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Original Scientific Paper

ON THE STARK BROADENING OF Os II SPECTRAL LINES

MILAN S. DIMITRIJEVIĆ[1,2,⋆]

[1]Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia
[2]Sorbonne Université, Observatoire de Paris, Université PSL, CNRS, LERMA, F-92190, Meudon, France

ABSTRACT

Stark broadening parameters, full widths at half maximum (FWHM) and shifts for 13 Os II lines have been calculated. The plasma parameters are: electron density of 10^{17} cm^{-3} and temperatures from 5 000 K to 80 000 K. Calculations have been performed with the simplified modified semiempirical (SMSE) approach. The results are also used for the consideration of Strak width and shift regularities within the Os II 6s^{6}D-6p^{6}D^o multiplet.

Keywords: Stark broadening, Spectral lines, Line profiles, Os II.

INTRODUCTION

Spectral line profiles in spectra emited 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. (Tankosić et al., 2003; Milovanović et al., 2004; Simić et al., 2006)), as well as for laboratory plasmas investigation and especially diagnostics (Konjević, 1999). Stark broadening data are also usefull for different investigations and modelling of fusion plasma (Griem, 1992), laser produced plasma diagnostic (Sorge et al., 2000) 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 Hoffman et al. (2006)). Such data are also needed for design and development of light sources using different plasmas (Dimitrijević & Sahal-Bréchot, 2014), as well as for development of laser devices (Csillag & Dimitrijević, 2004).

Osmium is a metal in the platinum group of chemical elements. Its alloys with platinum, iridium, and other platinum-group metals are used for fountain pen nib tipping, for electrical contacts, and in other different applications where extreme durability and hardness are needed, since it is the densest naturally occurring element. In stellar interiors, osmium is created by rapid neutron capture (r-process) and Os I and Os II lines are present in Solar and stellar spectra (Quinet et al., 2006). For example the abundance of osmium has been determined from an Os II line in chemically peculiar Ap star HR 465 (Cowley et al., 1973; Hartoog et al., 1973), in HgMn star HD 175640 of late B type (B9 V) (Castelli & Hubrig, 2004), Os II lines have been observed in peculiar A type stars HD 25354 and HD 5797 (Kuchowicz, 1973), in Ap stars HD2453, HD25354, HD42616, HD71866 and HD 137909 (Brandi & Jaschek, 1970), where and Os I spectral lines have been identified, and in the UV spectrum of the HgMn star κ Canc, where Bord & Davidson (1982) found that osmium is overabundant by a factor 10^4. The presence of Os I and Os II lines in the spectrum of α^2 CVn has been discussed by Cowley (1987) and Cowley et al. (2006) concluded that presence of Os II spectral lines in the spectrum of chemically peculiar star HD65949 is highy probable. Wahlgren et al. (1998) found several Os II lines in the spectrum of χ Lupi, and they stated that lines λ 2282.278 and 2067.229 Å are particularly suitable for osmium abundance determination. Ivarsson et al. (2004) experimentally determined oscillator strengths for 27 Os II lines and used them to establish osmium abundance for χ Lupi. Osmium has been found and in the spectrum of Vela supernova remnants (Wallerstein et al., 1995), and its spectral lines have been used for the investigation of ejecta of neutron star mergers (Tanaka et al., 2020), as well as for synthezis of the spectrum of ι Herculis, a B3 IV star (Castelli & Bonifacio, 1990).

For determination of abundances, radiative transfer calculations, stellar opacity calculations, modelling of stellar atmospheres and stellar spectra analysis and synthezis, Stark broadening data are needed for white dwarfs, where Stark broadening 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 stars and late B type (see for example Simić et al. (2005a,b, 2009)).

As we can see, Stark broadening data for Os II spectral lines are needed for various problems in astrophysics, but atomic data for osmium are scarce and there is neither experimental nor theoretical data for Stark broadening of its spectral lines. Consequently, in order to provide such data, we calculated here, Stark full widths at half maximum (FWHM - W) and shifts d for 13 Os II spectral lines by using the simplified modified semiempirical method (Dimitrijević & Konjević, 1987). The obtained results are used for investigation of regularity of behaviour of Stark broadening parameters within Os II 6s^{6}D-6p^{6}D^o multiplet.

The Stark broadening parameters for Os II spectral lines will be implemented in the STARK-B (Sahal-Bréchot et al., 2015, 2020) database.

