

## Regularities and systematic trends on Lu III Stark widths

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**Abstract.** Regularity and systematic trend analysis has been performed on the Stark widths of 27 Lu III spectral lines calculated elsewhere by modified semiempirical method. Possible correlation of those Stark widths with corresponding effective principal quantum numbers or effective ionization potentials have been also considered and discussed. Results obtained in such a way can be used for quick estimate of some other unknown Stark width data for the ions in the same homologous or isoelectronic sequence, especially if the conditions are not satisfied to use more accurate theoretical methods.

**Key words:** Atomic processes – Line: profiles – Plasmas

### 1. Introduction

Stark widths values are important in many fields of science and technology. For example, in astrophysics, line widths are useful for analysis, synthesis and interpretation of stellar spectra for all types of stars, investigation of chemical abundances of elements, solar opacity calculations and analysis of radiative transfer through the stellar atmospheres. (Majlinger et al., 2017b).

Regularities and systematic trends are common properties among the Stark widths and shifts (Wiese & Konjević, 1982). Those properties are very usually found among the atomic data, helping to interpolate or quickly estimate needed Stark broadening parameters.

Today the method producing the largest number of Stark broadening parameters is the semiclassical perturbation one (see e.g. Sahal-Bréchet, 1969a,b). If there are no atomic data to use this method adequately one can use the modified semiempirical method, MSE (Dimitrijević & Konjević, 1980). However, in the absence of data needed to calculate Stark broadening parameters, or if the conditions to use these methods are not satisfied, simple estimates become very useful tools, and sometimes become also the only way for finding Stark widths and shifts. Although we lose on accuracy when those estimates are performed,

they are still helpful when the great number of broadening parameters needs to be calculated, and if great accuracy of results is not necessary.

In this work we are focused on investigation of regularities and systematic trends based on Stark widths of 27 spectral lines of Lu III calculated elsewhere (Majlinger et al., 2015) by MSE method, in order to enable quick and simple estimations of the Stark widths.

## 2. Method

This study is purely empirical and it is performed as the similar statistical research for Stark broadening parameters of Zr IV spectral lines (Majlinger et al., 2017a). Estimation methods used here can be also divided into two groups:

- a) estimates based on theory – for example, Cowley’s formula (Cowley, 1971), or simplified MSE (Dimitrijević & Konjević, 1987), and
- b) estimates derived from purely statistical analysis of existing data, like the methods of Purić and Lakićević (see for example Purić & Šcepanović 1999, or Lakićević 1983), or estimates derived from systematic trends based on specific examples of Stark widths (Wiese & Konjević, 1982).

We search the estimation formula in same two versions as in paper mentioned above (Majlinger et al., 2017a). The first is in dependence on the so-called effective ionization potential (see for example Purić & Šcepanović 1999, or Lakićević 1983) for the atomic energy level  $j$ ,  $\chi_j = E_{ion} - E_j$ :

$$W_{E_1} = a_1 \cdot Z^{c_1} \cdot \lambda^2 \cdot N \cdot f(T) \cdot (\chi_j)^{-b_1} \quad (1)$$

where  $j = i, f$ , for upper - initial  $i$  or lower - final  $f$  atomic energy level, and the second in dependence on the effective principal quantum number  $n_j^*$

$$W_{E_2} = a_2 \cdot Z^{c_2} \cdot \lambda^2 \cdot N \cdot f(T) \cdot (n_j^*)^{-b_2} \quad (2)$$

The relation between effective principal quantum number and effective ionization potential  $\chi_j$  is given by:

$$n_j^{*2} = \frac{Z^2 E_H}{\chi_j}. \quad (3)$$

where  $Z - 1$  is ionic charge,  $n_j^*$  - effective principal quantum number of upper or lower level,  $W_E$  estimated Stark width in  $\text{\AA}$ ,  $\lambda$  wavelength in  $\text{\AA}$ ,  $N$  - perturber density in  $\text{m}^{-3}$ ,  $E_H$  - hydrogen atom ionization energy,  $E_{ion}$  - ionization energy,  $E_j$  - energy of upper or lower atomic energy level. Coefficients  $a$ ,  $b$  and  $c$  in equations (1) and (2) are independent of temperature, ionization potential and electron density for a given transition.

