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Stark Broadening of Cr III Spectral Lines: DO White Dwarfs

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Abstract: Using the modified semiempirical method of Dimitrijević and Konjević, Stark widths have been calculated for six Cr III transitions, for an electron density of 10^{17} cm^{-3} and for temperatures from 5000–80,000 K. Results have been used for the investigation of the influence of Stark broadening on spectral lines in cool DO white dwarf atmospheres. Calculated Stark widths will be implemented in the STARK-B database, which is also a part of the Virtual Atomic and Molecular Data Center (VAMDC).

Keywords: Stark broadening; line profiles; atomic data; DO white dwarfs; stellar spectra

1. Introduction

Stark broadening data are very useful for a number of applications, such as laboratory plasma diagnostics, the investigation and modelling of various plasmas in technology and inertial fusion, as well as for the research of laser-produced plasmas, and particularly in astrophysics, primarily for stellar plasma modelling, abundance determination, and stellar spectra analysis and synthesis.

Lines of chromium in various ionization stages are present and often observed in stellar spectra. Underhill [1] identified a great number of Cr II and Cr III lines, as well as a probable Cr IV line in the spectrum of B5 Ia type star η CMa recorded by Orbiting Astronomical Observatory OAO-3, also known as Copernicus. Underhill [2] also found a large number of Cr II and Cr III lines and concluded that Cr IV lines are probably present in the spectra of τ Her (B5 IV) and ζ Dra (B6 III), also obtained by the spectrometer on OAO-3. A feature of Cr III was found by Fahey et al. [3] in the spectrum of β Cephei obrtained by OAO-2. A number of Cr II and Cr III lines were also identified by Bauer and Bennett [4] in the spectrum of ζ Aurigae binary system 31 Cygni (K4 Ib + B4 V), obtained by the FUSE (Far Ultraviolet Spectroscopic Explorer) satellite. Generally, the iron group elements contribute very significantly to the observed opacity in stellar atmospheres [5], and doubly ionized spectra of this group—including Cr III—dominate the UV spectra of hot B stars [6–8].

Cr II lines have also been observed in the spectra of chemically peculiar A-type stars, where Stark broadening is the dominant pressure broadening mechanism, like 7 Sex [9] and ϕ Aqu [10], where 28 Cr II spectral lines have been identified. Chromium lines have been observed and in A-type star spectra of o Peg [11] and Przybylski's star [12]. In Ae/Be Herbig Star V 380 Ori, where Shevchenko [13] found 25 Cr II lines, ionized chromium spectral lines are before Fe II and Ti II in number and intensity. Ionized chromium lines were also found, e.g. in α UMi (Polaris) and HR 7308 by Andrievsky et al. [14], and in XX Oph [15], yet in 1951, Merrill [16] found 58 emission Cr II lines. With the development of high-resolution spectrographs, the assumption of the homogeneous distribution of an element in stellar atmosphere becomes less adequate, for example Babel and Lanz [17] investigated the influence of stratification on chromium lines in the spectrum of chemically peculiar Ap 53 Cam star, and Dimitrijević, M. S. et al. [18] in the Ap HD 133972.

Chromium in various ionization stages from Cr I to Cr VI has been observed and in the spectra of white dwarfs, where the Stark broadening is often the dominant broadening mechanism in wide layers of the atmosphere [19–27]. For example, Cr I has been found by Gianninas et al. [28] in an extremely low mass white dwarf in the SDSS J074511.56+194926.5 binary system and by Dufour et al. [29] in the spectrum of DZ white dwarf G165-7; Cr II spectral lines were identified by Klein et al. [30] in the spectrum of white dwarf GD 40, observed on the Keck I telescope at Mauna Kea Observatory; and, for example, Cr V and Cr VI by Rauch et al. [31] in the spectrum of the white dwarf central star of Sh 2-216.

In spite of the importance of chromium, theoretical data on Stark broadening parameters are scarce. Dimitrijević, M. S. et al. [32] used the semiclassical perturbation method—SCP [33–35]—to calculate electron-, proton-, and ionized helium-impact widths and shifts for nine Cr I spectral lines from the $4p^7P^o$–$4d^7D$ multiplet and used the obtained results to investigate the influence of Stark broadening on line shapes in the spectrum of Cr-rich Ap star β CrB atmosphere. By using the SCP method, Dimitrijević, M. S. et al. [18] obtained electron-, proton-, and ionized helium-impact widths and shifts for spectral lines of seven Cr II multiplets belonging to 4s–4p transitions. They applied obtained Stark broadening parameters to the analysis of Cr II line profiles observed in the spectrum of Cr-rich Ap-type star HD 133792, and found that the Stark broadening mechanism is very important and should be taken into account. Simić et al. [25] calculated Stark broadening parameters for an additional nine resonance Cr II multiplets from $3d^5$–$3d^44p$ transition array using the same method. For Cr I and Cr II there are also the estimates of Lakićević [36], based on regularities and systematic trends, for Stark width and shift of resonance lines Cr I 4289.7 Å and Cr II 2065.5 Å. A large number of Stark-damping constants from chromium lines may also be found in Kurucz [37]. For the Stark broadening of Cr III, Cr IV, and Cr V lines, there is no data in the literature. Electron-, proton-, and ionized helium-impact widths and shifts only exist for two multiplets of Cr VI [38].

