

Photoionization of Al IV (neon-type) from its ground $2s^2 2p^6 \ ^1S^e$ and excited $2s^2 2p^5 3p \ ^{3,1}P^0 \ ^3S^e$ states using the R -matrix method

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MS received 29 April 1999

Abstract. The R -matrix method is used to calculate the total photoionization cross-sections from the ground $2s^2 2p^6 \ ^1S^e$ and the first three excited $2s^2 2p^5 3p \ ^{3,1}P^0 \ ^3S^e$ states of Al IV, for photon energies ranging from the first ionization threshold to just above the second threshold of the residual ion Al V. The two lowest LS terms of Al V – $2s^2 2p^5 \ ^2P^0$, $2s^2 2p^6 \ ^2S^e$, $2s^2 2p^6 \ ^2S^e$, represented by sophisticated configuration interaction wavefunctions, are included in the R -matrix calculation. The resulting cross-sections are affected by Rydberg series of resonances converging to the $2s^2 2p^6 \ ^2S^e$ excited threshold.

Keywords. Photoionization; configuration interaction; R -matrix method.

PACS Nos 32.80 Fb; 32.80-t

1. Introduction

Photoionization cross-sections for ions are of increasing interest in atomic physics, since the use of laser-produced plasmas and synchrotron radiation sources which allows accurate cross-section measurements of them [1]. They are also of crucial importance in many astrophysical applications, e.g. in the calculation of the opacity of stellar envelopes [2–4].

In the present work, we use the R -matrix method [5] to calculate cross-sections for the photoionization of the ground $2s^2 2p^6 \ ^1P^e$ and the three lowest excited $2s^2 2p^5 3p \ ^{3,1}P^0 \ ^3S^e$ states of Al IV, allowing for the residual ion to be left in one of the 2 lowest LS states Al V : $2s^2 2p^5 \ ^2P^0$, $2s^2 2p^6 \ ^2S^e$.

These target states are represented by configuration interaction (CI) wavefunctions described in detail by Mohan and Hibbert [6]. Consistent close coupling expansions on these 2 target states are used to represent the initial state and the final continuum states. Within the electronic cloud of the residual ion, the collisional expansions are obtained by decomposition on a discrete R -matrix basis [7], while outside this region, the interaction of the

escaping electron with the residual ion is represented by Coulomb waves, perturbed by the residual multipolar interaction with the target [8].

2. Calculations

In the present paper, we have calculated the photoionization cross-sections for the ground $2s^2 2p^6 \ ^1S^e$ and excited $2s^2 2p^6 3p^3 \ ^1P^0 \ ^3S^e$ states of Al IV for photon energies ranging from the ground state ionization threshold. At these energies, only the channels associated to the first two Al V states $2s^2 2p^6 \ ^2P^0$ and $1s^2 2s^2 2p^6 \ ^2S^e$ are open. This photoionization processes from the three lowest states of Al IV up to the $^2S^e$ threshold of Al V can therefore be described as:

1. $h\nu + \text{Al IV } (1s^2 2s^2 2p^6 \ ^1S^e) \rightarrow [\text{Al V } (1s^2 2s^2 2p^5 \ ^2P^0) + e^-] \ ^1P^0$
 $\rightarrow [\text{Al V } (1s^2 2s^2 2p^6 \ ^2S^e) + e^-] \ ^1P^0,$
2. $h\nu + \text{Al IV } (1s^2 2s^2 2p^5 3p^3 \ ^1P^0) \rightarrow [\text{Al V } (1s^2 2s^2 2p^5 \ ^2P^0) + e^-] \ ^3S^e, \ ^3D^e$
 $\rightarrow [\text{Al V } (1s^2 2s^2 2p^6 \ ^2S^e) + e^-] \ ^3S^e, \ ^3D^e,$
3. $h\nu + \text{Al IV } (1s^2 2s^2 2p^5 3p^1 \ ^1P^0) \rightarrow [\text{Al V } (1s^2 2s^2 2p^5 \ ^2P^0) + e^-] \ ^1S^e, \ ^1D^e$
 $\rightarrow [\text{Al V } (1s^2 2s^2 2p^6 \ ^2S^e) + e^-] \ ^1S^e, \ ^1D^e,$
4. $h\nu + \text{Al IV } (1s^2 2s^2 2p^5 3p^3 \ ^3S^e) \rightarrow [\text{Al V } (1s^2 2s^2 2p^5 \ ^2P^e) + e^-] \ ^3P^0$
 $\rightarrow [\text{Al V } (1s^2 2s^2 2p^6 \ ^2S^e) + e^-] \ ^3P^0.$

