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► **To cite this version:**

R. Aloui, H. Elabidi, S. Sahal-Bréchet. Stark broadening and atomic data for Ar XVI. Contributions of the Astronomical Observatory Skalnaté Pleso, 2020, 50, pp.154-163. 10.31577/caosp.2020.50.1.154 . insu-03718060

HAL Id: insu-03718060

<https://insu.hal.science/insu-03718060v1>

Submitted on 8 Jul 2022

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Stark broadening and atomic data for Ar XVI

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Received: August 1, 2019; Accepted: August 16, 2019

Abstract. Stark broadening and atomic data calculations have been developed for the recent years, especially atomic and line broadening data for highly ionized ions of argon. We present in this paper atomic data (such as energy levels, line strengths, oscillator strengths and radiative decay rates) for Ar XVI ion and quantum Stark broadening calculations for 10 Ar XVI lines. Radiative atomic data for this ion have been calculated using the University College London (UCL) codes (SUPERSTRUCTURE, DISTORTED WAVE, JAJOM) and have been compared with other results. Using our quantum mechanical method, our Stark broadening calculations for Ar XVI lines are performed at electron density $N_e = 10^{20} \text{ cm}^{-3}$ and for electron temperature varying from 7.5×10^5 to 7.5×10^6 K. No Stark broadening results in the literature to compare with. So, our results come to fill this lack of data.

Key words: line:profiles– stars– atomic data– Stark line broadening.

1. Introduction

Lithium-like ions are of importance in astrophysical and magnetized plasmas. Many emission lines of highly ionized argon, such as Ar IX–XVIII, were studied in Dere et al. (2001). Many Li-like transitions were useful for the determination of chemical abundances (Lemen et al., 1986). The number of the previous publications shows the importance of the Li-like ions: In Aggarwal & Keenan (2013), the authors reported the atomic data for Li-like ions with $12 \leq Z \leq 20$. In Whiteford et al. (2002), the authors performed the calculations of energy levels for Ar XVI ion by using AUTOSTRUCTURE (AS) code of Badnell (1997). Recently, in McKeown et al. (2004), the authors calculated the energy levels and radiative rates for Ar XVI and Fe XXIV. Atomic and line broadening data of highly ionized atoms are required in plasma physics. These parameters are used in the opacity calculations. They were also required for the modelling of fusion

plasmas (Peacock et al., 1997) as many elements were presented as impurities in the reactor walls. They determined the chemical abundances of elements and they used to test various theoretical approximations (Dimitrijević, 2003). Theoretical atomic data for Ar XVI were required for the modelling and diagnostics of plasmas and not available from measurements (McKeown et al., 2004).

Argon ions played a great role in technological devices and plasma applications (Djurović et al., 2011). We choose to study Ar XVI because of its ground configuration $1s^2 2s^1$ (with one external electron on closed shells), this ion is like hydrogen, thus their atomic properties can be calculated *ab initio* with a great accuracy. Therefore we perform another calculations to assess a precision of the available data, and that results can be applied with confidence in plasma diagnostics. Despite the importance of these parameters for stellar plasma research, for the interpretation of high-resolution spectra from astrophysical sources, the line broadening data of Ar XVI are totally missing in the literature. To fill this lack, we calculated their parameters using our quantum mechanical method. We hope that our results enrich the databases of astrophysicists. In the present work, the calculations of atomic data are computed by the sequence of UCL (University College, London) atomic packages (SUPERSTRUCTURE (Eissner et al., 1974)/DW (Eissner, 1998)/JAJOM (Saraph, 1978)). In Elabidi et al. (2014); Elabidi & Sahal-Bréchet (2018); Aloui et al. (2018, 2019), the authors adapted these packages to provide Stark broadening data for several argon lines missing in the literature. This method gave acceptable results. In Aloui et al. (2018), we calculated the Stark widths for Ar VII spectral lines. In Aloui et al. (2019), we computed quantum Stark broadening data for Ar VIII and Ar IX lines.