Example of first type Eq.(1) estimation formula are Purić & Šćepanović (1999) or Lakićević (1983) estimates, while example of second type Eq.(2) is formula of Cowley. In our estimates in this work we assume that the condition:

$$\frac{3kT}{2|E_j - E_{j'}|} \leq 2, \quad (4)$$

where  $k$  is Boltzmann's constant and  $E_{j'}$  is the closest perturbing level, is satisfied. In that case, Gaunt factor from MSE theory is constant (Dimitrijević & Konjević 1980, and Griem 1968) and the use of temperature function

$$f(T) = T^{-1/2} \quad (5)$$

is a proper choice for spectral widths of isolated ion lines in the case of low temperatures (Elabidi et al. 2009, Elabidi & Sahal-Bréchet 2011). However, it is not recommended to use any of these estimates above temperature limit, and it is the reason why results of  $W_C$  mostly decrease faster with temperature than  $W_{MSE}$  in Table 2 (Majlinger et al., 2015). So we scaled all of our analysed widths on temperature  $T = 10000$  K, where we assume that lower temperature limit condition Eq.(4) is satisfied, at least in the case of our considered Lu III lines.

First, we compare the results obtained by Cowley formula (Cowley, 1971) and MSE results, both already published in Majlinger et al. (2015). Our experiences on Zr IV spectral lines show that modified Cowley formula (see, for example, Kilian et al. 1991, and Przybilla et al. 2016) which includes both upper and lower state influences gives better accuracy than old Cowley equation which is based only on upper state influence (for further detailed see Majlinger et al. 2017a). So we used Cowley's estimating formula in a form:

$$W_{E2A} = a_2 \cdot Z^{c_2} \cdot \lambda^2 \cdot N \cdot f(T) \cdot [(n_{upper*})^{b_2} + (n_{lower*})^{b_2}] \quad (6)$$

with parameters  $a_2 = 1.1075 \cdot 10^{-30}$ ,  $b_2 = 4$  and  $c_2 = -2$  (according to Kilian et al. 1991), instead in form (2).

Also we test the possibility to use the statistical estimates of Jagoš Purić for quick prediction of unknown Stark widths. Comparing the great amount of Stark width data from STARK-B database (Sahal-Bréchet et al. 2014; Sahal-Bréchet et al. 2015a), Purić and his co-workers found the correlation between Stark width and difference between ionization energy and energy of the upper state (which is, according to Purić, called upper effective ionization potential) and offered set of different estimating formulae.

### 3. Results and Discussion

We calculated Stark Full Width at Half intensity Maximum (FWHM) for 27 Lu III transitions by using the so-called "generalized" estimating formula (Purić

**Table 1.** Comparison of Stark Full widths at half intensity maximum for spectral lines of Lu III obtained by "generalized" method of Purić & Šćepanović (1999) for all types of transitions,  $W_{PS}$ , and the method of Purić et al. (2008), for 3s-3p transitions, applied here for all s-p transitions,  $W_P$ , with widths obtained by MSE method ( $W_{MSE}$ ) and with Cowleys method ( $W_C$ ) calculated in Majlinger et al. (2015). All estimates are done for temperature of  $T = 10000$  K and perturber density of  $N = 10^{23} \text{m}^{-3}$ .

