STARK PARAMETERS REGULARITIES OF MULTIPLY CHARGED IONS SPECTRAL LINES ORIGINATING FROM THE SAME TRANSITION ARRAY

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Abstract

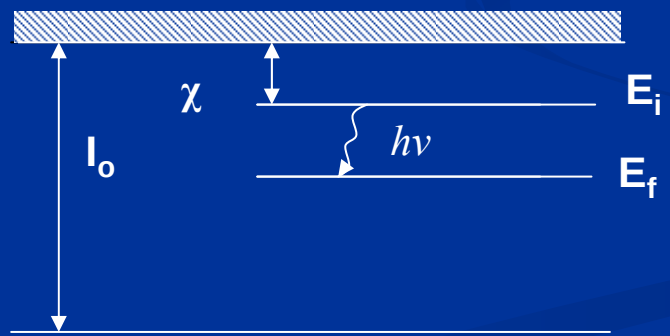
- Stark width and shift regularities of the multiply charged ion spectral lines have been studied
- The emphasis is on the Stark width and shift dependences on the upper level ionization potential and the rest core charge of the emitters
- The found regularities can be used for Stark widths and shifts predictions for the lines of multiply charged ions where not existing so far
- The accuracy of the obtained width and shift values are of the same order as the accuracies of the used data in the procedure of establishing regularities

Outline

- Introduction
- Different kinds of regularities
- Results and discussion
- Conclusions

Introduction

- In the last thirty five years Stark parameters of over thousand neutral and ion spectral lines up to fifteenth stage of the ionization of about fifty elements from Periodic table have been determined experimentally or theoretically calculated
- Stark parameters dependence on the upper level ionization potential has been theoretically evaluated and experimentally demonstrated and proved using the Stark parameters database available from NIST
- The present approach differs from earlier Stark broadening trend analyses primarily in the choice of the variable conveying atomic structure information; Stark parameters dependence on the upper level ionization potential is theoretical expected



Energy diagram and notation

In establishing the expected dependences the existing theoretical and experimental data were used:

- Theoretical data are taken from H. R. Griem, Spectral Line Broadening by Plasmas, New York Academic (1974) and Dimitrijević at al. and many other authors (see references)

- Experimental data are taken from review papers by N. Konjević, M. S. Dimitrijević and W. L. Wiese, J. Phys Chem. Ref. Data 13 (1984) 3, N. Konjević and W. L. Wiese, J. Phys Chem. Ref. Data 19 (1990) 6, N. Konjević, A. Lesage, J.R. Fuhr, W.L. Wiese, J. Phys. Chem. Ref. Data 31 (2002) 819

Different kinds of regularities have been found

- Within spectra of particular emitter
  - multiplet
  - supermultiplet
  - spectral series
  - transition array
- Within spectra of different emitters of the same stage of ionization
  - homologous sequences
  - lines originating from the same transition of all elements along the periodic table (resonance, off-resonances…)
- Within similar spectra of the same element in several different stages of ionization
  - isonuclear sequences
  - lines originating from the same transition array
- Within similar spectra of the different elements and different ionization stages
  - isoelectronic sequences
  - transition arrays of different elements

Theory

- Stark width and shift dependence on the ionization potential was firstly derived by J. Purić, I. Lakićević and V. Glavonjić Phys.Let. 76A (1980) 128, within semi empirical approach (H. R. Griem, Phys.Rev. 165 (1968) 258)

- According to Grime's semi classical approach Stark parameters are expressed in terms of atomic matrix elements. These in turn, can be related to quantum numbers as per equation (77) of Griem (1974):

$$\sum \left| \left\langle J' \left| r_i \right| J \right\rangle \right|^2 = \frac{a_0^2}{2J+1} S$$

  - a_0 is the Bohr radius
  - J is total orbital quantum number
  - S is the line strength - when LS coupling is assumed, S can be factored:

$$S = \sigma(M)\sigma(L)\sigma^2$$

  - Where $\sigma(M)$ and $\sigma(L)$ are tabulated (Allen 1963) multiplet and intramultiplet relative line strengths
  - σ is the integral of the radial wave function for the transition

It is acceptable to model the jumping electron as being under the influence of a screened central charge
In this Coulomb approximation (Bates & Daamgaard 1949):

$$\sigma\left(n_{l-1}^{*}, l-1, n_{l}^{*}, l\right)=\frac{1}{Z_c}\left[\frac{3n_{l}^{*}}{2}\left(\frac{\left|n_{l}^{*2}-l^{2}\right|}{4l^{2}-1}\right)^{1/2}\right]\varphi\left(n_{l-1}^{*}, n_{l}^{*}, l\right)$$

- l is the larger of azimuthal quantum numbers l_i, l_f
- $\varphi\left(n_{l-1}^{*}, n_{l}^{*}, l\right)$ is a tabulated correction factor (Oertel & Shomo 1968)
- n^* is the effective principle quantum number:

$$n^{*} \equiv Zc\left(\frac{E_H}{E_\infty - E}\right)^{1/2} \equiv Zc\left(\frac{E_H}{\chi}\right)^{1/2}$$

- E_H and E_∞ are the ionization potentials of hydrogen and the emitter
- E is the state energy
- Zc is the rest core charge of the emitter, as seen by the electron undergoing transition

- **Two cases can be considered (J. Purić, M. H. Miler and A. Lesage, Ap. J. 416 (1993) 825):**

$$n_l^{*2} = \frac{Z_c^2 E_H}{E_\infty - E_e} = \begin{cases} \dfrac{Z_c^2 E_H}{\chi_i}; l = l_i \\ Z_c^2 E_H \sum_{v=0}^{\infty} (-1)^v \dfrac{(E_i - E_f)^v}{\chi_i^{v+1}}; l = l_f \end{cases}$$

  - where the second version of equation is the Taylor expansion of $1/(E_\infty - E_l)$ for $\chi_i > E_i - E_f$
  - knowing that $E_\infty = \chi_i + E_i$, $E_l = E_f$

- The explicit dependence of the transition integral on the potential χ and the rest core charge Z_c of the emitter is obtained:

$$w, d = \left(\frac{Z_c E_H}{\chi}\right)^2 \sum_{v=0}^{\infty} A_v \left(\frac{Z_c}{\chi}\right)^v$$

- Usually a single term dominate the series in this equation

It has been shown that for ion lines Stark width and shift can be expressed as:

$$w = N_e f(T) a_1 Z_c^{c_1} \chi^{-b_1}$$

$$d = N_e f(T) a_2 Z_c^{c_2} \chi^{-b_2}$$

- a_1, b_1, c_1 and a_2, b_2 and c_2 are coefficients independent of
  - temperature
  - electron density
  - ionization potential

for particular transition

- Within the same stage of ionization (Z_c=const) of the emitters the above equations become:

$$w, d = a_{1,2}\chi^{-b_{1,2}}$$

- General form of this reduced dependence for widths in the case of ionized emitters in different ionization stages ($Z_c \neq$const):

$$w^* = w / Z_c^{c_1} = a_1 N_e f(T) \chi^{-b_1} = a\chi^{-b}$$

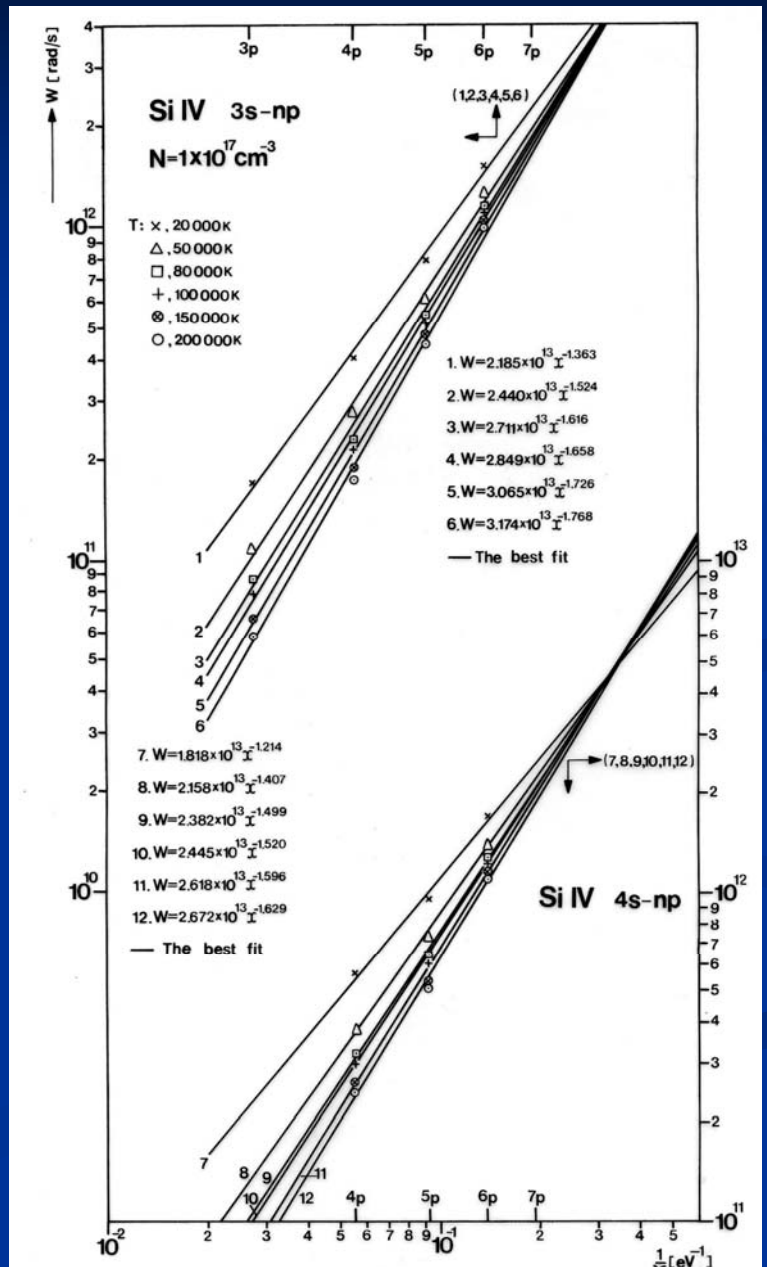
  - it has been found that the coefficient c_1 is constant approximately equal to 5.20

