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Calculation of Rates of 4p–4d Transitions in Ar II

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Abstract: Recent experimental work by Belmonte et al. (2014) has given rates for some 4p–4d transitions that are significantly at variance with the previous experimental work of Rudko and Tang (1967) recommended in the NIST tabulations. To date, there are no theoretical rates with which to compare. In this work, we provide such theoretical data. We have undertaken a substantial and systematic configuration interaction calculation, with an extrapolation process applied to ab initio mixing coefficients, which gives energy differences in agreement with experiment. The length and velocity forms give values that are within 10%–15% of each other. Our results are in sufficiently close agreement with those of Belmonte et al. that we can confidently recommend that their results are much more accurate than the early results of Rudko and Tang, and should be adopted in place of the latter.

Keywords: E1 transitions; configuration interaction calculaton; transition rates

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1. Introduction

Some years ago, we [1–3] studied transitions among Ar II levels arising from configurations $3s^23p^5$, $3s3p^6$, $3p^43d$, $3p^44s$, and $3p^44p$. That work was prompted by a range of conflicting experimental results and a limited amount of theoretical work. We found that our calculations gave transition rates in close agreement with the experimental values recommended by Vujnović and Wiese [4], and gave much closer agreement between length and velocity forms of transition rates than were obtained by the only other major theoretical work, conducted by Luyken[5]. The values cited in the NIST tabulations [6] are taken from Bennett et al. [7] where possible, in agreement with the recommended values given in [4], but for other 4p–4d transitions, it is the data of Rudko and Tang [8] which are quoted.

Recently, Belmonte et al. [9]—building on the work of Aparicio et al. [10]—extended the experimental study to 4p–4d (and a few other) transitions. They also included results for some transitions between the lower-lying levels previously studied in [2–4], and found that they were in much closer agreement with the experimental values recommended by Vujnović and Wiese [4], and with our previous calculations, than with other experimental work. By contrast, they found that their results differed by up to a factor of five from the experimental values of Rudko and Tang [8]. The purpose of the present work is to provide some theoretical corroboration (or otherwise) of the new experimental results.

2. Method of Calculation

The calculations in this work have been undertaken using the code CIV3 [11,12].

2.1. Basic Theory

We express the wave functions in terms of configuration interaction (CI) expansions:

$$\Psi(J) = \sum_{i=1}^{M} a_i \Phi_i(\alpha_i L_i S_i J) \tag{1}$$

where $\{\Phi_i\}$ are single-configuration functions (configuration state functions—CSFs) and the expansions in general include summations over L_i and S_i. For a specific choice of $\{\Phi_i\}$, the expansion coefficients $\{a_i\}$ are the eigenvector components of the diagonalized Hamiltonian with matrix elements $H_{ij} = < \Phi_i|H|\Phi_j >$. In this work, we take the Hamiltonian H to be the Schrödinger Hamiltonian plus the mass correction and Darwin terms, together with a modified spin-orbit term

$$H_{so} = \frac{1}{2}\alpha^2 \sum_{i=1}^{N} \frac{Z\zeta_l}{r_i^3}\mathbf{l_i}.\mathbf{s_i} \tag{2}$$

In (2), the sum is over the electrons, and the parameters $\{\zeta_l\}$ depend on the l-value of the electrons involved in the interaction (Hibbert and Hansen 1989) [2].

The ordered eigenvalues $\{E_i\}$ of the Hamiltonian matrix are upper bounds to the similarly-ordered energy levels:

$$E_i \geq E_i^{\text{exact}} \tag{3}$$

Hence, any of the eigenvalues may be used as the variational functional for optimisation of the radial parts of the one-electron orbitals from which the $\{\Phi_i\}$ are constructed. We express these radial functions as sums of normalised Slater-type orbitals (STOs):

$$P_{nl}(r) = \sum_{j=1}^{k} C_{jnl}\chi_{jnl}(r) \tag{4}$$

where the STOs are of the form

$$\chi_{jnl}(r) = \left[\frac{(2\xi_{jnl})^{2I_{jnl}+1}}{(2I_{jnl})!}\right]^{1/2} r^{I_{jnl}} \exp(-\xi_{jnl}r) \tag{5}$$

Being integers, the $\{I_{jnl}\}$ are kept fixed, but the exponents $\{\xi_{jnl}\}$ and the coefficients $\{C_{jnl}\}$ may be treated as variational parameters in (3), subject to the orthonormality conditions:

$$\int_0^\infty P_{nl}(r)P_{n'l}(r)dr = \delta_{nn'}; \qquad l < n' \leq n \tag{6}$$

2.2. Radial Function Parameters

Since we were adding to earlier work [3], we were able to use many of the radial functions we used previously. However, that work did not include 4d levels. The radial function parameters are determined by optimising the energy associated with different states; the optimisation is undertaken in LS coupling. The radial function parameters used in this work were optimised as displayed in Table 1. We comment here on the reasons underpinning the choice of procedure used for the functions new to this work.

