Revised and Extended Analysis of Five Times Ionized Argon (Ar VI)

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Abstract

The spectrum of five times ionized argon, (Ar VI), has been observed in the 280–2100 Å wavelength range. Eighty-seven lines have been identified as transitions between levels of the 3s23p, 3s3p2, 3p23d, 3p3, 3s3p3d, 3s24s, 3p24d and 3s3p4d configurations. For 33 of the lines the classification is new. Forty-one energy level values belonging to these configurations were analyzed and we propose 9 new energy level values for levels corresponding to odd parity configurations. The configurations are interpreted by fitting the theoretical energy expressions to the observed energy levels using least-squares techniques. The parameter values are compared with results from Hartree–Fock calculations.

1. Introduction

The ground-state configuration of five times ionized argon, (Ar5+), is 3s23p with the term 3P. Ar VI belongs to the Al I isoelectronic sequence. Excited states either belong to simple one-electron configuration of the type 3s'nl or to three-electron configurations such as 3s3p2, 3p3 and 3s3p(1,3P)nl etc., giving both doublets and quartets.

The spectra of the first, second and third elements in this sequence are presented in Atomic Energy Levels (AEL), Ref. [1]. Subsequent to this tabulation, the Al I spectrum was investigated by Eriksson and Isberg [2]. Results about Si II were published by Shenstone [3] and the P III spectrum was studied by Magnusson and Zetterberg [4]. Early results on the spectra of S IV and CI V have been published in AEL but later results of S IV were compiled by Martin et al., see Ref. [5] and references therein. The first results about the spectrum of Ar VI in the vacuum ultraviolet were published by Phillips and Parker [6]. Fawcett et al. [7] studied the spectra of multiple ionized inert gases, including Ar, and Schönheit [8] made a similar study finding a large quantity of new lines. Lines corresponding to the spin-forbidden resonance multiplet 3s23p2P–3s3p2P were reported by Ekberg and Svensson [9]. Using a Theta-Pinch light source Fawcett et al. [10] classified some lines of Ar VI. Using the beam-foil technique Livingston et al. [11] have studied the argon spectra from Ar V to Ar VIII and using the same technique Buchet–Poulizac et al. [12] have studied the argon spectra from Ar VI to Ar VIII. A few lines of Ar VI were classified in the work of De-Ye et al. [13].

Theoretical calculations for the Al I isoelectronic sequence were made by Fawcett [14]. Computed ab-initio transition probabilities and energy levels for Al I-like ions were made by Huang [15] and data about highly ionized copper and zinc, belonging to this sequence, were published by Sugar and Kaufman [16–17].

Recently, Träbert et al. [18–19] have studied the spectrum of argon and other ions in the vacuum ultraviolet. They searched for lines of Mg-, Al- and Si-like ions. Recoil ion spectroscopy was used by Lesteven–Vaïsse et al. [20] who have studied all argon spectra from Ar I to Ar IX. Some anomalies in resonance transitions in the Al I isoelectronic sequence were observed by Engström et al. [21] and a new work about energy levels and lifetimes of Ar VI was recently published by Pinnington et al. [22]. An extended analysis of spectra and term systems in Al-like Ca VIII to Ni XVI was published by Redfors and Litzén [23] and lifetimes of the 3s24s7S states for Al-like ions from S IV to Fe XIV were published by Thornbury et al. [24]. Transitions in spectra of highly ionized Kr and Mo belonging to the Al I isoelectronic sequence were recently reported by Jupén et al. [25]. In the present work we report a revised and extended analysis of Ar VI that includes 33 newly classified lines and 9 new energy level values.

Experiment

The light source used in the present work is a discharge tube built at the Centro de Investigaciones Opticas, (CIOp), to study highly ionized gases [26]. It is a 30 cm long Pyrex tube with an inner diameter of 3 mm. Gas excitation was produced by discharging a bank of low inductance capacitors varying between 2.5 and 100 nF and charged up to 19 kV through the tube. Light radiation emitted axially was analyzed using a 3 m normal incidence vacuum spectro-

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graph with a concave diffraction grating of 1200 lines/mm, blazed for 1200 Å. The plate factor in the first order is 2.77 Å/mm. Ilford Q-2 plates were used to record the spectra between 280–2100 Å. C III and N II [27], O III [28] and lines of Ar III–Ar V [27] were recorded as internal wavelength standards. Exposing the plates with 10⁴ shots we were able to obtain good spectra of argon below 300 Å. The lines were observed in the first, second, and in some cases, third order of diffraction.

