Research Article

Forbidden Transitions in the Ground State Configuration of Doubly Ionized Argon

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We have calculated forbidden transitions (M1 and E2) between fine structure levels in the ground state configuration $3s^2 3p^4$ of doubly ionized argon (Ar III) using the multiconfiguration Hartree-Fock approach within the framework of the Breit-Pauli Hamiltonian. The data for the analysis of forbidden lines in the spectrum is important for the study of the plasma in astrophysical objects and fusion devices. The results obtained from this work have been compared with other results available in the literature.

1. Introduction

Atomic radiative transition is one of the fundamental processes in plasmas. The numerical simulation of atomic kinetics in laboratory as well as astrophysical plasma requires accurate radiative transition rates [1]. Information about the term values and transition probabilities of highly stripped ions is required in astrophysics and plasma diagnostics. In plasma research, transitions in such ions can be used to determine temperature and density distributions. Forbidden transitions within the ground state configuration are particularly useful since their relatively long wavelengths make them convenient for spectroscopic studies [2]. Although the atomic kinetics depend on, in particular, optical allowed transitions (E1), the weak forbidden transitions (magnetic dipole, M1, and electric quadrupole, E2) have been linked to dominant features in the optical spectra of planetary nebulae and the aurora [3, 4]. Since the parity of upper and lower levels within the ground state configuration is the same, the electric dipole (E1) transitions are forbidden. The lowest-order metastable levels radiatively decay correspond to M1 and E2 transitions [5]. M1 and E2 transition rates are of several orders of magnitude smaller than those for E1 transitions with a similar energy-level separation.

Argon is one of the most abundant rare gases in the universe (its abundance is being $3.8 * 10^{-6}$ times smaller than that of hydrogen). Argon ion lines are observed in solar and astrophysical plasmas as well as in the laboratory [6]. The argon spectral lines are important in determining chemical abundances of elements and for estimation of the radiative transfer through stellar plasmas [7]. Argon plasma sources are required in various fields [8–11]. For this reason, the data on the transition parameters in multiply ionized argon ions is important for argon plasma modeling and laser physics [12, 13].

Some of the data for the energy levels and transition parameters on allowed and forbidden lines in Ar III can be found in NIST website [14]. M1 and E2 transition parameters for Ar III in NIST were compiled from the values reported by Czyak and Krueger [15], Naqvi [16], Bowen [17, 18], Kelly and Lacy [19], and Feuchtgruber et al. [20]. Saloman and Kim calculated magnetic dipole and electric quadrupole transition rates for S-like ions between ground state terms using multiconfiguration Dirac-Fock wave functions [2]. Calamai and Johnson measured the natural lifetimes of the $ns^2 np^4$ ($^1S_0$) metastable states for some rare gases (Ar^{2+}, Kr^{2+}, and Xe^{2+}) using an ion trapping technique [21]. Biémont and Hansen calculated energy levels and radiative transition probabilities in the ground configurations of the sulfur and selenium isoelectronic sequences up to molybdenum and silver, respectively, using HFR self-consistent method [22]. Prior observed M1 and E2 lines from trapped metastable Ar III and Cu II ions [23]. Mendoza and Zeippen calculated radiative transition probabilities for the forbidden lines in

