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Semi-empirical calculations of transition probabilities for atomic aluminium

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Abstract. We discuss the use of a semi-empirical method to obtain the energy values of 391 energy levels and dipolar-electric radiative transition probabilities in neutral aluminium. A relativistic Hartree-Fock atomic structure code allowing superposition of configurations coupled with a least-square fit procedure has been used for this purpose. Einstein coefficients for spontaneous emission not yet tabulated by the NIST atomic spectra database are reported for several transitions.

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1. Introduction

Aluminium is an important element both on earth and in astrophysics. Determination of its abundance may be of major interest for many purposes. In many situations, a proper evaluation of this abundance is based on the radiative properties of aluminium and this evaluation makes use of atomic data such as energy levels and transition probabilities (A values). Obtaining and discussing spectroscopic reference data for neutral aluminium (Al I) in particular, is strongly necessary to achieve this goal. Over the years, a significant amount of experimental and theoretical results concerning Al I has been obtained to analyze laboratory spectra or astrophysical observations. Even so, very few reliable measurements exist for the A values. In particular, taking the NIST atomic spectra database [1] as a reference source of information, very few values of transition probabilities exist in comparison with the important list of energy levels. These specific data come from a critical evaluation published in Ref. [2]. Besides this, only theoretical values of transition probabilities may be found, more or less scattered in the literature. Furthermore, the use of these values relies on a proper identification of the spectral lines, which is far from being guaranteed since the calculated energy of electronic levels may have large uncertainty. Thus, to determine accurate transition probabilities, a reliable identification of energy levels is crucial.

Al I is a neutral three valence electron system where correlation effects are important so that the configuration interaction (CI) has a large impact. This is particularly true for $3s\ 3p^2\ ^2D$ states which mix with many other $3s^2\ nd\ ^2D$ states. Accurate calculations of this complex system are possible using large scale MultiConfiguration Hartree-Fock [3] or MultiConfiguration Dirac-Fock [4] approaches. In the former case, calculations are often performed at the Breit-Pauli approximation in order to capture relativistic effects. Large CI calculations allow to consider valence and core-valence electron correlations, but this implies a specific procedure to define the large set of the necessary configurations [5]. Indeed correlation effects are taken into account by defining each *atomic state function* as an expansion over many *configuration state functions*. The convergence of this expansion toward accurate energy values of the electronic levels is difficult to control, so these *ab initio* calculations often rely on a comparison with precise experimental results, when they exist. One can mention that, in addition to the intra-valence correlations taken into account by a configuration expansion, a method to include also core-polarization effects i.e. core-valence correlations (without adding configurations in the expansion) by means of a core-polarization model potential has been proposed [6, 7]. This potential is directly proportional to a parameter α_d which is the atomic dipole polarizability (here of the ionic core). In Ref. [8], the value $\alpha_d = 0.259\ a_o^3$ is given for the $n=2$ core of aluminium (a_o being the Bohr radius). Such a value can be considered as small so that, in the case of Al I, polarization of the core is not supposed to be important.

With respect to the previous *ab initio* calculations, the other approach is semi-empirical (see for instance Ref. [9]). While only possible when some precise energy measurements are already available, this approach yields an accuracy for other energy levels which is competing with more advanced *ab initio* models which may require large computational resources in the case of large CI. Still working in the Racah-Slater theory of atomic structure, this semi-empirical approach consists in using a *reduced* set of configurations (although large enough to capture the main configuration mixing) in the atomic state function expansion, and modify some of the so-called Slater parameters (E_{av} , F^k , G^k) and the so-called Spin-Orbit integrals ζ (for a proper definition of these parameters, see atomic structure textbooks, e.g. Ref. [10]). In principle CI effects must be properly accounted by means of off-diagonal Slater parameters called CI integrals R^k . One may also vary these CI integrals R^k . Optimisation of the whole set of parameters is realized through a least-square fitting procedure with the existing and well identified measured energy levels. On the whole, the fitted parameters are expected to "absorb" CI effects from far-lying configurations. Once a good fit is obtained, one can compute a more or less important set of energy levels that makes use of these modified Slater parameters and one can proceed to the calculation of transition probabilities. Even so, the task is not easy. Indeed, before the optimization process, a correspondence must be found between the experimental and the theoretical level scheme preceding the optimization process. Also, as stated in Ref. [11], if parameters with a weak influence on energy levels are free to vary, they can converge to meaningless values, or even lead

to divergence of the whole system.

