$^3D_2$	3704.2	20	1.61	0.96
			25.2	1.41	0.85
			33	1.22	0.74

Table 4 – *continued*

Transition array	Multiplet	λ (Å)[a]	T (× 10^3 K)	ω (Å) This work	d (Å) This work
	$^1D_2$–$^3D_2$	4221.0	20	2.26	1.25
			25.2	1.99	1.11
			33	1.71	0.96
	$^3F_3$–$^3D_2$	4416.9	20	2.29	1.36
			25.2	2.01	1.20
			33	1.74	1.05
	$^1P_1$–$^3D_2$	5770.6	20	4.23	2.39
			25.2	3.71	2.11
			33	3.20	1.84
	$^3P_2$–$^3D_3$	2102.9	20	0.72	0.44
			25.2	0.64	0.39
			33	0.55	0.34
	$^3F_4$–$^3D_3$	3482.2	20	2.00	1.20
			25.2	1.76	1.06
			33	1.52	0.92
	$^3F_2$–$^3D_3$	3563.7	20	2.19	1.26
			25.2	1.92	1.11
			33	1.66	0.97
	$^1D_2$–$^3D_3$	4142.4	20	2.97	1.70
			25.2	2.61	1.50
			33	2.26	1.31
	$^3F_3$–$^3D_3$	4330.9	20	3.07	1.85
			25.2	2.70	1.63
			33	2.33	1.42
	$^3P_2$–$^1D_2$	2048.9	20	0.51	0.24
			25.2	0.45	0.21
			33	0.39	0.18
	$^3F_2$–$^1D_2$	3411.2	20	1.51	0.66
			25.2	1.33	0.59
			33	1.15	0.51
	$^3P_1$–$^1D_2$	3484.2	20	1.65	0.76
			25.2	1.45	0.67
			33	1.25	0.59
	$^1D_2$–$^1D_2$	3937.8	20	2.03	0.89
			25.2	1.78	0.79
			33	1.54	0.69
	$^3F_3$–$^1D_2$	4107.7	20	2.05	0.95
			25.2	1.80	0.85
			33	1.56	0.74
	$^1P_1$–$^1D_2$	5253.9	20	3.61	1.62
			25.2	3.17	1.44
			33	2.74	1.25

[a]Moore (1958). A positive shift is red.

The system considered is complex, with high Z, such that both relativistic and correlation effects are expected to be important. Least-squares fitting of experimental energy levels partially accounts for the correlation effects, which are not explicitly calculated in our work. The relatively good agreement between our previous experimental Stark parameters and the theoretical results obtained in this work shows that our IC mixing accounts for the correlation effects.

In most cases, the single configuration and Russell–Saunders scheme are sufficient to describe the Pb III. However, this scheme is not sufficient to describe the $5d^{10}$ 6s 6d and $5d^{10}$ $6p^2$configurations. In the above-mentioned work (Colón & Alonso-Medina 2000), we proposed a more detailed description. HFR calculations were performed using the Cowan code. The basis set used in this work consists of three configurations of even parity, namely $5d^{10}$ $6s^2$, $5d^{10}$ 6s 6d and $5d^{10}$ $6p^2$.

Some noticeable discrepancies were found in this previous work. The transition probability of the resonant 1048.9-Å spectral line was about twice the experimental value, as measured by Pinnington et al. (1988). Moreover, in this work the matrix elements for spectral lines involving $5d^9 6s^2$ 6p, $5d^{10}$6p 7s, and $5d^{10}$6p 6d configurations were not calculated.

In the present work, in order to calculate a complete set of atomic matrix elements, we have used six configurations of even parity, namely $5d^{10}$ $6s^2$, $5d^{10}$ $6p^2$, $5d^{10}$ 6s 6d, $5d^{10}$ 6s 7d, $5d^{10}$ 6s 8d and $5d^{10}$ 6s 9d, and seven configurations of odd parity, namely $5d^{10}$ 6s 6p, $5d^{10}$ 6s 7p, $5d^{10}$ 6s 8p, $5d^{10}$ 6s 5f, $5d^{10}$ 6s 9d, $5d^{10}$ 6p 7s, and $5d^{10}$ 6p 6d. In this way we obtained the LS composition of each level, the degree of configuration mixing, and the radial parts of the wavefunctions for the determination of the matrix elements. We have thus obtained a substantial improvement in the identification of the levels of the $5d^{10}$ 6p 7s and of the $5d^{10}$ 6p 6d configurations. We have also obtained a better agreement between the measured transition probabilities (Colón et al. 1999) and calculated (Colón & Alonso-Medina 2000) for several lines arising from the $5d^{10}$ 6s 7p configurations. As an example, we present in Table 1 the oscillator strengths corresponding to $7s\,^3S_1$-$7p\,^3P_{0,1,2}$. Fig. 1 shows an energy-level diagram of Pb III.