Experimental data exist only for Cr II lines. Rathore et al. [39] experimentally determined the widths and shifts of three lines within the Cr II multiplet $4s^4D$–$4p^4F^o$ and Aguilera et al. [40] measured the widths and shifts of 83 Cr II lines within 45 multiplets.

As we can see, data for the Stark broadening of Cr III lines observed and present in stellar atmospheres are completely missing. Data on the energy levels of Cr III are not complete, and it is not possible to perform a more sophisticated semiclassical perturbation calculation. So, in this work we will calculate full widths at half intensity maximum (FWHM) due to collisions with surrounding electrons for Cr III spectral lines, using the modified semiempirical method (MSE) [41–43]. As an example of the importance of of Stark broadening data for stellar spectra analysis and synthesis and stellar plasma investigation and modelling, we will compare Stark and thermal Doppler broadening importance using two models of white dwarf atmospheres.

2. The Modified Semiempirical Method

For the calculations of Stark full width at half-intensity maximum (FWHM), the modified semiempirical (MSE) approach [41] is used. It is explained in detail in [41–43], and only basic expressions needed for the understanding of the calculation method will be given here. The FWHM of an isolated ion line is given by the following equation:

$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\lambda^2}{\sqrt{3}}\cdot\Big\{\sum_{\ell_i\pm1}\sum_{L_{i'}J_{i'}}\vec{\Re}^2_{\ell_i,\ell_i\pm1}\widetilde{g}(x_{\ell_i,\ell_i\pm1})+$$

$$\sum_{\ell_f\pm1}\sum_{L_{f'}J_{f'}}\vec{\Re}^2_{\ell_f,\ell_f\pm1}\widetilde{g}(x_{\ell_f,\ell_f\pm1})+\Big(\sum_{i'}\vec{\Re}^2_{ii'}\Big)_{\Delta n\neq0}g(x_{n_i,n_i+1})+\Big(\sum_{f'}\vec{\Re}^2_{ff'}\Big)_{\Delta n\neq0}g(x_{n_f,n_f+1})\Big\}. \quad (1)$$

Here, i and f are for initial and final levels, respectively, $\vec{\Re}^2_{\ell_k,\ell_{k'}}$, $k = i, f$ is the square of the matrix element, and

$$(\sum_{k'} \vec{\Re}^2_{kk'})_{\Delta n \neq 0} = (\frac{3n_k^*}{2Z})^2 \frac{1}{9}(n_k^{*2} + 3\ell_k^2 + 3\ell_k + 11) \quad (2)$$

(in Coulomb approximation).

In Equation (1),

$$x_{l_k,l_{k'}} = \frac{E}{\Delta E_{l_k,l_{k'}}}, k = i, f,$$

where $E = \frac{3}{2}kT$ is the electron kinetic energy and $\Delta E_{l_k,l_{k'}} = |E_{l_k} - E_{l_{k'}}|$ is the energy difference between levels l_k and $l_k \pm 1$ ($k = i, f$),

$$x_{n_k,n_k+1} \approx \frac{E}{\Delta E_{n_k,n_k+1}},$$

where for $\Delta n \neq 0$ the energy difference between energy levels with n_k and $n_k + 1$, $\Delta E_{n_k,n_k+1}$, is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H / n_k^{*3}$. With $n_k^* = [E_H Z^2/(E_{ion} - E_k)]^{1/2}$ is denoted the effective principal quantum number, Z is the residual ionic charge (e.g., $Z = 1$ for neutral atoms), E_{ion} is the appropriate spectral series limit, N and T are electron density and temperature, respectively, while $g(x)$ [44] and $\widetilde{g}(x)$ [41] are the corresponding Gaunt factors.

3. Results and Discussion

The needed set of atomic energy levels was taken from Sugar and Corliss [45] (see also NIST database [46]), and the dipole matrix elements for considered transitions were calculated within Coulomb approximation [47]. Stark widths of Cr III spectral lines were calculated by using the modified semiempirical method [41] (see also the review of innovations and applications in [43]). The obtained results are shown in Table 1 for a perturber density of 10^{17} cm^{-3} and temperatures from 5000 K up to 80,000 K.

The presented data for Stark broadening of Cr III lines are the first, so there is no other experimental or theoretical data for comparison.

