# Stark Broadening of Se IV, Sn IV, Sb IV and Te IV Spectral Lines

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**Abstract:** Stark broadening parameters, line width and shift, are needed for investigations, analysis and modelling of astrophysical, laboratory, laser produced and technological plasmas. Especially in astrophysics, due to constantly increasing resolution of satellite borne spectrographs, and large terrestrial telescopes, data on trace elements, which were previously insignificant, now have increasing importance. Using the modified semiempirical method of Dimitrijević and Konjević, here, Stark widths have been calculated for 2 Se IV, 6 Sn IV, 2 Sb IV and 1 Te IV transitions. Results have been compared with existing theoretical data for Sn IV. Obtained results will be implemented in the STARK-B database, which is also a part of Virtual atomic and molecular data center (VAMDC).

**Keywords:** Stark broadening; line profiles; atomic data

## 1. Introduction

With the development of satellite-born spectrographs, the significance of trace elements, which have been without any particular importance for investigation of stellar spectra before the development of space astronomy, is becoming more and more increasing. For example, Rauch et al. [1] underlined that accurate Stark broadening data for spectral lines of as much as possible large number of atoms and ions "are of crucial importance for sophisticated analysis of stellar spectra by means of NLTE model atmospheres". High resolution spectra obtained from space born instruments contain different lines of trace elements and the corresponding Stark broadening data are important for their analysis and synthesis. But such data are also very useful for laboratory plasma diagnostics and for investigation and modelling of various plasmas in technology, inertial fusion, as well as for research of laser produced plasmas.

For example, Selenium (Se), which was previously without astrophysical significance, has been detected in the atmospheres of Am star $\rho$ Pup [2], in cool DO white dwarfs [3,4], and Se III emission has been identified in the planetary nebula (PN) NGC5315 [5]. Werner et al. [6] found Se, Sn and Te in the spectra of RE0503-289, a helium rich DO white dwarf. Presence of selenium in the stellar spectra is a confirmation that in subphotosperic layers, where Stark broadening is dominant broadening mechanism [7] it exists in various ionization stages. Consequently, the corresponding Stark broadening parameters for Se in various ionization stages, are useful for theoretical consideration and modelling of such layers, as well as for the calculation of radiative transfer in such conditions. Moreover, in DO white dwarfs, where effective temperatures are within the interval 45,000 K–120,000K, Stark broadening is usually larger than or comparable to Doppler broadening [8,9]. At such temperatures selenium is

mainly ionized and if one ionization stage is observed, certainly others also exist and will be observed in the future with new generations of space telescopes and large telescopes on the Earth. In spite of the fact that Stark broadening data for various ionization stages are needed for interpretation, analysis and synthesis of selenium spectral lines in astrophysical spectra, exist only data for Se I [10,11].

Tin (Sn) is also present in stellar spectra. As an example, Sn lines have been observed in the spectra of A-type stars [12] and in cool DO white dwarfs [3,4]. They mark the hot end of the so-called DB gap, which corresponds to an interval in effective temperatures from 45,000 K to 30,000 K [4]. For a wider analysis of the tin presence in stellar spectra see references in Alonso-Medina and Colón [13]. It is worth to note that Proffitt et al. [14] used the 1313.5-Å resonance line of Sn IV in order to determine the tin abundance of the early B main-sequence star, AV 304, in the Small Magellanic Cloud. Alonso-Medina and Colón [13] report also that Sn plasmas are a candidate for the extreme ultraviolet light source for next-generation microlithography [15,16]. Stark broadening of Sn II and Sn III lines has been measured by Kieft et al. [17], in order to investigate the pinched discharge plasmas in tin vapor as candidates for application in future semiconductor lithography. Stark broadening of seven Sn III spectral lines has been also measured by Djeniže [18]. Concerning the spectral lines of Sn IV, experimentally determined Stark broadening parameters of nine spectral lines have been published by Djeniže [18], and Burger et al. [19] measured again five of them. Results of theoretical calculations of Stark broadening parameters of Sn III lines can be found in [13,17,20]. For Sn IV, there is only one paper [21] with Stark widths and shifts for 66 spectral lines, calculated using semiempirical method of Griem [22] with atomic matrix elements obtained with the relativistic Hartree-Fock method and configuration interaction in an intermediate coupling scheme, by using the Cowan [23] approach and the COWAN code.

