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Stark broadening parameters for Kr II lines from 5s – 5p transitions*

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Abstract. With the development of space-borne spectroscopy, spectral line parameters for a large number of lines become of increasing interest for astrophysics. To provide Stark broadening data for ion lines from complex spectra, we present here calculated Stark widths for 37 Kr II lines from the 5s – 5p transition. The calculations were performed by using a modified semiempirical approach. The obtained Stark widths are on average in satisfactory agreement with available experimental data.

Key words: atomic data — lines, profiles

1. Introduction

Stark broadening data for many transitions of many atoms and ions are needed for diagnosis of laboratory and astrophysical plasmas. As an example, data for more than 10^6 transitions, including line-profile parameters, are needed for the calculation of stellar opacities (Seaton 1988). With the development of space-borne spectroscopy, interest increases even more for a large number of spectral line profile parameters. For example, Leckrone et al. (1993) stated that with the Goddard High Resolution Spectrograph (GHRS) on Hubble Space Telescope they "have doubled the number of heavy elements ($22 \leq Z \leq 80$) for which abundances in χ Lupi can be estimated, compared to ground-based data alone". Cardelli et al. (1991) have used the GHRS for investigation of spectra of the interstellar medium, which more accurately represents the pre-stellar material from which the Ap and Bp stars (where Stark broadening data are of interest) are formed (Leckrone et al. 1993). For the first time, they have begun to detect elements such as krypton and germanium.

Stark broadening for Kr II lines has additional theoretical interest for the investigation of regularities and systematic trends for singly-charged noble gas ions (e.g. Dimitrijević & Popović 1989; Di Rocco 1990; Purić et al. 1991; Bertuccelli & Di Rocco 1993). Stark broadening data for Xe II, which is homologous with Kr II, have been published recently (Popović & Dimitrijević 1996a). A consistent set of Stark broadening data for Kr II and Xe II enables the investigation and testing of regularities in the case of homologous atoms, as well as Stark width estimates for homologous sequences for noble gas ions.

Stark broadening of Kr II lines have been considered experimentally (see e.g. Brandt et al. 1981; Pittman & Konjević 1986; Vitel & Skowronek 1987; Uzelac & Konjević 1989; Lesage et al. 1989; Bertuccelli & Di Rocco 1991) and theoretically (see e.g. Bertuccelli & Di Rocco 1993). Bertuccelli & Di Rocco (1993) have calculated Kr II Stark widths for several lines by using analytical expressions for the cross sections and rate coefficients based on the Born approximation, with and without the empirical modification for the collision strength suggested by Robb and with the help of a semiempirical method (Griem 1968). Estimates also exist based on the dependence on atomic number and the upper level ionization potential, established from the consideration of regularities (Di Rocco 1990; Purić et al. 1991; Bertuccelli & Di Rocco 1991, 1993). Here we present Stark widths for 37 spectral lines from the 5s – 5p transition array of singly-charged krypton, calculated by using a modified semiempirical approach (Dimitrijević & Konjević 1980; Dimitrijević & Kršljanin 1986). Due to the complexity of the Kr II spectrum, calculations were performed as in Popović & Dimitrijević (1996b). Our results for Stark widths and shifts are compared with the available experimental and theoretical data.

2. Results and discusion

The atomic energy levels needed for the calculation were taken from Sugar & Musgrove (1991). Oscillator

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* Tables 1-4 are only available in electronic form via anonymous ftp 130.79.128.5 at the CDS in Strasbourg or via http://cdsweb.u-strasbg.fr/Abstract.html

strengths have been calculated using the method of Bates & Damgaard (1949). Our investigation of the influence of the departure from the LS coupling scheme on the Xe II Stark broadening parameters (Popović & Dimitrijević 1996a) has demonstrated that the differences between results obtained by using the LS and jK coupling schemes are relatively small in comparison with the accuracy of the modified semiempirical method (±50% in average). The differences for the homologous Kr II radiator should not be larger, so that the use of the LS coupling approximation should not influence the accuracy significantly, especially for transitions between lower levels. In Table 1 (accessible only in electronic form), we present Stark widths for 37 Kr II lines obtained for temperatures from 5000 K up to 50000 K and at an electron density of 10^{23} m^{-3}. Since we have found that the ion broadening contribution to the line widths is several percent, only the electron broadening contribution is given.