- The 6p function was newly introduced in this calculation. While retaining the 4p and 5p functions from previous work, the parameters for 6p were optimised on the ground state to improve the capture of the electron correlation effect in the n = 3 shell, and thereby improve the calculated separation between the ground and excited states.
- We retained the previous 3d and 4d functions, but reoptimised 5d and 6d. We considered the lowering of the energy of several different states brought about by the introduction of 5d. The effect was largest for the $3p^4 4d\ ^4F$ state. Similarly, the lowering of the energy of several different doublet states through the introduction of 6d was noted. There was a substantial difference in the mixings between doublet states, depending on the final LS symmetry chosen for the optimisation. As a consequence, we selected those obtained during the optimisation of the $3p^4(^3P)4d\ ^2D$ state.

- We reoptimised the 6s function on the 5s ^{4}P state, since the energy of that state lay in the region of those of the 4d states.

The set of parameters for all the radial functions used here is displayed in Table 2.

Table 1. Method of determining the radial functions.

Orbital	**Process of Optimisation**	
1s, 2s, 2p, 3s	Hartree–Fock orbitals of 3p^4 ^{1}D of Ar III (Clementi and Roetti (1974)) [13]	
3p	Exponents taken from the Hartree–Fock orbital of 3p^4 ^{1}D of Ar III; coefficients reoptimised on 3p^{4}4s ^{4}P of Ar II	
	Eigenvalue minimised	Configurations
3d	3s3p^6 ^{2}S	3s3p^6, 3s^{2}3p^{4}3d
4s	3p^{4}4s ^{4}P	3p^{4}4s
4p	3p^{4}4p ^{4}D^o	3p^{4}4p
4d	3p^{4}3d ^{4}D	3p^{4}3d, 3p^{4}4d
4f	3p^{4}3d ^{4}P	3p^{4}4s, 3p^{4}3d, 3p^{4}4d, 3p^{3}3d4f
5s	3p^{4}4p ^{4}D^o	3p^{4}4p, 3p^{3}4s5s
5p	3p^{4}4p ^{4}P^o	3p^{4}4p, 3p^{4}5p
5d	3p^{4}4d ^{4}F	3p^{4}3d, 3p^{4}4d, 3p^{4}5d
5f	3p^{4}4p ^{4}D^o	3p^{4}4p, 3p^{4}4f, 3p^{4}5f
6s	3p^{4}5s ^{4}P	3p^{4}4s, 3p^{4}5s, 3p^{4}6s
6p	3p^5 ^{2}P^o	3p^5, 3p^{4}4p, 3p^{4}5p, 3p^{4}6p
6d	3p^{4}4d(^{3}P) ^{2}D	3p^{4}3d, 3p^{4}4d,3p^{4}5d, 3p^{4}6d

2.3. *Choice of Configurations*

In our previous work [3], we included a limited range of configurations aimed at capturing the main correlation effects in the 3p^{4}3d/4s/4p states. This led to some difficulties, primarily that the degree of correlation included in the ground state was substantially greater than for the excited states, and the order of some 3d and 4s levels was incorrect.

Consequently, in this work, we have included all possible configurations that can be obtained by one- and two-orbital replacements from the 3*l* and 4*l* subshells to the full set of orbitals shown in Table 2, from the configurations of the following reference sets.

Odd	3p^5; 3p^{4}4p
Even	3s3p^6; 3p^{4}4s, 3p^{4}5s, 3p^{4}6s; 3p^{4}3d, 3p^{4}4d, 3p^{4}5d, 3p^{4}6d

The configurations of the reference sets were those with a significant CI coefficient in a relatively small CI calculation. For each possible LSπ symmetry, all CSFs were then constructed and combined to give a set of CSFs for each allowed J π symmetry, resulting in Hamiltonian matrices of the following sizes.