2. Outline of our line broadening method

To perform the present line broadening calculations, we have used our quantum mechanical method obtained in Elabidi et al. (2004, 2008). The expression of the full width at half-maximum (valid at temperatures and densities studied here), W is given by the following expression:

$$W = 2N \left(\frac{\hbar}{m} \right)^2 \left(\frac{2m\pi}{k_B T} \right)^{\frac{1}{2}} \times \int_0^{\infty} \Gamma_w(E) \exp\left(-\frac{\epsilon}{k_B T}\right) d\left(\frac{\epsilon}{k_B T}\right), \quad (1)$$

where the integration is over the Maxwellian velocity distribution, m is the electron mass, k_B is the Boltzmann constant, N is the electron density, T denotes

the electron temperature, ϵ is the incident electron energy, and

$$\begin{aligned} \Gamma_w(\epsilon) = & \sum_{J_i^T J_f^T l K_i K_f} \frac{[K_i, K_f, J_i^T, J_f^T]}{2} \\ & \times \left\{ \begin{matrix} J_i K_i l \\ K_f J_f 1 \end{matrix} \right\}^2 \left\{ \begin{matrix} K_i J_i^T s \\ J_f^T K_f 1 \end{matrix} \right\}^2 \\ & \times [1 - (\text{Re}(\mathbf{S}_i)\text{Re}(\mathbf{S}_f) + \text{Im}(\mathbf{S}_i)\text{Im}(\mathbf{S}_f))], \end{aligned} \quad (2)$$

where $L_i + S_i = J_i$, $J_i + l = K_i$ and $K_i + s = J_i^T$. L is the atomic orbital angular momentum, S is the spin of the target, l is the electron orbital momentum. The superscript T designates the operators of the total system (electron+ion). \mathbf{S}_i (\mathbf{S}_f) represent the scattering matrix elements for the initial (final) levels in intermediate coupling. $\text{Re}(\mathbf{S})$ and $\text{Im}(\mathbf{S})$ denotes the real and the imaginary parts of the \mathbf{S} -matrix, respectively. $\left\{ \begin{matrix} abc \\ def \end{matrix} \right\}$ designate 6-j symbols and we use the notation $[x, y, \dots] = (2x+1)(2y+1)\dots$

To calculate both \mathbf{S}_i and \mathbf{S}_f , we use the same incident electron energy $\epsilon = mv^2/2$. The SUPERSTRUCTURE (SST) code (Eissner et al., 1974) calculates the atomic structure in intermediate coupling, where configuration interaction and relativistic corrections (spin-orbit, mass, Darwin and one-body) are included according the Breit-Pauli approach (Bethe & Salpeter, 1957). The radial wave functions are determined by diagonalization of the non relativistic Hamiltonian using orbitals calculated in a scaled Thomas FermiDirac Amaldi (TFDA) potential. The potential depends on scaling parameters λ_l that have been obtained by a selfconsistent energy minimization on the term energies included in our calculations. The DISTORTED WAVE (DW) code (Eissner, 1998) performs the electron-ion scattering calculations and produces reaction matrices \mathbf{R} in LS coupling. The JAJOM code (Saraph, 1978) treats the scattering calculations in intermediate coupling. This code uses the term coupling coefficients (TCC) -resulting of SST calculations- and these matrices in LS coupling (obtained by DW) to calculate collision strengths and reactance matrices \mathbf{R} in intermediate coupling. This resulting matrices \mathbf{R} and the $\text{Re} \mathbf{S}(\text{Im} \mathbf{S})$ which are obtained using JAJPOLARI program -the transformed of JAJOM code- (Elabidi & Dubau, unpublished results) and RtoS program (Dubau, unpublished results) have been used as input data suitable for the formula (2). $\text{Re} \mathbf{S}$ and $\text{Im} \mathbf{S}$ are assessed by the expressions below:

$$\text{Re} \mathbf{S} = (1 - \mathbf{R}^2) (1 + \mathbf{R}^2)^{-1}, \text{Im} \mathbf{S} = 2\mathbf{R} (1 + \mathbf{R}^2)^{-1} \quad (3)$$