The subject of this article is an attempt to determine the Einstein coefficients of spontaneous emission for selected transitions in Al I by means of such an empirical method, based on the available experimental data compiled in the NIST database. The transitions have been chosen for their interest in the diagnostics of plasmas produced by laser ablation of aluminium alloys or other aluminium containing materials. In experimental conditions typical for laser-induced breakdown spectroscopy (LIBS), a low temperature plasma in local thermodynamical equilibrium (LTE) is generated, and temperature measurements via the Boltzmann plot method require accurate A values for the involved transitions. On the other hand, producing low temperature LTE plasmas allows one to obtain A values for high-lying excited states by means of the Boltzmann plot method applied to well-known low-lying states [12, 13, 14]. Thus, besides the 28 lowest states of Al I, we targeted our study to $3s3p3d$ and $3s3p4s$ states, and the spectral lines corresponding to their deexcitation towards the $3s3p^2$, $3s^23d$ (and $3s^2nd$) states.

2. Theory

For this work, we used a recently developed atomic structure code (named MASC-B). Initially, this code has been developed for the spectroscopy of plasmas submitted to magnetic fields of arbitrary strength B [15]. MASC-B follows the usual approach in which the N -electron Hamiltonian (here free of the B dependent part) is first divided into two parts: a *separable* part in which electrons are supposed independent in a central mean potential and a corrective part being considered by perturbation theory. In this framework, the multielectron states are formally a combination of Slater determinants. Thus, in this basis of Slater determinants, matrix elements of operators H , J^2 and J_z must be calculated, and the common eigenvectors of these operators obtained after diagonalisation, are the eigenstates of the atomic system. After identifying the *useful* Slater determinants belonging to a set of configurations, matrix elements of the previous operators are calculated using the Condon rules summarized in classical textbooks [16, 17]. After treating a list of configurations sequentially, it is still possible to diagonalize the atomic Hamiltonian in a basis of states belonging to all of the considered configurations, which is just the method known as the *superposition of configurations*. In the present code, the description is based on the non-relativistic Schrödinger equation, incorporating however the main relativistic corrections to the central potential [18, 10] in addition to an explicit treatment of the Spin-Orbit (SO) interaction. For a light element like aluminium, this treatment of the (weak) relativistic effects is more than sufficient. The central potential is built self-consistently, either in the framework of the optimized effective potential method [19], or in the framework of the Hartree+statistical Exchange (HX) method [10]. The latter method is used in the present calculations.

The multiconfiguration basis system used in this work contains 17 even and 15 odd configurations (see Table 1). This corresponds to 391 fine-structure levels.

In order to minimize discrepancies between existing experimental (E_{exp}^i) and

Table 1. The systems of even and odd configurations. The underlined configurations are those for which some Slater parameters have been varied or fixed (see text).

Even configurations	Odd configurations
<u>$3s3p^2$</u>	<u>$3s^23p$</u>
<u>$3s^2nd$</u> ($n = 3, 4, 5, 6$)	<u>$3s^2np$</u> ($n = 4, 5, 6$)
<u>$3s^2ns$</u> ($n = 4, 5, 6$)	<u>$3p^2np$</u> ($n = 3, 4, 5$)
<u>$3s^25g$</u>	<u>$3s^2nf$</u> ($n = 4, 5$)
<u>$3p^2ns$</u> ($n = 4, 5$)	<u>$3p^2nf$</u> ($n = 4, 5$)
<u>$3p^2nd$</u> ($n = 3, 4, 5$)	<u>$3p3d^2$</u>
<u>$3s3d^2$</u>	<u>$3s3p3d$</u>
<u>$3d^3$</u>	<u>$3s3p4s$</u>
<u>$3s3p4p$</u>	<u>$3s3p4d$</u>

