Electron impact excitation for Ar VI

Haykel Elabidi\textsuperscript{1,2}

\textsuperscript{1} Deanship of the Foundation Year, Department of Physics, Umm Al-Qura University, P.O. Box 715, Makkah, Saudi Arabia
\textsuperscript{2} Groupe de Recherche en Physique Atomique et Astrophysique, Faculté des Sciences de Bizerte, Université de Carthage, Tunisia

E-mail: haykel.elabidi@fsb.rnu.tn

Abstract. Radiative atomic and electron impact excitation data for Ar VI ion have been calculated using the AUTOSTRUCTURE code. The two-body non-fine structure operators of the Breit-Pauli Hamiltonian have been incorporated in AUTOSTRUCTURE, and for the collisional problem, we use the distorted wave approximation. We compare our radiative atomic results with the few available ones. To our best knowledge, there are no distorted wave collision strengths for Ar VI. Some discrepancies have been reported between our oscillator strengths and the only calculated ones using the MCHF method. We perform the same calculations with the UCL codes SST/DW/JAJOM and we compare with the present AUTOSTRUCTURE results.

1. Introduction

Atomic and collisional data are of great importance to accurate plasma modelling in astrophysics and in tokamaks. Many radiative processes, and many electron collision strengths are required for calculating level populations and spectral line intensities. These parameters can provide diagnostics of temperature and density of an emitting plasma, and of the abundance of elements in the plasma. Argon ions are important in astrophysics and in fusion [1, 2]. The Ar VI transition at $\lambda = 1303.87$ Å has been identified in [3] as an isolated line in the STIS spectrum of LSV+46\textdegree 21, and it was noted in [3] that is the first time that Ar VI has been detected in the photosphere of any star.

The first results about the spectrum of Ar VI in the vacuum ultraviolet were published in [4]. A list of many theoretical and experimental works dedicated to the Ar VI before 1992 was reported in [5]. Recently, a new analysis of the Ar VI spectrum in the vacuum ultraviolet region was reported in [6], where adjusted and new energy levels and new classified lines were obtained. The only calculations that provide oscillator strengths or transitions probabilities for Ar VI are presented in [7] where the authors used the multiconfiguration Hartree-Fock (MCHF) and the multiconfiguration Dirac-Hartree-Fock (MCDHF) methods. Electron impact excitation calculations have been done for the argon isoelectronic sequence in [8] using the first-order many-body perturbation theory and in [2] using the Breit-Pauli R-matrix method. The existing results are presented as effective collision strengths. To our best knowledge, there no distorted wave fine structure collision strengths for Ar VI. This is the main motivation of the present work.

We present in this work radiative atomic data and electron impact collision strengths for the five times ionized argon (Ar VI). Comparisons of energy levels have been made with the values compiled by NIST [9]. Our oscillator strengths have been compared with the only existing theoretical results [7] where the MCHF method has been used.
2. Atomic structure and electron-ion scattering

The atomic structure is calculated using the AUTOSTRUCTURE (AS) code [10] by constructing target wavefunctions using radial wavefunctions calculated in a scaled Thomas-Fermi-Dirac-Amaldi statistical model potential using the Breit-Pauli intermediate coupling [11]. Besides the one-body and the two-body fine structure interactions, the two-body non-fine structure operators of the Breit-Pauli Hamiltonian, namely contact spin-spin, two-body Darwin and orbit-orbit are incorporated. It is shown in [10] how these interactions have been incorporated.

Recently, the Breit-Pauli Distorted Wave (BPDW) approach for electron impact excitation of atomic ions has been implemented in the AUTOSTRUCTURE code [12], which is used in the present paper for the scattering problem. We note that the distorted wave approximation (DW) is adequate for moderately and highly charged ions and the agreement between the DW and MCHF [7] values, a "top up" for dipole transitions makes use of the sum rule of Burgess [13]. For higher multipoles, a geometric series in energy in combination with the degenerate energy limit [14] is used. We perform also the same calculations using the UCL codes SST/DW/JAJOM [15, 16, 17], where only the one-body and the two-body fine structure interactions are introduced in SST. We show the effect of the neglecting of these interactions on the structure and the collisional problems.

3. Results and discussions

16 configurations (3s²3p — 3s²5s, 3s3p², 3s3p3d — 3s3p5s, 3p³ and 3p²3d), yielding 155 fine structure levels, have been used to study the atomic structure and the collisional problem of the Ar VI ion. Results of the atomic structure are presented in tables 1 and 2.