The Stark broadened shape $F(\omega)$ of an isolated spectral line has Lorentzian form, and can be represented as:

$$F(\omega) = \frac{W/2\pi}{(\omega - \omega_{if} - d)^2 + (W/2)^2}.$$

Here,

$$\omega_{if} = \frac{E_i - E_f}{\hbar}.$$

In the upper equation E_i and E_f are energies of the initial and final states, while Stark FWHM (W) and shift (d) are in angular frequency units. For the difference of Stark width, were contributions of all term in Equation (1) are positive, for shift the analogous contributions of particular terms may be positive and negative. Additionally, the theoretical accuracy is smaller due to mutual cancellations of various terms. For s–p transitions considered here, the contribution of the lower s state is negative and the shift will be smaller than width, so it could be neglected. In order to obtain the line shape, one should transform results from Table 1 from Å-units to angular frequency units using the following expression:

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

where c is the speed of light.

Table 1. Full Width at Half intensity Maximum (FWHM, Å) for Cr III spectral lines, for a perturber density of 10^{17} cm^{-3} and temperatures from 5000 K to 80,000 K. Calculated wavelength (λ) of the transitions (in Å) is also given. 3kT/2ΔE is the ratio of the energy of free electron and of the energy difference to the closest perturbing level for T = 10,000 K.

Transition	T (K)	FWHM (Å)
CrIII $3d^3(^4F)4s\,^5F$–$3d^3(^4F)4p\,^5F^o$	5000	0.723E-01
	10,000	0.511E-01
λ = 2121.8 Å	20,000	0.361E-01
3kT/2ΔE = 0.234	40,000	0.256E-01
	80,000	0.181E-01
CrIII $3d^3(^4F)4s\,^5F$–$3d^3(^4F)4p\,^5G^o$	5000	0.791E-01
	10,000	0.559E-01
λ = 2241.9 Å	20,000	0.396E-01
3kT/2ΔE = 0.234	40,000	0.280E-01
	80,000	0.198E-01
CrIII $3d^3(^4F)4s\,^5F$–$3d^3(^4F)4p\,^5D^o$	5000	0.732E-01
	10,000	0.518E-01
λ = 2138.2 Å	20,000	0.366E-01
3kT/2ΔE = 0.234	40,000	0.259E-01
	80,000	0.183E-01
CrIII $3d^3(^4F)4s\,^3F$–$3d^3(^4F)4p\,^3F^o$	5000	0.850E-01
	10,000	0.601E-01
λ = 2235.6 Å	20,000	0.425E-01
3kT/2ΔE = 0.258	40,000	0.301E-01
	80,000	0.213E-01
CrIII $3d^3(^4F)4s\,^3F$–$3d^3(^4F)4p\,^3G^o$	5000	0.905E-01
	10,000	0.640E-01
λ = 2321.9 Å	20,000	0.453E-01
3kT/2ΔE = 0.258	40,000	0.320E-01
	80,000	0.226E-01
CrIII $3d^3(^4F)4s\,^3F$–$3d^3(^4F)4p\,^3D^o$	5000	0.101
	10,000	0.715E-01
λ = 2478.9 Å	20,000	0.505E-01
3kT/2ΔE = 0.258	40,000	0.357E-01
	80,000	0.253E-01

The obtained Stark widths will be used for an example of the importance of the Stark broadening mechanism in stellar atmospheres. Hamdi et al. [48] and Dimitrijević et al. [26] demonstrated that the Stark broadening is usually larger than or comparable to Doppler broadening in atmospheres of DO white dwarfs, where effective temperatures are within the interval 45,000–120,000 K. Here we will extend this to the cool DO white dwarfs, marking the hot end of the so-called DB gap, corresponding to an interval in effective temperatures from 30,000–45,000 K [49].

In Figure 1 are shown logarithms of Stark (SW) and thermal Doppler (DW) widths for Cr III $3d^3(^4F)4s\,^5F$–$3d^3(^4F)4p\,^5F^o$ (λ = 2121.8 Å) and $3d^3(^4F)4s\,^3F$–$3d^3(^4F)4p\,^3D^o$ (λ = 2478.9 Å) spectral lines as a function of Rosseland optical depth (τ_{Ros}), for an atmospheric model [50] with effective temperatures T_{eff} = 40,000 K, and log g = 6, where g is surface gravity. These two lines were chosen since they have the smallest and largest Stark width, so for all other lines the corresponding curves will be between the curves presented in Figure 1. In Figure 2, Stark and thermal Doppler widths are presented for the same spectral lines, but for a model with T_{eff} = 40,000 K, and log g = 9. We can see that there are large atmospheric layers where Stark broadening is dominant in comparison with thermal Doppler broadening. We can also see that the influence of Stark broadening increases with the increase of the value of Rosseland opacity, and that gravity becomes more important for atmospheric models with larger surface.