In the R -matrix formulation of photoionization, the initial bound state i of Al IV and the final continuum states f of the residual ion Al V plus an outgoing electron are expanded consistently on collisional-type R -matrix basis sets, expressed in terms of the states of the N -electron residual ion Al V.

The two lowest LS states of Al V, included in the present calculation, are represented by CI expansions of the form

$$\phi_n(LS) = \sum_{i=1}^M \phi_i(\alpha_i LS) b_{i,n}, \quad (1)$$

where the $\{\phi_i\}$ are single configuration functions in which the orbital and spin angular momenta of the electrons are coupled as specified by $\{\alpha_i\}$ to form an eigenstate of L^2 and S^2 respectively. The radial part of each orbital is written in analytic form as a sum of Slaster-type orbitals

$$P_{nl}(r) = \sum_{i=1}^k r^{p_i} \exp(-\zeta_i r) a_i. \quad (2)$$

The a_i, p_i, ζ_i parameters in (2) and the b_i mixing coefficients in (1) are determined variationally as described elsewhere [6].

Our calculation uses six orthogonal orbitals ($1s, 2s, 2p, 3s, 3p$ and $3d$). The $1s, 2s$ and $2p$ orbitals are the self consistent orbitals optimized on the Al V ground state by Clementi and Roetti [9], while the $n = 3$ orbitals were obtained using the CIV3 program of Hibbert [10], as described by Mohan and Hibbert [6]. In table 1, we have given the optimized values of the parameters a_i, p_i and ζ_i for the $3s, 3p$ and $3d$ orbitals. In table 2, we have

Table 1. Parameters of the $3l$ Slater-type orbitals.

Orbital	a_i	p_i	ζ_i
$3s$	0.14873	1	10.44923
	-0.59151	2	4.20370
	1.15639	3	2.18283
$3p$	0.40291	2	4.92276
	-1.04040	3	1.89893
$3d$	0.06417	3	4.43373
	0.96731	3	1.75757

Table 2. Configurations used in the CI expansion of Al V target states.

Target states	Key No.	Configurations used
$2P^0$	1	$[1s^2]2s^22p^5, 2s^22p^4(^3P)3p, 2p^4(^1D)3p,$ $2p^4(1S)3p, 2p^5(^2P^0)3s^2, 2p^5(^2P^0)3p^2$
$2S^e$	2	$[1s^2]2s2p^6, 2s2p^5(^3P^0)3p, 2p^5(^1P^0)3p,$ $2s^22p^4(1S)3s, 2p^6(^1S)3s^2, 2s^22P^4(^1D)3d$

Table 3. Excitation thresholds for Al V.

Key No.	Configuration	State	Energy in Rydberg	
			Theoretical	Experimental
1	$1s^22s^22p^5$	$2P^0$	0.0000	0.0000
2	$1s^22s^22p^6$	$2S^e$	3.3735	3.2384

listed the configurations used in the CI expansion of the Al V target states, while, in table 3, we have compared our theoretical energy separations between the Al V states included in the collisional calculation, with the experimental ones, compiled by Martin and Zalubas [11]. The agreement between them is reasonably good.

In the inner region of configuration space, the initial bound state Ψ_i and the final continuum states Ψ_{fE} for the $(N+1)$ -electron system are expanded in terms of discrete R -matrix basis Ψ_k of adequate LSII symmetry as

$$\Psi_1^{L_i S_i \Pi_i} = \sum_k \Psi_k^{L_i S_i \Pi_i} A_{k,i} \quad \text{and} \quad \Psi_{fE}^{L_f S_f \Pi_f} = \sum_k \Psi_k^{L_f S_f \Pi_f} A_{k,fE}^- \quad (3)$$