- In the course of establishing regularities one has to use Stark parameters data normalized to given electron density and temperature
- Stark parameters dependence on the electron densities for nonhydrogenic lines is linear
- Temperature dependence for ion lines is of the form:

$$f(T) = A + BT^{-C}$$

Results and discussion

- Spectra of particular emitter
  - spectral series



J. Puric, M.H. Miller, A. Lesage, ApJ. **416** (1993) 825.

- transition array

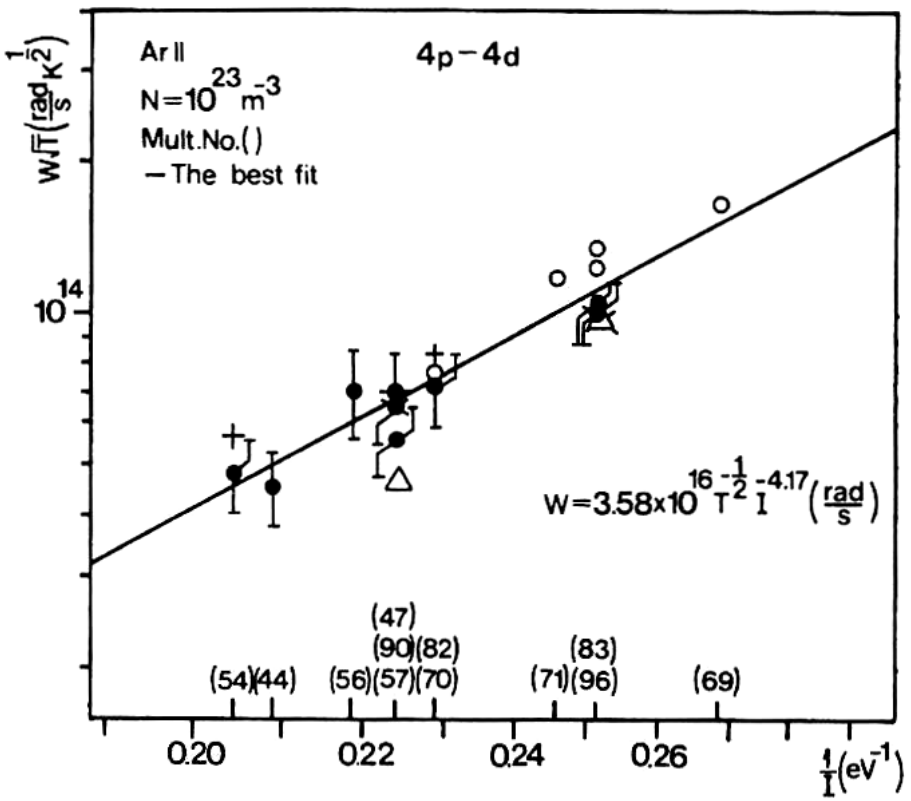


Fig. 2. Reduced Stark HWHM $w\sqrt{T}$ in rad $K^{1/2}$/sec vs the inverse values of the upper-level ionization potentials I in eV for the $4p$–$4d$ transition array at an electron density of $N = 1 \times 10^{23}$ m^{-3}; (●) our data and those of other authors; (○) Pittman and Konjević;[12] (△) experimental data of Behringer and Thoma;[8] theoretical values of Griem[15] (+) and of Dimitrijević and Truong-Bach[14] (×).

S. Djenize at al. J.Quant. Spectrosc. Radiat. Transfer 42 (1989) 429-435

- Spectra of different emitters in the same stage of ionization
  - homologous sequences

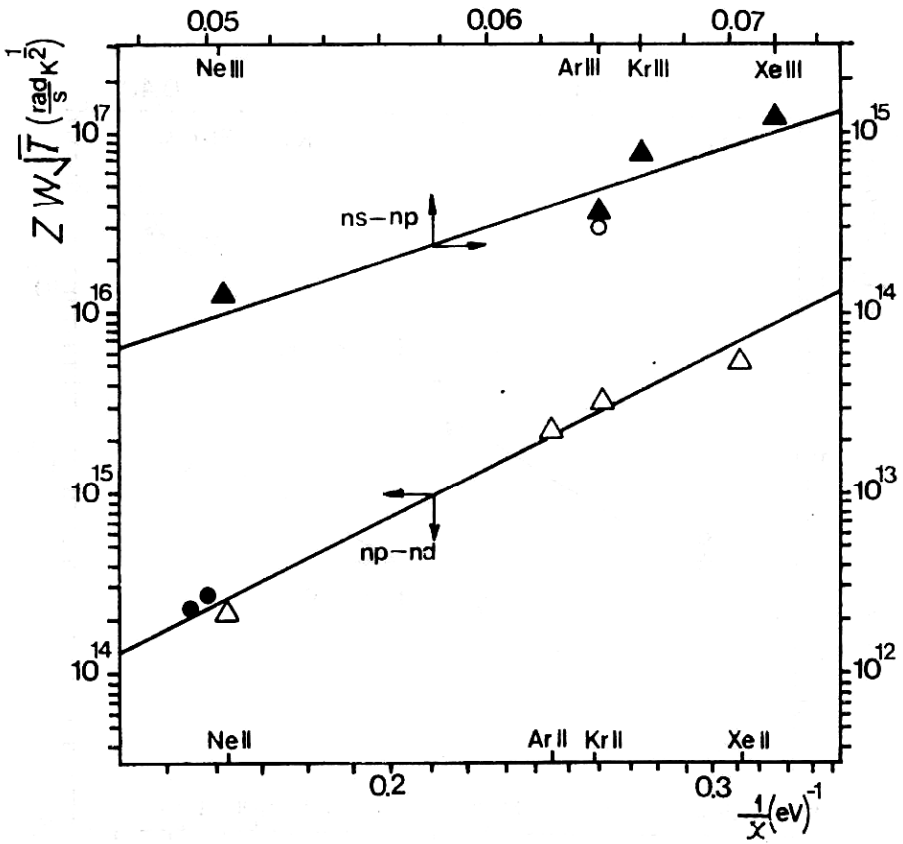
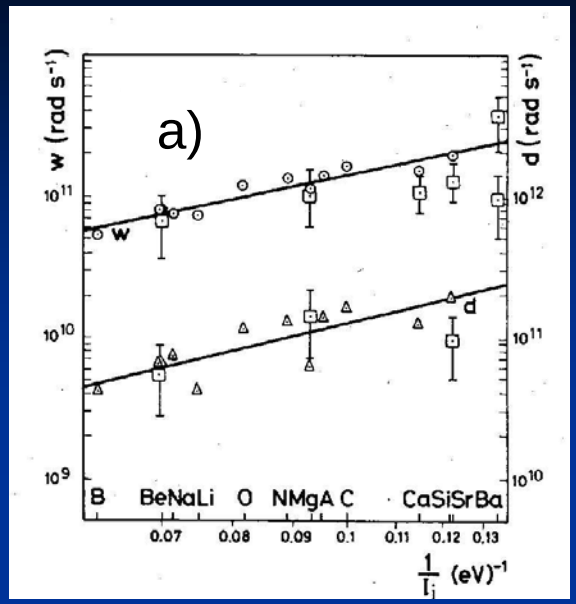
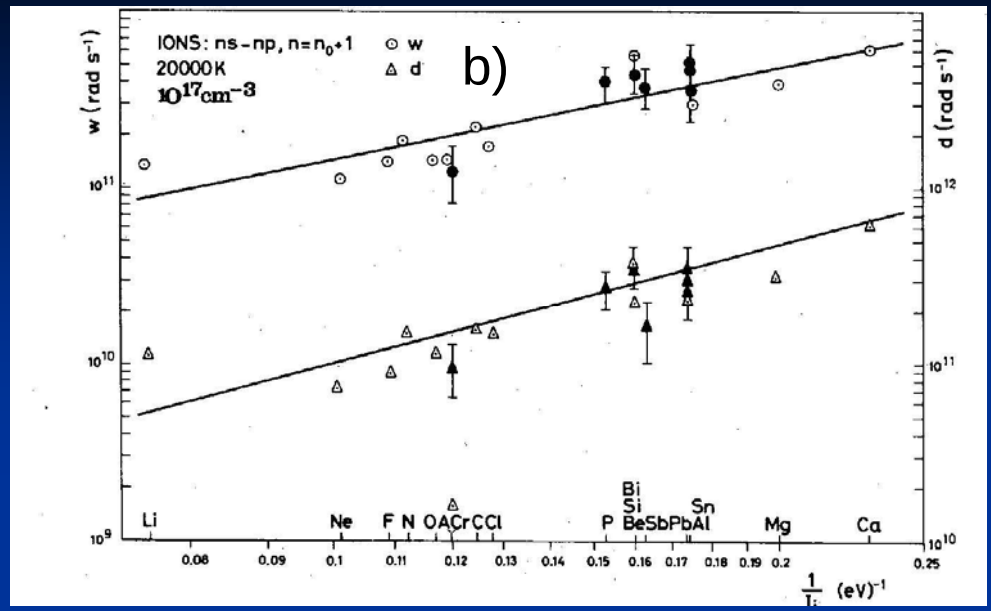