Our results for Stark widths have been compared in Table 2 (accessible only in electronic form) and Figs. 1-3 with available experimental data (Brandt et al. 1981; Vitel & Skowronek 1987; Uzelac & Konjević 1989; Lesage et al. 1989; Bertuccelli & Di Rocco 1990). The ratio of measured and calculated data varies between 0.73 and 1.97 (or 1.60 if we exclude the results of Bertuccelli & Di Rocco 1991). This is similar agreement as for the homologous 5s − 5p Xe II transitions, where this ratio varies between 0.7 and 1.4 (Popović & Dimitrijević 1996a). One can see from Table 2 that the largest disagreement exists between our theoretical Stark widths and the experimental data given by Bertuccelli & Di Rocco (1990) ($w_{\rm m}/w_{\rm th}$ vary from 0.73 up to 1.97). One should notice however, that they have not determined the electron density directly. They estimated the electron density by comparing the experimental widths of five selected lines with those obtained in Lesage et al. (1989) and Vitel & Skowronek (1987). The measured and calculated width ratios in the case of Uzelac & Konjević (1989), Brandt et al. (1981) and Vitel & Skowronek (1987) are well within the error bars of the modified semiempirical method (±50). This is the case for Lesage et al. (1989) as well, with the exception of the 461.9 nm line. Since all experimental data are within a narrow temperature range between 11000 K and 17400 K, where the Stark widths decrease quicker than for higher temperatures, it is significant to provide new reliable experimental data for higher temperatures in order to check the theoretical temperature dependence.

In Table 1, data are presented for each particular line within a multiplet. One should notice that the atomic energy level differences within the considered multiplets are comparable to the distances to the nearest perturbing level. Consequently, the line widths within a multiplet differ (Dimitrijević 1982). For example, for the lines $\lambda = 429.29$ nm ($5s^4P_{3/2} - 5p^4D^0_{3/2}$) and $\lambda = 476.57$ nm ($5s^4P_{3/2} - 5p^4D^0_{5/2}$), the lower ($5s^4P_{3/2}$) level is the same.

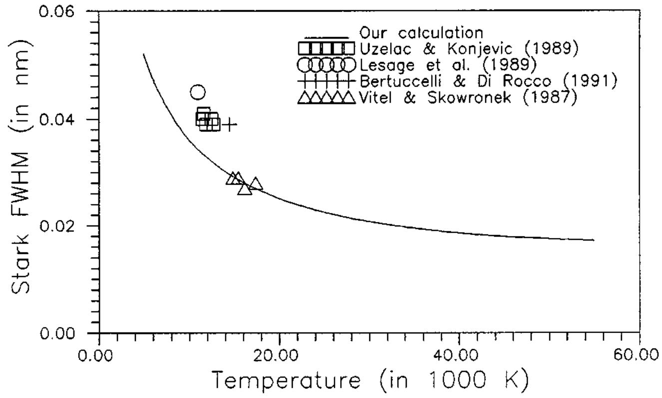

Fig. 1. Stark full-width (FWHM) for Kr II $\lambda = 465.9$ nm spectral line as a function of temperature, at an electron density of $N = 10^{23}$ m^{-3}