computed level energies (E_{th}^i), some of the Slater parameters mentioned above have been adjusted using a least-square fit procedure implemented in MASC-B and minimizing the mean error σ as defined first by Racah [20]

$$\sigma = \sum_{i=1}^{N_{lev}} (E_{exp}^i - E_{th}^i)^2 / (N_{lev} - N_{par}),$$

where N_{lev} and N_{par} are the numbers of experimental levels and of free parameters, respectively. The atomic structure parameters (Slater parameters and SO integrals) used in this minimisation procedure are given in next section. The initial guess starts from their *ab initio* values obtained by MASC-B. A generally accepted rule is that for obtaining a satisfactory fit, the number of known levels should be significantly greater than the number of varying parameters. Even for Al I, this condition is difficult to satisfy. So, in view of our objectives, we chose to select some configurations for which we varied Slater parameters. The selected 18 configurations are underlined in the list given in Table 1.

All other Slater parameters ($F^{(k)}, G^{(k)}$) were the *ab initio* values scaled down to 74%. It is also possible to freeze ratios of some judiciously chosen parameters (see Table 2). The configuration interaction integrals $R^{(k)}$ linking configuration $3s3p^2$ with configurations $3s^2nd$ ($n=3-6$) were fixed at 90% of their *ab initio* values. Other configuration interaction integrals were not modified and taken at their *ab initio* values.

3. Results

Here 59 known levels belonging to the underlined configurations of Table 1 were taken from the NIST compilation [1]. Level $3s3p4p \ ^2D_{3/2}$ at 70285.7 cm⁻¹ energy has been ignored in the calculations because of the difficulty to fit it adequately.

3.1. Parameters

Many different fitting runs where we slightly varied the set of parameters, have been performed. Our choice can be considered as a best compromise, i.e. leading to the lower σ . For most of the configurations underlined in Table 1, Slater parameters are just the center of gravity E_{av} and possibly a spin-orbit integral ζ_{3p} . The case of configurations $3s3p4s$, $3s3p3d$ or $3s3p4p$ is more complex since Slater integrals F^k and G^k must be considered. In the second case, besides $F^2(3p3d)$ and $G^1(3s3p)$ and $G^2(3s3d)$, we chose to freeze the ratios $G^1(3p3d)/F^2(3p3d)$, $G^2(3p3d)/F^2(3p3d)$, $G^3(3p3d)/F^2(3p3d)$. In the third case, besides $F^2(3p4p)$, $G^1(3s3p)$ and $G^1(3s4p)$, we chose to freeze the ratios $G^0(3p4p)/F^2(3p4p)$, $G^2(3p4p)/F^2(3p3d)$, $G^3(3p3d)/F^2(3p4p)$. Optimized parameters are listed in Table 2, they correspond to a standard deviation (as defined above) $\sigma = 693 \text{ cm}^{-1}$ ($N_{lev} = 59$). This value can be compared to the energy range of levels covered by the fit which is $\Delta E = E_{max} - E_{min} = 83877 \text{ cm}^{-1}$. We see that σ is less than 1% of ΔE and thus, the fit can be considered as good [10].

Table 2. Slater parameters deduced from the fit, for the selected configurations (underlined) of Table 1. The center of gravity E_{av} is relative to the ground state.

