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Quantum Stark broadening data for the C IV, N V, O VI, F VII and Ne VIII resonance doublets

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ABSTRACT

In this paper, we present new Stark electron impact widths of the 2s–2p resonance doublets of the C IV, N V, O VI, F VII and Ne VIII ions, obtained using our quantum mechanical method. The present results are required to develop future spectral analysis using non-local thermodynamic equilibrium model atmospheres, which can make the determination of photospheric properties more accurate. Results are presented for a large range of electron temperatures required for plasma modelling. These are compared to the available theoretical ones. They are also used to check the previously obtained semiclassical perturbation results, and very good agreement is found. The atomic structure and collision data, used for the calculations of line broadening for the five ions studied here, are also calculated and compared to available theoretical results. The agreement found between the two calculations ensures that our line-broadening procedure uses the adequate structure and collision data. Scalings of linewidths with effective charge Z are also studied.

Key words: atomic data – line: profiles – scattering – stars: atmospheres – white dwarfs.

1 INTRODUCTION

The Stark broadening mechanism is important in stellar spectroscopy and the analysis of astrophysical and laboratory plasmas. Its influence should be considered in opacity calculations, the modelling of stellar interiors, the estimation of radiative transfer through stellar plasmas and the determination of chemical abundances of elements. For such investigations, in particular for opacity and radiative transfer calculations, a very large number of lines of different elements and their ions are needed (Dimitrijević 2003). For example, Barstow, Hubeny & Holberg (1998) have shown that the analysis of white dwarf atmospheres, where Stark broadening is dominant in comparison with the thermal Doppler broadening, cannot always be accomplished properly with models that neglect the opacity of heavy elements (Popović, Dimitrijević & Tankosić 1999; Tankosić, Popović & Dimitrijević 2003). Consequently, atomic and line-broadening data for many elements are necessary for stellar plasma research.

Rauch et al. (2007) have stressed that many line-broadening data for many species and their ions have been missed in the literature. Some other data exist but they are absent for the required temperatures and electron densities. It has been necessary to extrapolate these to the temperatures and densities at the line-forming regions, especially the line cores. This procedure can provide inaccurate results, especially in the case of extrapolation to temperatures, because the temperature dependence of linewidths can be very different. This lack of data represents an obstacle for the development of spectral analysis using non-local thermodynamic equilibrium (NLTE) model atmosphere techniques.

Rauch et al. (2007) have reported many problems that they have encountered in their determination of element abundances: the line cores of the S VI resonance doublet appear too deep to match the observation and they are not well suited for an abundance determination. Rauch et al. (2007) attributed this problem to the fact that the line-broadening tables of Dimitrijević & Sahal-Bréchot (1993a) are presented for an insufficient range of temperatures and densities for the calculations of the corresponding element abundances. The same problem has also been encountered for the resonance doublet of N V (the tables of Dimitrijević & Sahal-Bréchot 1992b were used) and O VI (the tables of Dimitrijević & Sahal-Bréchot 1992a were used). There was another problem related to the oxygen; Rauch et al. (2007) reproduced all the oxygen lines in their synthetic spectra except for O V λ1371. The lack of line-broadening data for these species and the lack of accurate results are the origin

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of many discrepancies between the observations and synthetic line profiles in Rauch et al. (2007).

The Stark broadening calculations in this paper are based on a quantum mechanical approach. The quantum mechanical expression for electron impact broadening calculations for intermediate coupling was obtained from Elabidi, Ben Nessib & Sahal-Bréchot (2004). We performed the first applications for the 2s3s–2s3p transitions in Be-like ions from nitrogen to neon (Elabidi et al. 2007, 2008a) and for the 3s–3p transitions in Li-like ions from carbon to phosphor (Elabidi, Ben Nessib & Sahal-Bréchot 2008b; Elabidi, Sahal-Bréchot & Ben Nessib 2009). This approach was also used in Elabidi & Sahal-Bréchot (2011) to check the dependence on the upper-level ionization potential of electron impact widths. Our quantum approach is an *ab initio* method. That is, all the parameters required for the calculations of the line broadening, such as radiative atomic data (energy levels, oscillator strengths, etc.) or collisional data (collision strengths or cross-sections, scattering matrices, etc.) are evaluated during the calculation and are not taken from other data sources. We used the sequence of the UCL atomic codes SST/DW/JAJOM that have been used for many years to provide fine structure wavefunctions, energy levels, wavelengths, radiative probability rates and electron impact collision strengths. Recently, these have been adapted to perform line-broadening calculations (Elabidi et al. 2008a).

In order to provide new line-broadening data at a wide range of temperatures suitable for spectral analysis, and thus useful for a more accurate determination of photospheric properties, in this paper we apply our quantum mechanical method to calculate Stark electron impact widths for the resonant doublets of C IV, N V, O VI, F VII and Ne VIII ions. By providing these quantum results, we hope that we can partially contribute to the removal of some of the above-listed discrepancies between the observations and the synthetic profiles reported in Rauch et al. (2007). Other problems have been reported for some other ions and lines, which will be dealt with in future work.

The results obtained have been used to check the previous semiclassical perturbation (SCP) calculations (Dimitrijević, Sahal-Bréchot & Bommier 1991; Dimitrijević & Sahal-Bréchot 1992a,b, 1994) by comparison with quantum mechanical calculations obtained with a more sophisticated theoretical approach that includes more accurate oscillator strengths. Attention has been paid to the scaling of linewidths with the charge Z 'seen' by the optical electron: $Z = z + 1$ (where z is the ionic charge). There is a difference between the Z-scaling of theoretical and experimental Stark widths for homologous transitions (3s–3p and 2s3s–2s3p within Li-like and Be-like isoelectronic sequences, respectively; Glenzer, Uzelac & Kunze 1992, 1993; Blagojević et al. 1999; Hegazy et al. 2003; Elabidi, Sahal-Bréchot & Ben Nessib 2009). Here, we also study the Z-scaling of the 2s–2p linewidth, and we compare our results with the semiclassical results.

