Stark broadening data for spectral lines of rare-earth elements:
Example of Tb II and Tb IV

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Abstract. Stark full widths at half maximum (FWHM) for five multiplets of Tb II and 8 multiplets of Tb IV have been calculated for electron density of \(10^{17}\) cm\(^{-3}\) by using the simplified modified semiempirical (SMSE) method. The calculations were performed for temperatures from 5 000 K to 80 000 K, in the region where the used theory is applicable.

Key words: Spectral lines – Plasma – Atomic data – Stark broadening

1. Introduction

The lanthanides are a series of 15 chemical elements with atomic numbers 57 through 71, from lanthanum to lutetium. Along with the chemically similar elements scandium and yttrium, they are often collectively known as the rare earth elements (REE). Stark broadening of rare-earth atom and ion spectral lines is of considerable importance in astrophysics due to rare-earth peak of abundance distribution of chemical elements. Consequently, a lot of spectral lines of these elements have been and will be observed in stellar spectra, in particular due to the development of space astronomy. For example, instruments like the Goddard High Resolution Spectrograph (GHRS) on the Hubble Space Telescope, enable us to obtain spectral lines with unprecedented resolution and accuracy.

The data on Stark broadening of rare-earth elements are scarce, first because of the lack of reliable atomic data for the corresponding calculations. The semiclassical perturbation theory (SCP) for Stark broadening of isolated lines (Sahal-Bréchot, 1969a,b) can be used only for some scandium and yttrium ions. In some cases the modified semiempirical method (MSE - Dimitrijević & Konjević 1980) or the simplified modified semiempirical method (SMSA - Dimitrijević & Konjević 1987) can be applied, but in many cases there is not enough atomic data even for the simplest calculations and regularities and systematic trends can only be used for very rough estimates (Popović & Dimitrijević, 1998). Concerning Stark broadening data for REE spectral lines, up to now data are
published for six multiplets of Sc II, calculated by using MSE (Popović & Dimitrijević, 1996), ten of Sc III, using SCP (Dimitrijević & Sahal-Bréchot, 1992), four of Sc X and ten of Sc XI, using SCP (Dimitrijević & Sahal-Bréchot, 1998a), six of Y II using MSE (Popović & Dimitrijević, 1996), 32 of Y III, using SCP (Dimitrijević & Sahal-Bréchot, 1998b), three of La II, six of La III, 284 of Nd II, by using SMSE (Popović et al., 2001b) seven of Eu II, by using MSE, one of Eu III by using SMSE (Popović et al., 1999), four of Yb III, by using MSE (Dimitrijević, 2019), 27 of Lu III, by using MSE (Majlinger et al., 2015) and four of Lu IV, by using MSE, (Dimitrijević, 2019)

The significance of Stark broadening data, including data for REE elements, is increasing in astrophysics due to the increasing possibility of obtaining high resolution spectra. Rauch et al. (2007) underlined that they “are of crucial importance for sophisticated analysis of stellar spectra by means of NLTE model atmospheres”. Spectral lines of neutral and ionized terbium are present and observed in stellar spectra. For example, the terbium abundance was derived by Siqueira Mello et al. (2014) for the moderately r-process-enhanced star CS 30315-029, based on three weak Tb II lines. Elkin et al. (2015) found Tb III lines in ro Ap star HD 213637 and Sachkov et al. (2008) in ro Ap star 10 Aql. Tb I, Tb II and Tb III lines have been found and in the spectrum of the extreme roAp star HD 101065, known as Przybylski’s star (Cowley et al., 2000).

Since there is neither experimental or theoretical data for Stark broadening of Tb II and Tb IV, we calculated here Stark full widths at half maximum (FWHM) for five transitions of Tb II and eight transitions of Tb IV by using the simplified modified semiempirical method (Dimitrijević & Konjević, 1987), since there is not enough atomic data for more advanced calculations.

2. Notes about calculations

In cases when we do not have enough data for more sophisticated theoretical calculations, or when, for example in astrophysics for model atmosphere or radiative transfer calculations, a lot of spectral lines, with the corresponding data should be taken into account. Here the simplified modified semiempirical formula (Dimitrijević & Konjević, 1987) for Stark widths of isolated, singly, and multiply charged ion lines might be very useful. This formula may be used in the case when the nearest atomic energy level, having an allowed dipole transition from, or to, the initial or final energy level of the spectral line considered is far enough away so that the influence of elastic collisions is dominant.