Spectral lines of antimony (Sb) are also present in stellar spectra. For example, very strong absorption Sb II spectral lines are observed in the spectrum of HgMn star HR7775 where Stark broadening can not be neglected [24]. Besides the astrophysical importance, antimony is also significant in thin films and nanotechnologies [25–27], and as a laser medium [28]. Concerning antimony and its ionization stages, for Stark broadening in literature exist only experimental results for Sb III [29] and theoretical data for Sb II [30].

According to Cohen [31], the cosmic abundance of tellurium (Te) is larger than for any element with atomic number greater than 40, and its spectral lines are identified in stellar spectra. Yuschenko and Gopka [32] found tellurium line in the Procyon photosphere spectrum, Chayer et al. [3] identified tellurium lines in the cool DO white dwarfs HD199499 and HZ21, and Yuschenko et al. [2] detected tellurium in Am star $\rho$ Pup. We note that Stark broadening is important for Am stars and in particular for DO white dwarfs which have effective temperatures from approximately 45,000 K up to around 120,000 K [33]. So that Stark broadening parameters for Te in various ionization degrees are useful. It should be noted as well that tellurium is also interesting as a laser medium [28]. There is no experimental results for Stark broadening of Te spectral lines but exist a study [34] with Stark broadening parameters for four Te I multiplets.

In this work we will calculate full widths at half intensity maximum (FWHM), due to collisions with surrounding electrons, for Se IV, Sn IV, Sb IV and Te IV spectral lines, using the modified semiempirical method (MSE) [35–37] and will compare the obtained results with existing theoretical data.

## 2. The Modified Semiempirical Method

In accordance with the modified semiempirical (MSE) approach [35], the electron impact full width (FHWM) of an isolated ion line is given by the following equation:

$$w_{MSE} = N \frac{4\pi}{3c} \frac{\hbar^2}{m^2} \left(\frac{2m}{\pi kT}\right)^{1/2} \frac{\lambda^2}{\sqrt{3}} \cdot \{\sum_{\ell_i \pm 1} \sum_{L_{i'} J_{i'}} \vec{\mathfrak{R}}^2_{\ell_i, \ell_i \pm 1} \widetilde{g}(x_{\ell_i, \ell_i \pm 1}) +$$
$$\sum_{\ell_f \pm 1} \sum_{L_{f'} J_{f'}} \vec{\mathfrak{R}}^2_{\ell_f, \ell_f \pm 1} \widetilde{g}(x_{\ell_f, \ell_f \pm 1}) + \left(\sum_{i'} \vec{\mathfrak{R}}^2_{ii'}\right)_{\Delta n \neq 0} g(x_{n_i, n_i + 1}) + \left(\sum_{f'} \vec{\mathfrak{R}}^2_{ff'}\right)_{\Delta n \neq 0} g(x_{n_f, n_f + 1})\}. \tag{1}$$

Here, $i$ and $f$ are for initial and final levels, respectively, $\vec{\mathfrak{R}}^2_{\ell_k,\ell_{k'}}$, $k = i, f$ is the square of the matrix element, and

$$\left(\sum_{k'} \vec{\mathfrak{R}}^2_{kk'}\right)_{\Delta n \neq 0} = \left(\frac{3n_k^*}{2Z}\right)^2 \frac{1}{9}(n_k^{*2} + 3\ell_k^2 + 3\ell_k + 11) \tag{2}$$

(in Coulomb approximation).

In Equation (1)

$$x_{l_k,l_{k'}} = \frac{E}{\Delta E_{l_k,l_{k'}}}, k = i, f$$

where $E = \frac{3}{2}kT$ is the electron kinetic energy and $\Delta E_{l_k,l_{k'}} = |E_{l_k} - E_{l_{k'}}|$ is the energy difference between levels $l_k$ and $l_k \pm 1$ ($k = i, f$),

$$x_{n_k,n_k+1} \approx \frac{E}{\Delta E_{n_k,n_k+1}},$$

where for $\Delta n \neq 0$ the energy difference between energy leves with $n_k$ and $n_k+1$, $\Delta E_{n_k,n_k+1}$, is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H / n_k^{*3}$. With $n_k^* = [E_H Z^2 / (E_{ion} - E_k)]^{1/2}$ is denoted the effective principal quantum number, $Z$ is the residual ionic charge, for example $Z = 1$ for neutral atoms, $E_{ion}$ is the appropriate spectral series limit, $N$ and $T$ are electron density and temperature, while $g(x)$ [22] and $\widetilde{g}(x)$ [35] are the corresponding Gaunt factors.

