

# ON THE STARK BROADENING OF Ru III SPECTRAL LINES

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## ABSTRACT

**Stark broadening parameters, full widths at half maximum (FWHM) and shifts for spectral lines within six multiplets of doubly charged ruthenium ions have been calculated, for an electron density of  $10^{17} \text{ cm}^{-3}$  and temperature range from 10 000 K to 160 000 K. Calculations have been performed with the simplified modified semiempirical (SMSE) approach. In the case of two multiplets, it is possible to apply the full modified semiempirical method. The corresponding calculations have been performed and results are compared in order to test and determine the accuracy of the SMSE approach. The results are also used for the consideration of Stark width and shift regularities in Ru III spectrum.**

**Keywords:** Stark broadening, Spectral lines, Line profiles, Ru III.

## INTRODUCTION

Spectral line profiles in spectra emitted from various plasmas are very useful and precious source of informations about plasma conditions, like electron density, temperature and chemical composition. Among different line broadening mechanisms, Stark broadening due to interaction of emitter/absorber with surrounding charged particles has many useful applications in astrophysics (see e.g. Dimitrijević (2017)), as well as for laboratory plasmas investigation and especially diagnostics. Stark broadening data are also useful for different investigations and modelling of fusion plasma, laser produced plasma diagnostic and analysis, as well as for its different applications in industry and technology as for example for welding, melting and piercing of metals by laser produced plasmas (see for example Dimitrijević (2017) and references therein). Such data are also needed for design and development of light sources using different plasmas (Dimitrijević & Sahal-Bréchet, 2014), as well as for development of laser devices.

One of trace elements, which importance for stellar physics increases with the development of spectroscopic possibilities to obtain high resolution spectra using instruments on board of satellites and on large terrestrial telescopes is ruthenium, a transition metal belonging to the platinum group of the periodic table. In industry and technology, ruthenium is used for wear-resistant electrical contacts and thick-film resistors, as well as in platinum alloys and as a chemistry catalyst.

It is created in stellar interiors in r-process (rapid neutron capture) and it is present in stellar plasma. Yet Merrill (1947) found ruthenium lines in the spectrum of R Andromedae. Adelman et al. (1979) found that Ru I spectral lines are possibly present in gamma Equulei (HD 201601), an Ap star where Stark broadening might be of interest. Biémont et al. (1984) determined that solar abundance of ruthenium is 1.84. With the development of space astronomy and large telescopes of new generation, number of stars where

ruthenium is found increased. So Allen & Porto de Mello (2007) determined Ruthenium abundances in a large sample of giant and dwarf barium stars, within a wide range of plasma parameters. The effective temperatures were  $4300 \text{ K} < T_{eff} < 6500 \text{ K}$  and logarithm of surface gravity  $1.4 \leq \log g < 4.6$ . We note that for largest surface gravities and effective temperatures in this sample Stark broadening might be of interest. Roederer et al. (2010) found Ru I lines in the optical spectrum of r-process enriched metal-poor star BD +17 3248, obtained with the High Resolution Echelle Spectrograph on Keck telescope. Hansen et al. (2014) performed a large consistent study of ruthenium abundances in our Galaxy, using a sample of 52 stars with Ru I lines in their spectra. They underlined that ruthenium is important for nucleosynthetic diagnostics. Mishenina et al. (2019) found Ru I spectral lines and determined ruthenium abundance for a sample of 162 F-, G-, and K-stars belonging to different substructures of the Milky Way.

We can see that ruthenium is widely present in stellar plasma and the corresponding Stark broadening data are needed for determination of abundances, radiative transfer calculations, stellar opacity calculations, modelling of stellar atmospheres and stellar spectra analysis and synthesis. Such data are particularly needed for white dwarfs, where the condition for Stark broadening are very favorable so that it is the principal pressure broadening mechanism (Beauchamp et al., 1997; Tankosić et al., 2003; Milovanović et al., 2004; Simić et al., 2006). Stark broadening is often non negligible and in the case of A type and late B type stars (see for example Simić et al. (2005b,a, 2009)).