config.	parameter	value (cm ⁻¹)	
<u>3s²3p</u>	E_{av}	1080	
	$\zeta(3p)$	68	
<u>3s3p²</u>	E_{av}	40300	
	$F^2(3p3p)$	16734	
	$G^1(3s3p)$	27084	
	$\zeta(3p)$	14	
<u>3s²3d</u>	E_{av}	34092	
<u>3s²4s</u>	E_{av}	25672	
<u>3s²4p</u>	E_{av}	32544	
<u>3s²4d</u>	E_{av}	39176	
<u>3s²4f</u>	E_{av}	40940	
<u>3s3p4s</u>	E_{av}	65260	
	$G^2(3s3p)$	32721	
	$G^0(3s4s)$	2015	
	$G^1(3p4s)$	1493	
<u>3s3p3d</u>	E_{av}	73736	
	$F^2(3p3d)$	5807	
	$G^1(3s3p)$	31798	
	$G^2(3s3d)$	660	
	$G^1(3p3d)/F^2(3p3d)$	0.7125	fixed
	$G^3(3p3d)/F^2(3p3d)$	0.4127	fixed
	$\zeta(3p)$	225	
<u>3s²5s</u>	E_{av}	37296	
<u>3s²5p</u>	E_{av}	39704	
<u>3s²5d</u>	E_{av}	43984	
<u>3s²5f</u>	E_{av}	43420	
<u>3s²5g</u>	E_{av}	40396	
<u>3s²6s</u>	E_{av}	38648	
<u>3s²6p</u>	E_{av}	39768	
<u>3s²6d</u>	E_{av}	41156	
<u>3s3p4p</u>	E_{av}	70228	
	$F^2(3p4p)$	1557	
	$G^1(3s3p)$	16689	
	$G^1(3s4p)$	518	
	$G^0(3p4p)/F^2(3p4p)$	0.7687	fixed
	$G^2(3p4p)/F^2(3p4p)$	0.5187	fixed

3.2. Energy levels

The excitation energies for the lowest low-lying levels are displayed together with the observed excitation energies in Table 3. The full energy level set (391 levels) corresponding to the CI-mixed configuration set defined in Table 1 is available upon request (with the caution that the optimization concerns the levels belonging to the configurations underlined in Table 1). Labelling of levels is determined by the configuration having the largest coefficient in the CI expansion and the leading percentage compositions are reported in the last column. With this choice, the pair of levels $3s^24d$ 2D appears twice, i.e. levels (12, 13) and (19, 20) respectively. Labelling $3s^2nd$ y for levels (12, 13) by NIST is somewhat ambiguous since the label $3s^2nd$ y is more appropriate for levels (19, 20) according to the leading components listed in Table 3. Strong mixing of these levels between themselves and with the $3s3p^2$ levels is evidenced. This mixing is expected to be a source of uncertainty in the calculation of the transition probabilities from the $3s^2nd$ ($n=3$ to 6) levels.

3.3. Transition probabilities

Complete results concerning the dipolar electric (E1) transition probabilities (A values) between fine structure levels belonging to the CI-mixed configuration set defined in Table 1 (more precisely between the odd and the even parity sets) are available upon request. These transition probabilities have been calculated in the "length form". Following the idea of least-square fitting of the energy levels, it is possible to perform a similar LSF procedure to get the transition probabilities. Here, the procedure consists in using some of the dipolar integrals $\langle n\ell|r|n'\ell' \rangle$ (r being the electronic radial coordinate) as adjustable parameters [24, 25], instead of using their *ab initio* values. The method has been systematically used at large scale in a context where many measured A values are available [26, 25]. In the present case, the situation is less obvious because of the too small number of available (and accurately measured) A values for Al I in the NIST database. Nevertheless, it is still possible to adjust some radial dipolar integrals for some transitions like $5s - 3p$ in configuration $3s^25s$, $4p - 4s$ in configuration $3s^24p$ and $3d - 3p$ in configuration $3s^23d$. Because of the strong mixing of $3s^24d$ states, the case of transitions $4d - 3p$ is more complicated and the adjustment of the quantity $\langle 4d|r|3p \rangle$ is challenging. We also adjusted the $4s - 3p$ radial integral in the configurations $3s^24s$ and $3s3p4s$, respectively. In this last case, we took benefit from A values deduced from spectroscopic measurements of a plasma produced by laser ablation of aluminium and sapphire [13].

The computed transition probabilities are listed in Table 4 for the principal transitions ($> 10^6$ s^{-1}) together with measured values reported in literature. We noticed that the computed transition probabilities equal the measured values within the given uncertainty.

Table 5 contains predicted values of transition probabilities, sorted by wavelength for specific transitions in the UV range, corresponding to transitions of the kind

Table 3. Observed excitation energy taken from the NIST E_{obs} [1] and calculated excitation energy E_{calc} for the 28 lowest levels of Al I.