Although the transition probabilities obtained in this way are in good agreement in many cases with the experimental values, unfortunately the same is not true in the case of intercombination lines.

Curtis et al. (2001) carried out measurements and calculations in multi-configuration Dirac–Hartree–Fock (MCDHF) taking into account the effects of core polarization for the prediction of 1048-Å and 1553.0-Å radiative lifetimes. This inclusion corrected the above-mentioned problem of intercombination lines. This last result (experimental and calculated) is close to the multi-configuration relativistic Hartree-Fock (MCRHF) calculationcarried out by Migdalek & Baylis (1985), which also included core polarization effects.

In spite of these discrepancies we think that our calculations are adequate for the proposed objective of providing Stark-broadening parameters for the Pb III spectral lines. As can be seen in the formulae, matrix elements of practically all the allowed transitions are used for the calculation of the Stark parameters. In our calculations we use only a few overestimated matrix elements in front of a large number of matrix elements in good agreement with the experimental results.

3 RESULTS AND CONCLUSIONS

Our results for the Stark linewidth (FWHM) and lineshift at an electron density of 10^{17} cm^{-3} and a number of temperatures in the range $T = 11\,000$–$33\,000$ K are displayed in Tables 2–4. The first three columns denote the transition array, the multiplet, and the wavelength (in angstroms; Moore 1958) for each studied transition. Temperatures are shown in column four.

In Table 2 we present results for transitions arising from 5 d^{10} 6 s $np(n = 6, 7, 8)$. Stark broadening linewidths (in angstroms) are displayed in columns five and six (column five contains our results, and column six contains the rare experimental values to be found in the literature, together with their estimated relative uncertainties). The remaining column shows the theoretical Stark lineshift.

As can be seen, our results are in agreement with our previous experimental results, except for the values corresponding to

