Baltic Astronomy, vol. 20, 552–557, 2011

AB INITIO DETERMINATION OF ATOMIC STRUCTURE AND STARK BROADENING PARAMETERS: Pb IV AND RECENT RESULTS

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Received: 2011 August 8; accepted: 2011 August 15

Abstract. We present a review of our previous ab initio calculations of Stark broadening parameters using semi-classical perturbation method for the calculation of Stark widths and shifts, and the SUPERSTRUCURE (SST) code for the determination of atomic structure. SST code takes into account the configuration interactions and relativistic effects. New results are also presented for some spectral lines of Pb IV. Energy levels and oscillator strengths are calculated using Hartree-Fock relativistic approach, and the Stark broadening parameters are determined using a semiclassical perturbation approach.

Key words: atomic data – atomic processes – lines: formation

1. INTRODUCTION

In atomic structure study, ab initio calculation of energy levels and radiative parameters can be made, when no other data are taken from other sources, i.e., no semi-empirical adjustment of any parameter. Many methods can be used, as for example, Hartree-Fock with relativistic corrections of Cowan (1981), a scaled Thomas-Fermi-Dirac statistical potential employed in SST code (Eissner et al. 1974) and fully relativistic calculation based on multiconfiguration Dirac-Fock method employed in GRASP code (Grant et al. 1980).

Energy levels and oscillator strengths are the main input data for the Stark broadening parameter determination. Ab initio calculation of Stark broadening parameters can be made when the needed set of energy levels and oscillator strengths are determined during the calculation, not taken from other sources.

The lack of atomic data makes Stark broadening determination impossible, especially when we use the semiclassical perturbation method (Sahal-Bréchot 1969a,b). Indeed, this method needs a large set of energy levels and oscillator strengths com-

paring with other methods such as the modified semi-empirical approach (Dimitrijević & Konjević 1980). Therefore, ab initio determination of Stark widths and shifts is of great interest for ions for which the set of atomic data is not complete. This method allows us to treat a large number of ions and transitions, thereby, we contribute to the creation of a database as the STARK-B containing the calculated widths and shifts of isolated lines due to electron and ion collisions. This database is devoted for modeling and spectroscopic diagnostics of stellar atmospheres and envelopes.

In our previous work (Ben Nessib et al. 2004; Hamdi et al. 2007; Hamdi et al. 2010), we have performed ab initio calculation of Stark broadening parameters for Si V, Ne V and Ca V ions. Energy levels and oscillator strengths are determined using the SST code, and Stark widths and shifts are calculated using the semi-classical perturbation approach. All these results are reviewed in this paper. New results are also presented for spectral lines of triply ionized lead (Pb IV). Atomic data are determined using Hartree-Fock with relativistic correction method, and the Stark broadening parameters are calculated using the semi-classical perturbation method. Pb IV lines are of interest for modeling of hot star atmospheres, since Pb IV is characterized by a strong resonance line and it is a candidate for spectroscopic detection in DA white dwarfs (Vennes et al. 2005). The Pb IV resonance line is also detected in the photospheres of subdwarfs (O'Toole 2004).

2. AB INITIO DETERMINATION OF ATOMIC DATA

2.1. The SUPERSTRUCTURE code

The SST code was originally realized by Eissner et al. (1974). The wave functions are of configuration mixing type, and each configuration is expanded in terms of slater states. The radial functions P_{nl} are calculated in the scaled Thomas-Fermi statistical potential $V(\lambda_l)$ such that all P_{nl} of the same l are calculated in the same potential. The SST code was modified by Nussbaumer & Storey (1978) so that each P_{nl} is calculated in the separate potential $V(\lambda_{nl})$. Parameters λ_{nl} are determined variationally by optimizing the weighted sum of energy terms. Relativistic corrections are introduced by means of Breit-Pauli approximation in intermediate coupling. The Breit-Pauli Hamiltonian H_{BP} can be written

$$H_{BP} = H_{nr} + H_{rc}. \quad (1)$$

Here H_{nr} is the non relativistic Hamiltonian and H_{rc} is a sum of relativistic correction operators. H_{rc} contains the one electron operators for the mass correction, the Darwin contact term, the spin-orbit interaction in the field of the nucleus and two electron operators for spin-orbit, spin-other orbit and spin-spin interactions.