Pos.	config.	LSJ	$E_{obs}(\text{cm}^{-1})$	$E_{calc}(\text{cm}^{-1})$	Leading components (%)
1	$3s^23p$	$^2P_{1/2}^o$	0	0	94 $3s^23p$
2		$^2P_{3/2}^o$	112	104	94 $3s^23p$
3	$3s^24s$	$^2S_{1/2}$	25348	25348	95 $3s^24s$
4	$3s3p^2$	$^4P_{1/2}$	29020	29045	92 $3s3p^2$ + 7 $3s3p4p$
5		$^4P_{3/2}$	29067	29055	92 $3s3p^2$ + 7 $3s3p4p$
6		$^4P_{5/2}$	29143	29075	92 $3s3p^2$ + 7 $3s3p4p$
7	$3s^23d$	$^2D_{3/2}$	32435	32170	15 $3s3p^2$ + 71 $3s^23d$ + 4 $3s^24d$ + 5 $3s^26d$
8		$^2D_{5/2}$	32437	32177	15 $3s3p^2$ + 71 $3s^23d$ + 4 $3s^24d$ + 5 $3s^26d$
9	$3s^24p$	$^2P_{1/2}^o$	32950	32947	93 $3s^24p$
10		$^2P_{3/2}^o$	32966	32964	93 $3s^24p$
11	$3s^25s$	$^2S_{1/2}$	37689	37682	95 $3s^25s$
12	$3s^24d$	$^2D_{3/2}$	38929	38640	11 $3s3p^2$ + 16 $3s^23d$ + 66 $3s^24d$ (label NIST: $3s^2nd$ y)
13		$^2D_{5/2}$	38934	38640	11 $3s3p^2$ + 16 $3s^23d$ + 66 $3s^24d$ (label NIST: $3s^2nd$ y)
14	$3s^25p$	$^2P_{1/2}^o$	40272	40271	94 $3s^25p$
15		$^2P_{3/2}^o$	40278	40274	94 $3s^25p$
16	$3s^24f$	$^2F_{5/2}^o$	41319	41319	97 $3s^24f$
17		$^2F_{7/2}^o$	41319	41319	97 $3s^24f$
18	$3s^26s$	$^2S_{1/2}$	42144	42143	98 $3s^26s$
19	$3s^24d$	$^2D_{3/2}$	42234	42625	23 $3s3p^2$ + 8 $3s^23d$ + 24 $3s^24d$ + 23 $3s^25d$ + 16 $3s^26d$
20		$^2D_{5/2}$	42238	42625	23 $3s3p^2$ + 8 $3s^23d$ + 24 $3s^24d$ + 23 $3s^25d$ + 16 $3s^26d$
21	$3s^26p$	$^2P_{1/2}$	43335	43332	98 $3s^26p$
22		$^2P_{3/2}$	43338	43339	98 $3s^26p$
23	$3s^25f$	$^2F_{5/2}^o$	43831	43827	97 $3s^25f$
24		$^2F_{7/2}^o$	43831	43831	97 $3s^25f$
25	$3s^25g$	$^2G_{7/2}$	43876	43874	100 $3s^25g$
26		$^2G_{9/2}$	43876	43874	100 $3s^25g$
27	$3s^25d$	$^2D_{3/2}$	44166	44865	60 $3s^25d$ + 33 $3s^26d$
28		$^2D_{5/2}$	44169	44865	60 $3s^25d$ + 33 $3s^26d$

$3s3p3d \rightarrow 3s3p^2$. Transition probabilities were measured in LIBS plasmas using the Boltzmann plot technique [13]. These transitions are listed in the NIST database but A values are absent.

In Table 6 we report our computed transition probabilities for identified transitions listed in the NIST database (again no transition probabilities are given). Here, we performed three calculations of the A values. The first calculation uses the length form of the *ab initio* dipole operator, the second uses the velocity form, and the last one uses an adjusted value of the dipole integral coming from transitions of Table 4. The error $\delta A = |A_{length} - A_{velocity}| / \max(A_{length}, A_{velocity})$ is in the range 40% - 55%. Calculations using the adjusted value of the dipole integral (the last column) are always somewhere between. So, we estimate that 25% is a good value of the uncertainty associated to A values of this last column which are the *recommended* values.