<i>Transition</i>	$\lambda[\text{\AA}]$	$W_{PS}[\text{\AA}]$	$W_P[\text{\AA}]$	$W_{PS}/W_{MSE}$	$W_P/W_{MSE}$	$W_P/W_C$
$(^1S)5d^2D_{3/2} - (^1S)5f^2F_{5/2}^o$	1001.2	0.166		10.6		
$(^1S)5d^2D_{5/2} - (^1S)5f^2F_{5/2}^o$	1031.5	0.176		10.5		
$(^1S)5d^2D_{5/2} - (^1S)5f^2F_{7/2}^o$	1030.3	0.177		10.6		
$(^1S)5d^2D_{3/2} - (^1S)6p^2P_{1/2}^o$	3058.8	0.165		1.05		
$(^1S)5d^2D_{3/2} - (^1S)6p^2P_{3/2}^o$	2564.3	0.135		1.18		
$(^1S)5d^2D_{5/2} - (^1S)6p^2P_{1/2}^o$	2773.4	0.158		1.18		
$(^1S)5d^2D_{3/2} - (^1S)7p^2P_{1/2}^o$	1056.5	0.144		2.24		
$(^1S)5d^2D_{3/2} - (^1S)7p^2P_{3/2}^o$	1029.8	0.153		2.44		
$(^1S)5d^2D_{5/2} - (^1S)7p^2P_{3/2}^o$	1062.0	0.163		2.45		
$(^1S)5f^2F_{5/2}^o - (^1S)7d^2D_{3/2}$	5871.3	15.0		10.6		
$(^1S)5f^2F_{5/2}^o - (^1S)7d^2D_{5/2}$	5750.3	14.8		11.0		
$(^1S)5f^2F_{7/2}^o - (^1S)7d^2D_{5/2}$	5788.1	15.0		10.9		
$(^1S)6s^2S_{1/2} - (^1S)6p^2P_{1/2}^o$	2604.1	0.120	0.0926	0.83	0.643	0.73
$(^1S)6s^2S_{1/2} - (^1S)6p^2P_{3/2}^o$	2236.9	0.103	0.0684	0.94	0.628	0.67
$(^1S)6s^2S_{1/2} - (^1S)7p^2P_{1/2}^o$	996.4	0.128	0.0136	2.1	0.219	0.20
$(^1S)6s^2S_{1/2} - (^1S)7p^2P_{3/2}^o$	972.7	0.137	0.0129	2.3	0.215	0.19
$(^1S)6p^2P_{1/2}^o - (^1S)6d^2D_{3/2}$	1854.6	0.316		3.2		
$(^1S)6p^2P_{3/2}^o - (^1S)6d^2D_{3/2}$	2100.1	0.405		3.2		
$(^1S)6p^2P_{3/2}^o - (^1S)6d^2D_{5/2}$	2066.0	0.404		3.2		
$(^1S)6p^2P_{1/2}^o - (^1S)7s^2S_{1/2}$	2071.2	0.316	0.138	2.82	1.23	0.69
$(^1S)6p^2P_{3/2}^o - (^1S)7s^2S_{1/2}$	2382.3	0.418	0.216	2.75	1.42	0.82
$(^1S)6d^2D_{3/2} - (^1S)5f^2F_{5/2}^o$	7536.4	9.40		6.7		
$(^1S)6d^2D_{5/2} - (^1S)5f^2F_{5/2}^o$	8010.9	10.6		6.7		
$(^1S)6d^2D_{5/2} - (^1S)5f^2F_{7/2}^o$	7938.7	10.5		6.8		
$(^1S)7p^2P_{1/2}^o - (^1S)7d^2D_{3/2}$	4491.3	8.79		8.4		
$(^1S)7p^2P_{3/2}^o - (^1S)7d^2D_{3/2}$	5047.5	11.1		7.5		
$(^1S)7p^2P_{3/2}^o - (^1S)7d^2D_{5/2}$	4957.8	11.0		7.8		

& Šćepanović, 1999) derived from the large scale semiclassical perturbation and MSE calculations for all types of transitions, in order to test its applicability in the case of a complex ion like Lu III. We considered also the expression presented in (Purić et al. 2008, p. 805, Fig 1a), which is derived from large number of published theoretical and experimental data for Stark widths for multiply charged ions of different elements along the periodic table for transitions of type 3s – 3p. There is no such transitions in Lu III spectrum but in order to test its applicability to other transitions of the s-p type, we calculated also Stark widths for 6 s-p Lu III lines. After conversion of width from angular frequency units to