⋆ Corresponding author: mdimitrijevic@aob.rs

SIMPLIFIED MSE FORMULA

The simplified modified semiempirical method (Dimitrijević & Konjević, 1987), formulated for Stark broadening of isolated spectral lines of singly and multiply charged ions in plasma is convenient for Os II lines, since a set of atomic data, needed for more accurate semiclassical perturbation calculations (Sahal-Bréchot, 1969a,b; Sahal-Bréchot et al., 2014) does not exist. For the case of considered Os II lines we checked the validity condition

$$x_{jj'} = E/|E_{j'} - E_j| \leq 2 \tag{1}$$

and it is satisfied for electron temperatures less than 80000 K. Here, 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 with possibility to have an allowed dipole transition from or to the energy level i or f. According to (Dimitrijević & Konjević, 1987), full width at half intensity maximum is:

$$W(\text{Å}) = 2.2151 \times 10^{-8} \frac{\lambda^2(\text{cm}) N(\text{cm}^{-3})}{T^{1/2}(\text{K})} (0.9 - \frac{1.1}{Z}) \times$$

$$\times \sum_{j=i,f} (\frac{3n_j^*}{2Z})^2 (n_j^{*2} - \ell_j^2 - \ell_j - 1). \tag{2}$$

where N is the electron density, T temperature, $E = 3kT/2$ the energy of perturbing electron, $Z-1$ the ionic charge (charge seen by optical electron), n^{*2} the effective principal quantum number, ℓ_j (j=i,f) orbital angular momentum quantum number and λ the wavelength.

Similarly, in the case of the shift

$$d(\text{Å}) = 1.1076 \times 10^{-8} \frac{\lambda^2(\text{cm}) N(\text{cm}^{-3})}{T^{1/2}(\text{K})} (0.9 - \frac{1.1}{Z}) \frac{9}{4Z^2} \times$$

$$\times \sum_{j=i,f} \frac{n_j^{*2} \varepsilon_j}{2\ell_j + 1} \{(\ell_j + 1)[n_j^{*2} - (\ell_j + 1)^2] - \ell_j (n_j^{*2} - \ell_j^2)\}. \tag{3}$$

In the case when all levels $\ell_{i,f} \pm 1$ exist, an additional summation may be performed in Eq. (3) and we obtain:

$$d(\text{Å}) = 1.1076 \times 10^{-8} \frac{\lambda^2(\text{cm}) N(\text{cm}^{-3})}{T^{1/2}(\text{K})} (0.9 - \frac{1.1}{Z}) \frac{9}{4Z^2} \times$$

$$\times \sum_{j=i,f} \frac{n_j^{*2} \varepsilon_j}{2\ell_j + 1} (n_j^{*2} - 3\ell_j^2 - 3\ell_j - 1), \tag{4}$$

where $\varepsilon = +1$ for j = i and -1 for j = f.

RESULTS AND DISCUSSION

Atomic energy levels needed for calculation using the simplified modified semiempirical (SMSE) method (Dimitrijević & Konjević, 1987) have been taken from Kramida et al. (2020) and Moore (1971). Data on atomic energy levels for Os II are scarse so that the more accurate semiclassical perturbation method (Sahal-Bréchot, 1969a,b; Sahal-Bréchot et al., 2014) is not applicable in an adequate way. The best data are for the multiplet $6s^6D$-$6p^6D^o$ and SMSE is the most advanced method that could be successfully used for the corresponding calculations. The condition to apply so called "one electron approximation" (Griem, 1974), i.e. to average energies for energy levels within this multiplet and calculate Stark broadening parameters for the multiplet as a whole, is that the distance of energy levels in particular terms making this multiplet is much lower than the closest distance between two terms. In our case, largest separation of atomic energy levels in $6s^6D$ term is 6636.57 cm^{-1} and in $6p^6D^o$ term it is 4325.72 cm^{-1}. The smaller distance between two terms is 37165.79 cm^{-1} and the condition that this distance is much larger than the separation of levels within a term is not well satisfied. We calculate one value for the whole multiplet when this quantity is at least ten times larger, so here the accuracy will be better if we calculate Stark broadening parameters for each spectral line within the considered multiplet, separately.