## 3. Results and Discussion

All atomic energy levels needed for calculation of Se IV Stark line widths were found in Rao and Badami [38] and the newest value of ionization potential in Joshi and George [39]; for Sn IV, Sb IV and Te IV energy levels are taken from Moore [40], but the newest values for ionization potential have been taken for Sb IV [41] and for Te IV [42] as suggested in NIST database [43]. The needed matrix elements have been calculated within Coulomb approximation [44].

For the calculation of line width the modified semiempirical method [35] (see also the review of inovations and applications in [37]) has been used. The obtained results for 2 Se IV, 6 Sn IV, 2 Sb IV and 1 Te IV transitions are shown in Table 1 for perturber density of $10^{17}$ cm$^{-3}$ and temperatures from 10,000 K up to 160,000 K.

There is no experimental or theoretical data for comparison for Se IV, Sb IV and Te IV. For Sn IV exist four transitions where the comparison with semiempirical data of de Andrés-García et al. [21] is possible, while for other two there is no theoretical or experimental data in literature. There are two reasons to calculate Stark broadening for four tansitions already calculated by de Andrés-García et al. [21]. The first step is to compare with their results and to see if a systematic difference exist, so that user who needs also data for two transitions not calculated by [21], could eventualy perform the corresponding scaling or correction. The second reason is to check large difference between Stark widths within the multiplet $5p^2P^o$–$6s^2S$. For four transitions, existing in the paper of de Andrés-García et al. [21] we performed calculations for temperatures given in this article and compared the corresponding FWHM in Table 2. One can see that differences are up to factor of two and that they decrease towards higher temperatures. Since tin is a complex element and both methods are approximative in comparison with semiclassical perturbation method (see e.g., [45–47] these differences are more or less acceptable and obviously, more experimental date are needed in order to check and improve the theory, which works better for simpler spectra. The agreement is best for Sn IV $6s^2S_{1/2}$–$6p^2P^o_{1/2}$ line.

**Table 1.** FWHM - Full Width at Half intensity Maximum (Å) for Se IV, Sn IV, Sb IV and Te IV spectral lines, for a perturber density of $10^{17}$ cm$^{-3}$ and temperatures from 10,000 to 160,000 K. Calculated wavelength ($\lambda$) of the transitions (in Å) is also given.