2 OUTLINE OF THE THEORY AND COMPUTATIONAL PROCEDURE

Here, we present an outline of the quantum formalism of electron impact broadening. More details have been given elsewhere (Elabidi, Ben Nessib & Sahal-Bréchot 2004; Elabidi et al. 2008a). The calculations are performed within the frame of the impact approximation. This means that the time interval between collisions is much longer than the duration of a collision. The expression of the full width at half-maximum W obtained in Elabidi et al. (2008a) is

$$W = 2N_{\rm e}\left(\frac{\hbar}{m}\right)^2\left(\frac{2m\pi}{k_{\rm B}T}\right)^{1/2} \times \int_0^\infty \Gamma_w(\varepsilon)\exp\left(-\frac{\varepsilon}{k_{\rm B}T}\right)\,{\rm d}\left(\frac{\varepsilon}{k_{\rm B}T}\right). \quad (1)$$

Here, $k_{\rm B}$ is the Boltzmann constant, $N_{\rm e}$ is the electron density, T is the electron temperature and

$$\Gamma_w(\varepsilon) = \sum_{J_{\rm i}^{\rm T}J_{\rm f}^{\rm T}lK_{\rm i}K_{\rm f}} \frac{\left[K_{\rm i}, K_{\rm f}, J_{\rm i}^{\rm T}, J_{\rm f}^{\rm T}\right]}{2} \times \left\{\begin{array}{ccc} J_{\rm i} & K_{\rm i} & l \\ K_{\rm f} & J_{\rm f} & 1 \end{array}\right\}^2 \left\{\begin{array}{ccc} K_{\rm i} & J_{\rm i}^{\rm T} & s \\ J_{\rm f}^{\rm T} & K_{\rm f} & 1 \end{array}\right\}^2 \times \{1 - [{\rm Re}\,(S_{\rm i}){\rm Re}\,(S_{\rm f}) + {\rm Im}\,(S_{\rm i}){\rm Im}\,(S_{\rm f})]\}, \quad (2)$$

where $L_{\rm i} + S_{\rm i} = J_{\rm i}$, $J_{\rm i} + l = K_{\rm i}$ and $K_{\rm i} + s = J_{\rm i}^{\rm T}$. L and S represent the atomic orbital angular momentum and spin of the target, l is the electron orbital momentum and the superscript 'T' denotes the quantum numbers of the total electron+ion system. $S_{\rm i}$ ($S_{\rm f}$) are the scattering matrix elements for the initial (final) levels, expressed in the intermediate coupling approximation, and Re(S) and Im(S) are the real and imaginary parts, respectively, of the S-matrix element.

$$\left\{\begin{array}{ccc} a & b & c \\ d & e & f \end{array}\right\}$$

represent 6–j symbols, and we adopt the notation $[x, y, \ldots] = (2x + 1)(2y + 1)\ldots$. Both $S_{\rm i}$ and $S_{\rm f}$ are calculated for the same incident electron energy $\varepsilon = mv^2/2$. Equation (1) takes into account fine-structure effects and relativistic corrections resulting from the breakdown of the LS coupling approximation for the target.

The calculation starts with the study of the atomic structure in intermediate coupling, which is done using the SUPERSTRUCTURE code (SST; Eissner, Jones & Nussbaumer 1974). The scattering problem in LS coupling is carried out by the DISTORTED WAVE (DW) code (Eissner 1998), as in Elabidi et al. (2008a). This weak coupling approximation for the collision part assumed in DW is adequate for highly charged ions colliding with electrons, because the close collisions are of little importance. The JAJOM code (Saraph 1978) is used for the scattering problem in intermediate coupling. $\mathbf{R}$ matrices in intermediate coupling and the real (Re $\mathbf{S}$) and imaginary (Im $\mathbf{S}$) parts of the scattering matrix $\mathbf{S}$ have been calculated using the transformed version of JAJOM (Elabidi & Dubau, unpublished results) and the program RTOS (Dubau, unpublished results), respectively. The evaluation of Re $\mathbf{S}$ and Im $\mathbf{S}$ is carried out according to

$${\rm Re}\,\mathbf{S} = \left(1 - \mathbf{R}^2\right)\left(1 + \mathbf{R}^2\right)^{-1}, \qquad {\rm Im}\,\mathbf{S} = 2\mathbf{R}\left(1 + \mathbf{R}^2\right)^{-1}. \quad (3)$$

The relation $\mathbf{S} = (1 + i\mathbf{R})(1 - i\mathbf{R})^{-1}$ guarantees the unitarity of the $\mathbf{S}$ matrix.

3 RESULTS AND DISCUSSION

3.1 Structure and electron scattering data

We have used the $1s^2\ nl (2 \le n \le 5)$ configurations to study the atomic structure of the five Li-like ions from C IV to Ne VIII. This set of configurations gives rise to 24 fine-structure levels listed in Tables 1 and 2. We have used the SST code (Eissner, Jones &

Table 1. Our present energy levels (in Ry) for C IV, N V and O VI compared to those of NIST (Ralchenko et al. 2011), where *i* labels the 24 levels.