3. Results and discussions

3.1. Structure and radiative data

Structural and radiative atomic data have been calculated using the SUPERSTRUCTURE code of Eissner et al. (1974). We have used 6 configurations: $1s^2$ (2s, 2p, 3s, 3p, 3d and 4s). These configurations give rise to 6 terms and 9 levels of fine structure. The code (SST) provides also the scaling parameters ($\lambda_s = 1.3116$, $\lambda_p = 0.9392$ and $\lambda_d = 0.8683$). In Table 1, we display the present energy levels for Ar XVI in cm^{-1} and compare them with the experimental results of NIST (Kramida et al., 2018), with those calculated in McKeown et al. (2004) (GRASP) who used the GRASP (General purpose Relativistic Atomic Structure Package) code (Dyall et al., 1989), with those calculated from McKeown et al. (2004) (CIV3) who used the CIV3 code of Hibbert (1975), and with those from Whiteford et al. (2002) (AS) who used the AUTOSTRUCUTRE code (Badnell, 1997). As it is shown in Table 1, the average errors between our results and all the other ones are less than 1%.

The absorption oscillator strengths f_{ij} and radiative rates A_{ji} (in s^{-1}) for a transition $i \rightarrow j$ are related by the following expression (Aggarwal & Keenan, 2013):

$$f_{ij} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji}, \quad (4)$$

Table 1. Present fine structure energy levels E (in cm^{-1}) for Ar XVI ion compared with NIST values (Kramida et al., 2018), with GRASP values: the calculated results from McKeown et al. (2004) who used the GRASP code of Dyall et al. (1989), with CIV3 values: the results from McKeown et al. (2004) who used the CIV3 code from Hibbert (1975), and with AS values: the results obtained by Whiteford et al. (2002) who used the AS code (Badnell, 1997).

k	Level	E	NIST	GRASP	CIV3	AS
1	2s $^2S_{1/2}$	0.0	0.0	0.0	0.0	0.0
2	2p $^2P^{\circ}_{1/2}$	258659.	257026.	258563.03	259759.16	257860.71
3	2p $^2P^{\circ}_{3/2}$	283924.	282603.	285218.22	284263.50	283275.87
4	3s $^2S_{1/2}$	4176900.	4176030.	4176030.	4177350.	4179640.
5	3p $^2P^{\circ}_{1/2}$	4248504.	4246950.	4247060.	4248110.	4250730.
6	3p $^2P^{\circ}_{3/2}$	4255873.	4254180.	4255150.	4255370.	4258250.
7	3d $^2D_{3/2}$	4283042.	4281030.	4281730.	4282300.	4285880.
8	3d $^2D_{5/2}$	4285399.	4283560.	4284110.	4284660.	4288250.
9	4s $^2S_{1/2}$	5606962.	5605700.	5605740.	5607210.	5610400.

where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition wavelength in  , and ω_i and ω_j are the statistical weights of the lower (i) and upper (j) levels, respectively. Similarly, the oscillator strengths f_{ij} (dimensionless) and the line strength S (in atomic units, 1 a.u. = 6.460×10^{-36} cm² esu²) are related by the following standard equations for the electric dipole (E1) transitions:

$$A_{ji} = \frac{2.0261 \times 10^{18}}{\omega_j \lambda_{ji}^3} S^{E1} \text{ and } f_{ji} = \frac{303.75}{\omega_i \lambda_{ji}} S^{E1} \quad (5)$$

Table 2 displays present radiative decay rates A_{ji} (in s⁻¹) for Ar XVI transitions which are compared with GRASP and CIV3 results from McKeown et al. (2004), and with AS results from Whiteford et al. (2002). The difference between our results and these references (McKeown et al., 2004; Whiteford et al., 2002) varies from nearly 0% to 19%. The maximum error for radiative decay rates in CIV3 results (Δ_{CIV3} is about 19%) in the transition $4s \ ^2S_{1/2} - 2p \ ^2P_{1/2}^o$ (9-2). But the average value of errors still acceptable, is about 4%. According to this comparison we note that our A_{ji} values are relatively close to the other