Table 4. Computed wavelength λ_{calc} , dipolar integral $\langle n\ell|r|n'\ell' \rangle$, computed transition probability A_{calc} , measured transition probability A_{meas} and values reported in NIST for selected transitions in Al I.

Upper	Lower	λ_{calc} (nm)	$\langle n\ell r n'\ell' \rangle$ (a.u.)	A_{calc} (10^7 s^{-1})	A_{meas} (10^7 s^{-1})	A_{NIST} (10^7 s^{-1})
$3s^24s \ ^2S_{1/2}$	$3s^23p \ ^2P_{1/2}^o$	394.5	$\langle 4s r 3p \rangle = 3.25$	4.93	4.93^a	4.99
	$3s^23p \ ^2P_{3/2}^o$	396.1		9.79	9.8^a	9.85
$3s^25s \ ^2S_{1/2}$	$3s^23p \ ^2P_{1/2}^o$	265.3	$\langle 5s r 3p \rangle = 0.97$	1.32	1.33^a	1.42
	$3s^23p \ ^2P_{3/2}^o$	266.06		2.62	2.64^a	2.84
$3s^24p \ ^2P_{1/2}^o$	$3s^24s \ ^2S_{1/2}$	1316	$\langle 4p r 4s \rangle = -8.17$	1.69	1.69^b	1.59
$3s^24p \ ^2P_{3/2}^o$	$3s^24s \ ^2S_{1/2}$	1313		1.70	1.69^b	1.6
$3s^23d \ ^2D_{3/2}$	$3s^23p \ ^2P_{1/2}^o$	312.4	$\langle 3d r 3p \rangle = -3.19$	6.23	6.3^a	5.87
	$3s^23p \ ^2P_{3/2}^o$	313.46		1.24	-	1.16
$3s^23d \ ^2D_{5/2}$	$3s^23p \ ^2P_{3/2}^o$	313.4		7.43	7.4^a	7.29
$3s^2nd \ ^2D_{3/2}$	$3s^23p \ ^2P_{1/2}^o$	259	$\langle 4d r 3p \rangle = -1.31$	1.49	1.9^c	1.92
	$3s^23p \ ^2P_{3/2}^o$	259.7		0.29	0.38^c	0.599
$3s^2nd \ ^2D_{5/2}$	$3s^23p \ ^2P_{3/2}^o$	259.68		1.77	2.3^c	3.6
$3s^24d \ ^2D_{3/2}$	$3s^23p \ ^2P_{1/2}^o$	233.94		6.23	7.2^a	7.61
	$3s^23p \ ^2P_{3/2}^o$	234.5		1.23	1.4^a	1.51
$3s^24d \ ^2D_{5/2}$	$3s^23p \ ^2P_{3/2}^o$	234.51		7.43	8.6^a	9.07

^a Ref. [21], ^b Ref. [22], ^c Ref. [23]**Table 5.** Computed wavelength λ_{calc} with respect to the NIST values λ , computed transition probability A_{calc} for some measured transition probabilities A_{meas} in the UV range [13]. Last column (CF) is the calculated cancelation factor as defined by Cowan [10] (see text). Value of the dipolar integral is $\langle 4s|r|3p \rangle = 3.835$ (a.u.).

Upper	lower	λ_{calc} (nm)	λ_{NIST} (nm)	A_{calc} (10^7 s^{-1})	A_{meas} (10^7 s^{-1})	CF
$3s3p4s \ ^4P_{5/2}^o$	$3s3p^2 \ ^4P_{3/2}$	304.92	305.007	5.87	5.9^a	0.099
$3s3p4s \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{1/2}$	305.82	305.468	8.23	7.8^a	0.102
$3s3p4s \ ^4P_{5/2}^o$	$3s3p^2 \ ^4P_{5/2}$	305.10	305.714	13.98	14^a	0.100
$3s3p4s \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{3/2}$	305.92	305.903	2.64	2.8^a	0.092
$3s3p4s \ ^4P_{1/2}^o$	$3s3p^2 \ ^4P_{1/2}$	306.39	305.992	3.27	3.4^a	0.103
$3s3p4s \ ^4P_{1/2}^o$	$3s3p^2 \ ^4P_{3/2}$	306.48	306.429	16.3	16^a	0.102
$3s3p4s \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{5/2}$	306.10	306.614	8.9	9^a	0.102