	J = 0.5	J = 1.5	J = 2.5	J = 3.5	J = 4.5
Odd	13,082	18,144	17,603	9148	
Even	44,149	75,383	75,964	61,072	28,854

Table 2. Radial function parameters.

nl	C_{jnl}	I_{jnl}	ξ_{jnl}	***nl***	C_{jnl}	I_{jnl}	ξ_{jnl}
1s	0.926 94	1	17.332 10	2p	−0.011 17	3	3.102 81
	0.058 91	1	25.455 00		0.004 97	3	2.011 93
	0.007 82	2	7.657 68		0.145 75	3	5.190 03
	0.017 65	2	15.623 20		0.824 78	2	6.928 92
	0.000 90	3	3.237 31		0.087 03	2	13.042 40
	−0.000 47	3	2.296 92				
	−0.003 17	3	6.726 86	3p	0.530 23	3	3.102 81
					0.583 91	3	2.011 93
2s	−0.277 90	1	17.332 10		−0.074 28	3	5.190 03
	−0.008 62	1	25.455 00		−0.272 24	2	6.928 92
	0.816 64	2	7.657 68		−0.025 06	2	13.042 40
	−0.127 59	2	15.623 20				
	0.013 06	3	3.237 31	4p	0.744 05	4	0.995 10
	−0.003 71	3	2.296 92		0.297 40	4	0.775 02
	0.331 25	3	6.726 86		−0.296 30	3	2.508 00
					0.082 76	2	7.360 60
3s	−0.094 80	1	17.332 10				
	−0.001 41	1	25.455 00	5p	4.629 07	4	0.861 89
	0.289 14	2	7.657 68		−4.686 80	4	1.000 00
	−0.043 25	2	15.623 20		0.735 21	3	3.221 66
	−0.640 52	3	3.237 31		−0.403 55	2	3.473 69
	−0.494 62	3	2.296 92				
	0.216 65	3	6.726 86	6p	6.828 07	5	0.937 15
					−8.463 99	4	0.892 84
4s	0.487 62	4	1.299 90		3.198 41	4	1.697 71
	0.569 47	4	1.016 95		−1.193 75	3	2.716 06
	−0.384 57	3	2.931 16		0.308 57	2	8.508 55
	0.157 04	2	6.149 39				
	−0.042 15	1	14.064 49	3d	0.249 70	3	3.465 62
					0.821 57	3	1.684 33
5s	1.133 28	5	1.364 91				
	−2.125 95	4	2.019 60	4d	0.216 25	3	2.817 41
	1.487 29	3	2.884 30		0.300 37	3	1.891 60
	−0.468 68	2	5.897 16		−1.104 59	4	0.964 72
	0.113 37	1	14.178 86		0.067 82	4	0.570 20
6s	1.293 76	5	0.685 92	5d	0.438 75	3	2.189 96
	1.084 37	4	2.019 36		−1.653 12	3	0.717 04
	−1.350 12	4	1.180 83		1.981 83	4	0.612 62
	−0.458 59	3	2.844 45				
	0.120 74	2	5.635 72	6d	0.594 56	3	2.112 65
	−0.026 11	1	14.432 79		−3.249 46	3	0.719 43
					4.546 89	4	0.699 99
4f	1.000 00	4	2.154 77		−2.054 58	4	0.429 47
5f	0.522 16	4	2.573 22				
	−1.044 69	5	1.224 76				

2.4. Relativistic Effects

As in our earlier work [3], relativistic effects are included using the Breit–Pauli approximation, retaining in the Hamiltonian the mass correction and Darwin terms and a modified spin-orit term as given in (2). The parameters ζ_l—which depend only on the l-value of the electrons—were chosen to give the best fit to matrix elements of the full spin-orbit plus spin-other-orbit operators with respect to key CSFs. This led to the values 0.0, 0.856, 1.0, 1.0 for l = 0, 1, 2, 3, respectively. The d- and f-orbitals contribute little to the fine structure, most of which comes from configurations containing $3p^4(^3P)$.

3. Results

In our earlier work [3], we found that our choice of configurations resulted in the ground state being around 12,000 cm^{-1} too low when compared with the excited states. In the present work, with our more systematic choice of configurations, we find that our ab initio energy separations are in much better agreement with the experimental work of Minnhagen [14] and Saloman [15], given in the tabulations of NIST [6]. Most of the energy separations agree to within 1000 cm^{-1} with these experimental results, the exceptions being a few of the levels associated with states containing a 3p^4 ^{1}D core (within 3000 cm^{-1}) and those of 3p^4 ^1S 3d (about 4000 cm^{-1}). Moreover, the difficulty we encountered earlier with a very strong mixing between the 3p^4(^{1}D)4s and 3p^4(^{3}P)3d ^{2}D$_{3/2}$ levels is now sufficiently removed to clearly define the lower of the two as belonging to the 4s state, in agreement with experiment.