Table 2. Present radiative decay rates: A_{ij} (in s⁻¹), compared with GRASP values: the results from McKeown et al. (2004) who used the GRASP code of Dyaal et al. (1989), with CIV3 values: the results from McKeown et al. (2004) who used the CIV3 code of Hibbert (1975), and with AS values: the results from Whiteford et al. (2002) who used the AS code of Badnell (1997) for Ar XVI transitions. i and j are labelling the levels as in Table 1.

$i - j$	A_{ij}	GRASP	CIV3	AS	Δ_{GRASP}	Δ_{CIV3}	Δ_{AS}
2 - 1	1.179E+09	1.166E+09	1.195E+09	1.170E+09	1.10	1.36	0.76
3 - 1	1.564E+09	1.552E+09	1.573E+09	1.540E+09	0.77	0.58	1.53
4 - 2	1.836E+11	2.012E+11	1.880E+11	1.970E+11	9.59	2.40	7.30
4 - 3	3.879E+11	4.097E+11	3.900E+11	3.860E+11	5.62	0.54	0.49
5 - 1	1.433E+12	1.449E+12	1.440E+12	1.420E+12	1.12	0.49	0.91
5 - 4	1.530E+08	1.494E+08	1.468E+08	1.490E+08	2.35	4.05	2.61
6 - 1	1.423E+12	1.424E+12	1.425E+12	1.430E+12	0.07	0.14	0.49
6 - 4	2.051E+08	2.042E+08	1.974E+08	2.020E+08	0.44	3.75	1.51
7 - 2	3.619E+12	3.639E+12	3.630E+12	3.670E+12	0.55	0.30	1.41
7 - 3	7.203E+11	7.229E+11	7.219E+11	7.190E+11	0.36	0.22	0.18
7 - 5	1.111E+07	1.052E+07	1.073E+07	1.160E+07	5.31	3.42	4.41
7 - 6	1.079E+06	9.733E+05	1.047E+06	1.130E+06	9.80	2.97	4.73
8 - 3	4.330E+12	4.338E+12	4.335E+12	4.320E+12	0.18	0.12	0.23
8 - 6	8.308E+06	7.580E+06	8.088E+06	8.680E+06	8.76	2.65	4.48
9 - 2	8.715E+10	9.192E+10	7.044E+10	7.550E+10	5.47	19.17	13.37
9 - 3	1.649E+11	1.846E+11	1.514E+11	1.490E+11	11.95	8.19	9.64
9 - 5	5.693E+10	5.270E+10	5.268E+10	5.410E+10	7.43	7.47	4.97
9 - 6	1.121E+11	1.074E+11	1.086E+11	1.060E+11	4.19	3.12	5.44

ones (GRASP, CIV3, AS). Present absorption oscillator strengths f_{ij} ($i \rightarrow j$) and our line strengths S for Ar XVI transitions are reported in Table 3 and compared with GRASP results from McKeown et al. (2004). The percentage errors between the present two parameters (S and f_{ij}) and GRASP results vary from nearly 0% to 12%, for the both parameters. We found the maximum error in $4s\ 2S_{1/2}-2p\ 2P^{\circ}_{3/2}$ (9–3) transition nearly to 12%. Also the average value of errors still acceptable, is about 3%.

3.2. Line broadening results

We perform the calculations of Stark broadening for 10 Ar XVI lines. Quantum results W are calculated using our expression (1) and using 6 configurations. We use a range of electron temperature from 7.5×10^5 to 7.5×10^6 K and at electron density $N_e = 10^{20}$ cm $^{-3}$. Present calculations are reported in Table 4. We can prove that with the electron temperature and density values chosen in the present work, the condition of the impact approximation is valid: this approximation means that the duration τ of an interaction must be much smaller than the mean interval between two collision ΔT (Baranger, 1958):

$\tau \ll \Delta T$. τ can be expressed as $\tau \approx \frac{\rho_{typ}}{v_{typ}}$, where ρ_{typ} is a typical impact parameter, and v_{typ} presents a mean typical velocity. ΔT is of the order of the

Table 3. Present line strengths S and absorption oscillator strengths f_{ij} are compared with GRASP values: the results from McKeown et al. (2004) who used the GRASP code of Dyall et al. (1989) for Ar XVI transitions.