Level designation			C IV		N V		O VI	
i	Conf.	Level	Present	NIST	Present	NIST	Present	NIST
1	$1s^22s$	$^2S_{1/2}$	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000
2	$1s^22p$	$^2P^o_{1/2}$	0.58723	0.58762	0.73431	0.73324	0.88049	0.8782
3	$1s^22p$	$^2P^o_{3/2}$	0.58816	0.58860	0.73660	0.73559	0.88522	0.8831
4	$1s^23s$	$^2S_{1/2}$	2.75008	2.75976	4.14688	4.15653	5.82305	5.8325
5	$1s^23p$	$^2P^o_{1/2}$	2.90541	2.91651	4.34296	4.35372	6.05983	6.0701
6	$1s^23p$	$^2P^o_{3/2}$	2.90568	2.91680	4.34363	4.35442	6.06122	6.0715
7	$1s^23d$	$^2D_{3/2}$	2.94672	2.96052	4.40062	4.41422	6.13463	6.1476
8	$1s^23d$	$^2D_{5/2}$	2.94680	2.96062	4.40082	4.41442	6.13505	6.1481
9	$1s^24s$	$^2S_{1/2}$	3.64512	3.65735	5.51324	5.52546	7.75846	7.7703
10	$1s^24p$	$^2P^o_{1/2}$	3.70752	3.72081	5.59245	5.60558	7.85449	7.8673
11	$1s^24p$	$^2P^o_{3/2}$	3.70764	3.72092	5.59274	5.60588	7.85508	7.8679
12	$1s^24d$	$^2D_{3/2}$	3.72493	3.73926	5.61665	5.63087	7.88581	7.8996
13	$1s^24d$	$^2D_{5/2}$	3.72496	3.73929	5.61674	5.63095	7.88599	7.8998
14	$1s^24f$	$^2F^o_{5/2}$	3.72545	3.74015	5.61753	5.63217	7.88710	7.9014
15	$1s^24f$	$^2F^o_{7/2}$	3.72547	3.74015	5.61757	5.63221	7.88719	7.9015
16	$1s^25s$	$^2S_{1/2}$	4.04536	4.05850	6.12777	6.14090	8.63249	8.6451
17	$1s^25p$	$^2P^o_{1/2}$	4.07627	4.09028	6.16721	6.18113	8.68047	8.6942
18	$1s^25p$	$^2P^o_{3/2}$	4.07633	4.09034	6.16736	6.18128	8.68077	8.6942
19	$1s^25d$	$^2D_{3/2}$	4.08517	4.09968	6.17956	6.19400	8.69644	8.7104
20	$1s^25d$	$^2D_{5/2}$	4.08518	4.09970	6.17961	6.19404	8.69653	8.7104
21	$1s^25f$	$^2F^o_{5/2}$	4.08546	4.10015	6.18005	6.19471	8.69716	8.7115
22	$1s^25f$	$^2F^o_{7/2}$	4.08547	4.10015	6.18008	6.19471	8.69721	8.7115
23	$1s^25g$	$^2G_{7/2}$	4.08547	4.10023	6.18008	6.19481	8.69722	8.7116
24	$1s^25g$	$^2G_{9/2}$	4.08548	4.10023	6.18010	6.19481	8.69724	8.7116

Table 2. Same as in Table 1 but for F VII and Ne VIII.

Level designation			F VII		Ne VIII	
i	Conf.	Level	Present	NIST	Present	NIST
1	$1s^22s$	$^2S_{1/2}$	0.00000	0.00000	0.00000	0.00000
2	$1s^22p$	$^2P^o_{1/2}$	1.02632	1.02299	1.17210	1.16781
3	$1s^22p$	$^2P^o_{3/2}$	1.03503	1.03188	1.18689	1.18284
4	$1s^23s$	$^2S_{1/2}$	7.77889	7.78788	10.01479	10.02290
5	$1s^23p$	$^2P^o_{1/2}$	8.05640	8.06588	10.33311	10.34142
6	$1s^23p$	$^2P^o_{3/2}$	8.05897	8.06849	10.33747	10.34587
7	$1s^23d$	$^2D_{3/2}$	8.14910	8.16148	10.44455	10.45540
8	$1s^23d$	$^2D_{5/2}$	8.14989	8.16227	10.44589	10.45673
9	$1s^24s$	$^2S_{1/2}$	10.38114	10.39238	13.38177	13.39213
10	$1s^24p$	$^2P^o_{1/2}$	10.49403	10.50593	13.51157	13.52240
11	$1s^24p$	$^2P^o_{3/2}$	10.49511	10.50700	13.51340	13.52427
12	$1s^24d$	$^2D_{3/2}$	10.53277	10.54563	13.55808	13.56971
13	$1s^24d$	$^2D_{5/2}$	10.53310	10.54596	13.55865	13.57028
14	$1s^24f$	$^2F^o_{5/2}$	10.53458	10.54813	13.56049	13.57274
15	$1s^24f$	$^2F^o_{7/2}$	10.53474	10.54813	13.56078	13.57302
16	$1s^25s$	$^2S_{1/2}$	11.55989	11.57201	14.91051	14.92163
17	$1s^25p$	$^2P^o_{1/2}$	11.61644	11.62915	14.97566	14.98728
18	$1s^25p$	$^2P^o_{3/2}$	11.61699	11.62974	14.97660	14.98823
19	$1s^25d$	$^2D_{3/2}$	11.63618	11.64936	14.99934	15.01128
20	$1s^25d$	$^2D_{5/2}$	11.63635	11.64953	14.99963	15.01158
21	$1s^25f$	$^2F^o_{5/2}$	11.63718	11.65070	15.00067	15.01295
22	$1s^25f$	$^2F^o_{7/2}$	11.63727	11.65070	15.00082	15.01310
23	$1s^25g$	$^2G_{7/2}$	11.63728	11.65089	15.00083	15.01322
24	$1s^25g$	$^2G_{9/2}$	11.63733	11.65089	15.00092	15.01322

