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STARK BROADENING OF Tb III SPECTRAL LINES ORIGINATING FROM 6s-6p TRANSITIONS

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 full widths at half maximum (FWHM) for 26 6s-6p transitions in Tb III spectrum have been calculated for electron density of 10^{17} cm^{-3} within a temperature range of 5 000 K to 80 000 K, by using the simplified modified semiempirical (SMSE) method. The results obtained are used for the consideration of Strak width regularities within the investigated transition array.

Keywords: Stark broadening, Spectral lines, Line profiles, Tb III.

INTRODUCTION

Spectral line profiles, broadened by impacts with charged particles (Stark broadening) are useful for many topics as e.g. in astrophysics, laboratory plasma diagnostics, and for different plasma technologies.

For analysis of stellar atmospheres line broadening data for spectral lines of many atoms and ions are needed since the chemical composition of a stellar atmospheres is various and with development of space astronomy, spectrographs on board produce spectral line profiles with increasingly high resolution and accuracy. Consequently, even the data on spectral lines of trace elements become important.

Terbium belongs to lanthanides, a group of fifteen elements from lanthanum to lutetium. Their atomic numbers are from 57 to 71. They are also known as the rare earth elements (REE). Because of the rare-earth peak in the cosmic abundance distribution of chemical elements, data on Stark broadening of their spectral lines is of considerable significance in astrophysics, particularly for stellar atmospheres modelling and investigations and radiative transfer calculation.

The existence of terbium and its ions in stellar atmospheres is confirmed by observation of its spectral lines in stellar spectra. As an example, Siqueira Mello et al. (2014) derived, using three weak Tb II lines, the abundance of terbium for the moderately r-process-enhanced star CS 30315-029. Elkin et al. (2015) found Tb III lines in the spectrum of ro Ap star HD 213637 and Sachkov et al. (2008) in ro Ap star 10 Aql. The spectrum of HD 101065, known as Przybylski's star, an extreme roAp star, contains Tb I, Tb II and Tb III spectral lines (Cowley et al., 2000).

Stark full widths at half maximum (FWHM) for five multiplets of Tb II and 8 multiplets of Tb IV have been published in Dimitrijević (2020). Since for Tb III there is neither experimental nor theoretical data for Stark broadening, we calculated here, in order to provide such data, Stark full widths at half maximum (FWHM) for 26 s-p transitions of Tb III by using the simplified modified semiempirical method (Dimitrijević & Konjević, 1987), since there is no enough reliable atomic data for more sophysticated calculations.

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

SIMPLIFIED MSE FORMULA

For calculation of Stark line widths for Tb III the simplified modified semiempirical formula (Dimitrijević & Konjević, 1987) applicable to isolated, singly, and multiply charged ion lines is used. It is applicable for temperatures when the condition $x_{jj'} = E/|E_{j'} - E_j| \leq 2$ is satisfied. Here, j=i,f, where i denotes initial and f final atomic energy level forming the considered transition, $E_{j'}$ (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. In such a case, full width at half maximum is (Dimitrijević & Konjević, 1987):

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

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

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

RESULTS AND DISCUSSION

Here are calculated Full Stark wifths at half intensity maximum by using the simplified modified semiempirical (SMSE)

⋆ Corresponding author: mdimitrijevic@aob.rs

Table 1. This table gives electron-impact broadening (Stark broadening) Full Widths at Half Intensity Maximum (W) for Tb III spectral lines, for a perturber density of 10^{17} cm^{-3} and temperatures from 5 000 to 80 000 K. The configuration is $4f^8(^7F)n\ell$. 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. One value larger of two is given for better interpolation.