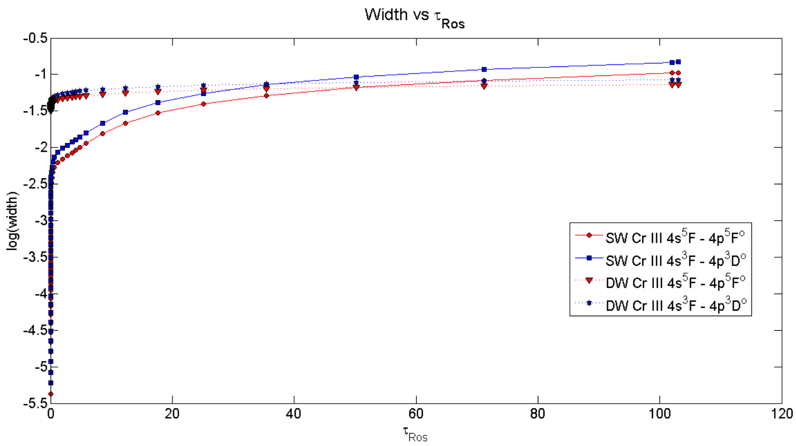

Figure 1. Stark (SW) and Doppler (DW) widths for Cr III 3d^3(^{4}F)4s^{5}F–3d^3(^{4}F)4p^{5}F^o (λ = 2121.8 Å) and 3d^3(^{4}F)4s^{3}F–3d^3(^{4}F)4p^{3}D^o (λ = 2478.9 Å) spectral lines as a function of Rosseland optical depth (τ_{Ros}). Stark and Doppler widths are shown for an atmospheric model [50] with effective temperatures T$_{eff}$ = 40,000 K, and log g = 6.

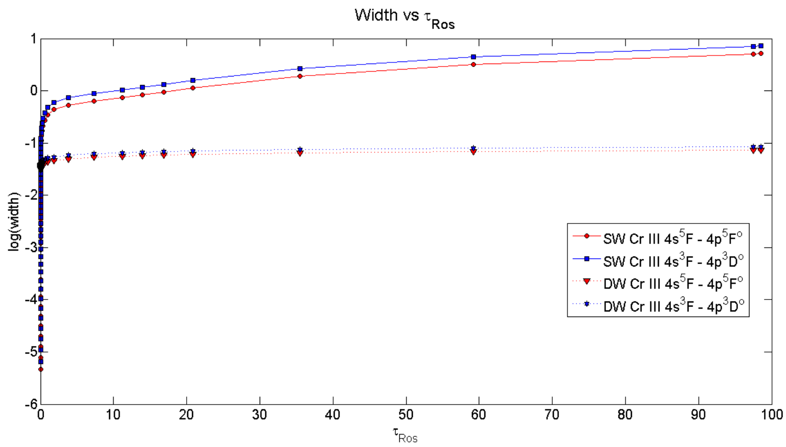

Figure 2. Stark (SW) and Doppler (DW) widths for Cr III 3d^3(^{4}F)4s^{5}F–3d^3(^{4}F)4p^{5}F^o (λ = 2121.8 Å) and 3d^3(^{4}F)4s^{3}F–3d^3(^{4}F)4p^{3}D^o (λ = 2478.9 Å) spectral lines as a function of Rosseland optical depth (τ_{Ros}). Stark and Doppler widths are shown for an atmospheric model [50] with effective temperatures T$_{eff}$ = 40,000 K, and log g = 9.

Seaton [51] underlines that Stark broadening is the dominant broadening mechanism in subphotospheric layers. If chromium exists in the stellar atmosphere, it also exists in various ionization stages in subphotospheric layers, since it is created in thermonuclear reactions in stellar interiors, and the corresponding Stark broadening parameters are useful for the theoretical consideration and modelling of such layers, as well as for the calculation of radiative transfer in such conditions even for cooler stars, where chromium is present but Stark broadening in the atmosphere is negligible.

The Stark widths of Cr III spectral lines, shown in Table 1, will be implemented in the STARK-B database [52,53], dedicated to the investigation, modelling, and diagnostics of the plasma of stellar atmospheres and for the diagnostics of laboratory plasmas, but also useful for investigation of laser-produced and inertial fusion plasma, as well as for plasma technologies. The STARK-B database is also included in the Virtual Atomic and Molecular Data Center (VAMDC) [54,55], created to enable an easier and more effective search of atomic and molecular data from different databases.

Stark line widths calculated in this work also contribute to the creation of a set of such data for as large as possible a number of spectral lines, since this is important for a number of problems such as stellar spectra analysis and synthesis, opacity calculations, and the modelling of stellar atmospheres.

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