By using the simplified modified semiempirical (SMSE) method (Dimitrijević & Konjević, 1987), the most advanced method applicable in present case due to the lack of a corresponding set of atomic data, we calculated Stark full widths at half maximum (FWHM) due to collisions with electrons, for five transitions of Tb II and eight of Tb IV, for an electron density of $10^{17} \text{ cm}^{-3}$ and for a temperature interval from $5000 \text{ K}$ up to $20000 \text{ K}$ or $40000 \text{ K}$, depending
on the limits of validity of the SMSE method, in the case of Tb II, while for Tb IV the temperature interval is from 5 000 K to 80 000 K. Energy levels and ionization potentials for these calculations have been taken from Martin et al. (1978) and Kramida et al. (2019).

3. Results and discussion

Table 1. This table gives electron-impact broadening (Stark broadening) Full Widths at Half Intensity Maximum (W) for Tb II spectral lines, for a perturber density of $10^{17}$ cm$^{-3}$ and temperatures from 5 000 to 40 000 K. Also is given quantity $3kT/2\Delta E$, where $\Delta E$ is the energy difference between closest perturbing level and the closer of initial and final levels.

| Transition | Temp. | W[Å] | $3kT/2\Delta E$ |
|------------|-------|------|-----------------|
| Tb II ($^6H_{15/2}^o$)6s$_{1/2}$(15/2,1/2) - ($^6H_{15/2}^o$)6p$_{1/2}$(15/2,1/2) | 5000. | 0.393 | 0.734 |
| 3934.1 | 10000. | 0.278 | 1.47 |
| | 20000. | 0.196 | 2.94 |
| Tb II ($^6H_{15/2}^o$)6s$_{1/2}$(15/2,1/2) - ($^6H_{15/2}^o$)6p$_{3/2}$(15/2,3/2) | 5000. | 0.350 | 0.556 |
| 3610.5 | 10000. | 0.247 | 1.11 |
| | 20000. | 0.175 | 2.22 |
| Tb II ($^6H_{13/2}^o$)6s$_{1/2}$(13/2,1/2) - ($^6H_{13/2}^o$)6p$_{1/2}$(13/2,1/2) | 5000. | 0.393 | 0.529 |
| 3938.3 | 10000. | 0.278 | 1.06 |
| | 20000. | 0.196 | 2.12 |
| Tb II ($^6H_{13/2}^o$)6s$_{1/2}$(13/2,1/2) - ($^6H_{13/2}^o$)6p$_{3/2}$(13/2,3/2) | 5000. | 0.344 | 0.417 |
| 3567.3 | 10000. | 0.243 | 0.834 |
| | 20000. | 0.172 | 1.67 |
| | 40000. | 0.122 | 3.34 |
| Tb II ($^6H_{11/2}^o$)6s$_{1/2}$(11/2,1/2) - ($^6H_{11/2}^o$)6p$_{1/2}$(11/2,1/2) | 5000. | 0.397 | 0.449 |
| 3966.1 | 10000. | 0.281 | 0.897 |
| | 20000. | 0.198 | 1.79 |
| | 40000. | 0.140 | 3.59 |

The results obtained for Stark widths for Tb II spectral lines are presented in Table 1 and those for Tb IV are in Table 2. The wavelengths given in Tables 1 and 2 are calculated from the energy levels used. In the last column is $3kT/2\Delta E$, representing the ratio of the average energy of free electrons, $E = 3kT/2$, and the energy difference between the initial ($i$) or final ($f$) and the closest perturbing
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Table 2. Same as in Table 1, but for Tb IV, for temperature interval 5000 - 80 000 K.