Nussbaumer 1974), where the wavefunctions are determined by diagonalization of the non-relativistic Hamiltonian using orbitals calculated in scaled Thomas–Fermi–Dirac–Amaldi (TFDA) potentials. The scaling parameters λ_l have been obtained by a self-consistent energy minimization procedure, in our case on all term energies of the 14 configurations. Relativistic corrections (spin-orbit, mass, Darwin and one-body) are introduced according to the Breit–Pauli approach (Bethe & Salpeter 1957) in intermediate coupling. In Tables 1 and 2, our level energies are compared to the experimental values compiled by the National Institute of Standards and Technology (NIST; Ralchenko et al. 2011). We find that the agreement between the two results is better than 1 per cent for all the ions studied here.

The oscillator strengths f_{ij} for some allowed transitions are presented in Tables 3 and 4 and are compared to the NIST values. The average agreement between them is about 3 per cent. However, we find for each ion that our oscillator strengths for some transitions are not in good agreement with those from NIST. For example, for the transitions $1s^22s\ ^2S_{1/2}$–$1s^24p\ ^2P^o_{1/2}$ (1–10), $1s^22s\ ^2S_{1/2}$–$1s^24p\ ^2P^o_{3/2}$ (1–11), $1s^23p\ ^2P^o_{1/2}$–$1s^24s\ ^2S_{1/2}$ (5–9) and $1s^23p\ ^2P^o_{3/2}$–$1s^24s\ ^2S_{1/2}$ (6–9), the agreements with the NIST values are 11, 11, 24 and 25 per cent, respectively. We find the same for the 1–10 and 1–11 transitions in the C IV ion.

Because our calculations are *ab initio*, the accuracy of the atomic structure (especially the oscillator strengths) is a prerequisite for the accuracy of the line-broadening results. From the above comparison, we can conclude that our atomic structure study is sufficiently accurate to be adopted in the scattering problem, and thus in the line-broadening calculations.

The electron scattering calculations in *LS* coupling have been performed in the distorted wave approximation through the DW code (Eissner 1998). Fine-structure collision strengths for low partial wave l of the incoming electron (l up to 29) have been obtained using the JAJOM code (Saraph 1978). This code transforms the transition matrix elements from *LS* coupling into intermediate ones using the term coupling coefficients (TCC)

Table 3. Oscillator strengths of some allowed transitions for C IV, N V and O VI compared to NIST values.

Transition	C IV		N V		O VI	
i–j	Present	NIST	Present	NIST	Present	NIST
1–2	0.0959	0.0953	0.0787	0.0780	0.0667	0.0661
1–3	0.1922	0.1905	0.1580	0.1563	0.1342	0.1327
1–5	0.0696	0.0678	0.0809	0.0794	0.0893	0.0885
1–6	0.1391	0.1355	0.1615	0.1588	0.1782	0.1770
1–10	0.0231	0.0204	0.0250	0.0230	0.0263	0.0247
1–11	0.0462	0.0408	0.0499	0.0459	0.0526	0.0494
2–4	0.0378	0.0375	0.0324	0.0323	0.0289	0.0289
2–7	0.6499	0.6456	0.6551	0.6531	0.6590	0.6576
2–9	0.0073	0.0070	0.0064	0.0062	0.0058	0.0057
3–4	0.0379	0.0377	0.0325	0.0323	0.0290	0.0290
3–7	0.0650	0.0646	0.0656	0.0652	0.0660	0.0656
3–8	0.5852	0.5807	0.5900	0.5874	0.5936	0.5915
3–9	0.0073	0.0070	0.0064	0.0062	0.0058	0.0057
4–5	0.1580	0.1599	0.1302	0.1312	0.1106	0.1114
4–6	0.3166	0.3199	0.2614	0.2630	0.2226	0.2239
4–10	0.0712	0.0678	0.0848	0.0818	0.0946	0.0922
4–11	0.1433	0.1358	0.1692	0.1637	0.1886	0.1849
5–7	0.0589	0.0628	0.0525	0.0552	0.0473	0.0492
5–9	0.0823	0.0815	0.0715	0.0708	0.0644	0.0637
6–7	–	0.0062	0.0052	0.0055	0.0046	0.0048
6–8	0.0528	0.0564	0.0469	0.0492	0.0420	0.0435
6–9	0.0825	0.0815	0.0717	0.0708	0.0647	0.0638
7–10	0.0136	0.0138	0.0131	0.0132	0.0127	0.0127
7–11	0.0027	0.0028	0.0026	0.0026	0.0025	0.0025

Table 4. Same as in Table 3 but for the F VII and Ne VIII transitions.