In spite of its wide presence in stellar plasma, the corresponding atomic data, needed for various problems in astrophysics and physics are scarce and neither experimental nor theoretical data on Stark broadening exist in literature. In order to provide some of the needed data we calculated here Stark full widths at half maximum (FWHM - W) and shifts the for six multiplets in

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the spectrum of doubly charged ruthenium ion by using the simplified modified semiempirical method - SMSE (Dimitrijević & Konjević, 1987). Additionally, for two multiplets, for which is possible to apply the full modified semiempirical method - MSE (Dimitrijević & Konjević, 1980; Dimitrijević & Kršljanin, 1986; Dimitrijević & Popović, 2001), analyzed in Dimitrijević (2017). The results obtained using both methods are compared in order to test the accuracy of SMSE method. The obtained results are also used for discussion of regularities of Stark broadening parameters. The obtained results for Ru III will be included in the STARK-B (Sahal-Bréchet et al., 2015; Sahal-Bréchet et al., 2020) database.

## NOTES ON CALCULATIONS

Ru III has atomic number 44 and belongs to the isoelectronic sequence of molybdenum. Atomic energy levels needed for the corresponding calculations have been taken from Kramida et al. (2020) and Moore (1971). The existing data for atomic energy levels are scarce and not complete. Consequently, it is not possible to use in appropriate way the more accurate semiclassical perturbation method (Sahal-Bréchet, 1969a,b; Sahal-Bréchet et al., 2014).

The modified semiempirical method (MSE) (Dimitrijević & Konjević, 1980; Dimitrijević & Kršljanin, 1986; Dimitrijević & Popović, 2001) is applicable only for two multiplets, for which we performed calculations of full width at half intensity maximum (FWHM)  $W$ . Since this method is presented recently in Dimitrijević (2017), we will not repeat this here.

For other four multiplets the simplified modified semiempirical (SMSE) method (Dimitrijević & Konjević, 1987) is the most advanced method that is applicable in an adequate way, without *ab initio* calculations when one first calculates the needed atomic energy levels. This method is applied to all six Ru III multiplets considered here. It is well described recently (Dimitrijević, 2020), so there is no need to describe it again.

For the case of the six Ru III multiplets we checked the validity condition of SMSE method (see e.g. Dimitrijević (2020)):

$$x_{j'j} = E/|E_{j'} - E_j| \leq 2 \quad (1)$$

Here,  $E = 3kT/2$ , is energy of free electron,  $j=i,f$ , where  $i$  is for initial atomic energy level of the considered spectral line and  $f$  for final,  $E_{j'}$  ( $j'=i'$  or  $f'$ ) is the nearest atomic energy level for which exists possibility of an allowed dipole transition from or to the energy level  $i$  or  $f$ . So  $X$  is ratio of energy of free electron and of energy difference between initial or final level and the nearest perturbing level. As the validity condition we take the higher  $x$  value of values for initial and final levels.

We can calculate one value for the whole multiplet if the so called "one electron approximation" (Griem, 1974) is valid, namely if the energy distance between atomic energy levels in particular terms making the considered multiplet is much lower than the closest energy distance between two considered terms. In

such a case we calculate an average energy of the term using the expression:

$$E = \frac{\sum_J (2J+1)E_J}{\sum_J (2J+1)}, \quad (2)$$

where  $E$  is the averaged energy and  $E_J$  and  $J$  energy and total angular momentum of a particular energy level.

If we want to obtain Stark broadening parameter, width or shift, for a particular spectral line within the considered multiplet, for the width, for example, we can use the expression:

$$W_{line} = (\lambda_{line}^2 / \lambda_{mult}^2) W_{mult} \quad (3)$$

where  $W_{line}$  and  $\lambda_{line}$  are width and wavelength of a particular line within multiplet, while  $W_{mult}$  and  $\lambda_{mult}$  are the corresponding values for the multiplet. The equation for the shift is analogous.

## RESULTS AND DISCUSSION

With the help of SMSE approach (Dimitrijević & Konjević, 1987) we calculated Full Stark widths at half intensity maximum ( $W$ ) and shifts ( $d$ ) for six multiplets of doubly charged ruthenium (Ru III) with spectral lines broadened due to collisions with electrons, for an electron density of  $10^{17} \text{ cm}^{-3}$  and plasma temperatures of 10 000, 20 000, 40 000, 80 000 and 160 000 K. Additionally, for multiplets  $5s^7S-5p^7P^o$  and  $5s^5S-5p^5P^o$  we calculated Stark widths using more sophisticated MSE method (Dimitrijević & Konjević, 1980), since only for those two multiplets application of this method is adequate.