Levels $i - j$	S			f_{ij}		
	Present	GRASP	$\Delta_{GRASP}(\%)$	Present	GRASP	$\Delta_{GRASP}(\%)$
2 – 1	0.067234	0.066430	1.20	2.641E–02	2.610E–02	1.17
3 – 1	0.134921	0.133900	0.76	5.818E–02	5.772E–02	0.79
4 – 2	0.003014	0.003309	9.79	1.793E–02	1.968E–02	9.76
4 – 3	0.006490	0.006869	5.84	1.919E–02	2.029E–02	5.73
5 – 1	0.018447	0.018690	1.32	1.190E–01	1.205E–01	1.26
5 – 4	0.411389	0.409700	0.41	4.474E–02	4.426E–02	1.07
6 – 1	0.036441	0.036530	0.24	2.356E–01	2.360E–01	0.17
6 – 4	0.822315	0.823300	0.12	9.863E–02	9.855E–02	0.08
7 – 2	0.109613	0.110500	0.81	6.700E–01	6.749E–01	0.73
7 – 3	0.022235	0.022380	0.65	6.753E–02	6.790E–02	0.55
7 – 5	0.532594	0.529100	0.66	2.794E–02	2.731E–02	2.25
7 – 6	0.106206	0.105700	0.48	2.190E–03	2.110E–03	3.65
8 – 3	0.200116	0.201100	0.49	6.081E–01	6.104E–01	0.38
8 – 6	0.955857	0.953300	0.27	2.143E–02	2.075E–02	3.17
9 – 2	0.000562	0.000594	5.69	4.570E–03	4.824E–03	5.56
9 – 3	0.001079	0.001210	12.14	4.360E–03	4.889E–03	12.13
9 – 5	0.022417	0.020760	7.39	4.625E–02	4.283E–02	7.39
9 – 6	0.044880	0.043020	4.14	4.605E–02	4.413E–02	4.17

Table 4. Present quantum Stark widths W for ten Ar XVI lines at electron density $N = 10^{20} \text{ cm}^{-3}$ for different temperatures, the wavelengths λ are taken from the SUPERSTRUCTURE (SST) code of Eissner et al. (1974).