Angstroms (see for example, Hamdi et al. 2013, p. 1045, Eq. 7), coefficient value  $a_1$  is recalculated to be  $a_1 = 1.134 \cdot 10^{-27}$  while  $b_1 = 3.33$  and  $c_1 = 5.2$  remain in relation (1) as in Purić et al. (2008). The comparison with our MSE results and calculations using Cowley's method, both from Majlinger et al. (2015) are presented in Table 1. These results are calculated for temperature of  $T = 10000$  K and perturber density of  $N = 10^{23} \text{m}^{-3}$ .

First of all, we can see the regularity of results for lines within the same multiplet. In such cases, we get approximately the same values of Stark broadening parameters, as expected. In the case of our calculation using the "generalized" expression of (Purić & Šćepanović, 1999), the average ratio with MSE results is 5.18 with extremes 11 and 0.83. The average ratio of Stark widths calculated according to Purić et al. 2008 and using MSE, for six s-p transitions is 0.73, with highest and lowest values of 1.30 and 0.215, while the average value for comparison with calculations using Cowley's formula is 0.55 with maximal and minimal value 0.82 and 0.19. We can conclude that the "general" method of Purić & Šćepanović (1999), derived for all types of transitions, is not reliable in the case of Lu III. However, if we make an analysis taking into account the type of transition we can see that the averaged ratio with MSE results is 9.4 for d-f, 3.65 for p-d and 1.96 for s-p transitions. In fact, only for s-p transitions we have a possibility for rough estimate of Stark widths which are not available.

We have already noticed (Majlinger et al., 2015) that method of Purić & Šćepanović (1999), derived from statistical analysis for ions of all elements in the periodic table and all known transitions (rearranged coefficients using in Eq. 1 are in this case  $a_1 = 3.27 \times 10^{-28}$ ,  $b_1 = 3.1$  and  $c_1 = 5.2$ ), is expected to be more accurate for very small ionic charge (e.g.  $Z = 1$ ) and for very large ionic charge (e.g.  $Z = 5$ ), where results of their statistics is standing in the lower or higher end of correlation line in Fig. 1 in Purić & Šćepanović (1999), e.g. for the smallest and for the greatest values of Stark widths. For Lu III  $Z = 3$ , our 27 Stark widths of spectral lines lie in the middle of this correlation line, where maximal standard deviation is observed. This is one reason why method of Purić & Šćepanović (1999) give better results in comparison with MSE for Zr IV (Majlinger et al., 2017a,b) while in the present case differences are even an order of magnitude for d-f transitions. Moreover, Purić & Šćepanović (1999) did their statistical analysis on the great amount of theoretical data, including the results obtained with different theories and for all types of transitions. On our opinion, this mixture of different methods, as well as different types of transitions which are not equally represented (smaller number of data for transitions with higher  $\ell$ ), can produce a large statistical noise, resulting with so large discrepancy of data, because every method, theoretical or empirical, has its own different accuracy, and the theoretical details for different types of transitions are different.

And finally, we try to find estimation based on systematic trend among 27 calculated MSE results. Any systematic trend we found is log-log correlation

between Stark widths and corresponding wavelengths of spectral lines:

$$\log W_{MSE} = 2.245 \log \lambda - 8.403 \quad (7)$$

with correlation coefficient of around 96.5%.

#### 4. Conclusion

We confirmed the possibility to use for s-p transitions of Lu III approximate formula for Stark width estimation given in reference Purić et al. (2008), comparing results for Stark widths of 6 spectral lines of Lu III, obtained by those formula and MSE results calculated and published elsewhere (Majlinger et al., 2015) as well as with calculations from Majlinger et al. (2015) using the method of Cowley (1971), but see also Kilian et al. (1991). The method of Purić et al. (2008) is not applicable for d-f and p-d transitions of Lu III, but for s-p transitions can provide a very rough estimate.

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