Transition	F VII		Ne VIII	
i–j	Present	NIST	Present	NIST
1–2	0.0578	0.0558	0.0510	0.0502
1–3	0.1167	0.1125	0.1034	0.1019
1–5	0.0957	0.0955	0.1008	0.1009
1–6	0.1909	0.1910	0.2008	0.2009
1–10	0.0273	0.0242	0.0280	0.0270
1–11	0.0545	0.0483	0.0559	0.0541
2–4	0.0264	0.0240	0.0246	0.0247
2–7	0.6621	0.6652	0.6646	0.6652
2–9	0.0053	0.0047	0.0050	0.0050
3–4	0.0266	0.0239	0.0249	0.0249
3–7	0.0663	0.0667	0.0666	0.0664
3–8	0.5967	0.5983	0.5992	0.5970
3–9	0.0054	0.0047	0.0051	0.0050
4–5	0.0962	0.0955	0.0850	0.0855
4–6	0.1942	0.1927	0.1725	0.1659
4–10	0.1022	0.1074	0.1082	–
4–11	0.2035	0.2143	0.2152	–
5–7	0.0430	0.0439	0.0395	0.0340
5–9	0.0594	0.0449	0.0557	–
6–7	0.0042	0.0043	0.0038	0.0037
6–8	0.0380	0.0388	0.0346	0.0324
6–9	0.0598	0.0448	0.0562	–
7–10	0.0123	–	0.0120	–
7–11	0.0024	–	0.0024	–

provided by SST. It is known that, for highly charged ions, the distorted wave approach is sufficiently accurate and the agreement between DW and more sophisticated methods (e.g. close coupling) is good.

For large l values, the above method becomes cumbersome and inaccurate, but the contributions of these values of l to collision strengths cannot be neglected. For $30 \leq l \leq 50$, we have adopted two different procedures. For allowed transitions, the contribution has been taken into account using the JAJOM–CBE code (Dubau, unpublished results) based upon the Coulomb–Bethe formulation of Burgess & Sheorey (1974) and adapted to the JAJOM approximation. For forbidden transitions, the contribution has been estimated by the SERIE-GEOM code, assuming a geometric series behaviour for high partial wave collision strengths (Chidichimo & Haig 1989; Chidichimo 1992).

We compare our collision strengths with those obtained by Aggarwal & Keenan (2004a,b) and Aggarwal, Keenan & Heeter (2010) using the Dirac atomic R-matrix code (DARC) of Norrington & Grant (private communication). This is a fully relativistic program, taking into account relativistic effects in both the target and the scattering study. This code is based on the *jj* coupling scheme and uses the Dirac–Coulomb Hamiltonian in the R-matrix approach. Table 5 presents collision strengths for C IV and O VI ions for transitions from the ground and the two first excited levels to the 10 first excited levels. In Table 6, we also present the collision strengths for N V, F VII and Ne VIII ions for transitions from the ground level to all the other levels. From Table 5, we find that the average relative difference between the two collision strengths ($\Delta\Omega/\Omega$) is about 36 per cent for C IV and 26 per cent for O VI. Table 6 shows that this difference is about 39 per cent for N V, 26 per cent for F VII and 17 per cent for Ne VIII. These results show clearly that our method is more adequate to highly charged ions. Thus, our results could converge to the more sophisticated R-matrix results for highly ionized atoms. The greatest disagreement between the two calculations is found

Table 5. Collision strengths for some transitions compared to the R-matrix (DARC) calculations: C IV (Aggarwal & Keenan 2004a); O VI (Aggarwal & Keenan 2004b).

Transition	C IV (06 Ry)		O VI (15 Ry)	
i–j	Present	DARC	Present	DARC
1–2	5.1181	4.9960	2.7505	2.8460
1–3	10.4218	9.9880	5.5515	5.6850
1–4	0.2514	0.3909	0.1384	0.1982
1–5	0.0678	0.0808	0.0583	0.0640
1–6	0.1363	0.1613	0.1175	0.1272
1–7	0.2846	0.2760	0.1602	0.1618
1–8	0.4278	0.4139	0.2410	0.2427
1–9	0.0442	0.0796	0.0256	0.0038
1–10	0.0150	0.0297	0.0116	0.0170
2–3	0.4900	0.6494	0.2078	0.2793
2–4	0.0904	0.1057	0.0317	0.0373
2–5	0.3042	0.4366	0.1519	0.2161
2–6	0.0975	0.1055	0.0428	0.0450
2–7	2.1122	2.1040	1.1306	1.1590
2–8	0.1561	0.1664	0.0604	0.0656
2–9	0.0151	0.0292	0.0055	0.0087
2–10	0.0515	0.0916	0.0274	0.0418
3–4	0.1790	0.2118	0.0641	0.0749
3–5	0.0974	0.1057	0.0430	0.0452
3–6	0.7260	0.9789	0.3568	0.0478
3–7	0.5740	1.0340	0.2843	0.3113
3–8	4.0250	3.9250	2.1278	2.1450
3–9	0.0297	0.0584	0.0111	0.0175
3–10	0.0253	0.0402	0.0110	0.0141

Table 6. Same as in Table 5 but for N v, F vii and Ne viii. Comparison is made with the R-matrix results of Aggarwal, Keenan & Heeter (2010).