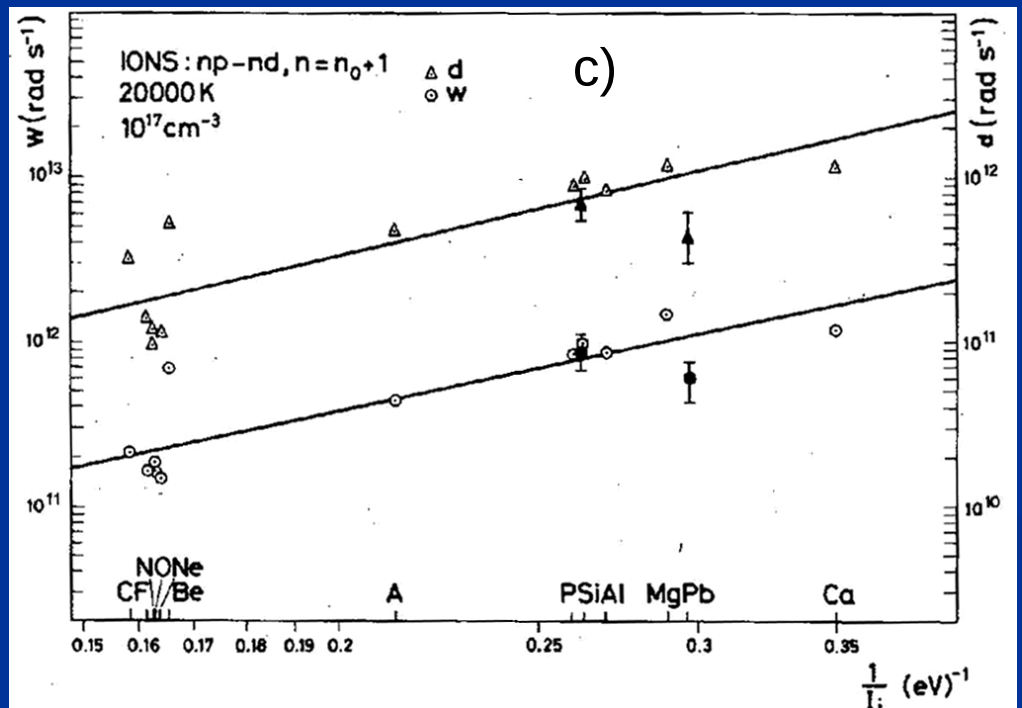
Fig. 2. Reduced Stark HWHM ($Z\omega\sqrt{T}$) vs inverse value of the upper-level ionization potential (I) for homologous sequences at $N = 1 \times 10^{23}$ m^{-3} electron density: ●, Ref. 13; ○, Ref. 14; △, Ref. 15; ▲, Ref. 16; —, The best fit.

Puric at al. Fizika 20 (1988) 485

- lines originating from the same transition of all elements along the periodic table (resonance, off-resonances…)







a) singly charged ion resonances

b) and c) off-resonance ion lines

Puric at al. Phys. Rev. A 32 (1985) 1106

- Similar spectra of the same element in several different stages of ionization
  - isonuclear sequences

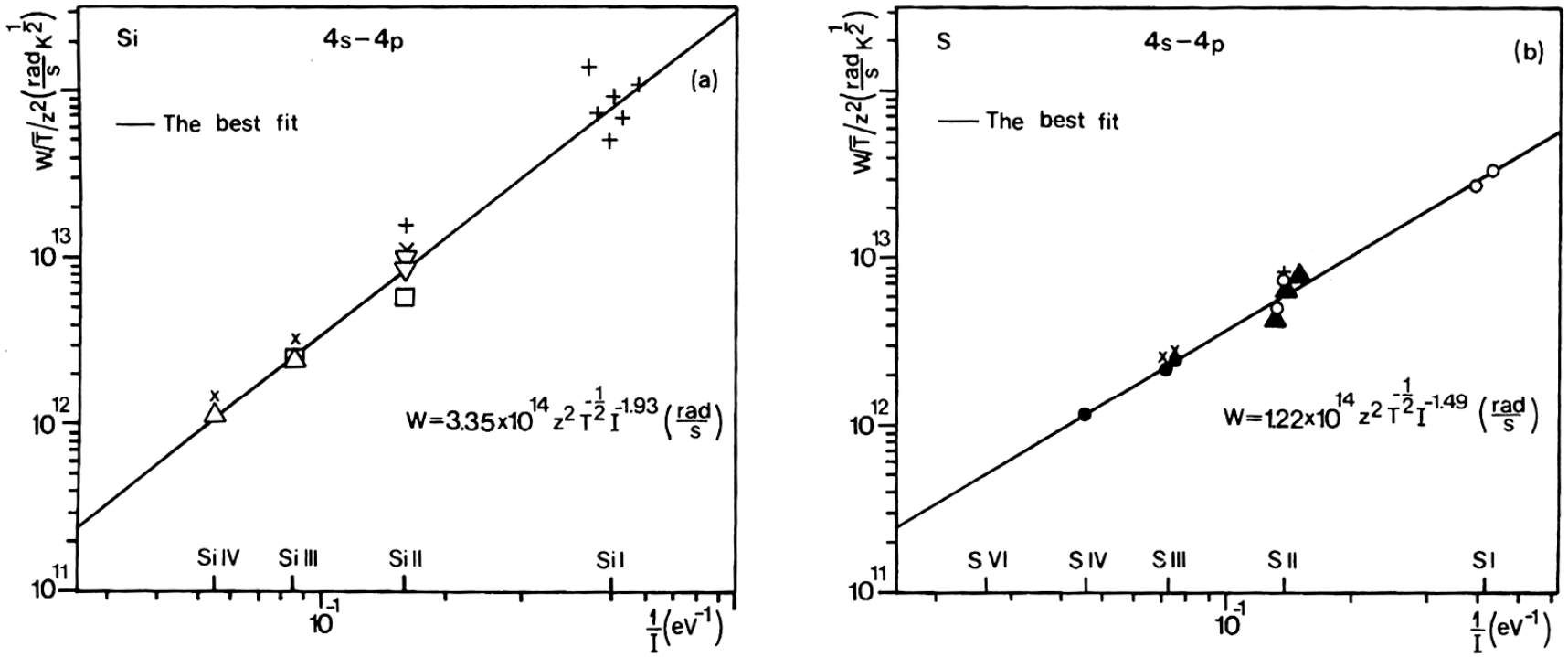


Fig. 1a and b. Reduced Stark HWHM ($w T^{1/2}/z^2$) vs inverse value of the upper-level ionization potential for $4s-4p$ transition array for: (**a**) Si I, Si II, Si III and Si IV; and (**b**) S I, S II, S III and S IV at electron density $1 \times 10^{23}\,m^{-3}$: □, Purić et al. [11]; ▽, Lesage et al. [13]; △, Platiša et al. [12]; ○, Bridges and Wiese [23]; ●, Platiša et al. [14]; ▲, Miller [24]; +, Griem's theory [20] and ×, Dimitrijević and Konjević [16]