^a Ref. [13]

Table 6. Computed transition rates A for some identified transitions of the NIST database in the UV range. A_{length} , $A_{velocity}$ correspond to the rate calculated with the length form and the velocity form of the dipole operator, respectively. A_{calc} is the recommended value, calculated with the dipolar integral $\langle 3d|r|3p \rangle = -3.19$ (a.u.). Last column (CF) is the calculated cancelation factor as defined by Cowan [10]. Estimated uncertainty is 25%.

Upper	Lower	λ (NIST) (nm)	A_{length} ($10^7 s^{-1}$)	$A_{velocity}$ ($10^7 s^{-1}$)	A_{calc} ($10^7 s^{-1}$)	CF
$3s3p3d \ ^4P_{1/2}^o$	$3s3p^2 \ ^4P_{1/2}$	231.103	3.29	1.44	2.06	0.119
$3s3p3d \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{1/2}$	231.249	9.22	4.11	5.76	0.121
$3s3p3d \ ^4P_{1/2}^o$	$3s3p^2 \ ^4P_{3/2}$	231.352	23.3	10.56	14.44	0.112
$3s3p3d \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{3/2}$	231.498	4.77	2.21	2.93	0.087
$3s3p3d \ ^4P_{5/2}^o$	$3s3p^2 \ ^4P_{3/2}$	231.748	5.6	2.43	3.52	0.119
$3s3p3d \ ^4P_{3/2}^o$	$3s3p^2 \ ^4P_{5/2}$	231.905	12.5	5.68	7.75	0.115
$3s3p3d \ ^4P_{5/2}^o$	$3s3p^2 \ ^4P_{5/2}$	232.150	21.11	9.63	13.06	0.114
$3s3p3d \ ^4D_{3/2}^o$	$3s3p^2 \ ^4P_{1/2}$	236.761	15.6	8.81	8.95	0.101
$3s3p3d \ ^4D_{1/2}^o$	$3s3p^2 \ ^4P_{1/2}$	236.810	29.3	16.49	16.74	0.103
$3s3p3d \ ^4D_{5/2}^o$	$3s3p^2 \ ^4P_{3/2}$	236.930	25.9	14.47	14.8	0.100
$3s3p3d \ ^4D_{3/2}^o$	$3s3p^2 \ ^4P_{3/2}$	237.022	16.8	9.5	9.54	0.101
$3s3p3d \ ^4D_{1/2}^o$	$3s3p^2 \ ^4P_{3/2}$	237.072	4.61	2.5	2.6	0.097
$3s3p3d \ ^4D_{5/2}^o$	$3s3p^2 \ ^4P_{5/2}$	237.357	7.92	4.52	4.47	0.096
$3s3p3d \ ^4D_{3/2}^o$	$3s3p^2 \ ^4P_{5/2}$	237.449	1.12	0.66	0.63	0.090

4. Conclusion

In the present work, a semi-empirical approach for atomic structure calculations was used to compute Einstein coefficients of spontaneous emission for transitions in Al I. In the Al I system, the calculation of the radiative properties is challenging due to the strong interaction between $3s3p^2$ and $3s^2nd$ states. The performed calculations take benefit from the experimental excitation energies provided by the NIST database in which, however, very few transition probabilities are available for the Al I system. For some transitions, no A values are given by NIST. The computed transition probabilities were therefore compared to A values deduced from spectroscopic measurements of a plasma produced by laser ablation of aluminium. At the end, a good agreement between experimental and calculated energy values has been obtained for the 28 lowest energy levels. When possible, some transition integrals considered as free parameters have been used in a subsequent least-square fit procedure to obtain accurate transition probabilities. This analysis allowed us to predict transition probabilities between other levels.

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