The obtained results for Stark widths ( $W$ ) and shifts ( $d$ ) are presented in Table 1. We note that for high densities linear dependence of Stark widths and shifts in function of density of electrons, may be influenced by Debye screening. In the last column the validity condition of the SMSE method, given by Eq. (1) is presented. We can see that for  $T = 160\,000 \text{ K}$  validity condition for SMSE method is not satisfied. These values are given for better interpolation for temperatures larger than 80 000 K.

If we compare the SMSE width with more sophisticated MSE calculations, we can see that in the case of  $5s^7S-5p^7P^o$  multiplet at the temperature of 10 000 K, SMSE width is 14% larger than MSE width and for 160 000 this difference is only 5.3%. In the case of  $5s^5S-5p^5P^o$  multiplet, these values are 13.5% and 1.6% respectively. First of all this confirms that more approximate SMSE results are acceptable. An interesting result is that for temperature of 160 000 K, where validity condition is not satisfied the obtained results are even in better mutual agreement which implies that all results for  $T = 160\,000 \text{ K}$  in Table 1 are acceptable.

Besides Stark broadening parameters in Å units, which is common presentation, in Table 1 they are given and in angular frequency units ( $s^{-1}$ ). This is more suitable for discussion of regularities because in such a way the influence of wavelength is avoided. The relation between Stark widths in Å units and in  $s^{-1}$  units is:

**Table 1.** This table gives electron-impact broadening (Stark broadening) Full Widths at Half Intensity Maximum ( $W$ ) and shifts ( $d$ ) for Ru III spectral lines, for a perturber density of  $10^{17} \text{ cm}^{-3}$  and temperatures from 10 000 to 160 000 K. Also, the  $3kT/2\Delta E$ , quantity is given, where  $\Delta E$  is the energy difference between closest perturbing level and the closer of initial and final levels. In order that the used method is valid, this quantity should be less or equal two.

Transition	T(K)	$W[\text{\AA}]$	$d[\text{\AA}]$	$W[10^{12} \text{ s}^{-1}]$	$d[10^{12} \text{ s}^{-1}]$	$W_{MSE}[\text{\AA}]$	$3kT/2\Delta E$
Ru III $5s^7S-5p^7P^o$ $\lambda = 1988.0 \text{ \AA}$	10000.	0.478E-01	-0.116E-01	0.228	-0.553E-01	0.419E-01	0.207
	20000.	0.338E-01	-0.821E-02	0.161	-0.391E-01	0.296E-01	0.415
	40000.	0.239E-01	-0.580E-02	0.114	-0.277E-01	0.210E-01	0.829
	80000.	0.169E-01	-0.410E-02	0.805E-01	-0.196E-01	0.148E-01	1.66
	160000.	0.119E-01	-0.290E-02	0.569E-01	-0.138E-01	0.113E-01	3.32
Ru III $5p^7P^o-5d^7D$ $\lambda = 1669.2 \text{ \AA}$	10000.	0.495E-01	-0.684E-02	0.335	-0.462E-01		0.207
	20000.	0.350E-01	-0.484E-02	0.237	-0.327E-01		0.415
	40000.	0.248E-01	-0.342E-02	0.167	-0.231E-01		0.829
	80000.	0.175E-01	-0.242E-02	0.118	-0.164E-01		1.66
	160000.	0.124E-01	-0.171E-02	0.837E-01	-0.116E-01		3.32
Ru III $5p^7P^o-6s^7S$ $\lambda = 1666.2 \text{ \AA}$	10000.	0.102	0.422E-01	0.690	0.286		0.207
	20000.	0.719E-01	0.298E-01	0.488	0.202		0.415
	40000.	0.508E-01	0.211E-01	0.345	0.143		0.829
	80000.	0.359E-01	0.149E-01	0.244	0.101		1.66
	160000.	0.254E-01	0.105E-01	0.172	0.716E-01		3.32
Ru III $5s^5S-5p^5P^o$ $\lambda = 2314.1 \text{ \AA}$	10000.	0.747E-01	-0.178E-01	0.263	-0.626E-01	0.658E-01	0.241
	20000.	0.528E-01	-0.126E-01	0.186	-0.443E-01	0.465E-01	0.483
	40000.	0.374E-01	-0.890E-02	0.131	-0.313E-01	0.329E-01	0.965
	80000.	0.264E-01	-0.629E-02	0.929E-01	-0.221E-01	0.233E-01	1.93
	160000.	0.187E-01	-0.445E-02	0.657E-01	-0.156E-01	0.184E-01	3.86
Ru III $5p^5P^o-5d^5D$ $\lambda = 1782.3 \text{ \AA}$	10000.	0.643E-01	-0.801E-02	0.381	-0.475E-01		0.241
	20000.	0.454E-01	-0.566E-02	0.269	-0.336E-01		0.483
	40000.	0.321E-01	-0.400E-02	0.191	-0.237E-01		0.965
	80000.	0.227E-01	-0.283E-02	0.135	-0.168E-01		1.93
	160000.	0.161E-01	-0.200E-02	0.953E-01	-0.119E-01		3.86
Ru III $5p^5P^o-6s^5S$ $\lambda = 1806.1 \text{ \AA}$	10000.	0.127	0.518E-01	0.736	0.299		0.241
	20000.	0.901E-01	0.366E-01	0.521	0.212		0.483
	40000.	0.637E-01	0.259E-01	0.368	0.150		0.965
	80000.	0.451E-01	0.183E-01	0.260	0.106		1.93
	160000.	0.319E-01	0.130E-01	0.184	0.748E-01		3.86