Puric at al. Z. Phys. D – Atoms, Molecules and Clusters 10 (1988) 431

- similar spectra of the different elements and different ionization stages
  - isoelectronic sequences

a) Lithium – like isoelectonic sequence

b) Sodium – like isoelectonic sequence

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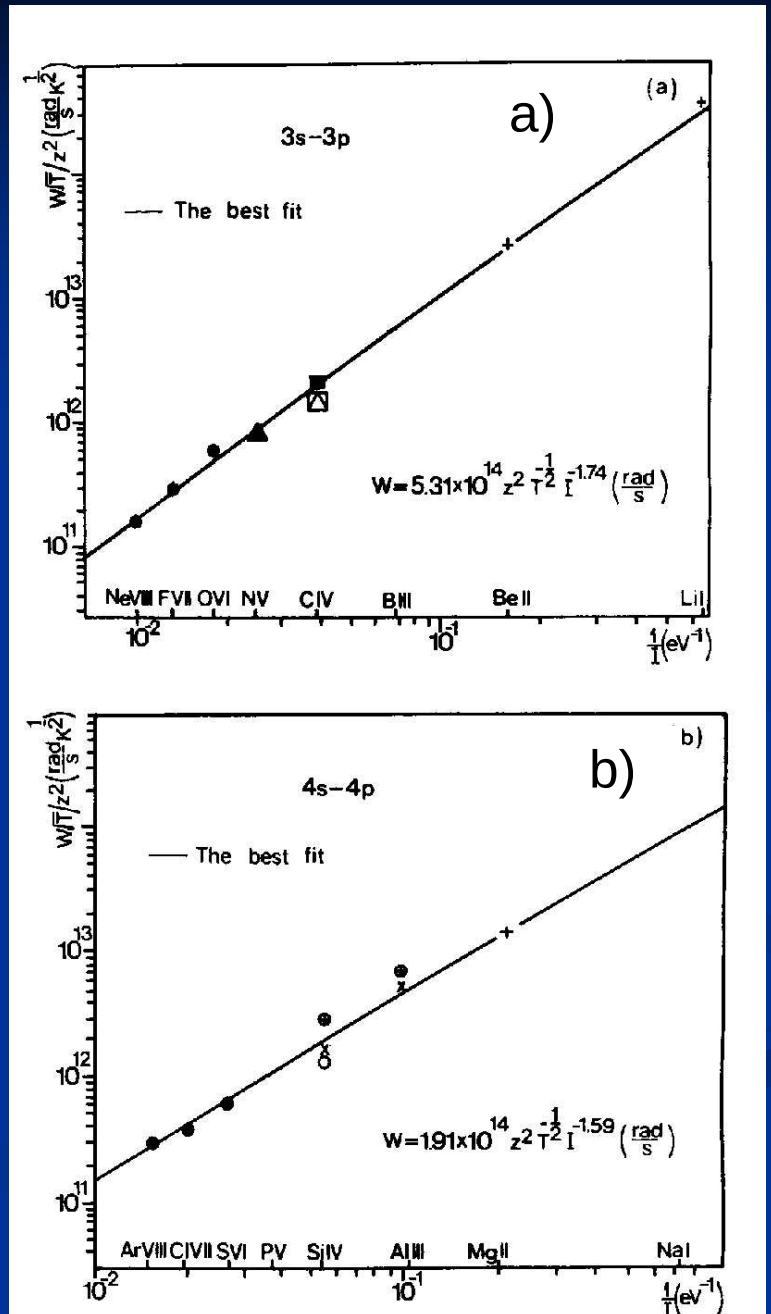

- The most general case: all transitions of all elements in different stages of ionization

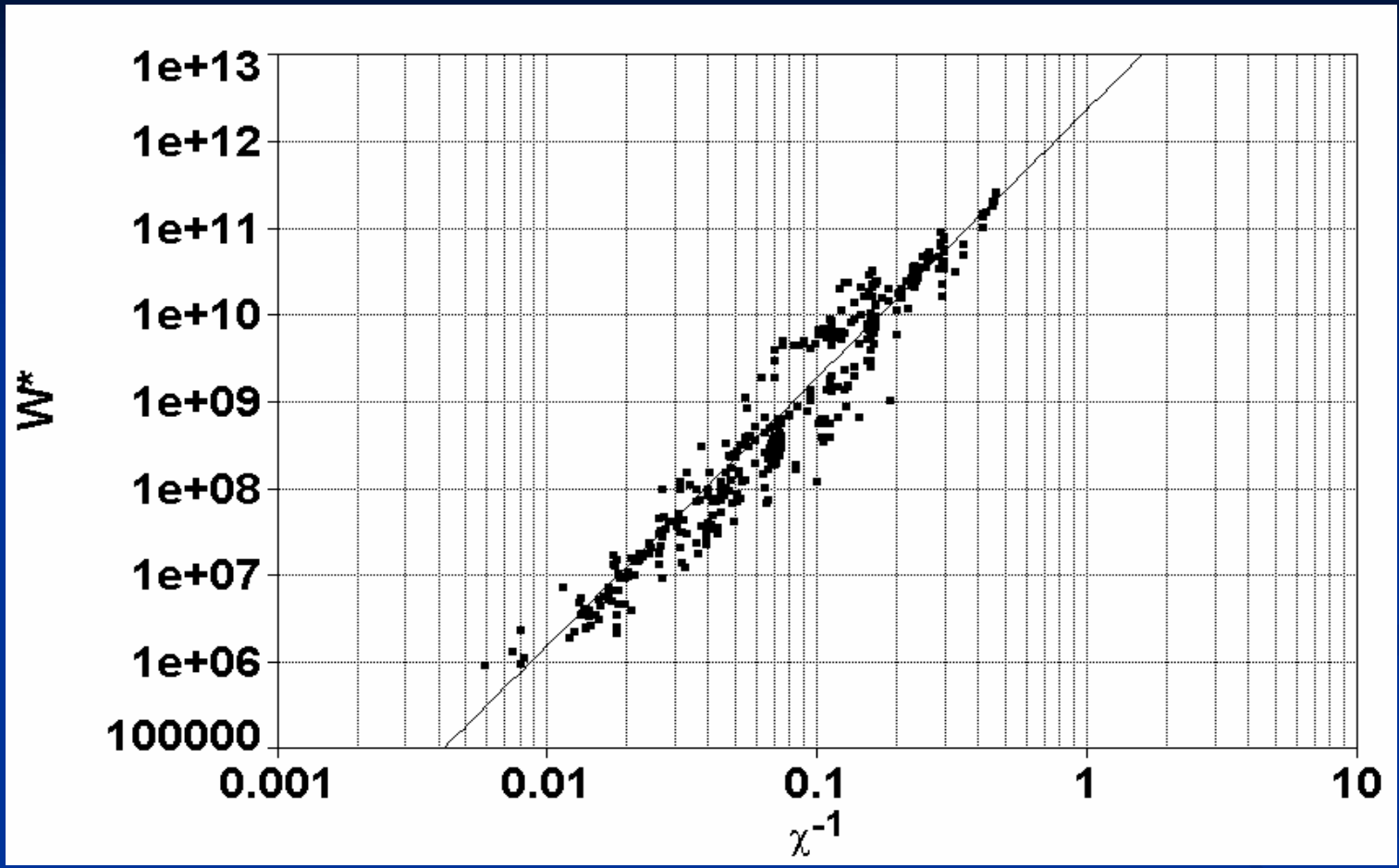

Fig.2.-Reduced Stark width W* (rad s-1) vs. inverse value of upper level ionization potential χ (eV) of the multiply charged ion of different elements along the periodic table

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a) Transition array 3s-3p

b) Transition array 3p-3d

c) Transition arrays 3s-3p and 3p-3d

experimental (square)

theoretical (triangle) data;

general trend dashed line

M. Scepanovic and J. Puric J.Quant. Spectrosc. Radiat. Transfer 78 (2003) 197-202

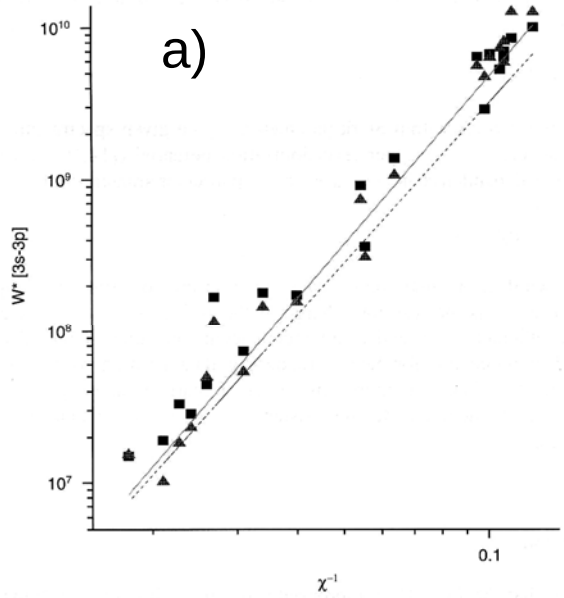


Fig. 1. Reduced Stark width W^* (rad/s) versus inverse value of upper level ionization potential χ (eV) of the multiply charged ion of different elements for $3s$–$3p$ transition array, square for experimental width, up triangle for calculated width, line for trend ($3s$–$3p$) and dash line for general trend.

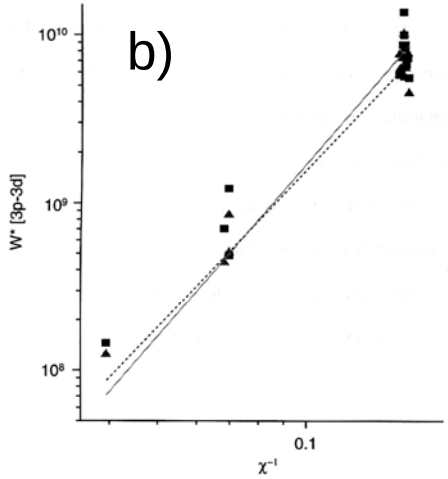


Fig. 2. Reduced Stark width W^* (rad/s) versus inverse value of upper level ionization potential χ (eV) of the multiply charged ion of different elements for $3p$–$3d$ transition array, square for experimental width, up triangle for calculated width, line for trend ($3p$–$3d$) and dash line for general trend.