The gas pressure, the discharge voltage, and the capacitance were varied to distinguish between different stages of ionization. A well developed Ar VI spectrum was obtained with the following parameters: 120 mTorr, 18 kV and 20 nF. The positions of spectral lines on the plates were determined with a rotating prism photoelectric automatic Grant comparator whose precision is 1 µm. The uncertainty in determining the wavelength of unperturbed lines by this procedure is estimated to be ±0.01 Å in the first diffraction order.

Analysis

The Ar VI lines observed in the present work are given in Table I, 33 of them being without previous classification. The intensities of the lines given in the table are based on visual estimates and the values given in the calculated column are deduced from the optimized level values. The optimized energy values derived from the observed lines are given in Table II and the general structure of the term system is shown in Fig. 1. The level values were determined in an iterative procedure where the wavenumbers of the observed lines are weighted according to their estimated uncertainties. Theoretical predictions of the structure of the configurations made at the Department of Physics, University of Lund, were also used in the analysis. The predictions were obtained by diagonalizing the energy matrices with appropriately scaled Hartree–Fock (HF) values for the energy parameters. The computer code developed by Cowan [29] was used. All levels designations in Table II are in LS notation, and in the same table we present the percentage composition of the levels.

A comparison with the level system given by Pinnington et al. [22] shows that six of their level values have been confirmed, although the accuracy has been considerably improved. However, for seven levels we propose new identifications as discussed below.

The observed structure of the configurations 3p³, 3s3p3d and 3s3p4s is shown in Fig. 2. For the level 3s3p3d 3P½ 3d½, we propose the new value 344 307.9 cm⁻¹. This level is established by five new lines that are given in Table I. For the level 3s3p3d 3P½ 3d½ we propose the new value 346 073.4 cm⁻¹ determined by two new lines, see Table I. Both level values fit well with the extrapolation that can be done from the isoelectronic data published in Ref. [23].

For the level 3s3p3d 3P½ 3d½ we propose the new value 375 657.6 cm⁻¹. This level is determined by four new lines, see Table I. The level value fits very well with the isoelectronic trend from Ref. [23]. The isoelectronic graph gives for the 3s3p3d 3P½ 3d½ level a probable value near 376 300 cm⁻¹. We were not able to find the transitions establishing this level, but according to the extrapolated values mentioned above and our theoretical predictions we reject the experimental value published in the work of Pinnington et al. [22] for this level.
For the levels 3s3p(1P)3d2D3/2 and 3s3p(1P)3d2D5/2, we propose the new values 395.4920 cm\(^{-1}\) and 395.8041 cm\(^{-1}\) respectively. These level values are in accordance with the values obtained along the isoelectronic sequence using data of Ref. [23] and with our theoretical predictions. The 3s3p(1P)3d2D5/2 level is determined by four new lines, see Table I. For the other level of the same multiplet we classified three lines that are given in the same table.

For the 3s3p(1P)3d2F7/2 level we propose the new value 376.4717 cm\(^{-1}\). This level is determined by a new line at 410.10\(\AA\), classified as 3s3p2D5/2–3s3p(1P)3d2F7/2 and another new line at 633.85\(\AA\), classified as 3s3d2D5/2–3s3p(1P)3d2F7/2. For the 3s3p(1P)3d2F5/2 level we propose the new value 376.9015 cm\(^{-1}\). The level is determined by four new lines that are classified in Table I. Both level values of this multiplet are in good agreement with our theoretical predictions and with the graphic extrapolation along the isoelectronic sequence based on the work of Ref. [23].