For the considered transitions of Os II one additional simplification is possible. Namely, if we look at the perturbing levels for each particular line within multiplet the one electron approximation is always satisfied. For example, in the case of the line $6s^6D_{7/2}$-$6p^6D^o_{5/2}$, perturbing levels for $6s^6D_{7/2}$ level are $6p^6D^o_{9/2}$, $6p^6D^o_{7/2}$ and $6p^6D^o_{5/2}$ and the distance between them is 2571.15 cm^{-1}. In the case of the upper level, perturbing levels are $6s^6D_{7/2}$, $6s^6D_{5/2}$ and $6s^6D_{3/2}$ and the distance is 1998.9 cm^{-1}. Since the smaller distance between two sets of perturbing levels, i. e. between $6s^6D_{3/2}$ and $6p^6D^o_{7/2}$ is 38210.31 cm^{-1} we can see that this value is more than ten times larger than the distances of perturbing levels for each of perturbed levels. Consequently, we can average not all levels in the multiplet but only perturbing levels of each perturbed level. An additional difficulty is that all atomic energy levels belonging to $6s^6L$-$6p^6L'^o$ supermultiplet are not known. So we take this averaged perturbing level as representative of other missing levels. Investigations of Wiese & Konjević (1982) demonstrated that Stark widths within a supermultiplet should be not different more than 30%. So, the error introduced by this approximation would be within these limits.

For calculation of averaged energies we used the expression:

$$E = \frac{\sum_J (2J+1) E_J}{\sum_J (2J+1)}, \tag{5}$$

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

Table 1. This table gives electron-impact broadening (Stark broadening) Full Widths at Half Intensity Maximum (W) and shifts (d) for Os II spectral lines, for a perturber density of 10^{17} cm^{-3} and temperatures from 5 000 to 80 000 K.Also, the $3kT/2\Delta E$, quantity is given, where ΔE 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[Å]	d[Å]	W[10^{12} s^{-1}]	d[10^{12} s^{-1}]	3kT/2ΔE
Os II $6s^6D_{9/2}$-$6p^6D^o_{7/2}$	5000.	0.486E-01	-0.171E-01	0.176	-0.619E-01	0.131
λ = 2282.279 Å	10000.	0.344E-01	-0.121E-01	0.124	-0.438E-01	0.262
	20000.	0.243E-01	-0.856E-02	0.878E-01	-0.310E-01	0.523
	40000.	0.172E-01	-0.606E-02	0.621E-01	-0.219E-01	1.05
	80000.	0.121E-01	-0.428E-02	0.439E-01	-0.155E-01	2.09
Os II $6s^6D_{9/2}$-$6p^6D^o_{9/2}$	5000.	0.480E-01	-0.167E-01	0.178	-0.618E-01	0.128
λ = 2256.6 Å	10000.	0.339E-01	-0.118E-01	0.126	-0.437E-01	0.256
	20000.	0.240E-01	-0.835E-02	0.888E-01	-0.309E-01	0.512
	40000.	0.170E-01	-0.590E-02	0.628E-01	-0.218E-01	1.02
	80000.	0.120E-01	-0.418E-02	0.444E-01	-0.154E-01	2.05
Os II $6s^6D_{7/2}$-$6p^6D^o_{7/2}$	5000.	0.595E-01	-0.212E-01	0.181	-0.647E-01	0.131
λ = 2486.247 Å	10000.	0.420E-01	-0.150E-01	0.128	-0.457E-01	0.262
	20000.	0.297E-01	-0.106E-01	0.906E-01	-0.323E-01	0.523
	40000.	0.210E-01	-0.751E-02	0.640E-01	-0.229E-01	1.05
	80000.	0.149E-01	-0.531E-02	0.453E-01	-0.162E-01	2.09
Os II $6s^6D_{7/2}$-$6p^6D^o_{9/2}$	5000.	0.586E-01	-0.207E-01	0.183	-0.645E-01	0.130
λ = 2455.7 Å	10000.	0.414E-01	-0.146E-01	0.129	-0.456E-01	0.259
	20000.	0.293E-01	-0.103E-01	0.915E-01	-0.323E-01	0.519
	40000.	0.207E-01	-0.730E-02	0.647E-01	-0.228E-01	1.04
	80000.	0.147E-01	-0.516E-02	0.458E-01	-0.161E-01	2.07
Os II $6s^6D_{7/2}$-$6p^6D^o_{5/2}$	5000.	0.555E-01	-0.186E-01	0.191	-0.640E-01	0.130
λ = 2336.807	10000.	0.392E-01	-0.131E-01	0.135	-0.453E-01	0.259
	20000.	0.277E-01	-0.928E-02	0.956E-01	-0.320E-01	0.519
	40000.	0.196E-01	-0.656E-02	0.676E-01	-0.226E-01	1.04
	80000.	0.139E-01	-0.464E-02	0.478E-01	-0.160E-01	2.07
Os II $6s^6D_{5/2}$-$6p^6D^o_{7/2}$	5000.	0.607E-01	-0.217E-01	0.182	-0.649E-01	0.131
λ = 2507.185 Å	10000.	0.429E-01	-0.153E-01	0.128	-0.459E-01	0.262
	20000.	0.303E-01	-0.108E-01	0.908E-01	-0.325E-01	0.523
	40000.	0.214E-01	-0.766E-02	0.642E-01	-0.230E-01	1.05
	80000.	0.152E-01	-0.542E-02	0.454E-01	-0.162E-01	2.09
Os II $6s^6D_{5/2}$-$6p^6D^o_{3/2}$	5000.	0.568E-01	-0.192E-01	0.191	-0.643E-01	0.132
λ = 2367.360 Å	10000.	0.402E-01	-0.135E-01	0.135	-0.455E-01	0.264
	20000.	0.284E-01	-0.958E-02	0.955E-01	-0.322E-01	0.528
	40000.	0.201E-01	-0.677E-02	0.675E-01	-0.227E-01	1.06
	80000.	0.142E-01	-0.479E-02	0.477E-01	-0.161E-01	2.11
Os II $6s^6D_{5/2}$-$6p^6D^o_{5/2}$	5000.	0.565E-01	-0.189E-01	0.192	-0.643E-01	0.131
λ = 2355.295 Å	10000.	0.400E-01	-0.134E-01	0.136	-0.454E-01	0.262
	20000.	0.283E-01	-0.947E-02	0.959E-01	-0.321E-01	0.523
	40000.	0.200E-01	-0.670E-02	0.678E-01	-0.227E-01	1.05
	80000.	0.141E-01	-0.473E-02	0.480E-01	-0.161E-01	2.09
Os II $6s^6D_{3/2}$-$6p^6D^o_{3/2}$	5000.	0.625E-01	-0.212E-01	0.194	-0.657E-01	0.132
λ = 2465.2 Å	10000.	0.442E-01	-0.150E-01	0.137	-0.465E-01	0.264
	20000.	0.312E-01	-0.106E-01	0.968E-01	-0.328E-01	0.528
	40000.	0.221E-01	-0.749E-02	0.685E-01	-0.232E-01	1.06
	80000.	0.156E-01	-0.530E-02	0.484E-01	-0.164E-01	2.11
Os II $6s^6D_{3/2}$-$6p^6D^o_{5/2}$	5000.	0.621E-01	-0.210E-01	0.195	-0.656E-01	0.131
λ = 2451.370 Å	10000.	0.439E-01	-0.148E-01	0.138	-0.464E-01	0.262

Table 1. Continued.

Os II $6s^6D_{3/2}$-$6p^6D^o_{5/2}$	20000.	0.311E-01	-0.105E-01	0.973E-01	-0.328E-01	0.525
	40000.	0.220E-01	-0.741E-02	0.688E-01	-0.232E-01	1.05
	80000.	0.155E-01	-0.524E-02	0.486E-01	-0.164E-01	2.10
Transition	T(K)	W[Å]	d[Å]	W[10^{12} s^{-1}]	d[10^{12} s^{-1}]	3kT/2ΔE
Os II $6s^6D_{3/2}$-$6p^6D^o_{1/2}$	5000.	0.593E-01	-0.191E-01	0.202	-0.651E-01	0.129
λ = 2350.240 Å	10000.	0.419E-01	-0.135E-01	0.143	-0.460E-01	0.257
	20000.	0.296E-01	-0.955E-02	0.101	-0.326E-01	0.514
	40000.	0.210E-01	-0.676E-02	0.714E-01	-0.230E-01	1.03
	80000.	0.148E-01	-0.478E-02	0.505E-01	-0.163E-01	2.06
Os II $6s^6D_{1/2}$-$6p^6D^o_{3/2}$	5000.	0.664E-01	-0.226E-01	0.195	-0.666E-01	0.132
λ = 2529.568 Å	10000.	0.470E-01	-0.160E-01	0.138	-0.471E-01	0.264
	20000.	0.332E-01	-0.113E-01	0.977E-01	-0.333E-01	0.528
	40000.	0.235E-01	-0.800E-02	0.691E-01	-0.235E-01	1.06
	80000.	0.166E-01	-0.566E-02	0.489E-01	-0.166E-01	2.11
Os II $6s^6D_{1/2}$-$6p^6D^o_{1/2}$	5000.	0.629E-01	-0.204E-01	0.204	-0.660E-01	0.132
λ = 2409.398 Å	10000.	0.445E-01	-0.144E-01	0.144	-0.467E-01	0.264
	20000.	0.314E-01	-0.102E-01	0.102	-0.330E-01	0.528
	40000.	0.222E-01	-0.720E-02	0.721E-01	-0.233E-01	1.06
	80000.	0.157E-01	-0.509E-02	0.510E-01	-0.165E-01	2.11