Transition	N v (10 Ry)		F vii (20 Ry)		Ne viii (40 Ry)	
i–j	Present	DARC	Present	DARC	Present	DARC
1–2	3.6838	3.7070	2.1094	2.2310	1.6683	1.9940
1–3	7.4581	7.4010	4.2512	4.4440	3.3492	3.9660
1–4	0.1846	0.2708	0.1052	0.1502	0.0946	0.1252
1–5	0.0644	0.0723	0.0491	0.0538	0.0638	0.0658
1–6	0.1297	0.1440	0.0989	0.1068	0.1274	0.1304
1–7	0.2101	0.2090	0.1237	0.1260	0.1133	0.1180
1–8	0.3160	0.3135	0.1861	0.1890	0.1705	0.1770
1–9	0.0339	0.0533	0.0194	0.0288	0.0179	0.0240
1–10	0.0132	0.0217	0.0096	0.0134	0.0125	0.0147
1–11	0.0269	0.0432	0.0195	0.0267	0.0253	0.0292
1–12	0.0353	0.0422	0.0197	0.0229	0.0173	0.0196
1–13	0.0531	0.0633	0.0296	0.0343	0.0260	0.0294
1–14	0.0156	0.0185	0.0093	0.0104	0.0078	0.0085
1–15	0.0210	0.0247	0.0125	0.0139	0.0106	0.0113
1–16	0.0127	0.0222	0.0072	0.0116	0.0068	0.0093
1–17	0.0053	0.0116	0.0037	0.0062	0.0047	0.0062
1–18	0.0107	0.0231	0.0075	0.0124	0.0096	0.0123
1–19	0.0125	0.0182	0.0069	0.0092	0.0059	0.0072
1–20	0.0188	0.0273	0.0104	0.0138	0.0089	0.0108
1–21	0.0084	0.0109	0.0049	0.0057	0.0040	0.0043
1–22	0.0112	0.0145	0.0065	0.0077	0.0054	0.0058
1–23	0.0007	0.0011	0.0004	0.0005	0.0003	0.0003
1–24	0.0009	0.0013	0.0005	0.0006	0.0003	0.0004

for the 1–16, 1–17 and 1–18 transitions and also for 1–4 and 1–9 transitions. All these transitions are optically forbidden, except for the two transitions 1–17 and 1–18. We also note that in Aggarwal, Keenan & Heeter (2010), the highest difference between the R-matrix results and those obtained by the fully relativistic distorted wave code (FAC) of Gu (2003) is found for the 1–9, 1–10 and 1–11 transitions.

In general, the two sets of collision strengths agree within 28 per cent for the five ions. We note that besides the comparison of our linewidths with experimental and other theoretical linewidths, the comparison of our scattering parameters with other results can be another tool to ensure that our line-broadening calculations are sufficiently accurate. This is because the scattering problem provides scattering matrices that are used in the line-broadening calculations. A comparison with experimental scattering parameters (cross-sections or collision strengths) should be more efficient for this purpose. Such a comparison can be found in Elabidi, Sahal-Bréchot & Ben Nessib (2011).

3.2 Line-broadening data

Except for the C iv ion, there are no experimental results for the resonance line 2s–2p. In Table 7, we present our C iv linewidths compared to the measured linewidths and to other theoretical data. The present quantum mechanical calculations are always in agreement (within less than 1 per cent) with the semiclassical results (Dimitrijević, Sahal-Bréchot & Bommier 1991), but they are two times higher than the close coupling (CC) results (Seaton 1988). The modified semi-empirical widths (MSEs) are in agreement with the CC results within 23 per cent. If we now compare our widths (W) and the CC widths (W_{CC}) to the experimental values (W_m), we find $(W/W_m)_{av} = 1.71$ and $(W_{CC}/W_m)_{av} = 1.36$. It is perhaps not easy to make a conclusion about this last comparison, and new measurements for the C iv 2s–2p linewidths should be made in order to update the two last experiments (Bogen 1972; El-Farra & Hughes 1983).

Table 7. Present FWHM (in Å) of the C iv 2s ^{2}S–2p ^{2}P^o resonance line compared to the experimental results and to other theoretical results. SCP denotes semiclassical perturbation calculations (Dimitrijević, Sahal-Bréchot & Bommier 1991), MSE denotes modified semi-empirical calculations (Dimitrijević & Konjević 1981) and CC denotes close-coupling calculations (Seaton 1988).

T	W	W_{exp}	W/W_{SCP}	W/W_{CC}	W/W_{MSE}
2.0	1.18E−02	–	1.03	–	–
4.0	8.44E−03	–	–	1.90	2.33
5.0	7.60E−03	–	1.05	–	–
5.3[a]	7.40E−03	3.34E−03	–	1.92	–
6.0[b]	7.00E−03	5.83E−03	–	1.88	–
8.0	6.16E−03	–	1.07	1.96	2.4
10.0	5.61E−03	–	1.08	–	–
15.0	4.78E−03	_	1.11	–	–
20.0	4.30E−03	–	1.13	–	–

[a]El-Farra & Hughes (1983).
[b]Bogen (1972).

In Table 8, some of our results for the N v, O vi, F vii and Ne viii ions are compared to the available semiclassical results (Dimitrijević & Sahal-Bréchot 1992a,b, 1993b, 1994). The agreement between the two calculations is better for N v and O vi (the averaged value of the ratio W/W_{SCP} is about 1.04) than for the F vii and Ne viii cases (W/W_{SCP} is about 0.77). In Tables 9 and 10, we also present the Stark electron impact widths (W) of the C iv, N v, O vi, F vii and Ne viii resonance doublets for a wide range of electron temperatures (10^4–5×10^6 K) and at an electron density of 10^{17} cm^{-3}. Such temperatures are of interest for some hot star atmospheres, such as for PG 1195 stars and DO white dwarfs, subphotospheric layers, soft X-ray lasers and laser-produced plasmas. They are also important for fusion plasmas and stellar interiors. The wavelengths are taken from NIST (Ralchenko et al. 2011).

The results presented for the C iv, N v, O vi, F vii and Ne viii resonance linewidths will be of great interest in the development of spectral analysis using the NLTE model atmosphere techniques because they extend the missing broadening data to a wide range of temperatures and electron densities. For example, Stark broadening parameters for the considered ions are needed for the modelling and theoretical considerations of subphotospheric layers (Seaton 1987) and for the interpretation and modelling of some hot star spectra, such as, for example, PG 1159-type stars (Werner, Heber & Hunger 1991).