2.2. The Cowan code

For theoretical calculations of atomic parameters needed for spectral line calculations, we can use the Cowan code (Cowan 1981) structure package for atomic calculations. The Cowan code consists of the following three programs:

1. RCN calculates the single configuration radial wave functions. In RCN, there is a choice of four approximations to the true Hartree-Fock method, namely, Hartree (H), Hartree-Fock-Slater (HFS), Hartree plus statistical exchange (HX) and Hartree-Slater (HS). HX is the normal option since it is most efficient in computations.

2. RCN2 calculates the multiple-configuration radial integrals, dipole integrals and Bessel integrals.

3. RCG calculates the angular factors, radiative data and collision strengths.

For the electric dipole transition, total transition probability from a state $\gamma' J' M'$ to all states M of the level γJ is given by (Cowan 1981):

$$A = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h(2J'+1)}\mathbf{S}, \tag{2}$$

where $\sigma = \frac{|E(\gamma')-E(\gamma)|}{hc}$, c is the light velocity, h is Plank's constant, e is elementary charge, a_0 is the Bohr radius and $\mathbf{S}$ is the dipole line strength defined as :

$$\mathbf{S} = \left| \left\langle \gamma J \left\| \mathbf{P}^{(1)} \right\| \gamma' J' \right\rangle \right|^2, \tag{3}$$

where $\mathbf{P}^{(1)}$ is the classical dipole moment of the atom measured in units of $-ea_0$. The weighted oscillator strength is given by :

$$gf = \frac{8\pi^2 mca_0^2\sigma}{3h}\mathbf{S}. \tag{4}$$

In order to calculate gf, the corresponding value of the line strength must be computed. The wavefunction $|\gamma J\rangle$ is expanded in terms of a suitable set of the basis functions $|\beta J\rangle$.

$$|\gamma J\rangle = \sum_{\beta} Y^{\gamma}_{\beta J} |\beta J\rangle \tag{5}$$

3. AB INITIO DETERMINATION OF STARK BROADENING PARAMETERS

Using the calculated set of atomic data and the semiclassical perturbation (SCP) method (Sahal-Bréchot 1969a,b) for the determination of Stark broadening parameters, ab initio Stark widths and shifts can be obtained.

In the SCP approach, the full width at half maximum (W) can be expressed in terms of inelastic cross-section and elastic processes as

$$W = N \int v f(v) dv \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el}(v) \right),$$

where N is the density of colliding perturber, $f(v)$ is the Maxwell distribution of the relative atom-perturber velocity v, $\sigma_{ii'}$ and $\sigma_{ff'}$ are the inelastic cross-sections between the initial level i (resp. f final level) and the perturbing levels i' (resp. f') of $i - f$ transition. $\sigma_{el}(v)$ represents the contribution of elastic collisions and include Feshbach resonances when ion-electron [...???] are studied.

In Ben Nessib et al. (2004), ab initio Stark broadening parameters were obtained for 16 multiplet of Si V. The energy levels and oscillator strengths were calculated using the SST code (Eissner et al. 1974). Scaling parameters λ_l were obtained by self-consistent energy minimization procedure on all term energies of the eleven configurations: $2s^2 2p^6$, $2s^2 2p^5$ 3ℓ, $2s$ $2p^6$ 3ℓ, $2s^2 2p$Results were obtained

for collisions with electrons and compared with the values calculated with Bates & Damgaard (1949) approximation oscillator strengths. The broadening parameters for proton, ionized helium and Si II were also given.

In Hamdi et al. (2007), Stark broadening parameters were calculated for 26 multiplets of Ne V. Atomic data were carried out using the SST code. The adopted atomic model includes 17 configurations: $2s^22p^2$, 2s $2p^3$, $2p^4$, $2s^22p$ 3ℓ, 2s $2p^2$ 3ℓ, $2s^22p$ 4ℓ, 2s $2p^2$ 4ℓ ($\ell \leq n-1$). The results are given for broadening by electron, proton and singly and doubly charged helium ion collisions. Comparison between the Stark widths obtained using the SST oscillator strengths and the Bates and Damgaard approximation oscillator strengths show that the difference is tolerable. The set of oscillator strength obtained using Bates and Damgaard approximation may then be useful for the Stark broadening calculations when more reliable data are not available. The Stark width for 3s $^3P^\circ$ – 3p ^3D was compared with theoretical and experimental results from Uzelac et al. (1993). We have found the best agreement with the measured width.