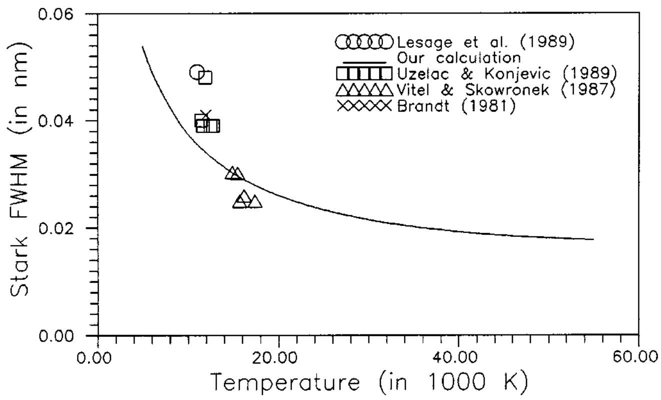

Fig. 2. Same as in Fig. 1, but for line $\lambda = 473.9$ nm

On the other hand, the upper level of the 476.57 line, i.e. $5p^4D^0_{5/2}$, is much closer to the 4d perturbing levels and especially to the $4d^4P_{5/2}$ and $4d^4P_{3/2}$ perturbing levels than the upper level ($5p^4D^0_{3/2}$) of the 429.29 nm line. Consequently, the 476.57 nm line width should be larger than the 429.29 nm line width. Indeed, the ratio of the corresponding widths is $w_{476.57}/w_{429.29} = 1.34$ from our calculations, $w_{476.57}/w_{429.29} = 1.7$ (Lesage et al. 1989) and $w_{476.57}/w_{429.29} = 1.16$ (Bertuccelli & Di Rocco 1991) from experiment.

The averaged value of the experimental and the theoretical data ratio is $w_{\rm exp}/w_{\rm th} = 1.25 \pm 0.05$, where the indicated error is an average quadratic error calculated in the same way as in Popović & Dimitrijević (1996a). If there are several values at different temperatures from the same reference for the same line, these values have been averaged before making an average ratio for the line. As one can see, the calculated Stark widths give a satisfactory agreement with experimental values on average.

The theoretical Stark widths for several lines are given in Bertuccelli & Di Rocco (1993). They have calculated Stark widths (only for $T = 10000$ and $N_{\rm e} = 10^{23}$ m^{-3}) by

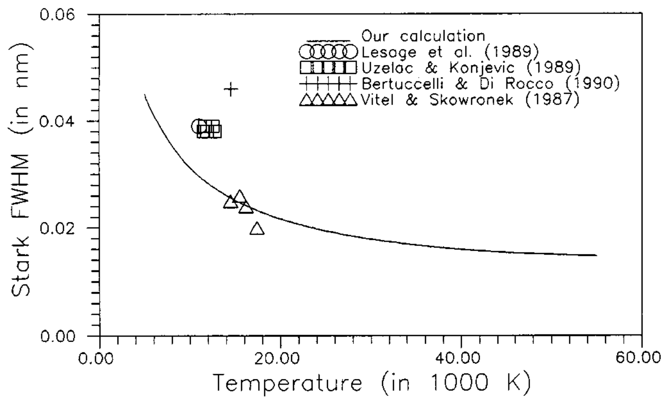

Fig. 3. Same as in Fig. 1, but for line $\lambda = 435.5$ nm

using Griem's semiempirical formula (Griem 1968) and by using the approach based on the Born approximation with and without the empirical modification for the collision strength suggested by Robb (see Bertuccelli & Di Rocco 1993). In Table 3 (accessible only in electronic form), we have compared our theoretical data with the theoretical data calculated by Bertucceli & Di Rocco (1993) and with the experimental data (Brandt et al. 1981; Vitel & Skowronek 1987; Uzelac & Konjević 1989; Lesage et al. 1989; Bertuccelli & Di Rocco 1991) for several lines. Data presented for a particular line are averaged if several values exist. As one can see, the ratios of calculations performed by Bertuccelli & Di Rocco (1993) and our calculations are 1.95, 1.76 and 1.56 for the calculations by using the approach based on the Born approximation with and without the empirical modification for the collision strength suggested by Robb and by using the Griem's semiempirical approach, respectively. Also, their calculations are significantly larger in comparison with experimental data.

There are Stark shift experimental data for three Kr II lines (Vitel & Skowronek 1987). The comparison between our calculations and experimental Stark shifts is shown in Table 4 (accessible only in electronic form). One should notice that the theoretical shifts are generally of lower accuracy than widths (see e.g. Dimitrijević et al. 1981; Popović et al. 1993). Namely, the contributions from different perturbing levels to the shift have different signs. If contributions with both signs are similar, shift accuracy is much lower. In view of these facts, the agreement between calculated and experimental shifts is satisfactory with the exception of the 435.55 nm line. The calculated data for Stark shifts can be obtained on request from the authors.

We hope that the presented data set on Kr II Stark widths will be of help for the analysis of the trace element spectral lines and abundances (especially by using spaceborne telescopes and instruments such as HST/GHRS), as well as for the investigation of regularities within homologous atom/ion sequences and their use for the interpolation of new data.

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