$$W(\text{\AA}) = \frac{\lambda^2}{2\pi c} W(\text{s}^{-1}), \quad (4)$$

where  $c$  is the speed of light. The corresponding relation for the shifts is analogous.

It is useful to consider regularities of Stark widths and shifts, since when they exist, we can use this for estimates of the unknown values from the known ones. Wiese & Konjević (1982) and Wiese & Konjević (1992) demonstrated that the differences between Stark widths or between shifts, expressed in angular frequency units, are less than 40% within a transitions array, namely the transition of the type  $n\ell - n'\ell'$ , where  $n$  is principal quantum number and  $\ell$  orbital angular momentum quantum number. In the case of considered Ru III multiplets, for  $5s-5p$  transition array the width for septet is 15.4% larger from the width of quintuplet at 10 000 K and 15.5% at 160 000 K. For the shift these values are

13.2% and 13.0% respectively. For  $5p - 5d$  transition array these values are 13.7% and 13.9% for the width as well as 2.81% and 2.59% for the shift. In the case of  $5p - 6s$  transition array we have 6.7% and 6.98% for the width as well as 4.55% and 4.47% for the shift. In all cases these values are well within the limits of  $\pm 40\%$  predicted by Wiese & Konjević (1982) and Wiese & Konjević (1992). We can also see that the differences are approximately the same at 10 000 K and 160 000 K. These findings can be used for the estimate of missing widths and shifts from the considered transition arrays.

## CONCLUSION

With the help of SMSE theoretical method we have calculated Stark full widths at half intensity maximum and shifts for six Ru III multiplets. For two of them calculations of the line widths have

been performed also using more accurate MSE method. Comparison of MSE and SMSE values confirms that SMSE approach gives correct results even for temperatures slightly beyond the domain of validity of SMSE approach. We investigated also regularities of Stark broadening parameters within Ru III transition arrays and found that differences are within the limits of 15.5%, so that calculated values could be used to estimate the missing ones from the considered transition arrays. The Stark broadening parameters for multiplets of doubly charged ruthenium, obtained in this work, will be implemented in the STARK-B database (Sahal-Bréchet et al., 2015; Sahal-Bréchet et al., 2020) which also can be accessed through the portal (<http://portal.vamdc.eu>) of the European Virtual Atomic and Molecular Data Center - VAMDC (Dubernet et al., 2010; Rixon et al., 2011; Dubernet et al., 2016; Albert et al., 2020).

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