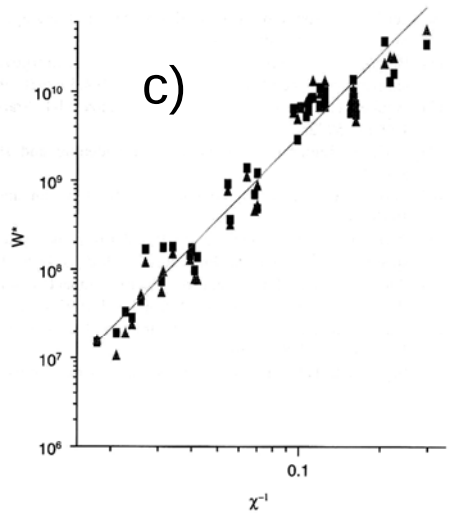


Fig. 3. Reduced Stark width W^* (rad/s) versus inverse value of upper level ionization potential χ (eV) of the multiply charged ion of different elements for $3s$–$3p$ and $3p$–$3d$ transition array, square for experimental width, up triangle for calculated width and line for trend.

- Regularities within 3s-3p transition arrays of different elements in different ionization stages (up to twelfth):
  - Theoretical data are taken from H.R. Griem, Spectral Line Broadening by Plasmas, New York Academic (1974) and Dimitrijević at al. and many other authors

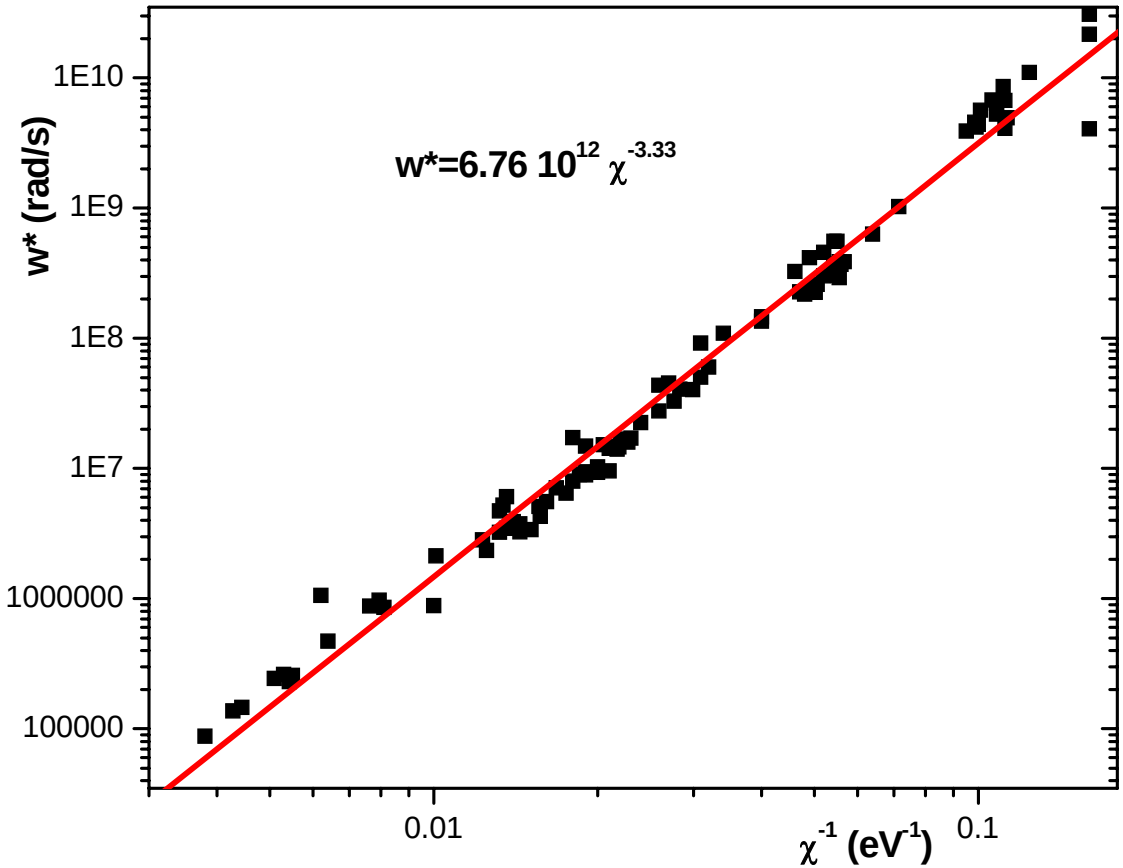


Fig.1. Reduced theoretical Stark width w^* (rad·s^{-1}) vs. inverse value of the upper level ionization potential χ (eV) of the multiply charged ions of different elements along the Periodic table (Puric at al. to be published)

- Experimental data are taken from N. Konjević, M. S. Dimitrijević and W. L. Wiese, J. Phys Chem. Ref. Data 13 (1984) 3, N. Konjević and W. L. Wiese, J. Phys Chem. Ref. Data 19 (1990) 6, N. Konjević, A. Lesage, J.R. Fuhr, W.L. Wiese, J. Phys. Chem. Ref. Data 31 (2002) 819 (and references therein)

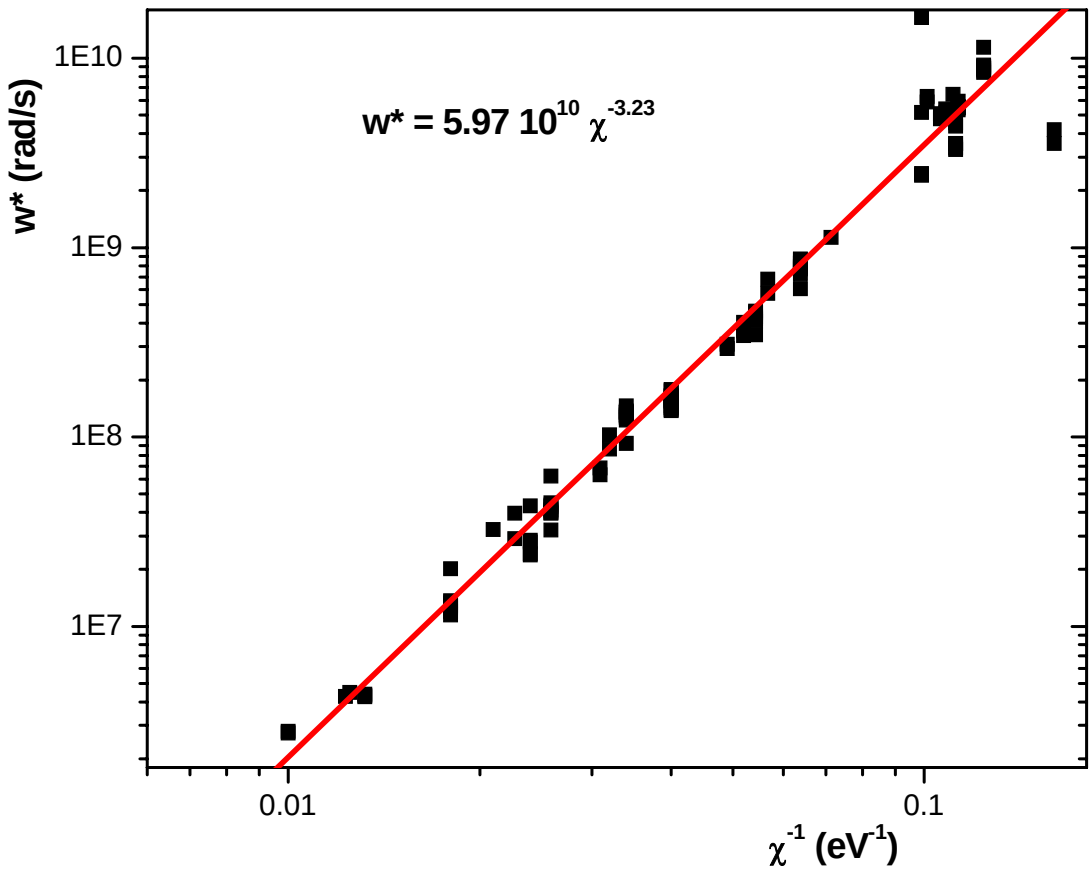


Fig.2. Reduced experimental Stark width w^* (rad·s^{-1}) vs. inverse value of the upper level ionization potential χ (eV) of the multiply charged ions of different elements along the Periodic table