Table 1. Some Ar VI energy levels calculated with AS and SST compared with the MCHF [7] and the NIST [9] values.

| i  | Conf. | level  | E_AS | E_SST | E_MCHF | E_NIST |
|----|-------|--------|------|-------|--------|--------|
| 1  | 3s²3p | ²P₀ | 0.0  | 0.0   | 0.0    | 0.0    |
| 2  | 3s²3p | ²P² | 98521.41 | 103170 | 98746.57 | 100 157.5 |
| 3  | 3s³p² | ²P₀ | 99320.29 | 105001 | 99486.49 | 100 957.6 |
| 4  | 3s³p² | ²P₃/₂ | 100563.05 | 10619.02 | 102 191.6 |
| 5  | 3s³p² | ²P₅/₂ | 132593.05 | 138268 | 131753.79 | 132 462.7 |
| 6  | 3s³p² | ²D₌/₂ | 132698.44 | 138351 | 131850.54 | 132 574.7 |
| 7  | 3s³p² | ²D₅/₂ | 182217.67 | 185889* | 170176.45 | 169 803.9 |
| 8  | 3s³p² | ²S₁/₂ | 186863.48 | 183493* | 184439.40 | 182 182.1 |
| 9  | 3s³p² | ²P₁/₂ | 188027.59 | 186563 | 185742.72 | 183 577.3 |
| 10 | 3s³p² | ²P₃/₂ | 224874.85 | 241708 | 220425.89 | 220 655.8 |
| 11 | 3s²3d | ²D₃/₂ | 224998.12 | 241553 | 220303.14 | 220 068.7 |
| 12 | 3s²3d | ²D₅/₂ | 259822.93 | 261109 | 260240.43 | 260 683.7 |
| 13 | 3p³ | ²D₀/₂ | 260028.71 | 261268 | 260438.99 | 260 272.9 |
| 14 | 3p³ | ²D₅/₂ | 276336.59 | 271030 | 271519.72 | 270 511.8 |
| 15 | 3p³ | ²S₀/₂ | 290035.74 | 300117* | 298923.12 | — |
| 16 | 3s³p₃d | ²F₀/₂ | 290479.99 | 300508* | 290245.49 | — |
| 17 | 3s³p₃d | ²F₂/₃ | 291113.84 | 301060* | 290847.72 | — |
| 18 | 3s³p₃d | ²F₄/₅ | 291950.14 | 301780* | — | — |
| 19 | 3s³p₃d | ²F₆/₇ | 301977.11 | 300330* | 294030.80 | 294086.0 |
| 20 | 3p³ | ²P₀ | 302144.00 | 299410* | 294908.42 | 294101.3 |
Table 2. Oscillator strengths and transition probabilities for some Ar VI allowed transitions calculated with AS and SST and compared with MCHF [7] and NIST [9].

| $i-j$ | $f_{AS}$ | $f_{SST}$ | $f_{MCHF}$ | $f_{NIST}$ | $A_{AS}$ | $A_{SST}$ | $A_{MCHF}$ | $A_{NIST}$ |
|-------|----------|-----------|------------|------------|---------|----------|-----------|----------|
| 1-3   | 0.00004  | 0.00004   | 0.00004    | 2.573E+05  | 2.381E+05| 2.894E+5 |           |          |
| 1-4   | 0.00000  | –         | 0.00002    | 4.716E+03  | –       | 6.038E+3 |           |          |
| 1-6   | 0.05603  | 0.09715   | 0.11724    | 4.815E+09  | 4.182E+09| 2.265E+09|           |          |
| 1-8   | 0.21743  | 0.18970   | 0.11724    | 7.208E+09  | 6.019E+08| 4.125E+08|           |          |
| 1-9   | 0.30949  | 0.09715   | 0.11724    | 7.208E+09  | 6.019E+08| 4.125E+08|           |          |
| 2-3   | 0.00001  | 0.00001   | 0.00002    | 1.523E+05  | 1.514E+05| 2.039E+05|           |          |
| 2-4   | 0.00001  | –         | 0.00002    | 9.188E+04  | –       | 8.414E+04|           |          |
| 2-5   | 0.00388  | 0.00734   | 0.00523    | 2.337E+05  | 2.263E+05| 2.409E+05|           |          |
| 2-6   | 0.04663  | 0.08223   | 0.05965    | 3.530E+09  | 6.019E+08| 4.125E+09|           |          |
| 2-7   | 0.15854  | 0.14983   | 0.12320    | 7.211E+09  | 6.889E+09| 5.468E+09|           |          |
| 2-8   | 0.54280  | 0.57812   | 0.54630    | 1.250E+10  | 1.297E+10| 1.224E+10|           |          |
| 2-9   | 0.10163  | 0.09713   | 0.09748    | 3.361E+09  | 3.563E+09| 3.130E+09|           |          |
| 3-13  | 0.00001  | 0.00002   | –          | 1.291E+05  | 2.256E+05| 2.229E+05|           |          |
| 3-15  | 0.22926  | 0.25299   | 0.22390    | 2.418E+09  | 2.694E+09| 2.229E+09|           |          |
| 3-16  | 0.00070  | 0.00007   | –          | 8.585E+05  | 1.029E+06| 8.222E+05|           |          |