the ground configuration of all the members of the sulfur isoelectronic sequence [24]. Fine structure splitting in Ar III was calculated using the *R*-matrix method by Stancalie et al. [6]. Träbert discussed some examples of measurements and calculations of the radiative lifetime of the $np^4 {}^1S_0$ level in Ne^{2+}, Ar^{2+}, Kr^{2+}, and Xe^{2+} ions [25]. Pasternack reported the transition probabilities of forbidden lines for atoms in the p^2, p^3, p^4, d^2, and d^3 configurations [26, 27]. Burger et al. presented 38 Ar III and 14 Ar IV A values obtained on the basis of the relative line intensity ratio method in the wavelength interval between 240 nm and 308 nm [7]. The weighted oscillator strengths (gf) and the lifetimes for Ar III were presented using a multiconfiguration Hartree-Fock relativistic (HFR) approach by Luna et al. [28]. Nandi et al. presented a comprehensive analysis of beam-foil and beam-gas excited spectrum of argon observed in small wavelength region, 2965–3090 Å, using Ar^+ and Ar^{2+} ions in the energy range 200–650 keV [29]. Ultraviolet and visible spectra of the symbiotic nova RR Telescopii were used to derive reference wavelengths for many forbidden and intercombination transitions of ions +1 to +6 of elements C, N, O, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, and Ca by Young et al. [30]. The transition probabilities of spontaneous emission of eight transitions in Ar III and seventeen transitions in Ar IV spectrum were obtained using the relative line intensity ratios method by Djeniže and Bukvić [31]. The radiative lifetime of the $3s^2 3p^4 {}^1S_0$ level in Ar^{2+} ions was measured via time resolved observation of the magnetic dipole (M1) transition to the $ns^2 np^4 {}^3P_1$ level, on ions circulating in a heavy-ion storage ring by Träbert and Gwinner [5]. Fischer et al. investigated the fine structure levels of $3s^2 3p^3 3d\ {}^3D$ for Ar III using nonorthogonal spline CI, multiconfiguration Hartree-Fock (MCHF), and multiconfiguration Dirac-Hartree-Fock (MCDHF) methods [32]. Theoretical energy levels and transition probabilities were presented for 47 low-lying levels of sulfur-like ions for all $Z \geq 18$ using the multiconfiguration Dirac-Fock method by Chou et al. [33]. Using a compilation of experimental energy levels, Verner et al. derived accurate wavelengths for 5599 lines of 1828 ground-term multiplets *gf*-values calculated in the Opacity Project and they recalculated the Opacity Project multiplet *gf*-values to oscillator strengths and transition probabilities of individual lines [34]. The energy levels and observed spectral lines of ionized argon atoms in all stages of ionization were presented by Saloman [35]. Johnson and Kingston calculated collision strengths for electron excitation of the $3s^2 3p^4$ levels of Ar III using the *R*-matrix method [36]. Munoz Burgos et al. calculated electron-impact excitation of Ar^{2+} including excitation up to the 5s subshell using *R*-matrix method [37].

The aim of this work is to investigate the forbidden transitions (M1 and E2) between energy levels within the ground state configuration of doubly ionized argon (Ar III) using multiconfiguration Hartree-Fock approach within the framework of Breit-Pauli Hamiltonian [38]. We have obtained the M1 and E2 transition parameters such as transition energies, line strengths, and transition probabilities (or rates) using the MCHF atomic structure code [39]. Although Ar is not a heavy element, the relativistic contributions to

the wave functions and energies of levels must be involved. Also an accurate atomic structure via large configuration interaction (CI) basis is required. Therefore, our calculations include the relativistic contributions and correlation effects. For considering the correlation effects in this work, the configurations of $3s^2 3p^4$, $3p^6$, $3s^2 3p^3 4p$, $3p^5 4p$, $3s 3p^4 3d$, $3s^2 3p^2 3d^2$, and $3p^4 3d^2$ have been considered.

2. Calculation Method

Radiative properties of atoms are described with an electromagnetic transition between two states which is characterized by the angular momentum and parity of the corresponding photon. They are very useful in the fields of quantum electronic, atomic physics and laser spectroscopy, plasma physics, and astrophysics. Hence, the reliability of the values of these parameters is mainly based on the performance of the calculation methods used. A detail of theoretical background can be found in the literature [38, 39]. We have here presented some formulas. Briefly, if the emitted or observed photon has angular momentum k and parity $\pi = (-1)^k$, the transition is an electric multipole transition (Ek), while the transition from absorbed photon with parity $\pi = (-1)^{k+1}$ is magnetic multipole transition (Mk).