| Transition | Temp. | W[Å] | 3kT/2ΔE |
|------------|-------|------|---------|
| Tb IV (8S\(^{o}\)5d \(7^{o}\)D\(^{-}\) - (8S\(^{7/2}\))6p\(_{1/2}\)(7/2,1/2)\(_{3}\) 1338.7 | 5000. | 0.275E-01 | 0.122 |
| | 10000. | 0.195E-01 | 0.243 |
| | 20000. | 0.138E-01 | 0.486 |
| | 40000. | 0.974E-02 | 0.973 |
| | 80000. | 0.689E-02 | 1.95 |
| Tb IV (8S\(^{o}\)5d \(8^{o}\)D\(^{-}\) - (8S\(^{7/2}\))6p\(_{1/2}\)(7/2,1/2)\(_{4}\) 1324.5 | 5000. | 0.273E-01 | 0.119 |
| | 10000. | 0.193E-01 | 0.239 |
| | 20000. | 0.136E-01 | 0.477 |
| | 40000. | 0.964E-02 | 0.973 |
| | 80000. | 0.682E-02 | 1.91 |
| Tb IV (8S\(^{o}\)5d \(8^{o}\)S\(^{o}\) - (8S\(^{7/2}\))6p\(_{1/2}\)(7/2,1/2)\(_{5}\) 1323.3 | 5000. | 0.255E-01 | 0.106 |
| | 10000. | 0.180E-01 | 0.211 |
| | 20000. | 0.128E-01 | 0.423 |
| | 40000. | 0.902E-02 | 0.845 |
| | 80000. | 0.638E-02 | 1.69 |
| Tb IV (8S\(^{o}\)6s \(9^{o}\)S\(^{o}\) - (8S\(^{7/2}\))6p\(_{1/2}\)(7/2,1/2)\(_{3}\) 2331.8 | 5000. | 0.161 | 0.122 |
| | 10000. | 0.114 | 0.243 |
| | 20000. | 0.807E-01 | 0.486 |
| | 40000. | 0.570E-01 | 0.973 |
| | 80000. | 0.403E-01 | 1.95 |
| Tb IV (8S\(^{o}\)6s \(9^{o}\)S\(^{o}\) - (8S\(^{7/2}\))6p\(_{3/2}\)(7/2,1/2)\(_{4}\) 2289.3 | 5000. | 0.156 | 0.122 |
| | 10000. | 0.111 | 0.243 |
| | 20000. | 0.782E-01 | 0.486 |
| | 40000. | 0.553E-01 | 0.973 |
| | 80000. | 0.391E-01 | 1.95 |
| Tb IV (8S\(^{o}\)6s \(9^{o}\)S\(^{o}\) - (8S\(^{7/2}\))6p\(_{3/2}\)(7/2,1/2)\(_{5}\) 2027.1 | 5000. | 0.128 | 0.122 |
| | 10000. | 0.904E-01 | 0.243 |
| | 20000. | 0.639E-01 | 0.486 |
| | 40000. | 0.452E-01 | 0.973 |
| | 80000. | 0.319E-01 | 1.95 |
| Tb IV (8S\(^{o}\)6s \(9^{o}\)S\(^{o}\) - (8S\(^{7/2}\))6p\(_{3/2}\)(7/2,3/2) 1203.8 | 5000. | 0.250E-01 | 0.107 |
| | 10000. | 0.177E-01 | 0.214 |
| | 20000. | 0.125E-01 | 0.429 |
| | 40000. | 0.884E-02 | 0.858 |
| | 80000. | 0.625E-02 | 1.72 |
| Tb IV (8S\(^{o}\)5d \(7^{o}\)D\(^{-}\) - (8S\(^{7/2}\))6p\(_{3/2}\)(7/2,3/2) 2056.2 | 5000. | 0.135 | 0.107 |
| | 10000. | 0.953E-01 | 0.214 |
| | 20000. | 0.674E-01 | 0.429 |
| | 40000. | 0.477E-01 | 0.858 |
| | 80000. | 0.337E-01 | 1.72 |
level ($i'$ or $f'$). Here, $T$ is the temperature and $k$ Boltzmann constant. The larger of these values for the initial and final levels are taken, i.e.:

$$\Delta E = \text{Max}[E/\Delta E_{i,i'}, E/\Delta E_{f,f'}]$$ (2)

This is the validity condition for the SMSE method used. The $3kT/2\Delta E$ is equal to one at the threshold for the corresponding inelastic transition. If it is lower, then elastic collisions are dominant and the SMSE method is completely applicable and valid. For values larger than one, the inelastic collisions start become more and more important with its increase. Up to the value of around two, the results are acceptable. Data for the slightly higher values in Table 1, are given in order to enable better interpolation. The behavior of Stark widths with electron density is linear within the limits of validity of the SMSE method. These are the first published data for Stark width of Tb II and Tb IV and there is no other theoretical or experimental data to compare with.

4. Conclusion

New Stark FWHM for five lines of singly charged, and eight lines for triply charged terbium ion have been calculated in this work using the simplified modified semiempirical formula (Dimitrijević & Konjević, 1987). There is no other theoretical or experimental Stark broadening data for these emitters, so that the data presented are of interest for stellar plasma analysis, as well as for laboratory plasma diagnostics and laser produced plasma investigation.

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