Transition	$T(10^5 \text{ K})$	$W(\text{Å})$	Transition	$T(10^5 \text{ K})$	$W(\text{Å})$
$2p \ ^2P^{\circ}_{1/2} - 2s \ ^2S_{1/2}$ $\lambda = 386.61 \text{ Å}$ 2-1	7.5	1.216E-02	$3p \ ^2P^{\circ}_{3/2} - 2s \ ^2S_{1/2}$ $\lambda = 23.50 \text{ Å}$ 6-1	7.5	1.735E-04
	10	1.065E-02		10	1.496E-04
	15	8.854E-03		15	1.212E-04
	30	6.510E-03		30	8.474E-05
	50	5.205E-03		50	6.452E-05
	75	4.338E-03		75	5.109E-05
$2p \ ^2P^{\circ}_{3/2} - 2s \ ^2S_{1/2}$ $\lambda = 352.21 \text{ Å}$ 3-1	7.5	1.002E-02	$3d \ ^2D_{3/2} - 2p \ ^2P^{\circ}_{1/2}$ $\lambda = 24.85 \text{ Å}$ 7-2	7.5	2.144E-03
	10	8.782E-03		10	1.594E-03
	15	7.304E-03		15	1.012E-03
	30	5.377E-03		30	4.361E-04
	50	4.302E-03		50	2.293E-04
	75	3.588E-03		75	1.380E-04
$3s \ ^2S_{1/2} - 2p \ ^2P^{\circ}_{1/2}$ $\lambda = 25.52 \text{ Å}$ 4-2	7.5	2.434E-04	$3d \ ^2D_{3/2} - 2p \ ^2P^{\circ}_{3/2}$ $\lambda = 25.01 \text{ Å}$ 7-3	7.5	1.968E-03
	10	2.098E-04		10	1.465E-03
	15	1.697E-04		15	9.326E-04
	30	1.170E-04		30	4.040E-04
	50	8.832E-05		50	2.137E-04
	75	6.996E-05		75	1.292E-04
$3s \ ^2S_{1/2} - 2p \ ^2P^{\circ}_{3/2}$ $\lambda = 25.69 \text{ Å}$ 4-3	7.5	2.467E-04	$4s \ ^2S_{1/2} - 2p \ ^2P^{\circ}_{3/2}$ $\lambda = 18.79 \text{ Å}$ 9-3	7.5	9.741E-05
	10	2.128E-04		10	8.428E-05
	15	1.722E-04		15	6.858E-05
	30	1.187E-04		30	4.807E-05
	50	8.953E-05		50	3.697E-05
	75	7.089E-05		75	2.996E-05
$3p \ ^2P^{\circ}_{1/2} - 2s \ ^2S_{1/2}$ $\lambda = 23.54 \text{ Å}$ 5-1	7.5	1.756E-04	$4s \ ^2S_{1/2} - 3p \ ^2P^{\circ}_{3/2}$ $\lambda = 74.01 \text{ Å}$ 9-6	7.5	2.940E-02
	10	1.516E-04		10	2.412E-02
	15	1.235E-04		15	1.735E-02
	30	8.836E-05		30	8.672E-03
	50	6.704E-05		50	4.831E-03
	75	5.245E-05		75	2.969E-03

inverse of collisional line width, which can be roughly expressed as equal to $N_e v_{typ} \rho_{typ}^2$. Thus, the validity condition of the impact approximation can be written as $\rho_{typ} \ll N_e^{-1/3}$. ρ_{typ}^3 is called the 'collision volume' that must be smaller than the volume of perturber N_e^{-1} . The condition of the impact approximation can be written in terms of temperature and the orbital momentum of the perturber. The classical angular momentum $L = \rho m v$ can be related to the eigenvalues of the corresponding quantum-mechanical operator \mathbf{L}^2 by $L^2 = (\rho m v)^2 = \hbar^2 l(l+1) \implies \rho^2 = \frac{\hbar^2 l(l+1)}{(m v)^2}$, using that $E = \frac{1}{2} m v^2 = \frac{3}{2} k_B T$, we find $\rho_{typ} = \frac{\hbar l_{typ}}{\sqrt{m k_B T_{typ}}} \approx 3 \times 10^{-10} \text{ m}$. We use $T_{typ} = 7.5 \times 10^6$, and with $N_e = 10^{20} \text{ cm}^{-3}$, we see that $\rho_{typ} \ll N_e^{-1/3} = 10^{-6.67} \text{ m}$. There are no other results in the literature to compare with the present Stark width calculations. The good agreement found between our atomic data and other results shows that our line broadening calculations have acceptable accuracy. Other experimental or theoretical results of Ar XVI line broadening would be very helpful to confirm our calculations.

4. Conclusions

In the present paper, we have performed quantum Stark broadening calculations for 10 Ar XVI lines for the range of electron temperatures from 7.5×10^5 to 7.5×10^6 K and an electron density of $N_e = 10^{20} \text{ cm}^{-3}$. Six configurations have been used in our calculations. The present structural and radiative parameters have been calculated using the UCL (SST/DW/JAJOM) codes. These parameters have been used in our line broadening calculations. To the best of our knowledge, there are no other results for the Stark broadening in the literature to compare with them. New calculations or measurements of line widths for this ion may be interesting for checking our calculations.

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