The transition probability for the emission from the upper level to the lower level is given by

$$A^{\pi k}\left(\gamma' J', \gamma J\right) = 2C_k \left[\alpha \left(E_{\gamma' J'} - E_{\gamma J}\right)\right]^{2k+1} \frac{S^{\pi k}\left(\gamma' J', \gamma J\right)}{g_{J'}},\tag{1}$$

where $S^{\pi k}$ is line strength,

$$S^{\pi k}\left(\gamma' J', \gamma J\right) = \left|\left\langle \gamma J \left\| \mathbf{O}^{\pi(k)} \right\| \gamma' J' \right\rangle\right|^2,\tag{2}$$

$C_k = (2k+1)(k+1)/k((2k+1)!!)^2$, and $\mathbf{O}^{\pi(k)}$ is transition operator. The transition rates (or probabilities) for forbidden transitions depend on the third (in M1 transition) or fifth (in E2 transition) power of transition energy.

3. Results and Discussion

In this work, the transition energies, line strengths, and transition probabilities (or rates) for forbidden transitions (magnetic dipole, M1, and electric quadrupole, E2) between the levels in the ground state configuration for doubly ionized argon (Ar III) have been calculated using the multiconfiguration Hartree-Fock atomic structure code [39] based on the multiconfiguration Hartree-Fock approach within the Breit-Pauli relativistic corrections [38]. In the calculations, the configurations of $3s^2 3p^4$, $3p^6$, $3s^2 3p^3 4p$, $3p^5 4p$, $3s 3p^4 3d$, $3s^2 3p^2 3d^2$, and $3p^4 3d^2$ are included due to considering correlation effects. Table 1 displays the results including transition energies, line strengths, and transition probabilities (or rates) for M1 and E2 transitions in the ground state configuration $[Ne]3s^2 3p^4$. In table, we have omitted the core and have only given the levels excited of $3s^2 3p^4$.

TABLE 1: Transition energies, ΔE (cm^{-1}), line strengths, S (a.u.), and transition probabilities, A_{ki} (s^{-1}), for forbidden transitions (M1 and E2) of the ground state $3s^2 3p^4$ configuration for Ar III. In table, $a(b)$ denotes $a \times 10^b$.

Transitions	ΔE		S		A_{ki}	
	This work	Other works	This work	Other works	This work	Other works
M1 transitions						
$^3P_1$-$^1S_0$	33734.36	32153.53[a] 32135[d] 32155[e] 30688[g] 30122.89[h]	3.36 (−3)	4.48 (−3)[a]	3.48	4.02[a] 3.972[d] 3.91[f]
$^3P_2$-$^1D_2$	—	14010.0[a] 13972[d] 14010[e] 17305.26[g] 16328.91[h]	—	2.16 (−3)[a]	—	3.21 (−2)[a] 4.5 (−1)[b] 3.2 (−1)[c] 3.23 (−1)[d] 3.13 (−1)[f]
$^3P_1$-$^1D_2$	14914.19	12897.83[a] 12865[d] 12898[e] 17647.36[g] 15275.43[h]	4.70 (−3)	7.2 (−3)[a]	8.41 (−2)	8.3 (−2)[a] 12 (−2)[b] 8.5 (−2)[c] 8.43 (−2)[d] 8.22 (−2)[f]
$^3P_2$-$^3P_1$	1008.28	1112.17[a] 1107[d] 1112[e] 1131.74[g] 1053.41[h]	2.50	2.50[a]	2.30 (−2)	3.1 (−2)[a] 3.1 (−2)[c] 3.054 (−2)[d] 3.08 (−2)[f]
$^3P_1$-$^3P_0$	428.35	458.06[a] 463[d] 458[e] 468.96[g] 449.92[h]	2.00	2.00[a]	4.23 (−3)	5.19 (−3)[a] 5.2 (−3)[c] 5.354 (−3)[d] 5.17 (−3)[f]
E2 transitions						
$^3P_2$-$^1S_0$	34742.64	33265.7[a] 33242[d] 33267[e] 31819.69[g] 31176.37[h]	4.46 (−3)	9.4 (−3)[a]	2.53 (−2)	4.3 (−2)[a] 3.493 (−2)[d] 4.17 (−2)[f]
$^1D_2$-$^1S_0$	18820.16	19255.7[a] 19271[d] 19257[e] 14514.43[g] 14847.46[h]	0.87 (1)	1.05 (1)[a]	2.30	3.10[a] 2.693[d] 2.59[f]
$^3P_2$-$^1D_2$	—	14010.0[a] 13972[d] 14010[e] 16328.91[h]	—	1.2 (−1)[a]	—	1.4 (−3)[a] 2.9(−3)[c] 1.362 (−3)[d] 1.14 (−3)[f]
$^3P_1$-$^1D_2$	14914.19	12897.83[a] 12865[d] 12898[e] 15704.55[g] 15275.43[h]	1.08 (−2)	1.6 (−2)[a]	1.78 (−4)	1.3 (−4)[a] 2.7 (−4)[c] 1.349 (−4)[d] 1.14 (−4)[f]
$^3P_0$-$^1D_2$	14485.85	12439.77[a] 12402[d] 12440[e] 14825.51[h]	3.17 (−3)	4.3 (−3)[a]	4.52 (−5)	2.9 (−5)[a] 7.0 (−5)[b] 5.8 (−5)[c] 2.038 (−5)[d] 2.21 (−5)[f]