Transition	T(K)	W[Å]	3kT/2ΔE
Tb III $6s^8F_{13/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.254	0.215
λ = 2900.4 Å	10000.	0.180	0.431
	20000.	0.127	0.861
	40000.	0.899E-01	1.72
	80000.	0.636E-01	3.45
Tb III $6s^8F_{13/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.204	0.177
λ = 2517.1 Å	10000.	0.144	0.354
	20000.	0.102	0.708
	40000.	0.721E-01	1.42
	80000.	0.510E-01	2.83
Tb III $6s^8F_{11/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.281	0.215
λ = 3032.8 Å	10000.	0.198	0.431
	20000.	0.140	0.861
	40000.	0.992E-01	1.72
	80000.	0.702E-01	3.45
Tb III $6s^8F_{11/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.222	0.177
λ = 2616.1 Å	10000.	0.157	0.354
	20000.	0.111	0.708
	40000.	0.786E-01	1.42
	80000.	0.556E-01	2.83
Tb III $6s^8F_{9/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.310	0.215
λ = 3174.1 Å	10000.	0.219	0.431
	20000.	0.155	0.861
	40000.	0.110	1.72
	80000.	0.776E-01	3.45
Tb III $6s^8F_{9/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.243	0.177
λ = 2720.6 Å	10000.	0.171	0.354
	20000.	0.121	0.708
	40000.	0.857E-01	1.42
	80000.	0.606E-01	2.83
Tb III $6s^8F_{7/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.333	0.215
λ = 3277.4 Å	10000.	0.235	0.431
	20000.	0.167	0.861
	40000.	0.118	1.72
	80000.	0.833E-01	3.45
Tb III $6s^8F_{7/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.258	0.177
λ = 2796.2 Å	10000.	0.182	0.354
	20000.	0.129	0.708
	40000.	0.911E-01	1.42
	80000.	0.644E-01	2.83
Tb III $6s^8F_{5/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.352	0.215
λ = 3359.2 Å	10000.	0.249	0.431
	20000.	0.176	0.861
	40000.	0.124	1.72
	80000.	0.879E-01	3.45

Table 1. Continued.

Transition	T(K)	W[Å]	3kT/2ΔE
Tb III $6s^8F_{5/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.270	0.177
λ = 2855.5 Å	10000.	0.191	0.354
	20000.	0.135	0.708
	40000.	0.955E-01	1.42
	80000.	0.675E-01	2.83
Tb III $6s^8F_{3/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.365	0.215
λ = 3418.1 Å	10000.	0.258	0.431
	20000.	0.183	0.861
	40000.	0.129	1.72
	80000.	0.913E-01	3.45
Tb III $6s^8F_{3/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.279	0.179
λ = 2898.0 Å	10000.	0.197	0.358
	20000.	0.140	0.716
	40000.	0.987E-01	1.43
	80000.	0.698E-01	2.86
Tb III $6s^8F_{1/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.374	0.215
λ = 3454.2 Å	10000.	0.264	0.431
	20000.	0.187	0.861
	40000.	0.132	1.72
	80000.	0.934E-01	3.45
Tb III $6s^8F_{1/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.285	0.181
λ = 2923.8 Å	10000.	0.201	0.362
	20000.	0.142	0.723
	40000.	0.101	1.45
	80000.	0.711E-01	2.89
Tb III $6s^6F_{11/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.303	0.215
λ = 3141.0 Å	10000.	0.214	0.431
	20000.	0.152	0.861
	40000.	0.107	1.72
	80000.	0.758E-01	3.45
Tb III $6s^6F_{11/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.238	0.177
λ = 2696.3 Å	10000.	0.168	0.354
	20000.	0.119	0.708
	40000.	0.840E-01	1.42
	80000.	0.594E-01	2.83
Tb III $6s^6F_{9/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.354	0.215
λ = 3369.4 Å	10000.	0.250	0.431
	20000.	0.177	0.861
	40000.	0.125	1.72
	80000.	0.885E-01	3.45
Tb III $6s^6F_{9/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.272	0.177
λ = 2862.9 Å	10000.	0.192	0.354
	20000.	0.136	0.708
	40000.	0.960E-01	1.42
	80000.	0.679E-01	2.83
Tb III $6s^6F_{7/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.378	0.215
λ = 3472.6 Å	10000.	0.267	0.431
	20000.	0.189	0.861
	40000.	0.134	1.72
	80000.	0.945E-01	3.45

Table 1. Continued.

Transition	T(K)	W[Å]	3kT/2ΔE
Tb III $6s^6F_{7/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.287	0.182
λ = 2937.1 Å	10000.	0.203	0.364
	20000.	0.144	0.727
	40000.	0.102	1.45
	80000.	0.719E-01	2.91
Tb III $6s^6F_{5/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.407	0.215
λ = 3591.1 Å	10000.	0.288	0.431
	20000.	0.204	0.861
	40000.	0.144	1.72
	80000.	0.102	3.45
Tb III $6s^6F_{5/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.306	0.188
λ = 3021.3 Å	10000.	0.216	0.376
	20000.	0.153	0.752
	40000.	0.108	1.50
	80000.	0.765E-01	3.01
Tb III $6s^6F_{3/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.425	0.215
λ = 3664.1 Å	10000.	0.301	0.431
	20000.	0.213	0.861
	40000.	0.150	1.72
	80000.	0.106	3.45
Tb III $6s^6F_{3/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.318	0.192
λ = 3072.9 Å	10000.	0.225	0.384
	20000.	0.159	0.767
	40000.	0.112	1.53
	80000.	0.794E-01	3.07
Tb III $6s^6F_{1/2}$-$6p_{1/2}(6,1/2)^o$	5000.	0.439	0.215
λ = 3715.7 Å	10000.	0.310	0.431
	20000.	0.219	0.861
	40000.	0.155	1.72
	80000.	0.110	3.45
Tb III $6s^6F_{1/2}$-$6p_{3/2}(6,3/2)^o$	5000.	0.326	0.195
λ = 3109.1 Å	10000.	0.231	0.389
	20000.	0.163	0.778
	40000.	0.115	1.56
	80000.	0.815E-01	3.11