Ab initio SCP Stark broadening parameters were also calculated for Ca V lines (Hamdi et al. 2010). The needed set of atomic data was obtained using the SST code and 12 configurations of the atomic model. Such data may be of astrophysical interest, since calcium in different ionization stages is observed in the atmospheres of white dwarfs.

Triply ionized lead Pb IV belongs to gold isoelectronic sequence, its ground state configuration is $4f^{14}5d^{10}6s$. This is an interesting isoelectronic sequence with filled subshells and a single electron in the outer shell. This ion is characterized by a strong resonance line, and it is a candidate for spectroscopic detection in hot DA white dwarfs (Vennes et al. 2005). O'Toole (2004) reported the discovery of strong photospheric resonance lines of several heavy elements in the UV spectra of more than two dozen sdB and sdOB stars at temperatures ranging from 22 000 K to 40 000 K. Among these lines, several correspond to Pb IV ones. Pb IV 1313.1 Å resonance line was detected by Proffitt et al. (2001) in the main-sequence B star AV 304.

Using the SCP approach, ab initio Stark broadening parameters are determined for 11 transitions of Pb IV of the type $5d^{10}nl$ – $5d^{10}n'l'$. The energy levels and oscillator strengths were carried out in the Hatree-Fock relativistic (HFR) approach using the Cowan code. We adopt an atomic model including 43 configurations: $5d^96s^2$, $5d^96p^2$, $5d^{10}ns$ ($6\leq n \leq 11$), $5d^{10}nd$ ($6\leq n \leq 11$), $5d^{10}ng$ ($5\leq n \leq 11$), $5d^96s7s$, $5d^96s6d$ (even parity) and $5d^{10}np$ ($6\leq n \leq 11$), $5d^{10}nf$ ($5\leq n \leq 11$), $5d^{10}nh$ ($6\leq n \leq 11$), $5d^96s6p$ (odd parity).

Stark widths and shifts are shown in Table 1 for the perturber density $N{=}10^{17}$ cm^{-3} and temperatures from 20 000 K up to 400 000 K for collisions with electrons, protons and singly charged helium. Such temperatures are of interest for modeling of sdB, sdBO and hot white dwarf atmospheres. We also specify a parameter C (Dimitrijević & Sahal-Bréchot 1984), which gives an estimate for the maximal perturber density for which the line may be treated as isolated. For each value given in Table 1, the collision volume V multiplied by the perturber density N is much less than 1, and the impact approximation is valid.

ACKNOWLEDGMENTS. This work is a part of the Project 146001, "Influence of collisional processes on astrophysical plasma lineshapes" supported by the Ministry of Science and Technological Development of Serbia.

Table 1. This table gives electron, proton and singly-charged helium impact broadening parameters for Pb IV lines, for a perturber density of 10^{17} cm^{-3} and temperatures in the range of 20 000 to 400 000 K. Transitions, wavelengths (in Å) and the parameter C are also given. This parameter when divided to the corresponding Stark width gives an estimate for the maximal perturber density for which the line may be treated as isolated. W_e is the electron-impact full Stark width at half maximum, d_e is the electron-impact Stark shift, W_{H^+} is the proton-impact full Stark width at half maximum, d_{H^+} is the proton-impact Stark shift, W_{He^+} is the singly charged helium-impact full Stark width at half maximum, d_{He^+} is the singly charged helium-impact Stark shift.