where R -matrix basis functions are chosen as

$$\Psi_k^{LS\Pi}(z_1, \dots, x_{N+1}) = A \sum_{ij} \bar{\Psi}_i^{LS\Pi}(x_1, \dots, x_N, \hat{r}_{N+1}, \sigma_{N-1}) u_{ij}(r_{N-1}) c_{ij,k} + \sum_i \bar{\Psi}_i^{LS\Pi}(x_1, \dots, x_{N+1}) d_{j,k}, \quad (4)$$

where A is the antisymmetrisation operator, the $\{\bar{\Psi}_i^{LS\Pi}\}$ are channel functions consisting of the CI wavefunction for a residual ionic state coupled with spin-angle function $\chi(\sigma_{N+1}, \hat{r}_{N+1})$ for the $(N + 1)$ th electron to give an eigenstate of L, S and Π . The u_{ij} are continuum radial orbitals, obtained by solving the zero-order radial differential equation [5,7]:

$$\left[-\frac{d^2}{dr^2} + \frac{l_i(l_i - 1)}{r^2} + V(r) - k_j^2 \right] u_{ij}(r) = \sum_n \lambda_{ij,n} P_{nl}(r) \delta_{li} \quad (5)$$

subject to the boundary conditions:

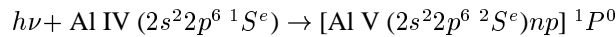
$$u_{ij}(r = 0) = 0 \quad \text{and} \quad \frac{a}{u_{ij}} \frac{du_{ij}}{dr} \Big|_{r=a} = 0. \quad (6)$$

The Lagrange multipliers $\lambda_{ij,n}$ ensure that the continuum orbitals are orthogonal to the physical orbitals of the ground ionic state having the same orbital momentum l_i . Finally, the whole set of bound P_{ni} and continuum u_{ij} orbitals for a given angular symmetry l_i is Schmidt orthogonalized in order to form an orthonormal set in the internal region. As a consequence, bound configurations of the $(N + 1)$ -electron system $\Phi_j^{LS\Pi}(x_1, \dots, x_{N+1})$ are included in the R -matrix expansion (4) in order to account for the orthogonality between the bound P_{nl} and continuum u_{ij} orbitals having the same symmetry and eventually, to include additional short range correlations.

The coefficients $\{c_{ijk}\}$ and $\{d_{jk}\}$, as well as the corresponding eigenvalues E_k , are determined by diagonalising the $(N + 1)$ electron Hamiltonian in the internal region. The coefficients $A_{k,i}$ and $A_{k,fE}$ in (3) are finally obtained [5] by matching at the inner region radius a , to an external solution satisfying the adequate asymptotic boundary conditions for the initial state i or the final continuum states fE .

3. Results and discussion

The present calculations were performed in LS coupling. Figure 1 shows the total photoionization cross-section of Al IV from its ground state $[1s^2]2s^22p^6 \ ^1S^e$, in the photon energy range from $[1s^2]2s^22p^5 \ ^2P^0$ threshold to just above the second threshold $[1s^2]2s^22p^6 \ ^2S^e$. Only the length results are given throughout the paper, since the discrepancy between length and velocity value is less than 10%. For photoabsorption from $2s^22p^6 \ ^1S^e$ there is only one final $LS\Pi$ state i.e. $\ ^1P^0$ is allowed by selection rule which leads to a single Rydberg series of autoionised resonances Al IV $[(2s^22p^6 \ ^2S^e)np \ ^1P^0]$ converging to $\ ^2S^e$ valence excited state. This process can be represented by



which clearly corresponds to one photon jump $2s$ to $2p$ from the inner shell. The first autoionised member of the series i.e. Al IV $[(2s2p^6 \ ^2S^e)3p \ ^1P^0]$ appearing on the figure 1 has a resonances position 9.63332 Ryd and effective quantum number 2.53 which is quite close to the experimental resonance position 9.53610 Ryd [12] and experimental effective quantum number 2.50. We have identified the higher members of the series up to $n = 8$. In table 4, we list their position and effective quantum numbers and we compare them.