Table 1: Continued.

Transitions	ΔE		S		A_{ki}	
	This work	Other works	This work	Other works	This work	Other works
$^3P_2$-$^3P_0$	1436.63	1570.23[a] 1570[d] 1570[e] 1600.70[g] 1503.41[h]	2.46	2.54[a]	1.69 (−6)	2.72 (−6)[a] 5.6 (−5)[c] 2.784 (−6)[d] 2.37 (−6)[f]
$^3P_2$-$^3P_1$	1008.28	1112.17[a] 1107[d] 1112[e] 1131.74[g] 1053.48[h]	5.50	5.7[a]	2.14 (−7)	3.6 (−7)[a] 7.4 (−7)[c] 3.617 (−7)[d] 3.13 (−7)[f]

[a]Ref. [14], [b]Ref. [27], [c]Ref. [26], [d]Ref. [22], [e]Ref. [40], [f]Ref. [24], [g]Ref. [6], and [h]Ref. [37].

The results obtained from this work are generally in agreement with other works. In M1 transitions, the transition energies for $^3P_1$-$^1D_2$, $^3P_2$-$^3P_1$, and $^3P_1$-$^3P_0$ are in agreement with the values reported in [37]. $^3P_1$-$^1S_0$ transition energy is in agreement with [14, 22, 40]. We have compared our line strength values with those in NIST [14]. Only the line strength for $^3P_1$-$^1D_2$ transition is somewhat poor. There is also good agreement in transition probabilities. In E2 transitions, the transition energies for $^3P_2$-$^1S_0$, $^1D_2$-$^1S_0$, $^3P_1$-$^1D_2$, $^3P_0$-$^1D_2$, $^3P_2$-$^3P_0$, and $^3P_2$-$^3P_1$ are in good agreement with [6, 14, 22, 37]. The line strengths are also in agreement with the values of NIST. Moreover, the transition probabilities for this transition type are in agreement with other works. It is noted that the values reported by Pasternack within the other works are somewhat poor. It is seen in first column that there is no values for M1 transition of $^3P_2$-$^1D_2$ and E2 transition of $^3P_2$-$^1D_2$. We have not obtained these transitions in this work due to the forbiddenness of $J - J' = 0$ transitions in this computer code.

In conclusion, the aim of this work is to investigate the transitions between excited levels of ground state configuration in doubly ionized argon (Ar III) using the approach within the framework of the Breit-Pauli Hamiltonian. Such excited states, known as metastable states, perform weak spectral lines, and they decay via magnetic dipole (M1) and electric quadrupole (E2) transitions. The values for transition energies, line strengths, and transition probabilities are fundamental quantities for many scientific applications. Especially, forbidden transitions such as M1 and E2 are of great interest for plasma diagnostics and modeling. Therefore, we hope that our results on M1 and E2 transitions in Ar III will provide the supports to further researches for this ion.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

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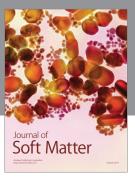
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