Transition	$T(kK)$	W_e	d_e	W_{H^+}	d_{H^+}	W_{He^+}	d_{He^+}
	20	0.66E-02	-0.85E-04	0.31E-03	-0.24E-04	0.39E-03	-0.23E-04
$6s\ ^2S_{1/2} - 8p\ ^2P_{3/2}$	30	0.58E-02	-0.39E-04	0.39E-03	-0.34E-04	0.47E-03	-0.32E-04
$\lambda = 385,5$ Å	50	0.51E-02	-0.53E-04	0.48E-03	-0.51E-04	0.52E-03	-0.45E-04
C= 0.20E+19	100	0.45E-02	-0.32E-04	0.55E-03	-0.72E-04	0.59E-03	-0.62E-04
	200	0.41E-02	-0.29E-04	0.61E-03	-0.91E-04	0.64E-03	-0.75E-04
	400	0.37E-02	-0.35E-04	0.65E-03	-0.11E-03	0.66E-03	-0.89E-04
	20	0.71E-02	-0.11E-03	0.30E-03	-0.88E-04	0.38E-03	-0.81E-04
$6s\ ^2S_{1/2} - 8p\ ^2P_{1/2}$	30	0.62E-02	-0.42E-04	0.37E-03	-0.12E-03	0.45E-03	-0.10E-03
389.9 Å	50	0.54E-02	-0.12E-03	0.47E-03	-0.16E-03	0.51E-03	-0.14E-03
C= 0.17E+19	100	0.47E-02	-0.80E-04	0.55E-03	-0.21E-03	0.58E-03	-0.17E-03
	200	0.42E-02	-0.67E-04	0.62E-03	-0.25E-03	0.63E-03	-0.21E-03
	400	0.38E-02	-0.72E-04	0.67E-03	-0.30E-03	0.66E-03	-0.24E-03
	20	0.52-E02	-0.13E-03	0.14E-03	-0.28E-05	0.20E-03	-0.28E-05
	30	0.44E-02	-0.82E-04	0.19E-03	-0.44E-05	0.25E-03	-0.43E-05
$6s\ ^2S_{1/2} - 7p\ ^2P_{3/2}$	50	0.36E-02	-0.48E-04	0.25E-03	-0.73E-05	0.31E-03	-0.71E-05
474.4 Å	100	0.29E-02	-0.53E-04	0.33E-03	-0.13E-04	0.36E-03	-0.12E-04
C= 0.67E+19	200	0.23E-02	-0.35E-04	0.38E-03	-0.20E-04	0.40E-03	-0.17E-04
	400	0.20E-02	-0.39E-04	0.41E-03	-0.27E-04	0.43E-03	-0.22E-0
	20	0.55E-02	-0.99E-04	0.13E-03	-0.11E-04	0.19E-03	-0.11E-04
$6s\ ^2S_{1/2} - 7p\ ^2P_{1/2}$	30	0.47E-02	-0.74E-04	0.18E-03	-0.16E-04	0.24E-03	-0.16E-04
484.8 Å	50	0.38E-02	-0.11E-04	0.24E-03	-0.26E-04	0.30E-03	-0.24E-04
C= 0.60E+19	100	0.30E-02	-0.46E-04	0.32E-03	-0.41E-04	0.35E-03	-0.35E-04
	200	0.25E-02	-0.11E-04	0.36E-03	-0.57E-04	0.39E-03	-0.48E-04
	400	0.21E-02	-0.24E-04	0.41E-03	-0.71E-04	0.42E-03	-0.57E-04
	20	0.15E-01	0.16E-02	0.80E-03	0.70E-03	0.92E-03	0.60E-03
$6p\ ^2P_{1/2} - 8d\ ^2D_{3/2}$	30	0.13E-01	0.14E-02	0.11E-02	0.89E-03	0.11E-02	0.74E-03
500.8 Å	50	0.11E-01	0.16E-02	0.13E-02	0.11E-02	0.13E-02	0.88E-03
C= 0.15E+19	100	0.99E-02	0.14E-02	0.16E-02	0.13E-02	0.15E-02	0.11E-02
	200	0.85E-02	0.13E-02	0.20E-02	0.16E-02	0.17E-02	0.13E-02
	400	0.73E-02	0.11E-02	0.23E-02	0.18E-02	0.20E-02	0.14E-02
	20	0.212E-01	0.62E-02	0.13E-02	0.13E-02	0.14E-02	0.11E-02
$6p\ ^2P_{3/2} - 8d\ ^2D_{5/2}$	30	0.19E-01	0.53E-02	0.17E-02	0.16E-02	0.17E-02	0.13E-02
552.1 Å	50	0.17E-01	0.46E-02	0.22E-02	0.19E-02	0.19E-02	0.16E-02
C= 0.19E+19	100	0.16E-01	0.37E-02	0.27E-02	0.24E-02	0.24E-02	0.19E-02
	200	0.15E-01	0.31E-02	0.33E-02	0.28E-02	0.27E-02	0.22E-02
	400	0.14E-01	0.27E-02	0.38E-02	0.32E-02	0.33E-02	0.25E-02
	20	0.18E-01	0.20E-02	0.97E-03	0.85E-03	0.11E-02	0.73E-03
$6p\ ^2P_{3/2} - 8d\ ^2D_{3/2}$	30	0.16E-01	0.17E-02	0.13E-02	0.11E-02	0.13E-02	0.90E-03
553.0 A	50	0.14E-01	0.20E-02	0.16E-02	0.13E-02	0.15E-02	0.11E-02
C= 0.18E+19	100	0.12E-01	0.17E-02	0.20E-02	0.16E-02	0.18E-02	0.13E-02
	200	0.10E-01	0.16E-02	0.24E-02	0.19E-02	0.21E-02	0.15E-02
	400	0.89E-02	0.14E-02	0.28E-02	0.22E-02	0.24E-02	0.18E-02