- Theoretical and experimental data

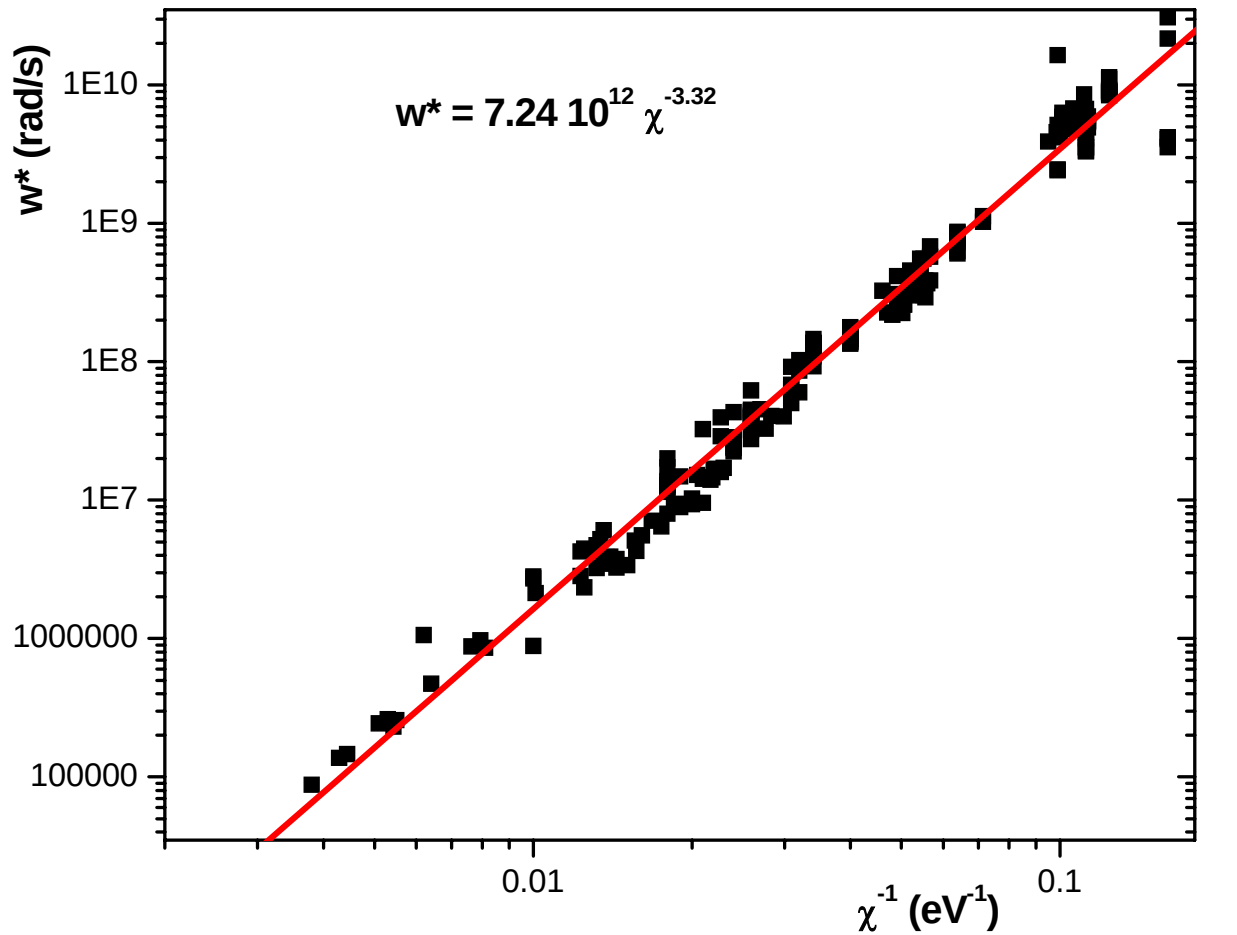


Fig.3. Reduced theoretical and experimental Stark width w^* (rad·s^{-1}) vs. inverse value of the upper level ionization potential χ (eV) of the multiply charged ions of different elements along the Periodic table

Data presented in figures 1-3 are normalized to electron density $N_e=10^{17}$ cm^{-3} electron temperature T=100 000 K

- The obtained equations can be used for predicting data where not available but originating from the same type of transition
- The accuracy of predicted data is comparable to the accuracies of the data used in the procedure of the establishing regularities:

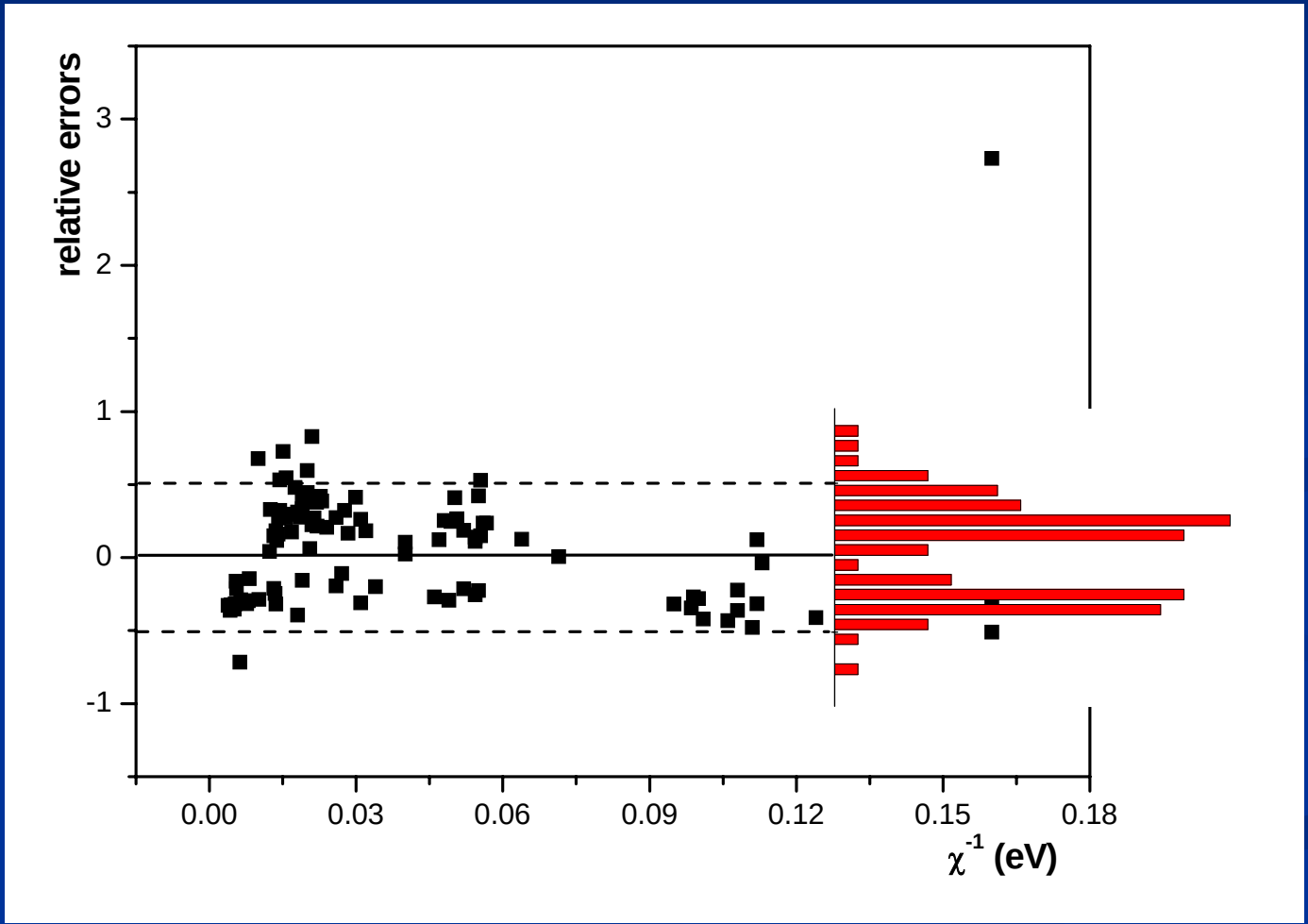


Fig. 4 Relative errors of theoretical data fit

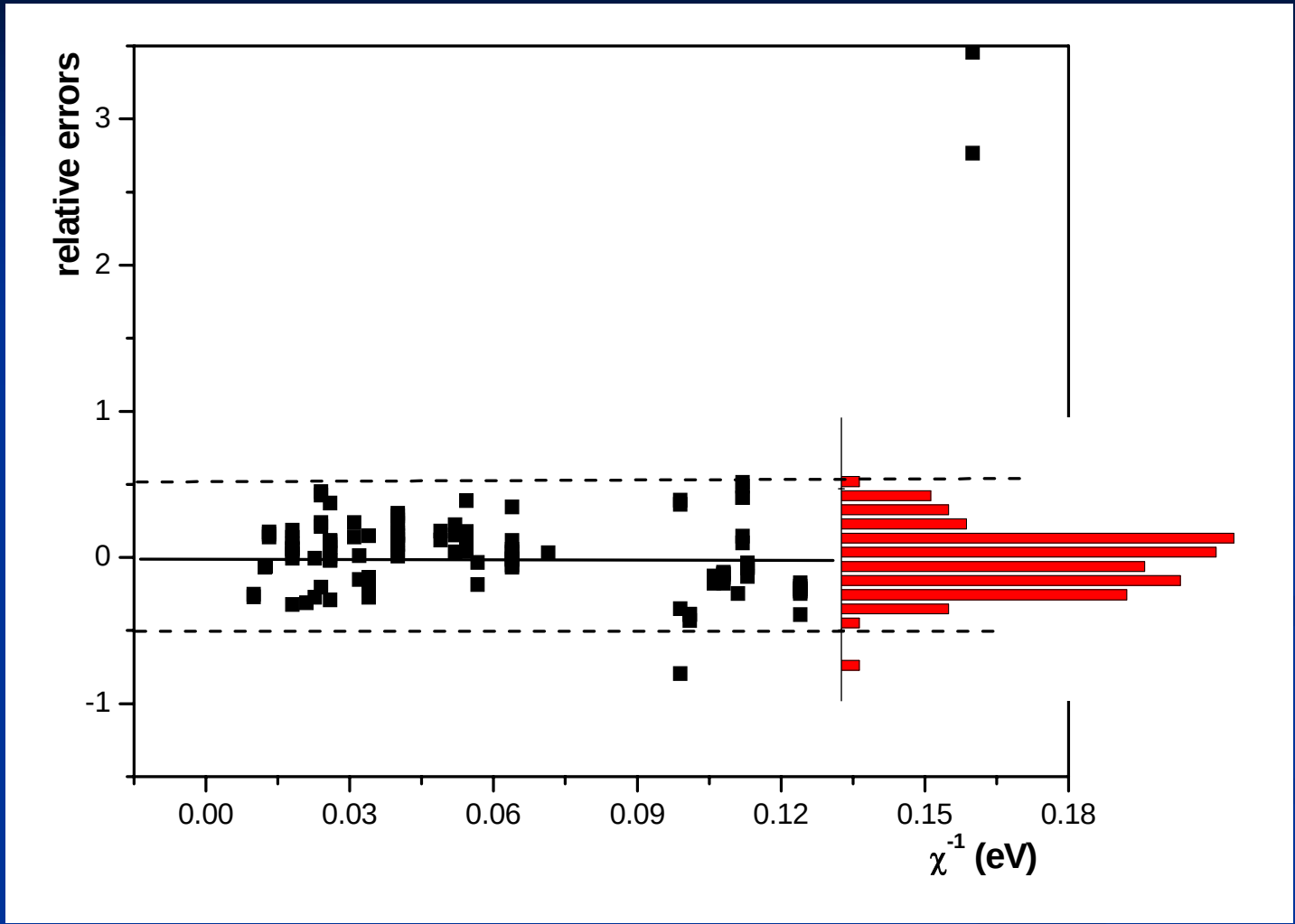


Fig. 5 Relative errors of experimental data fit

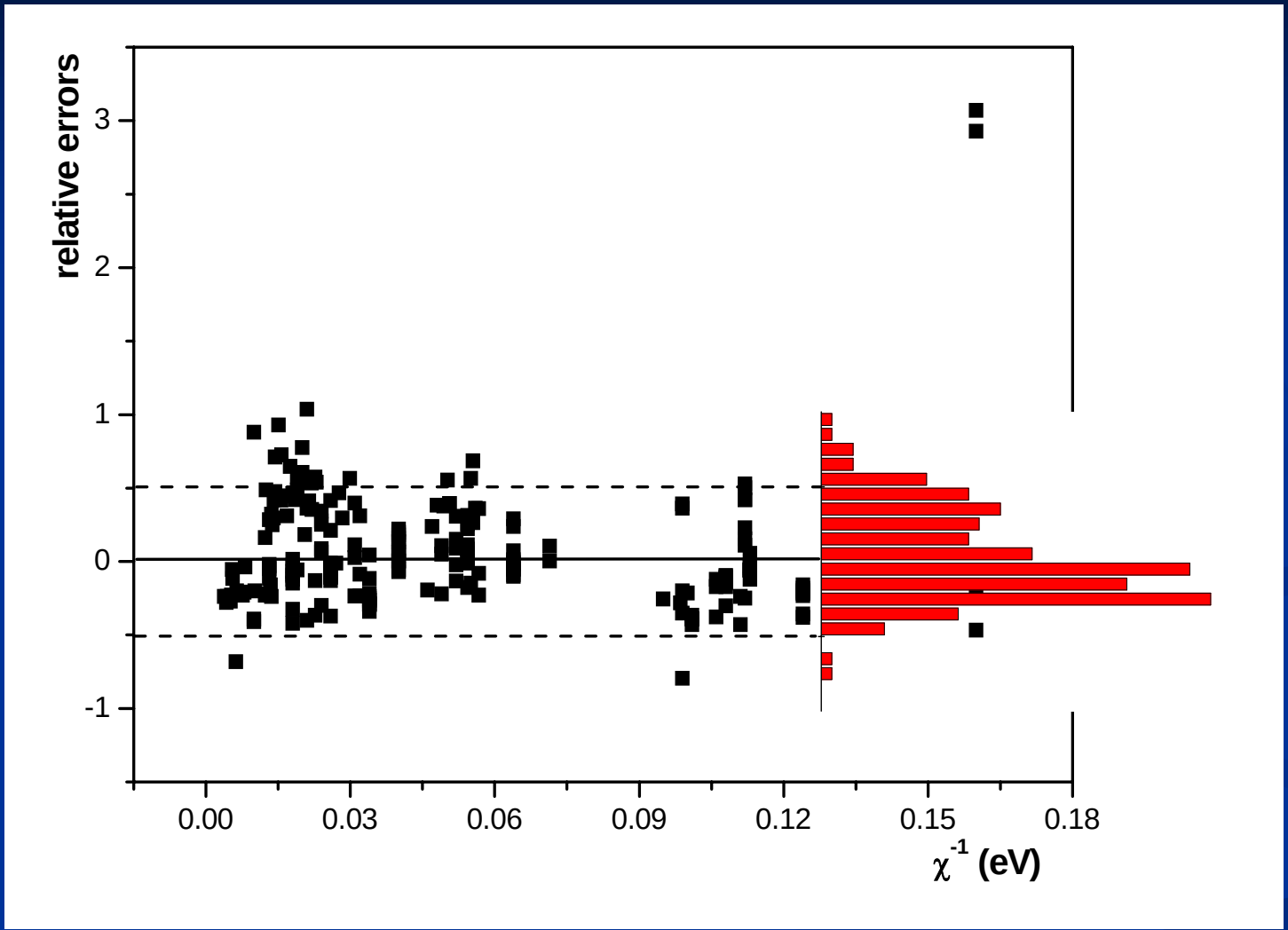


Fig. 6 Relative errors of theoretical and experimental data fit

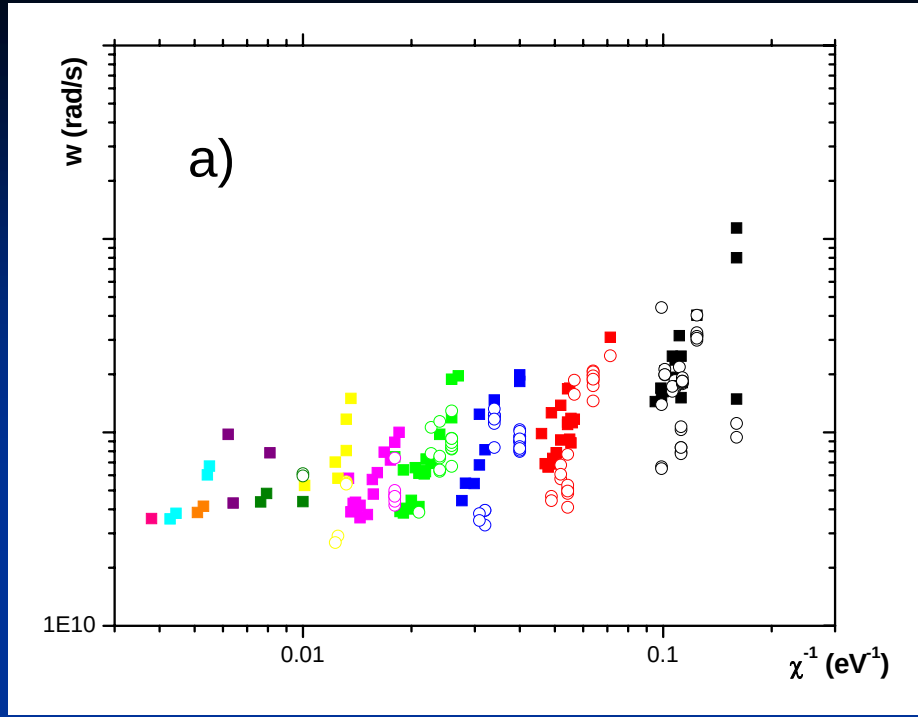
3s-3p transition array from different ionization stages

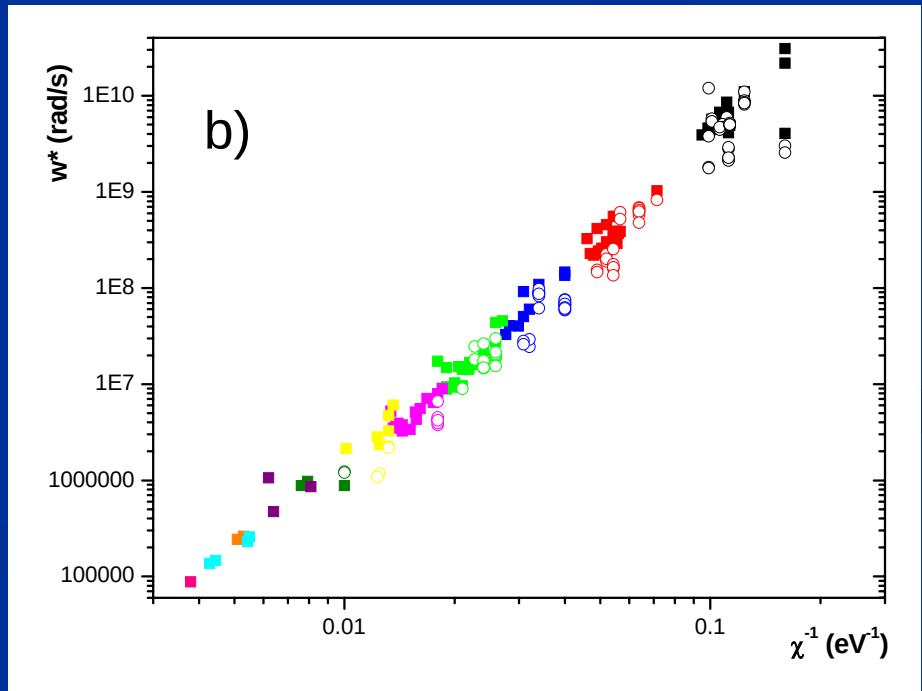
a) Experimental (circles) and theoretical (squares) Stark widths

b) Reduced Experimental (circles) and theoretical (squares) Stark widths

Different ionization stages:

II (black), III (red), IV (blue), V (green), VI (magenta), VII (yellow), VIII (olive), IX (purple), X (orange), XI (cyan) and XII (pink)





Conclusions

- Theoretically expected Stark parameters regularities within multiplet, supermultiplet, spectral series, transition arrays, homologous, isonuclear and isoelectronic sequences, same transition (e.g. resonance or off-resonance…) of atoms or ions of all elements along Periodic table can be explained on the bases of Stark widths and shift dependences of the upper level ionization potential and the rest core charge of the emitter

- These dependences on the rest core charge of the emitter (seeing by the electron undergoing transition) and the upper level ionization potential established using existing experimental and theoretical data can be used for prediction of Stark widths and shifts for the lines not calculated or measured so far

- The accuracy of the obtained data is the same as the accuracies of the data used in the procedure of establishing these dependences

References

[1] H.R. Griem, Spectral Line Broadening by Plasmas, New York Academic (1974).

[2] N. Konjević, A. Lesage, J.R. Fuhr, W.L. Wiese, J. Phys. Chem. Ref. Data **31** (2002) 819.

[3] J. Puric, M. Cuk, I.S. Lakicevic, Phys. Rev. A **32** (1985) 1106.

[4] J. Puric, I.S. Lakicevic, V. Glavonjic, Phys. Lett. **76A** (1980) 128.

[5] W.L. Wiese, N. Konjević, J.Q.S.R.T. **28** (1982) 185.

[6] W.L. Wiese, N. Konjević, J.Q.S.R.T. **47** (1992) 185.

[7] J. Puric, M.H. Miller, A. Lesage, ApJ. **416** (1993) 825.

[8] D.R. Inglis, E. Teller, ApJ. **90** (1939) 439.

[9] J. Purić, M. Šćepanović, ApJ. **521** (1999) 490.

[10] M. Šćepanović, J. Purić, J.Q.S.R.T **78** (2003) 197.

[11] J. Purić, M. Ćuk, M. Dimitrijević, A. Lesage, ApJ. **382** (1991) 353.

[12] N.J. Peacock, M.F. Stamp, J.D. Silver, Physica Scripta **T8** (1984) 10.

[13] J. Purić, S. Djeniže, A. Srećković, M. Ćuk, J. Labat, M. Platiša, Z. Phys. D **10** (1988) 431.

[14] M. Ivkovic, N. Ben Nessib, N. Konjević, J. Phys. B: At. Mol. Opt. Phys. 38 (2005) 715.
[15] M. S. Dimitrijević, S. Sahal-Br´echot, Serb. Astron. J. 160 (1999) 15.
[16] Yu.V. Ralchenko, H.R. Griem, I. Bray, J.Q.S.R.T. 81 (2003) 371.
[17] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. 128 (1998) 359.
[18] V. Milosavljević, M.S. Dimitrijević, S. Đeniže, Astrophys. J. Suppl. Ser. 135 (2001) 115.
[19] H. Elabidi, N. Ben Nessib, M.S. Dimitrijević, Mem. S. A. It. 7 (2005) 213.
[20] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. 129 (1998) 155.
[21] Z. Simić, M.S. Dimitrijević, L.Č. Popović, M.D. Dačić, J. Appl. Spectroscopy 72 (2005) 3.
[22] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. 133 (1998) 227.
[23] A. Srećković, M.S. Dimitrijević, S. Djeniže, A&A 371 (2001) 354.
[24] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. 107 (1994) 349.

[25] N. Ben Nessib, M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. **423** (2004) 397.

[26] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. **131** (1998) 141.

[27] M.S. Dimitrijević, S. Sahal-Brechot, Physica Scripta **61** (2000) 319.

[28] M.S. Dimitrijević, S. Sahal-Brechot, Astron. Astrophys. Suppl. Ser. **131** (1998) 143.

[29] B. Blagojevic, M. V. Popovic, N. Konjevic, M. S. Dimitrijevic, J. Quant. Spectrosc. Radiat. Transf. 61 (1999) 361.

[30] B. Blagojević, M. V. Popović, N. Konjević, Phys. Scr. 59 (1999) 374.

[31] A. Srećković, V. Drincić, S. Bukvić, S. Djenize, J. Phys. B 33 (2000) 4873.

[32] E. V. Sarandaev, M. Kh. Salakhov, J. Quant. Spectrosc. Radiat. Transf. 54 (1995) 827.

[33] S. Djenize, L. Č. Popović, J. Labat, A. Srećković, M. Platiša, Contrib. Plasma Phys. 33 (1993) 103.

[34] B. Blagojevic, M. V. Popovic, N. Konjevic, J. Quant. Spectrosc. Radiat. Transf. 67 (2000) 9.

[35] S. Djenize, J. Labat, A. Srećković, M. Platiša, J. Purić Phys. Scr. 44 (1991) 148.

[36] N. I. Uzelac, S. Glenzer, N.Konjević, J. D. Hey, H. -J. Kunze, Phys. Rev. E 47 (1993).

[37] J. A. Del Val, J. A. Aparicio, S. Mar, Astrophys. J. 536 (2000) 998.

[38] Th. Wrubel, I. Ahmad, S. Büscher, H. -J. Kunze, S. H. Glenzer, Phys. Rev. E 57 (1998) 5972.

[39] S. Glenzer, N. I. Uzelac, H. -J. Kunze, Phys. Rev. A 45 (1992) 8795.

[40] S. Mar, J. A. Aparicio, M. I. de la Rosa, J. A. del Val, M. A. Gigososs, V. R. Gonzalez, C. Perez, J. Phys. B 33 (2000) 1169.

[41] S. Djenize, A. Srećković, J. Labat, Astron. Astrphys. 253 (1992) 632.

[42] V. Milosavljević, S. Djenize, Astron.Astrophys., Suppl. Ser. 128 (1998) 197.

[43] J. A. Del Val, J. A. Aparicio, V. Gonzales, S. Mar, Astron. Astrophys. Suppl. Ser. 140 (1999) 171.

[44] S. Djenize, V. Milosavljević, A. Srećković, J. Quant. Spectrosc. Radiat. Transf. 59 (1998) 71.

[45] S. Glenzer, J. D. Hey, H. -J. Kunze, J. Phys. B 27 (1994) 413.

[46] G. S. Romanov, K. L. Stepanov, M. I. Sirkin, Opt. Spetrosc. (USSR) 47 (1979) 476.

[47] N. Konjević, T. L. Pittman, J. Quant. Spectrosc. Radiat. Transfer 37 (1987) 311.

[48] J. Purić, S. Djeniže, A. Srećković, M. Ćuk, J. Labat, M. Platiša, Z. Phys. D 8 (1988) 343.

[49] J. Purić, A. Srećković, S. Djeniže, M. Platiša, Phys. Rev. A 36 (1987) 3957.

[50] F. Böttcher, P. Breger, J. D. Hey, H. -J. Kunze, Phys. Rev. A 38 (1988) 2690.

[51] J. Purić, S. Djeniže, A. Srećković, M. Platiša, J. Labat, Phys. Rev. A 37 (1988) 498 .

[52] P. Bogen, Z. Naturforsch, Teil A 27 (1972) 210.

[53] M. Platiša, M. S. Dimitrijević, M. Popović, N. Konjević, Astron. Astrophys. 54 (1977) 837.

[54] M. Platiša, M. S. Dimitrijević, N. Konjević, Astron. Astrophys. 67 (1978) 103.

[55] M. Platiša, M. Popović, N. Konjević, Astron. Astrophys. 45 (1975) 325.

[56] J. Puric, M.H. Miller, A. Lesage, ApJ. **416** (1993) 825.

[57] S. Djenize at al. J.Quant. Spectrosc. Radiat. Transfer 42 (1989) 429-435.

[58] Puric at al. Fizika 20 (1988) 485.

[59] Puric at al. Phys. Rev. A 32 (1985) 1106.

[60] Puric at al. Z. Phys. D – Atoms, Molecules and Clusters 10 (1988) 431.

[61] Puric at al. Z. Phys. D – Atoms, Molecules and Clusters 10 (1988) 431.

[62] Puric and Scepanovic ApJ 521 (1999)353.