Using SMSE method and above explained approximations we calculated Full Stark widths at half intensity maximum (W) and shifts (d) for 13 spectral lines of singly charged osmium (Os II) broadened by impacts with electrons, for an electron density of 10^{17} cm^{-3} while temperatures are 5 000, 10 000, 20 000, 40 000 and 80 000 K.

The obtained Stark broadening paramerers, W and d, are shown in Table 1. One should take into account that the linear dependence of Stark broadening parameters in function of electron density, for high densities may be influenced by Debye screening. The wavelengths shown in Table 1 are the observed ones from Ivarsson et al. (2004). In the last column the validity condition $3kT/2\Delta E$ is given, representing the ratio of the average energy of free electrons, $E = 3kT/2$, and the smaller of energy differences between the initial or final and the closest perturbing level i.e.:

$$\mathrm{Max}[E/\Delta E_{i,i'}, E/\Delta E_{f,f'}] \tag{5}$$

Namely the SMSE method is valid if elastic collisions dominate. Since the threshold for the corresponding inelastic transition is $3kT/2\Delta E = 1$, we can see that for values lower than one and close to one elastic collisions dominate and the method is valid. We use that for values larger than two there are already a significant contribution of inelastic collisions and the method becomes unreliable. Stark broadening parameters for values slightly larger than two are useful for better interpolation.

Stark broadening parameters are presented in Table 1 in Å-, which is the usual presentation and in angular frequency units, which is convenient for discussion of regularities since the influence of wavelength is eliminated. Stark widths and shifts are transformed to angular frequency units, using the expression:

$$W(\mathring{A}) = \frac{\lambda^2}{2\pi c} W(s^{-1}), \tag{6}$$

where c is the speed of light.

The investigations of regularities is useful because if they exist, they can be used for estimates of missing values from the known ones. The Stark widths obtained here, belong to the Os II $6s^6D$-$6p^6D^o$ multiplet. Wiese & Konjević (1982) and Wiese & Konjević (1992) demonstrated that Stark line widths in angular frequency units, are very similar in a multiplet, while shifts are within ± 10%. If we look at values in angular frequency units in Table 1, we can see that for T = 5000 K, the maximal value for the width is 15.9% higher than the minimal one. In the case of the shift, this is 7.77%. At the temperature of 80000 K, these differences are 16.2%for the width and 7.79% for the shift. Consequently, difference within the considered Os II multiplet are higher than predicted by Wiese & Konjević (1982), while for shift are within the limits predicted by Wiese & Konjević (1992). Also, we can see that these differences practically do not change with temperature.

CONCLUSION

By using the SMSE theoretical approach we have calculated Stark full widths at half intensity maximum and shifts for 13 Os II spectral lines within the $6s^6D$-$6p^6D^o$ for electrons as perturbers. The considered temperature range has been from 5000 K up to 80000 K and electron density is 10^{17} cm^{-3} . We examined the similarities of Stark broadening parameters for spectral lines within this multiplet and found that the differences for the widths are within the limits of 16.2% and for the shifts within 7.79%. The obtainrd data will be implemented in the STARK-B database (Sahal-

Bréchot et al., 2015, 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). Other experimental or theoretical data for Stark broadening parameters of Os II lines are missing in the literature, so that the obtained data may be of interest for investigation of stellar spectral lines of ionized osmium and determination of abundances, in particular for white dwarfs and A type stars, as well as for laboratory plasma investigations and diagnostics.

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