method for 26 s-p transitions of Tb III. Calculations has been performed for an electron density of 10^{17} cm^{-3} and for temperature interval from 5 000 K to 80 000 K, for broadening of spectral lines by collisions with electrons. The needed energy levels and the ionization energy have been taken from Martin et al. (1978) and Kramida et al. (2020). The data on Tb III energy levels are not sufficient for a more sophysticated calculations, so that SMSE method, needing less atomic data, is the most advanced that could be successfully applied.

The additional complication with Tb III energy level system is that 6s levels are described with LS coupling and 6p levels with J_1j coupling. Moreover, in 6p terms only a part of energy levels is known. Consequently we calculated averaged term energies for $6p_{1/2}(6,1/2)^o$ and $6p_{3/2}(6,3/2)^o$ using existing energy levels and expression:

$$E = \frac{\sum_{\mathrm{J}}(2\mathrm{J}+1)E_{\mathrm{J}}}{\sum_{\mathrm{J}}(2\mathrm{J}+1)}, \qquad (2)$$

where E is the averaged energy and E_{J} and J energy and total angular momentum of a particular energy level. An average energy obtained for the term $6p_{1/2}(6,1/2)^o$ is 52154.1 cm^{-1} and for $6p_{3/2}(6,3/2)^o$ 57405.3 cm^{-1}. Also, we assumed that the perturber with $\Delta n = 0$ of the lower level is the upper level of the considered transition. Since the contribution of the lower level is smaller in comparison with the upper one, and the averaged energy is ob-

Table 2. This table gives electron-impact broadening (Stark broadening) Full Widths at Half Intensity Maximum (W) for Tb III $(^7F)6s^{(2S+1)}F_{j_1/2}$-$(^7F)6p_{j_2/2}(6,j_2/2)^o$ transition array, for a perturber density of 10^{17} cm^{-3} and temperature of 10 000 K, in [Å] and in [10^{12}s^{-1}] units.

Transition	W[Å]	W[10^{12} s^{-1}]
Tb III $6s^8F_{13/2}$-$6p_{1/2}(6,1/2)^o$ λ = 2900.4 Å	0.180	0.403
Tb III $6s^8F_{13/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2517.1 Å	0.144	0.428
Tb III $6s^8F_{11/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3032.8 Å	0.198	0.405
Tb III $6s^8F_{11/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2616.1 Å	0.157	0.432
Tb III $6s^8F_{9/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3174.1 Å	0.219	0.409
Tb III $6s^8F_{9/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2720.6 Å	0.171	0.435
Tb III $6s^8F_{7/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3277.4 Å	0.235	0.412
Tb III $6s^8F_{7/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2796.2 Å	0.182	0.438
Tb III $6s^8F_{5/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3359.2 Å	0.249	0.416
Tb III $6s^8F_{5/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2855.5 Å	0.191	0.441
Tb III $6s^8F_{3/2}$-$6p_{1/2}$ $(6,1/2)^o$ λ = 3418.1 Å	0.258	0.416
Tb III $6s^8F_{3/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2898.0 Å	0.197	0.442
Tb III $6s^8F_{1/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3454.2 Å	0.264	0.417
Tb III $6s^8F_{1/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2923.8 Å	0.201	0.443
Tb III $6s^6F_{11/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3141.0 Å	0.214	0.409
Tb III $6s^6F_{11/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2696.3 Å	0.168	0.435
Tb III $6s^6F_{9/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3369.4 Å	0.250	0.415
Tb III $6s^6F_{9/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2862.9 Å	0.192	0.441
Tb III $6s^6F_{7/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3472.6 Å	0.267	0.417
Tb III $6s^6F_{7/2}$-$6p_{3/2}(6,3/2)^o$ λ = 2937.1 Å	0.203	0.443
Tb III $6s^6F_{5/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3591.1 Å	0.288	0.421
Tb III $6s^6F_{5/2}$-$6p_{3/2}(6,3/2)^o$ λ = 3021.3 Å	0.216	0.446
Tb III $6s^6F_{3/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3664.1 Å	0.301	0.422
Tb III $6s^6F_{3/2}$-$6p_{3/2}(6,3/2)^o$ λ = 3072.9 Å	0.225	0.449
Tb III $6s^6F_{1/2}$-$6p_{1/2}(6,1/2)^o$ λ = 3715.7 Å	0.310	0.423
Tb III $6s^6F_{1/2}$-$6p_{3/2}(6,3/2)^o$ λ = 3109.1 Å	0.231	0.450

tained without missing energy levels, we assume that the introduced error is acceptable.