3.3 *Z*-scaling of linewidths

Elabidi, Sahal-Bréchot & Ben Nessib (2009) have studied the Z-scaling problem (where Z is the charge 'seen' by the optical electron) for the 3s–3p transitions in 10 Li-like ions from C iv to P xiii. We have found that our calculations give widths that are related to the charge by $W \propto Z^{-1.84}$, and that semiclassical calculations give $W \propto Z^{-1.43}$. This problem has been dealt with in some other experimental works. Blagojević et al. (1999) have found that the measured widths are related to the charge by $W \propto Z^{-0.79}$ for Li-like ions (only C iv, N v and O vi). Glenzer, Uzelac & Kunze (1992, 1993) and Hegazy et al. (2003) found $W \propto Z^{-1.13}$. This shows that there are still discrepancies between the experimental and the theoretical predictions of the Z-scaling of widths. In the present work, we try to look for the same Z-scaling, but for the 2s–2p resonance

Table 8. Present FWHM W (in Å) of the N V, O VI and Ne VIII 2s $^2S_{1/2}$–2p $^2P^o_{3/2}$ lines compared to the semiclassical perturbation results W_{SCP}: N V (Dimitrijević & Sahal-Bréchot 1992b); O VI (Dimitrijević & Sahal-Bréchot 1992a); F VII (Dimitrijević & Sahal-Bréchot 1993b); Ne VIII (Dimitrijević & Sahal-Bréchot 1994). Temperature values are given in 10^5 K and the electron density is 10^{17} cm^{-3}.

	N V		O VI		F VII		Ne VIII	
T	W	W/W_{SCP}	W	W/W_{SCP}	W	W/W_{SCP}	W	W/W_{SCP}
0.5	3.44E−03	0.96	–	–	–	–	–	–
1	2.49E−03	0.98	1.45E−03	0.99	7.20E-04	0.81	–	–
2	1.85E−03	1.01	1.07E−03	1.02	5.21E-04	0.81	3.14E−04	0.72
4	–	–	–	–	–	–	–	–
5	1.30E−03	1.04	7.67E−03	1.11	3.50E-04	0.82	2.07E−04	0.73
8	–	–	6.24E−03	1.09	–	–	–	–
10	–	–	–	–	2.64E-04	0.83	1.55E−04	0.74
20	–	–	–	–	–	–	1.15E−04	0.73

Table 9. Stark electron impact widths (FWHM) in Å of the 2s $^2S_{1/2}$–2p $^2P^o_{3/2}$ line for C IV, N V, O VI, F VII and Ne VIII. Temperature values are given in 10^5 K and the electron density is 10^{17} cm^{-3}.

	C IV	N V	O VI	F VII	Ne VIII
T	1548.19	1238.82	1031.91	883.10	770.41
0.1	1.65E−02	7.54E−03	3.91E−03	2.22E−03	1.35E−03
0.3	9.66E−03	4.39E−03	2.27E−03	1.29E−03	7.81E−04
0.5	7.60E−03	3.44E−03	1.77E−03	1.00E−03	6.08E−04
1.0	5.61E−03	2.49E−03	1.28E−03	7.20E−04	4.35E−04
3.0	3.72E−03	1.58E−03	7.90E−04	4.35E−04	2.60E−04
5.0	3.09E−03	1.30E−03	6.58E−04	3.50E−04	2.07E−04
10.0	2.34E−03	9.92E−04	5.06E−04	2.64E−04	1.55E−04
50.0	9.65E−04	4.38E−04	2.26E−04	1.25E−04	7.46E−05

Table 10. Same as in Table 9 but for the 2s $^2S_{1/2}$–2p $^2P^o_{1/2}$ line.

	C IV	N V	O VI	F VII	Ne VIII
T	1550.77	1242.80	1037.61	890.76	780.32
0.1	1.68E−02	7.68E−03	4.00E−03	2.28E−03	1.40E−03
0.3	9.82E−03	4.47E−03	2.32E−03	1.32E−03	8.09E−04
0.5	7.72E−03	3.50E−03	1.81E−03	1.03E−03	6.30E−04
1.0	5.68E−03	2.53E−03	1.30E−03	7.39E−04	4.50E−04
3.0	3.76E−03	1.60E−03	8.01E−04	4.46E−04	2.69E−04
5.0	3.12E−03	1.32E−03	6.57E−04	3.59E−04	2.14E−04
10.0	2.35E−03	1.00E−03	5.02E−04	2.70E−04	1.60E−04
50.0	9.69E−04	4.42E−04	2.28E−04	1.28E−04	7.68E−05

transitions of Li-like ions. There are not enough experimental widths at the required temperatures for the transitions of ions studied here (except for C IV). Therefore, we cannot perform an experimental Z-scaling for comparison. In Fig. 1, we present the behaviour of $\log_{10}(W)$ and $\log_{10}(W_{SCP})$ as a function of $\log_{10}(Z)$. The widths are expressed in angular frequency units. We find that the dependence of the linewidths with the charge Z can be expressed as $W \propto Z^{-\alpha}$ with $\alpha = 1.67$ for our values and $\alpha_{SCP} = 1.13$ for the semiclassical values. We also note that these values of α can be different for different chosen temperatures. Fig. 2 displays the same Z-scaling of linewidths, but at temperature $T = 2 \times 10^5$ K and for the same electron density as in Fig. 1. We find $\alpha = 1.76$ and $\alpha_{SCP} = 1.11$. To decide about the validity and utility of this scaling, more experimental linewidths are needed for the resonance transitions of the five studied ions.