Before calculating the electric dipole transition rates between all these levels, we refined the CI mixing coefficients by making small adjustments to some diagonal elements of the Hamiltonian matrices, and then rediagonalising the adjusted matrices. In this way, we were able to bring the calculated eigenvalue differences into agreement with the experimental energy separations. From past experience, we have found that, while the mixing coefficients are improved by this process, there is a tendency for the coefficients to be somewhat over-corrected. However, since most of the matrix corrections are quite small, and many of the levels are spectroscopically fairly pure, the principal effect of this fine-tuning process will be to allow the use of experimental energy separations, with some modifications to the interactions between levels in a limited number of cases.

In Table 3, we present our calculated transition rates in both length and velocity gauges for those 4p–4d transitions for which experimental values are given by [9]. The corresponding results from the experimental determinations of [7,8] are also listed. Belmonte et al. [9] also give estimates of the uncertainties in their results, which they obtain not only from the customary standard deviation of experimental measurements, but also from a detailed and careful analysis of a range of other factors which could lead to uncertainties. As a result of this analysis, they are able to provide uncertainties, most of which lie in the 10%–20% range, with a small proportion having higher uncertainties. Table 3 quotes those uncertainties.

Table 3. *A*-values (10^8 s^{-1}) for 4p–4d transitions in Ar II.

Transition		**This Work**					
4p *	4d	Wavelength (nm)	A_l	A_v	[9]	[7]	[8]
$^4P^o_{5/2}$	$^4F_{3/2}$	319.423	0.074	0.066	0.086 (12%) †		0.236
$^4P^o_{1/2}$	$^4F_{3/2}$	326.357	0.105	0.094	0.13 (11%)	0.155	0.348
$^4P^o_{5/2}$	$^4F_{7/2}$	326.899	0.0031	0.0026	0.002 (84%)		
$^4P^o_{5/2}$	$^4P_{5/2}$	313.902	0.625	0.551	0.49 (18%)	0.52	1.00
$^4P^o_{3/2}$	$^4P_{5/2}$	316.967	0.524	0.455	0.43 (18%)	0.49	0.817
$^4P^o_{5/2}$	$^4P_{3/2}$	318.104	0.469	0.421	0.36 (12%)	0.37	0.627
$^4P^o_{3/2}$	$^4P_{1/2}$	324.369	1.18	1.05	1.07 (11%)	1.1	1.99
$^4P^o_{1/2}$	$^4P_{3/2}$	324.980	0.763	0.678	0.60 (14%)	0.63	1.00
$^4P^o_{1/2}$	$^4P_{1/2}$	328.170	0.459	0.405	0.41 (11%)	0.42	0.733
$^4D^o_{3/2}$	$^4D_{1/2}$	384.152	0.258	0.235	0.19 (12%)	0.269	0.267
$^4D^o_{5/2}$	$^4D_{7/2}$	384.473	0.051	0.046	0.049 (17%)	0.048	0.047
$^4D^o_{5/2}$	$^4D_{5/2}$	382.681	0.325	0.297	0.30 (15%)	0.281	0.345
$^4D^o_{5/2}$	$^4D_{3/2}$	379.938	0.221	0.199	0.22 (13%)	0.17	0.23
$^2D^o_{3/2}$	$^2P_{3/2}$	320.432	0.176	0.171	0.24 (12%)		0.402
$^2D^o_{3/2}$	$^2P_{1/2}$	327.332	0.172	0.158	0.20 (16%)		0.371
$^2D^o_{3/2}$	$^4D_{1/2}$	403.138	0.039	0.033	0.07 (60%)	0.075	
$^2D^o_{5/2}$	$^2D_{5/2}$	295.539	0.325	0.297	0.19 (13%)		