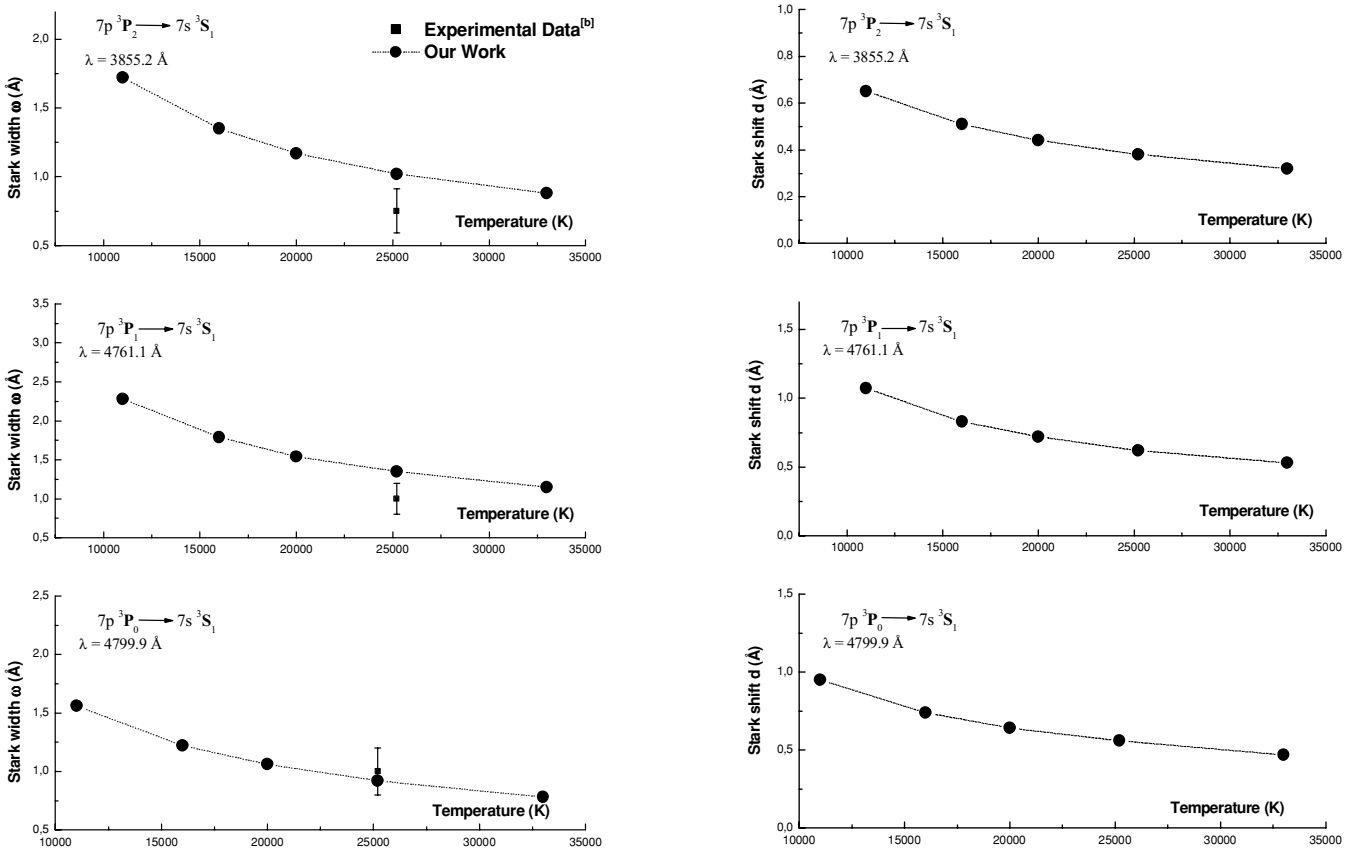

Figure 2. Measured ([b] Alonso-Medina & Colón 2007) and calculated Stark width FWHM (ω(Å)) and Stark lineshift (d(Å)) versus temperature for 3855.2-, 4761.1- and 4799.9-Å Pb III lines.

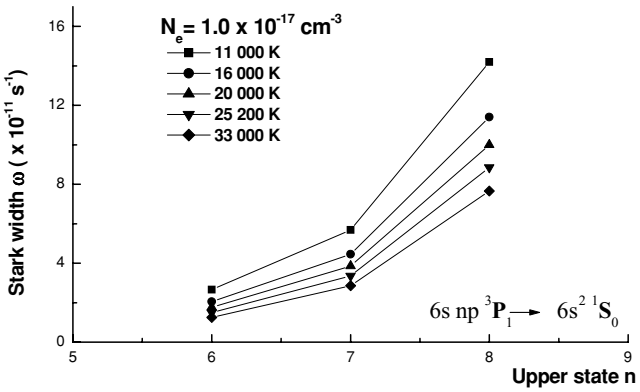

Figure 3. Stark width FWHM ($\omega(s^{-1})$) for the $6s^{21}S_0 - 6snp\,^3P_1$ lines of Pb III versus the principal quantum number of the upper state.

intercombination lines. This discrepancy can be accounted for by our experimental fitting method.

Fig. 2 shows measured and calculated Stark widths FWHM (ω(Å)) and Stark lineshifts (d(Å)) versus temperature for 3855.2-, 4761.1- and 4799.9-Å Pb III lines. In these cases our values are in agreement, within the margins of Griem's semi-empirical calculations, with the existing experimental data.

There are no experimental data for Stark widths of 1553.0- and 1048.9-Å resonant lines with evident astrophysical interest. As can be seen in Table 1, Stark broadening of 1553.0- and 1048.9-Å lines is close to 0.04 Å in both cases. The theoretical transition probabilities of these lines are overestimated by a factor of 2. On carrying out calculations considering the experimental transition probabilities as measured by other authors, these values are affected by only about 0.001Å. In both cases we can consider that our calculations provide an adjusted estimate.

The Stark systematic trends of linewidths FWHM (ω) for resonant transitions $6\,s^2\,^1S_0 - 6\,s\,np\,^3P_1$ (1553.0-, 584.5- and 483.1-Å lines) versus the principal quantum number of the upper state are presented. Clear trends in the Stark widths are seen in our results.

Tables 3 and 4 include results for transitions arising from $5d^{10}6s\,ns$ and $5d^{10}6s\,nd$ configurations, respectively. Stark broadening linewidths (in Å) are displayed in column 5. The remaining column displays the theoretical Stark lineshift. We have not found any experimental results in the literature concerning these transitions.

As can be seen, there are differences between the widths and shifts of the various fine-structure lines of a given multiplet. Although the effects of the fine structure of the multiplets in the interaction with the electrons can be neglected, the effects of different taxes of other configurations cannot be omitted in lines of the same multiplet but with different J. In this way, different widths and shifts are possible where the simple LS model is not the appropriate, as is the case for the Pb III.

This work provides theoretical Stark width and shift parameters for 122 spectral lines of Pb III, of astrophysical interest appearing in the UV and visible regions, arising from $5d^{10}\,6s\,mp$, $5d^{10}\,6s\,ns$ and $5d^{10}\,6s\,nd$ configurations. Experimental data are available on the Stark widths of 10 lines.

Our data are given for an electron density of 10^{17} cm^{-3} and several temperatures. As can be seen, some clear trends in the Stark width appear in our results. These data add to our knowledge of the atomic database of Pb III.

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