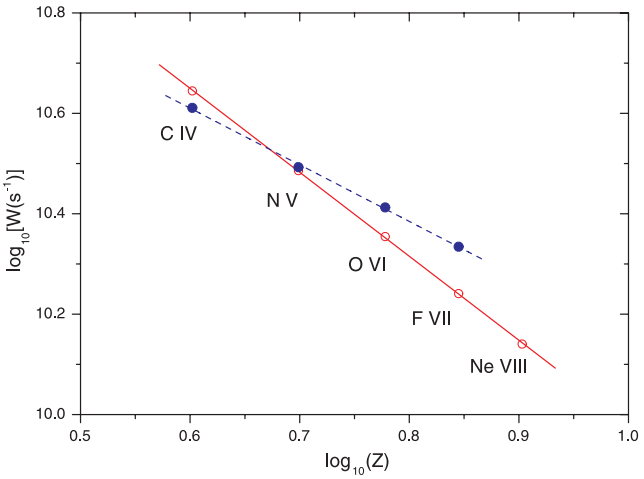

Figure 1. Our Stark width in angular frequency units W (open circles) of the 2s $^2S_{1/2}$–2p $^2P^o_{3/2}$ transition for the C IV, N V, O VI, F VII and Ne VIII ions as a function of Z compared with the semiclassical widths W_{SCP} (solid circles). The solid and dashed lines are the linear fits of the W and W_{SCP} widths, respectively. $T = 10^5$ K and $N_e = 10^{17}$ cm^{-3}.

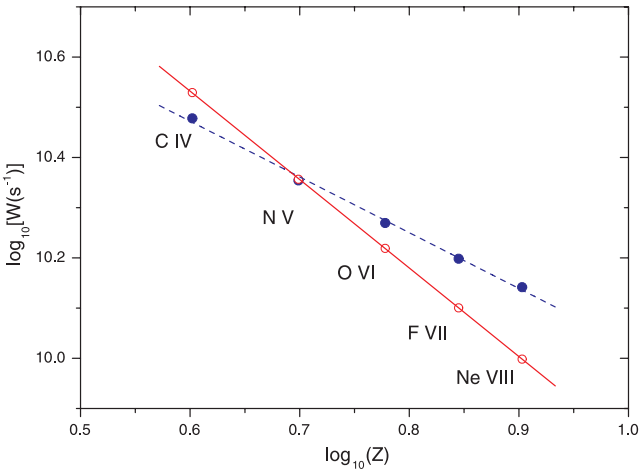

Figure 2. Same as in Fig. 1, but for $T = 2 \times 10^5$ K.

4 SUMMARY OF THE RESULTS AND CONCLUSION

We have performed quantum mechanical calculations of Stark electron impact widths for the resonance doublets of the C IV, N V, O VI,

F VII and Ne VIII ions. Our results are presented within the wide range of temperatures required for the development of spectral analysis using the NLTE model atmospheres. Our calculated data can solve some of the problems that have been encountered and reported by Rauch et al. (2007) when calculating the element abundance by filling in the missing line-broadening data. Thus, it is no longer necessary to extrapolate the existing data, as was done for some cases in Rauch et al. (2007). Our quantum linewidths have also been compared to the SCP results in order to check the previous SCP calculations. A good agreement has been found between them (within 1 per cent).

A confirmation of previous SCP results using more sophisticated quantum mechanical results is important as such data are often used for stellar spectra modelling and interpretation. In some cases (e.g. hot white dwarfs) the Stark broadening is the dominant broadening mechanism, and the accuracy of used data might be important.

Our results are also compared to the only experimental results for C IV lines (El-Farra & Hughes 1983; Bogen 1972). We find that our calculations give linewidths that are 71 per cent higher than those measured. The CC (Seaton 1988) and MSE results (Dimitrijević & Konjević 1981) agree well; regarding the lines investigated here, they exist only for the C IV lines. More measurements of the resonance lines for these ions would be very useful for checking the previous and present calculations.

Part of this work has been dedicated to the Z-scaling of linewidths. As in previous papers (Glenzer, Uzelac & Kunze 1992, 1993; Blagojević et al. 1999; Elabidi, Sahal-Bréchot & Ben Nessib 2009), the scaling with Z is different from one approach to another. We find that widths are related to Z by $W \propto Z^{-\alpha}$ when $\alpha = 1.67$ for our calculations and $\alpha_{\rm SCP} = 1.13$ for the SCP calculations for $T = 10^5$ K. These values of α can change with temperature (e.g. for $T = 2 \times 10^5$ K, we find $\alpha = 1.76$ and $\alpha_{\rm SCP} = 1.11$). Because there are not enough experimental results for these lines, we cannot make any conclusions about this scaling.

We have also calculated the atomic structure and collision data for the five ions. A comparison with the NIST values (Ralchenko et al. 2011) for the atomic structure shows an agreement better than 1 per cent for level energies, and within 3 per cent for the oscillator strengths. Our distorted wave collision strengths have been compared to the R-matrix results (Aggarwal & Keenan 2004a,b; Aggarwal, Keenan & Heeter 2010) at different electron energies. We find an average relative difference (over the five ions) between the two approaches of about 28 per cent. We confirm that the distorted wave method is more adequate for highly charged ions. Because in our line-broadening calculation procedure we use atomic structure (level energies and oscillator strengths) and collision data (collision strengths, scattering matrices), this comparison might be another tool to check our line-broadening results, besides a comparison of widths with those measured.

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