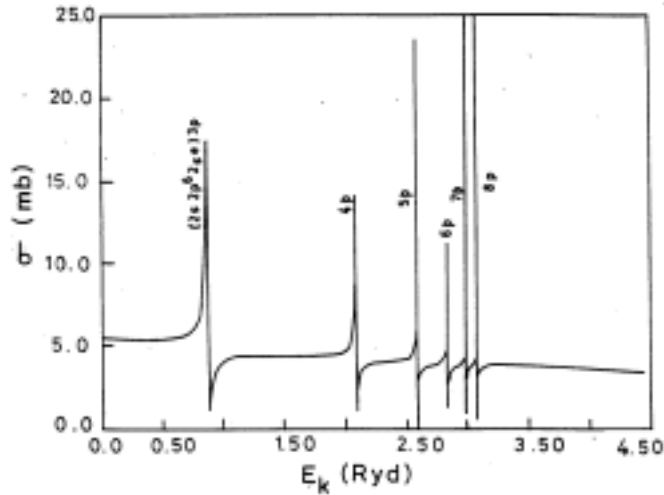


Figure 1. The cross-section in mb for photoionization from the Al IV ($1s^2 2s^2 2p^6 \ ^1S^e$). The figure shows the cross-section against the energy of the ejected electron, E_k (in Ryd.) in the region from the first ionisation threshold, $2s^2 2p^5 \ ^2P^0$, to just above the second threshold, $2s^2 2p^6 \ ^2S^e$.

Table 4. Resonance positions and effective quantum numbers for the Al IV [$2s^2 2p^6 \ ^2S^e \ np \ ^1P^0$] Rydberg series converging to the ($2s^2 2p^6$) $^2S^e$ limit of Al IV. Also given ionisation potential of Al V ($2s^2 2p^6 \ ^1S^e$) and threshold of Al V ($2s^2 2p^5 \ ^2S^e$).

Ionisation potential of Al V ($1s^2 2s^2 2p^6$) (Ryd.)		Threshold of Al V ($1s^2 2s^2 2p^5 \ ^2S^e$) (Ryd.)	
Theory	Experiment	Theory	Experiment
8.76799	8.81930	12.13180	12.08910

Series	Limit	Configuration	Resonance position E_n	
			Experiment	Theory
$^1P^0$	$[1s^2] 2s^2 2p^6 \ ^2S^e$	$[1s^2] 2s^2 2p^6 \ ^2S^e \ 3p$	9.53610	9.6332
		$[1s^2] 2s^2 2p^6 \ ^2S^e \ 4p$	10.79959	10.84015
		$[1s^2] 2s^2 2p^6 \ ^2S^e \ 5p$	11.30888	11.35162
		$[1s^2] 2s^2 2p^6 \ ^2S^e \ 6p$	11.56580	11.60817
		$[1s^2] 2s^2 2p^6 \ ^2S^e \ 7p$	11.71449	11.75737
		$[1s^2] 2s^2 2p^6 \ ^2S^e \ 8p$	11.80707	11.85010

Figures 2 and 3 displays the total photoionization cross section from the $2s^2 2p^5 2s \ ^3P^0$ first excited state of Al IV. Here, we find two Rydberg series Al IV [$(2s^2 2p^6 \ ^2S^e) ns \ ^3S^e$] and Al IV [$(2s^2 2p^6 \ ^2S^e) nd \ ^3D^e$] converging on the $^2S^e$ threshold. These are the only two Rydberg series accessible in this energy range by dipole photoabsorption from the $^3P^0$

state. The position and effective quantum for these resonances are given in table 5. Here in figure 3 we find one interesting phenomena that the first peak corresponding to autoionised resonance $(2s2p^6)^2S^e3s^3S^e$ is very large as compared to other peaks corresponding to other ns and nd resonances. This particular member corresponds to the following process