For the level 3s3p(1P)4s2P3/2 we propose the new value 525.043 cm\(^{-1}\). The level is determined by a new line at 326.32\(\AA\), classified as 3s3d2D5/2–3s3p(1P)4s2P3/2, and
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Table 11. Energy levels of Ar VI

| Designation | Energy (cm⁻¹) | Percentage composition* |
|-------------|---------------|-------------------------|
| 3s3p⁴ 2D P₁/₂ | 0.0 | 97 |
| 3s3p⁴ 2P P₁/₂ | 2207.1 | 97 |
| 3s3p⁴ 4P P₁/₂ | 100158.2 | 99 |
| 3s3p⁴ 4P P₅/₂ | 100954.8 | 99 |
| 3s3p⁴ 5D P₁/₂ | 101218.2 | 99 |
| 3s3p⁴ 5D P₅/₂ | 132461.4 | 87 |
| 3s3p⁴ 7D P₁/₂ | 132574.1 | 87 |
| 3s3p⁴ 7D P₅/₂ | 169803.7 | 99 |
| 3s3p⁴ 2P P₁/₂ | 182181.1 | 99 |
| 3s3p⁴ 2P P₅/₂ | 183576.1 | 99 |
| 3s3p⁴ 3D P₁/₂ | 218593.0 | 87 |
| 3s3p⁴ 3D P₅/₂ | 218652.8 | 87 |
| 3s3p⁴ 6P P₁/₂ | 260066.9 | 64 |
| 3s3p⁴ 6P P₅/₂ | 260271.4 | 64 |
| 3s3p⁴ 4S P₁/₂ | 270510.4 | 99 |
| 3s3p⁴ 4S P₅/₂ | 294084.8 | 99 |
| 3s3p⁴ 4S P₇/₂ | 294099.5 | 94 |
| 3s3p⁴ 3S P₁/₂ | 3197903.9 | 99 |
| 3s3p⁴ 3S P₅/₂ | 328958.8 | 47 |
| 3s3p⁴ 3S P₇/₂ | 328989.9 | 47 |
| 3s3p⁴ 4S P₁/₂ | 342302.8 | 99 |
| 3s3p⁴ 4S P₅/₂ | 344307.9 | 71 |
| 3s3p⁴ 3S P₁/₂ | 375657.6 | 78 |
| 3s3p⁴ 3S P₅/₂ | 376417.2 | 71 |
| 3s3p⁴ 3S P₇/₂ | 376901.5 | 71 |
| 3s3p⁴ 3S P₉/₂ | 395492.0 | 66 |
| 3s3p⁴ 3S P₅/₂ | 395804.1 | 67 |
| 3s3p⁴ 3S P₇/₂ | 345410.8 | 99 |
| 3s3p⁴ 3S P₉/₂ | 345745.6 | 99 |
| 3s3p⁴ 3S P₁/₂ | 345798.8 | 99 |
| 3s3p⁴ 3S P₅/₂ | 345872.5 | 99 |
| 3s3p⁴ 3S P₇/₂ | 456271.6 | 99 |
| 3s3p⁴ 3S P₉/₂ | 525043.6 | 99 |
| 3s3p⁴ 3S P₁/₂ | 525191.3 | 98 |

* Percentages lower than 5% are omitted

Theoretical Interpretation

The level structure was theoretically interpreted by a least-squares fit of the energy parameters to the experimental level values. For this purpose the computer code developed by Cowan [29] was used.

The scaled Hartree–Fock factor was 0.85 for all parameters, except for \( \zeta_{n} \), where the scaled factor was 0.95 and for \( E_{av} \) where the scaled factor was 1.00. These scaled factors were taken in this form because the computed energy-level intervals agree better with the experimental ones.

In order to obtain a better interpretation of the levels it was necessary to introduce the 3s3p configuration. The results of the parametric calculations are presented in Table III.

The \( \alpha \) parameter was kept free because all the levels of the 3p configuration are known. The first three configuration interaction integrals were held fixed in the calculation scaled at 0.75, 0.95 and 0.95 of their Hartree–Fock values. The rest of the configuration interaction integrals were held fixed at 0.75, 0.95 and 0.95 of their Hartree–Fock values.

For the level 3s3p⁴ 4s² 3p₂, we propose the new value 525,191.3 cm⁻¹. This level is supported by three new lines that are classified in Table I.

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We report two new lines at 508.918, and 509.128 classified as 3s3p⁴ 4s² 3p₂ 2D and 3s3p⁴ 4s² 3p₂ 2P transitions. These lines confirm the previously observed values of the 3s3p⁴ 4s² 3p₂ doublet, see Ref. [22].