Energies of the first 21 excited levels are presented in table 1 and compared with the present SST results, with the MCHF [7] and with the NIST [9] ones. Our energies from (AS) and the MCHF ones are closer to the NIST values (1%) than those calculated by SST (4%). An inversion is found between the 3s3p3d 4F levels (which are not provided by NIST) and the 3p32P0 ones for SST and AS results (levels with asterisks in table 1). New and adjusted energy levels are reported in a revision study of Ar VI [6], but they are not yet taken into account by NIST. These new values are in agreement with the present results. The only calculated oscillator strengths and transition probabilities are those presented in [7] using the MCHF method. Within the 104 lines provided by NIST, there are only 3 lines with oscillator strength and transition probability values that are in disagreement with all the other results (AS, SST and MCHF). Sometimes there is a factor of 10 between them. Table 2 shows that the averaged difference between SST/AS and MCHF oscillator strengths is about 16%, but the major disagreement is found to be for transitions involving the four levels: 6, 7, 8 and 9 (see table for explanation of levels) where the difference can reach 40%. The line at 1303.87 Å has been defined in [18] (and precedent papers) and has been used in [3] as 3s3p2P3/2 − 3p3/2D5/2 but in the revision study [6], it was defined as 3s3p(3P)3d 2P0o/3 3P3/2 − 3p2(3P)3d 2P3/2. In our calculations with AS, the 3s3p2P3/2 − 3p3/2D5/2 line is at 1388.87 Å and the 3s3p(3P)3d 2P0o/3 3P3/2 one is at 1351.71 Å which is closer to the experimental wavelength 1303.87 Å. More calculations of oscillator strengths and radiative decay rates are required to decide about some of the above disagreements.

We present in table 3 fine structure collision strengths for transitions from the ground and the first excited level to the first 10 lowest levels. To our best knowledge, there are no distorted wave fine structure collision strengths in the literature to compare with. Some discrepancies have been found between the AS and the SST results: at high energy (160 Ry) almost all the
Table 3. Fine structure collision strengths for the Ar VI (1 – j) and (2 – j) transitions (j from 2 to 10) calculated with AS and UCL-DW. Levels j are defined in Table 1.

| Transition | 10 Ry | 40 Ry | 160 Ry |
|------------|-------|-------|--------|
| i j        | AS    | UCL   | AS     | UCL   | AS     | UCL   |
| 1 2        | 6.04E-01 | 6.12E-01 | 5.79E-01 | 5.44E-01 | 5.72E-01 | 3.83E-01 |
| 1 3        | 1.58E-02 | 1.88E-02 | 3.65E-03 | 3.48E-03 | 2.43E-03 | 1.63E-03 |
| 1 4        | 2.10E-02 | 2.56E-02 | 2.82E-03 | 2.94E-03 | 1.51E-04 | 2.79E-04 |
| 1 5        | 1.30E-02 | 1.56E-02 | 1.73E-03 | 1.77E-03 | 6.95E-05 | 1.47E-04 |
| 1 6        | 1.15E+00 | 2.04E+00 | 1.58E+00 | 2.73E+00 | 2.29E+00 | 2.52E+00 |
| 1 7        | 6.49E-02 | 6.81E-02 | 4.26E-02 | 3.28E-02 | 4.47E-02 | 2.75E-02 |
| 1 8        | 2.66E+00 | 2.19E+00 | 3.62E+00 | 3.18E+00 | 5.64E+00 | 3.25E+00 |
| 1 9        | 3.67E+00 | 5.28E+00 | 5.00E+00 | 7.64E+00 | 7.80E+00 | 7.80E+00 |
| 1 10       | 2.64E+00 | 3.02E+00 | 3.58E+00 | 4.36E+00 | 5.60E+00 | 4.47E+00 |
| 2 3        | 9.64E-03 | 1.13E-02 | 2.26E-03 | 2.10E-03 | 1.54E-03 | 9.94E-04 |
| 2 4        | 2.68E-02 | 3.25E-02 | 4.72E-03 | 4.78E-03 | 1.88E-03 | 1.47E-03 |
| 2 5        | 6.07E-02 | 7.30E-02 | 1.23E-02 | 1.23E-02 | 6.76E-03 | 4.82E-03 |
| 2 6        | 2.45E-01 | 3.98E-01 | 2.77E-01 | 4.56E-01 | 3.75E-01 | 4.04E-01 |
| 2 7        | 2.01E+00 | 3.54E+00 | 2.72E+00 | 4.67E+00 | 3.92E+00 | 4.30E+00 |
| 2 8        | 1.01E+00 | 2.15E+00 | 1.37E+00 | 3.03E+00 | 2.13E+00 | 8.16E+00 |
| 2 9        | 3.81E+00 | 5.44E+00 | 5.19E+00 | 8.09E+00 | 8.09E+00 | 3.08E-01 |
| 2 10       | 1.29E+01 | 1.53E+01 | 1.76E+01 | 2.21E+01 | 2.75E+01 | 2.26E+01 |

UCL-DW results are lower than the AS ones. It seems to be a consequence of the neglect in SST of the two-body non-fine structure interactions. Nevertheless, collision strengths calculated with other approaches should be very important to conclude about this last interpretation.

Acknowledgments
This work has been supported by the Tunisian research unit 05/UR/12-04 and "the Faculté des Sciences de Bizerte".

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