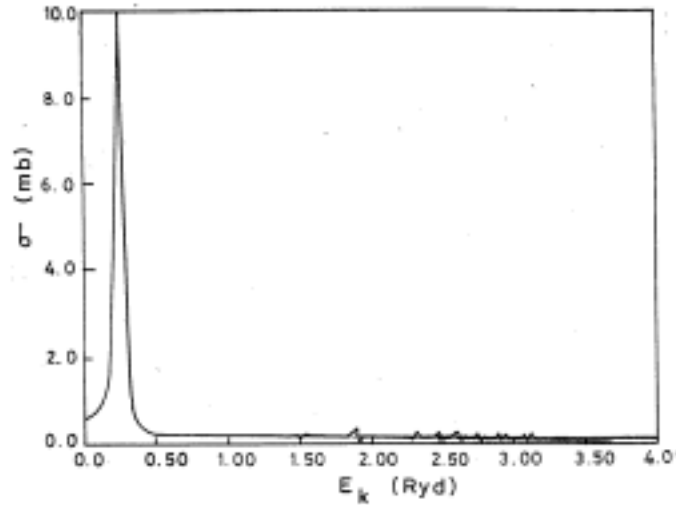
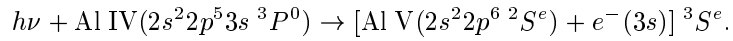


Figure 2. Cross-section photoionization from Al IV $(2s^22p^53p^3P^0)$ against energy, E_k (in Ryd.) in the region from the first ionisation threshold, $2s^22p^5^2P^0$, to just above the second threshold, $2s^22p^6^2S^e$.

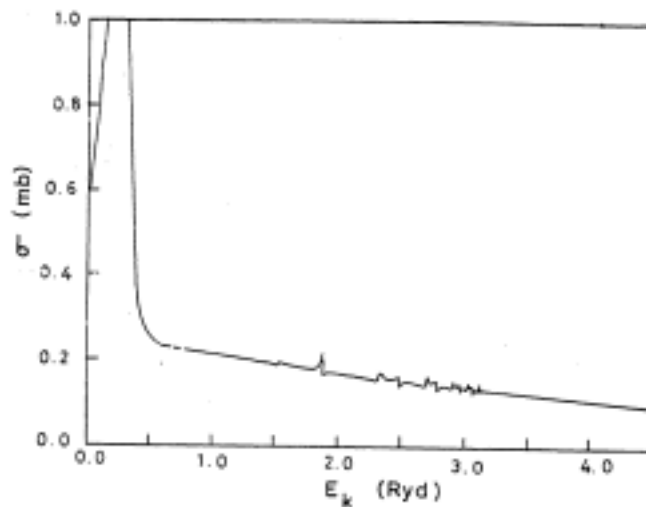


Figure 3. Same as in figure 2, but expanded view.

Table 5. Resonance positions and effective quantum numbers for the Rydberg series Al IV [$2s2p^6\ ^2S^e\ ns\ ^3S^e$] and Al IV [$2s2p^63p\ ^2S^e\ nd\ ^3D^e$] converging to the $(2s^2p^6)^2S^e$ limit of Al V.

Ionisation potential of Al V ($1s^22s^22p^5\ 3p\ ^3P^0$) (Ryd.)		Threshold of Al V ($1s^22s2p^5\ ^2S^e$) (Ryd.)		
Theory 3.17427		Theory 6.5381		
Series	Limit	Configuration	Resonance position	
			E_n	n^*
$^3S^e$	$[1s^2]2s2p^6\ ^2S^e$	$[1s^2]2s2p^6\ 3s$	3.43533	2.27083
		$[1s^2]2s2p^6\ 4s$	5.04149	3.26967
		$[1s^2]2s2p^6\ 5s$	5.65996	4.26852
		$[1s^2]2s2p^6\ 6s$	5.92361	5.27735
		$[1s^2]2s2p^6\ 7s$	6.131929	6.27621
		$[1s^2]2s2p^6\ 8s$	6.235809	7.27506
$^3D^e$	$[1s^2]2s2p^6\ ^2S^e$	$[1s^2]2s2p^6\ 3d$	4.72426	2.97002
		$[1s^2]2s2p^6\ 4d$	5.50159	3.92891
		$[1s^2]2s2p^6\ 5d$	5.87920	4.92776
		$[1s^2]2s2p^6\ 6d$	6.08259	5.92660
		$[1s^2]2s2p^6\ 7d$	6.20355	6.91547
		$[1s^2]2s2p^6\ 8d$	6.28267	7.91434

Table 6. Resonance positions and effective quantum numbers for the Rydberg series Al IV ($2s2p^63p\ ^2S^e$) and Al IV [$2s2p^63p\ ^2S^e\ nd\ ^1D^e$] converging to the $(2s^2p^6)^2S^e$ limit of Al V.