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Table III. Energy parameters (cm\(^{-1}\)) for the 3s\(^2\)3p, 3s\(^2\)4p, 3p\(^3\), 3s3p3d, 3s3p4s configurations of Ar VI

| Configuration | Parameter | Scaled HF Value | Fitted Value* | SHF Value |
|---------------|-----------|----------------|---------------|-----------|
| 3s\(^2\)3p    | \(E_\alpha^*\) | 0              | 13738         |           |
| 3s\(^2\)3p    | \(\zeta_{3p}\) | 1307           | 1512          | 1.157     |
| 3s\(^2\)3p    | \(E_{\alpha}\) | 391438         | 393887        | 1.006     |
| 3s\(^2\)4p    | \(\zeta_{4p}\) | 394            | 394 (FIX)     |           |
| 3p\(^1\)      | \(E_{\alpha}\) | 287614         | 294987        | 1.026     |
| 3p\(^1\)      | \(F(3p,3p)\) | 66962          | 68868         | 1.028     |
| 3p\(^1\)      | \(\sigma(3p,3p)\) | -112          |              |           |
| 3s3p3d       | \(E_\alpha\) | 323495         | 332094        | 1.027     |
| 3s3p3d       | \(F(3p,3d)\) | 63506          | 63334         | 0.997     |
| 3s3p3d       | \(G(3s,3p)\) | 48916          | 44557         | 0.911     |
| 3s3p3d       | \(G(3p,3d)\) | 1319           | 1797          | 1.362     |
| 3s3p3d       | \(\zeta_{3d}\) | 60             | 60 (FIX)      |           |
| 3s3p4s       | \(E_\alpha\) | 463784         | 475779        | 1.026     |
| 3s3p4s       | \(G(3s,3p)\) | 82900          | 95501         | 1.152     |
| 3s3p4s       | \(G(3s,4s)\) | 5896           | 6137          | 1.041     |
| 3s3p4s       | \(G(3p,4s)\) | 1405           | 1420          | 1.011     |

| Configuration | Interaction Integrals |
|---------------|-----------------------|
| 3s\(^2\)3p    | - 3p\(^1\)            | \(R(3s,3p,3p)\) | 79351 | 79351 (FIX) |
| 3s\(^2\)3p    | - 3s3p3d             | \(R(3s,3p,3d)\) | 92765 | 92765 (FIX) |
| 3s\(^2\)3p    | - 3s3p3d             | \(R(3s,3p,3d)\) | 70775 | 70775 (FIX) |
| 3s\(^2\)3p    | - 3s3p4s             | \(R(3s,3p,3p)\) | 4725  | 4725 (FIX)  |
| 3s\(^2\)3p    | - 3s3p4s             | \(R(3s,3p,3d)\) | 7557  | 7557 (FIX)  |
| 3s\(^2\)3p    | - 3s3p4s             | \(R(3s,3p,3d)\) | 1368  | 1368 (FIT)  |
| 3s\(^2\)4p    | - 3s3p3d             | \(R(3s,4p,3d)\) | 8998  | 8998 (FIT)  |
| 3s\(^2\)4p    | - 3s3p3d             | \(R(3s,4p,3d)\) | 10777 | 10777 (FIT) |
| 3s\(^2\)4p    | - 3s3p4s             | \(R(3s,4p,3p)\) | 38098 | 38098 (FIT) |
| 3s\(^2\)4p    | - 3s3p4s             | \(R(3s,4p,3d)\) | 6074  | 6074 (FIT)  |
| 3p\(^3\)     | - 3s3p3d             | \(R(3s,3s,3d)\) | 82900 | 82900 (FIT) |
| 3p\(^3\)     | - 3s3p3d             | \(R(3s,3s,3d)\) | 7384  | 7384 (FIT)  |
| 3s3p3d - 3s3p3d | \(R(3s,3d,3s)\)     | 2974  | 2974 (FIT)  |
| 3s3p4s - 3s3p4s | \(R(3s,4s,4p)\)     | 5010  | 5010 (FIT)  |

* The RMS deviation of the fit is 210 cm\(^{-1}\) for 28 observed levels.

...the standard 85% of the Hartree–Fock values. The standard-deviation for the 28 observed levels was 210 cm\(^{-1}\).

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