| Element | Transition | $\lambda$(Å) | T(K) = 10,000 | 20,000 | 40,000 | 80,000 | 160,000 |
|---|---|---|---|---|---|---|---|
| | | | **FWHM(Å)** | | | | |
| Se IV | $4p^2P^o$–$4d^2D$ | 654.8 | $0.224 \times 10^{-2}$ | $0.159 \times 10^{-2}$ | $0.112 \times 10^{-2}$ | $0.794 \times 10^{-3}$ | $0.600 \times 10^{-3}$ |
| Se IV | $5s^2S$–$5p^2P^o$ | 2987.7 | 0.230 | 0.163 | 0.115 | $0.831 \times 10^{-1}$ | $0.697 \times 10^{-1}$ |
| Sn IV | $5s^2S_{1/2}$–$6p^2P^o_{1/2}$ | 505.4 | $0.581 \times 10^{-2}$ | $0.411 \times 10^{-2}$ | $0.290 \times 10^{-2}$ | $0.215 \times 10^{-2}$ | $0.182 \times 10^{-2}$ |
| Sn IV | $5s^2S_{1/2}$–$6p^2P^o_{3/2}$ | 499.9 | $0.592 \times 10^{-2}$ | $0.419 \times 10^{-2}$ | $0.296 \times 10^{-2}$ | $0.218 \times 10^{-2}$ | $0.183 \times 10^{-2}$ |
| Sn IV | $6s^2S_{1/2}$–$6p^2P^o_{1/2}$ | 4217.3 | 0.687 | 0.486 | 0.344 | 0.263 | 0.229 |
| Sn IV | $6s^2S_{1/2}$–$6p^2P^o_{3/2}$ | 3862.2 | 0.591 | 0.418 | 0.295 | 0.225 | 0.196 |
| Sn IV | $5p^2P^o_{1/2}$–$6s^2S_{1/2}$ | 956.3 | $0.142 \times 10^{-1}$ | $0.101 \times 10^{-1}$ | $0.712 \times 10^{-2}$ | $0.541 \times 10^{-2}$ | $0.460 \times 10^{-2}$ |
| Sn IV | $5p^2P^o_{3/2}$–$6s^2S_{1/2}$ | 1019.7 | $0.167 \times 10^{-1}$ | $0.118 \times 10^{-1}$ | $0.834 \times 10^{-2}$ | $0.633 \times 10^{-2}$ | $0.536 \times 10^{-2}$ |
| Sb IV | $5s^1S$–$5p^1P^o$ | 1042.2 | $0.623 \times 10^{-2}$ | $0.441 \times 10^{-2}$ | $0.312 \times 10^{-2}$ | $0.220 \times 10^{-2}$ | $0.167 \times 10^{-2}$ |
| Sb IV | $6s^3S$–$6p^3P^o$ | 3543.2 | 0.429 | 0.303 | 0.214 | 0.158 | 0.135 |
| Te IV | $6s^2S$–$6p^2P^o$ | 3375.0 | 0.366 | 0.259 | 0.183 | 0.134 | 0.114 |

**Table 2.** Comparison between FWHM - Full Width at Half intensity Maximum (Å) for Sn IV calculated in this work ($W_{TW}$) and in de Andrés-García et al. [21] ($W_{AAC}$), for a perturber density of $10^{17}$ cm$^{-3}$.

| Element | Transition | T(K) | $W_{TW}$(Å) | $W_{AAC}$(Å) |
|---|---|---|---|---|
| Sn IV | $5s^2S_{1/2}$–$6p^2P^o_{1/2}$ | 11,000 | $0.554 \times 10^{-2}$ | $0.121 \times 10^{-1}$ |
| | | 17,500 | $0.439 \times 10^{-2}$ | $0.880 \times 10^{-2}$ |
| | $\lambda = 505.4$ Å | 20,000 | $0.411 \times 10^{-2}$ | $0.810 \times 10^{-2}$ |
| | | 30,000 | $0.335 \times 10^{-2}$ | $0.620 \times 10^{-2}$ |
| | | 50,000 | $0.261 \times 10^{-2}$ | $0.450 \times 10^{-2}$ |
| Sn IV | $6s^2S_{1/2}$–$6p^2P^o_{1/2}$ | 11,000 | 0.655 | 0.888 |
| | | 17,500 | 0.520 | 0.656 |
| | $\lambda = 4217.3$ Å | 20,000 | 0.486 | 0.603 |
| | | 30,000 | 0.397 | 0.469 |
| | | 50,000 | 0.310 | 0.348 |
| Sn IV | $5p^2P^o_{1/2}$–$6s^2S_{1/2}$ | 11,000 | $0.136 \times 10^{-1}$ | $0.290 \times 10^{-1}$ |
| | | 17,500 | $0.108 \times 10^{-1}$ | $0.213 \times 10^{-1}$ |
| | $\lambda = 956.3$ Å | 20,000 | $0.101 \times 10^{-1}$ | $0.195 \times 10^{-1}$ |
| | | 30,000 | $0.822 \times 10^{-2}$ | $0.151 \times 10^{-1}$ |
| | | 50,000 | $0.642 \times 10^{-2}$ | $0.111 \times 10^{-1}$ |
| Sn IV | $5p^2P^o_{3/2}$–$6s^2S_{1/2}$ | 11,000 | $0.159 \times 10^{-1}$ | $0.433 \times 10^{-1}$ |
| | | 17,500 | $0.126 \times 10^{-1}$ | $0.317 \times 10^{-1}$ |
| | $\lambda = 1019.7$ Å | 20,000 | $0.118 \times 10^{-1}$ | $0.290 \times 10^{-1}$ |
| | | 30,000 | $0.963 \times 10^{-2}$ | $0.223 \times 10^{-1}$ |
| | | 50,000 | $0.752 \times 10^{-2}$ | $0.163 \times 10^{-1}$ |