Ionisation potential of Al V ($1s^22s^22p^6\ ^1S^e$) (Ryd.)		Threshold of Al V ($1s^22s2p^5\ ^2S^e$) (Ryd.)		
3.1131005		6.47690		
Series	Limit	Configuration	Resonance position	
			E_n	n^*
$^1S^e$	$[1s^2]2s2p^6\ ^2S^e$	$[1s^2]2s2p^6\ 3s$	3.45446	2.30079
		$[1s^2]2s2p^6\ 4s$	5.01623	3.30962
		$[1s^2]2s2p^6\ 5s$	5.61898	4.31846
		$[1s^2]2s2p^6\ 6s$	5.91104	5.31730
		$[1s^2]2s2p^6\ 7s$	6.077139	6.32613
$^1D^e$	$[1s^2]2s2p^6\ ^2S^e$	$[1s^2]2s2p^6\ 4d$	5.45088	3.94888
		$[1s^2]2s2p^6\ 5d$	5.82069	4.93774
		$[1s^2]2s2p^6\ 6d$	6.02295	5.93658
		$[1s^2]2s2p^6\ 7d$	6.11430	6.93543
		$[1s^2]2s2p^6\ 8d$	6.22278	7.93427

Clearly this process involves only one electron jump from $2s$ to $2p$ from the inner shell therefore occurs with higher probability as compared to other resonances Al V ($2s2p^62S^e$) ns , $n > 3$ and Al V($2s2p^6\ ^2S^e$) nd , $n \geq 3$ which involves two electrons jumps.

Table 7. Resonance positions and effective quantum numbers for the Rydberg series Al IV ($2s2p^6\ ^2S^e\ np\ ^3P^0$) converging to the ($2s^2p^6$) limit of Al V.

Ionisation potential of Al V ($1s^22s^22p^6\ ^1S^e$) (Ryd.)		Threshold of Al V ($1s^22s2p^5\ ^2S^e$) (Ryd.)		
2.69227		6.0561		

Series	Limit	Configuration	Resonance position	
			E_n	n^*
$^3P^0$	$[1s^2]2s2p^6\ ^2S^e$	$[1s^2]2s2p^6\ ^2S^e\ 3p$	3.51759	2.51055
		$[1s^2]2s2p^6\ ^2S^e\ 4p$	4.76433	3.51938
		$[1s^2]2s2p^6\ ^2S^e\ 5p$	5.27580	4.52821
		$[1s^2]2s2p^6\ ^2S^e\ 6p$	5.53235	5.52705
		$[1s^2]2s2p^6\ ^2S^e\ 7p$	5.68155	6.53588
		$[1s^2]2s2p^6\ ^2S^e\ 8p$	5.77428	7.53474

Resonances of this type involving one electron jump are also noted by Yan and Seaton [2] and are referred as PEC resonances.

The total photoionization cross-section from the $2s^22p^63s\ ^1P^0$ state of Al IV. Again, we get two Rydberg series Al IV [$(2s2p^6\ ^2S^e)ns\ ^1S^e$] and Al IV [$(2s2p^6\ ^2S^e)nd\ ^1D^e$], which are autoionized for $n^* \geq 3$ ($3d, 4s, \dots$). Their positions are listed in table 6 for comparison with any future experiment. Here again we find the peak for the first member of the Rydberg series Al IV [$(2s2p^6\ ^2S^e)3s\ ^1S^e$] is quite high as compared to other. This resonance is again PEC as it involves one electron jump i.e. $2s$ to $2p$ (core excitation).

In the last, for the total photoionization cross-section from the fourth excited state $2s2p^52p\ ^3S^e$, here like in ground state $^1S^e$ only single final $^3P^0$ symmetry is allowed, leading to one Rydberg series Al IV [$(2s2p^6\ ^2S^e)np\ ^3P^0$] converging on to the $^2S^e$ threshold.

To conclude, we expect our results to be quite reliable, as we have taken all the important physical effects like exchange, channel coupling and short-range correlation into account.

Acknowledgement

MM is thankful to UGC and DST, India. SERC (UK) and ICTP, Trieste (Italy) for financial support.

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