Table 3. *Cont.*

Transition			This Work				
$^2D^o_{5/2}$	$^2D_{5/2}$	301.448	0.036	0.034	0.039 (19%)		
$^2P^o_{3/2}$	$^4F_{3/2}$	383.017	0.0008	0.0009	0.042 (27%)		
$^2P^o_{3/2}$	$^2F_{5/2}$	365.528	0.326	0.316	0.37 (13%)		0.232
$^2P^o_{3/2}$	$^2P_{3/2}$	329.364	0.899	0.847	0.59 (17%)		1.73
$^2P^o_{1/2}$	$^2P_{1/2}$	330.723	1.44	1.38	1.43 (11%)		3.35
$^2P^o_{3/2}$	$^2P_{1/2}$	336.658	0.271	0.255	0.24 (15%)		0.409
$^2S^o_{1/2}$	$^2P_{3/2}$	338.853	0.761	0.795	0.81 (12%)		1.91
$^2S^o_{1/2}$	$^2D_{3/2}$	316.137	0.370	0.368	0.35 (45%)		1.837
4p′	4d′	Wavelength (nm)	A_l	A_v	[9]	[7]	[8]
$^2F^o_{5/2}$	$^2F_{5/2}$	335.092	0.929	0.815	0.90 (13%)		1.48
$^2F^o_{7/2}$	$^2F_{5/2}$	336.552	0.073	0.066	0.075 (18%)		0.131
$^2F^o_{7/2}$	$^2F_{7/2}$	337.644	0.860	0.764	0.74 (13%)		1.49
$^2P^o_{3/2}$	$^2P_{3/2}$	366.044	0.741	0.693	0.73 (11%)		2.22
$^2P^o_{3/2}$	$^2P_{1/2}$	367.101	0.199	0.191	0.23 (31%)		0.709
$^2P^o_{1/2}$	$^2D_{3/2}$	368.006	0.031	0.007	0.59 (19%)		1.15
$^2P^o_{3/2}$	$^2S_{1/2}$	302.675	0.600	0.679	1.03 (21%)		
$^2D^o_{3/2}$	$^2D_{5/2}$	379.659	0.141	0.132	0.18 (23%)		0.250
$^2D^o_{5/2}$	$^2D_{5/2}$	380.317	0.978	0.902	0.89 (12%)		1.53
$^2D^o_{3/2}$	$^2P_{3/2}$	381.902	0.244	0.172	0.15 (49%)		0.0036
$^2D^o_{5/2}$	$^2P_{3/2}$	382.567	0.384	0.356	0.33 (55%)		0.756

* *nl* denotes $3p^4(^3P)nl$; *nl*′ denotes $3p^4(^1D)nl$; † estimated uncertainty.

4. Discussion

The accuracy of theoretical energy differences and transition rates can only be estimated: there is no monotonic convergence of these quantities, even as the wave functions are systematically improved. Instead, it is necessary to refer to a number of *indicators* of accuracy, as explained in [16]. These indicators include a comparison between calculated and experimental energy levels, the convergence of results as the wave functions are improved, the degree of agreement between different forms of the transition rates (typically length and velocity), comparison with other calculations, and of course, comparison with experiment.

In this work, we have adopted our fine-tuning process, which ensures that we are using accurate transition energies and that the CI mixing coefficients are as accurate as we can obtain within the limitations of our finite configuration lists. We have not undertaken a sequence of calculations of different complexity, as would be necessary if we were to establish the degree of convergence of the results, but as many of the levels are fairly pure spectroscopically, we do not believe that this would have a major influence on the level of accuracy achieved. There are no other theoretical transition rates available in the literature for these transitions. That leaves two major factors to be taken into account in assessing the accuracy of our calculations.

It can be observed from Table 3 that the length and velocity forms of our calculated transition rates differ fairly consistently by about 10%–15%, the length form mostly giving the larger of the two. This discrepancy is an indication of either insufficient treatment of electron correlation in the $3p^4$ core, or (given the strong state-dependency of the valence orbitals) insufficient flexibility in the form of the radial functions of the valence orbitals; that is, there may be too few basis functions in the expansions (4).

However, in spite of these limitations, the important thing to note is the comparison between our calculated *A*-values and the experimental values recently determined by Belmonte et al. [9]. For most transitions listed in Table 3, our results lie quite close to the experimental values of [9], bearing in mind the uncertainty of both sets of results. Similar good agreement is found with the experimental results of [7], which are the values recommended in the critical compilation of [4].

By contrast, the experimental results of Rudko and Tang [8] are substantially different from both the recent experimental values and our calculations.

In view of these considerations, we would anticipate that for most of the transitions listed in Table 3, our results are accurate to about 20%–25%, or better.

5. Conclusions

We have undertaken a substantial calculation of 4p–4d transitions in Ar II, using a systematic configuration interaction process. These results provide the only theoretical corroboration with which the recent experimental results given in [9] and in other earlier work may be compared. It is clear that our calculations substantially support the results of Belmonte et al. [9], and of Bennett et al. [7] (where comparison is possible), but are in substantial disagreement with the experimental data of Rudko and Tang [8] for many of the transitions considered here. However, until the recent work of [9], the only available data for the doublet transitions was that of [8], and for those transitions, it is the values of [8] which are quoted in the NIST tabulations [6]. We therefore recommend that—where possible—the transition rates of [9] are adopted instead.

Conflicts of Interest: The author declares no conflict of interest.

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