Concerning the big difference of Stark widths within some multiplets of de Andrés-García et al. [21], we have data for three Sn IV multiplets enabling to check how similar are Stark broadening parameters. Wiese and Konjević [48] concluded in their article where regularities and similarities in plasma broadened spectral line widths have been considered that "line widths in multiplets usually agree within a few per cent". In order to see how it is in the case of Sn IV for multiplets considered in this work. First of all we should convert results from Å units to angular frequency units. For this purpose the following formula can be used:

$$W(\mathring{A}) = \frac{\lambda^2}{2\pi c} W(s^{-1}) \tag{2}$$

where $c$ is the speed of light.

For the multiplet 5s$^2$S–6p$^2$P$^o$, for $T$ = 20,000 K, we obtain in units $10^{12}$ s$^{-1}$ 0.303 for $\lambda$ = 505.4 Å and 0.316 for $\lambda$ = 499.9 Å , so that the difference is 4.1%. For the multiplet 6s$^2$S–6p$^2$P$^o$, the corresponding Stark width for $\lambda$ = 4217.3 Å is 0.515 and for $\lambda$ = 3862.2 Å 0.529, so that the difference is 2.6%. For the multiplet 5p$^2$P$^o$–6s$^2$S, the result for $\lambda$ = 956.3 Å is 0.208 and for $\lambda$ = 1019.7 Å , 0.214 i.e., the difference is 2.8%, which is in accordance with the conclusion of Wiese and Konjević [48]. Contrary, the corresponding values in de Andrés-García et al. [21] are 0.402 and 0.526, respectively, so that the difference is 24%.

We note also that Se IV and Te IV are homologous ions and if we look at Stark widths expressed in angular frequency units for homologous transitions, 5s$^2$S–5p$^2$P$^o$ for Se IV and 6s$^2$S–6p$^2$P$^o$ for Te IV widths are only for 11% smaller for Se IV at 10,000 K, and for 30% at 160,000K. Consequently for a rough estimation of Stark width, we could use the value for corresponding transition in homologous atom or ion, nearest to the considered one.

It is worth to add that the theoretical resolving power of the high-resolution echelle spectrometer for the Keck Ten—Meter Telescope is of the order of > 250,000. However, practical realizations may be approximately 36,000. Resolution needed for Stark widths shown in Table 1 may be divided in two groups. For lines between 4217.3 Å and 2987.7 Å needed resolutions are 6,139–12,990 for 10,000 K and 16,035–35,953 for 80,000 K. For lines between 1042.2 Å and 505.4 Å needed resolutions are 61,060–292,321 for 10,000 K and 161,090–824,685 for 80,000 K. It is important that for Sn IV 4217.3 Å line, which is in the visible, needed resolution is 6,139 at 10,000 K and 16,035 at 80,000 K, so that the influence of Stark broadening can be observed with large terrestrial telescopes. For this line, thermal Doppler width is 0.0277 Å and Stark 0.687 Å for $T$ = 10,000 K. The corresponding values for 80,000 K are 0.0784 Å and 0.263 Å respectively.

The obtained Se IV, Sn IV, Sb IV and Te IV Stark widths presented in Table 1, will be implemented as well in the STARK-B database [49,50], which is first of all dedicated for the investigations, modelling and diagnostics of the plasma of stellar atmospheres, but this collection of Stark broadening parameters is also useful for diagnostics of laboratory plasmas, as well as for investigation of laser produced, inertial fusion plasma and for plasma technologies.

We note that STARK-B database participates in the Virtual Atomic and Molecular Data Center—VAMDC [51,52], which enables a more effective search and mining of atomic and molecular data from different databases.

Stark line widths calculated in this work contribute also to the creation of a set of such data for the largest possible number of spectral lines, since this is of importance for a number of problems like stellar spectra analysis and synthesis, opacity calculations and modelling of stellar atmospheres.

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