The obtained results of our theoretical determination of Stark widths for spectral lines of doubly charged terbium ion are shown in Table 1. The extrapolation towards lower electron densities than 10^{17} cm^{-3} is linear while for higher it is linear if the influence of Debye screening is negligible or reasonably small. The wavelengths shown in Tables 1 and 2 are the calculated ones from the lower energy level and the averaged upper one, so that they are not equal with the observed ones. In the Table 1 the quantity $3kT/2\Delta E$ is given in the last column. This is the ratio of the average energy of free electrons, $E = 3kT/2$, and the larger of energy differences between the initial or final and the closest perturbing level.

$$\Delta E = \mathrm{Max}[E/\Delta E_{i,i'}, E/\Delta E_{f,f'}] \tag{3}$$

This ratio is one of the validity conditions for the used, simplified modified semiempirical method. Namely, the threshold for the corresponding inelastic transition is $3kT/2\Delta E = 1$. For values lower than one, elastic collisions dominate and the SMSE method is convenient and valid. In the case of values larger than one the inelastic collisions start to be more and more important but up to the value around two it is acceptable to neglect their influence. In Table 1, for the Stark width at T = 80 000 K, this value is higher than two. The width for this temperature is just a point for better interpolation.

The Stark widths obtained here, all belong to the 6s-6p transition array what enables to compare them in order to check their similarities. When such similarities exist, this gives possibility to use them for estimates of missing values, using the known ones. Wiese & Konjević (1982) demonstrated that Stark line widths, if expressed in angular frequency units, are usually very similar in a multiplet, in a supermultiplet they agree within about 30 per cent and, within up to 40 per cent within a transition array. In order to check their similarities within Tb III 6s-6p transition array we transformed the Stark widths expressed in Å-units to angular frequency units, using the expression:

$$W(\mathring{A}) = \frac{\lambda^2}{2\pi c} W(s^{-1}), \tag{4}$$

where c is the speed of light.

In Table 2 are shown Stark widths expressed in Å and in s^{-1} for a temperature of 10 000 K. We can see that values expressed in s^{-1} are much closer because they are liberated from the influence of wavelength. If expressed in Å, the highest value in the considered transition array is more than two times (115%) higher from the smallest one, while in angular frequeny units (s^{-1}) this difference is only 12%. If we look separately sextets and octets, the difference is in both groups 10%. For a fixed lower level, the difference betwen transitions with upper level $6p_{1/2}(6,1/2)^o$ and $6p_{3/2}(6,3/2)^o$ is 6-7% and for transitions with $6p_{1/2}$ only 5% as well as for the case of $6p_{1/2}$, even smaller if we separate octets and sextets, so that we look at multiplets. Than the difference is only 3.5%. In all considered cases the agreement is well within the maximal limits predicted by Wiese & Konjević (1982).

The results obtained in this investigation - Stark widths of Tb III spectral lines will be included in the STARK-B database (Sahal-Bréchot et al., 2015, 2020). This database is also one of the 33 databases entering in the european Virtual Atomic and Molecular Data Center - VAMDC (Dubernet et al., 2010; Rixon et al., 2011; Dubernet et al., 2016), which can be found on the web site http://portal.vamdc.eu.

CONCLUSION

With the help of the SMSE method we have calculated Stark widths for 26 Tb III transitions within the 6s-6p transition array as a function of temperature, for an electron density of 10^{17} cm^{-3} . The consideration of their similarities within the 6s-6p transition array of Tb III show that their differences are within 12 per cent for the transition array as a whole and up to 3.5% for multiplets. This can be used for the estimate of missing values in Tb III multiplets and transition arrays on the basis of the known ones. These data will be implemented in STARK-B database containing the calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions. There is no other experimental or theoretical data for Stark broadening of Tb III lines so that it is not possible to make a comparison with other results. The new Stark broadening data for Tb III obtained in this work may be of interest for stellar physics and plasma diagnostics, especially for investigation of spectral lines and abundances of rare earth elements in atmospheres of white dwarfs and chemically peculiar stars .

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