Table 1. Continued

Transition	$T(kK)$	W_e	d_e	W_{H+}	d_{H+}	W_{He+}	d_{He+}
	20	0.14E-01	0.17E-02	0.42E-03	0.42E-03	0.51E-03	0.37E-03
$6p\ ^2P_{1/2} - 7d\ ^2D_{3/2}$	30	0.12E-01	0.13E-02	0.57E-03	0.53E-03	0.65E-03	0.46E-03
592.7 Å	50	0.99E-02	0.12E-02	0.80E-03	0.70E-03	0.81E-03	0.58E-03
C= 0.17E+19	100	0.85E-02	0.12E-02	0.10E-02	0.87E-03	0.99E-03	0.71E-03
	200	0.74E-02	0.11E-02	0.13E-02	0.10E-02	0.12E-02	0.84E-03
	400	0.64E-02	0.10E-02	0.16E-02	0.12E-02	0.13E-02	0.97E-03
	20	0.12E-01	0.32E-02	0.27E-03	0.51E-03	0.29E-03	0.44E-03
$6p\ ^2P_{1/2} - 8s\ ^2S_{1/2}$	30	0.11E-01	0.28E-02	0.42E-03	0.64E-03	0.41E-03	0.55E-03
594.7 Å	50	0.93E-02	0.21E-02	0.66E-03	0.84E-03	0.62E-03	0.68E-03
C= 0.21E+19	100	0.81E-02	0.19E-02	0.97E-03	0.10E-02	0.82E-03	0.84E-03
	200	0.70E-02	0.16E-02	0.12E-02	0.12E-02	0.10E-02	0.99E-03
	400	0.61E-02	0.13E-02	0.16E-02	0.14E-02	0.12E-02	0.11E-02
	20	0.16E-01	0.21E-02	0.55E-03	0.55E-03	0.66E-03	0.47E-03
$6p\ ^2P_{3/2} - 7d\ ^2D_{5/2}$	30	0.14E-01	0.16E-02	0.73E-03	0.69E-03	0.85E-03	0.60E-03
663.4 Å	50	0.12E-01	0.15E-02	0.10E-02	0.91E-03	0.10E-02	0.75E-03
C= 0.56E+19	100	0.11E-01	0.16E-02	0.14E-02	0.11E-02	0.13E-02	0.91E-03
	200	0.92E-02	0.14E-02	0.16E-02	0.13E-02	0.15E-02	0.11E-02
	400	0.80E-02	0.13E-02	0.19E-02	0.15E-02	0.17E-02	0.13E-02
	20	0.17E-01	0.21E-02	0.54E-03	0.53E-03	0.65E-03	0.46E-03
$6p\ ^2P_{3/2} - 7d\ ^2D_{3/2}$	30	0.15E-01	0.15E-02	0.72E-03	0.67E-03	0.84E-03	0.59E-03
667.0 Å	50	0.13E-01	0.14E-02	0.10E-02	0.89E-03	0.10E-02	0.73E-03
C= 0.21E+19	100	0.11E-01	0.15E-02	0.13E-02	0.11E-02	0.13E-02	0.89E-03
	200	0.93E-02	0.14E-02	0.16E-02	0.13E-02	0.15E-02	0.11E-02
	400	0.81E-02	0.12E-02	0.20E-02	0.15E-02	0.17E-02	0.12E-02

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