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Effective collision strengths for electron-impact excitation of Al^{10+}

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Abstract. Electron collision strengths for electron-impact excitation of the Li-like Al ion are evaluated in the close-coupling approximation using the multichannel R-matrix method. Five *LS* target eigenstates are included in the expansion of the total wave function, consisting of the two n =2 states with configurations $1s^2 2s$, $1s^2 2p$, and the three n =3 states with configurations $1s^2 3s$, $1s^2 3p$, $1s^2 3d$. These five ionic states correspond to eight fine-structure levels leading to a total of 18 independent transitions. The collision strengths for all possible allowed transitions are tabulated for electron energies in the range of 0.19 –0.3 Ry, which are the temperatures of interest for many plasma applications.

1. Introduction

A very limited number of collision strength calculations have been published for Al^{10+}. Up to now, only the results obtained by Burgess *et. all* [1] for compact effective collision strengths for 2s –*n*s, *nd*, refer to forbidden transitions in Al XI. These authors fit the extensive tables of collision strengths in Li-like ions with Z = 8,14, 22, 30, 42, 56, 74, 93, for non-optically allowed transitions, to get values for Li-like ions of charge 1 to 23 in a compact form. The atomic data themselves are not available through this work. Our previously works [2,3] have reported atomic data for forbidden transitions in Al XI. They used the configuration interaction structure code CIV3[4] to output electric –dipole, -quadrupole and octupole fine-structure line strengths in *jj* coupling, for transition modes of type $1s^2 nl_j - 1s^2 nl_j$, with $n \leq 5$, and the generalised oscillator strength.

In the present work, calculation uses atomic data from the SUPERSTRUCTURE (SST) program by Eissner *et. al*. [5] and Breit-Pauli R-matrix [6] method and code for the scattering problem. The SST code is based on a scaled Thomas-Fermi-Dirac-Amadi potential. The scaling parameters are different for each angular momentum *l*. These parameters are iterated to give a minimum energy of a term or a group of terms. Optimum Thomas-Fermi potential is obtained by minimizing the sum of the term energies. It should be noted that this

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method does not take into account correlation effects properly, which explains the disagreement of present results on atomic data with the previously reported, for some states.

2. Method of calculation

An initial calculation of a full-exchange *LS* R-matrix code has been performed. Using the configurations $1s^2 2s$, $1s^2 2p$, $1s^2 3s$, and $1s^2 3p$ $1s^2 3d$ in the SST program, the corresponding eight levels were calculated in intermediate coupling scheme. The results on the energy levels in intermediate coupling, are shown in *Table 1*. Comparisons are provided with calculations using direct SCF method and those by Froese Fischer using MCHF [7].

Table 1*: Calculated energies for the lowest states of type $1s^2 nl_j(^2L_j)$ in Al^{10+}*

k	$1s^2$ $nl_j(^2L_j)$	E_k *(a.u.)* *this work*	E_k*(a.u.)* SCF method	E_k*(a.u.)* MCHF method
1	$2s_{1/2}(^2S_{1/2})$	*-177.5340841*	-177.566110	-177.63005568
2	$2p_{1/2}(^2P_{1/2})$	*-176.7110185*	-176.765500	-176.82918022
3	$2p_{3/2}(^2P_{3/2})$	*-176.6875292*	-176.735900	-176.80259640
4	$3s_{1/2}(^2S_{1/2})$	*-168.2608506*	-168.366100	-168.41724452
5	$3p_{1/2}(^2P_{1/2})$	*-168.0949646*	-168.146500	-168.19862568

The line strengths have been calculated for electric dipole and quadrupole transitions involving all states with n=2 and n=3 configurations. Only dipole radiative transition probabilities are reported in *Table 2* for comparison. The atomic system of Al XI is most appropriate to MCHF method, because the energy level fine-structure is mainly dominated by the spin-orbit splitting, and by correlation effects that multiconfigurational description can account for.

Table 2*: Comparisons between electric-dipole transition probability (s^{-1}) results*

transition no.	upper level (*k*)	lower level (*j*)	A_{kj} *(s^{-1})* *this work*	A_{kj} (s^{-1}) SCF	A_{ki}(s^{-1}) MCHF
1.	$2p_{1/2}(^2P_{1/2})$	$2s_{1/2}(^2S_{1/2})$	7.777^{08}	7.1400^{08}	7.6853^{08}
2.	$2p_{3/2}(^2P_{3/2})$	$2s_{1/2}(^2S_{1/2})$	8.570^{08}	8.0100^{08}	8.4937^{08}
3.	$3s_{1/2}(^2S_{1/2})$	$2p_{1/2}(^2P_{1/2})$	4.883^{10}	4.7618^{10}	4.9611^{10}
4.	$3s_{1/2}(^2S_{1/2})$	$2p_{3/2}(^2P_{3/2})$	9.674^{10}	9.6293^{10}	9.8847^{10}
5.	$3p_{1/2}(^2P_{1/2})$	$2s_{1/2}(^2S_{1/2})$	3.076^{11}	3.1605^{11}	3.2062^{11}

Some of the transitions considered into *Table 2* are likely to be affected by cancellation effects in forming the radial integral. For these transitions the cancellation factor as defined by Cowan code [8] is very small indicating that the corresponding probability must

be considered with care. Reactance matrices are calculated in *LS* coupling and transformed to intermediate coupling by using term-coupling coefficients obtained from SST program. The N-electron Breit-Pauli Hamiltonian including spin-orbit interaction is diagonalized in intermediate coupling to output values of the total collision strengths. High energy Born collision strengths for forbidden transitions are calculated and compared with those reported by other works. Finally, the effective collision strength as function of temperature, have been obtained up to a temperature that does not exceed half of the maximum energy in the R-matrix run. The higher energy of the R-matrix calculation, the larger the number of basis orbitals required to represent the continuum. The need for effective collision strengths at higher temperature was balanced against the size of the resulting calculations. In general, the highest energy for which accurate collision strengths can be calculated is about half the maximum eigen-energy of the continuum basis orbitals. Comparison between present results and those obtained from the compact representation in Ref. [1] is shown in *Table 3.*

Table 3*: High energy Born collision strengths*

transition type $E\lambda$	Ω(nlj – n'l'j')	
$nl_j \rightarrow n'l'_{j'}$	this work	Ref.[1]
(E0) $2s_{1/2} \rightarrow 3s_{1/2}$	7.293^{-02}	1.396^{-01}
(E2) $2s_{1/2} \rightarrow 3d_{3/2}$	9.010^{-02}	1.604^{-01}
(E2) $2s_{1/2} \rightarrow 3d_{5/2}$	1.351^{-01}	2.407^{-01}

Selected results on the effective collision strengths results from non-exchange R-matrix theory and code,including forbidden transitions in excitation from the ground are presented in *Table 4*.

Table 4*: Effective collision strengths for transitions* $2s_{1/2}$ *– nlj,* Ω*(nlj), non-exchange*

energy $\times 10^{-01}$ *ryd*	$\Omega(2p_{1/2})$ $\times 10^{-01}$	$\Omega(2p_{3/2})$ $\times 10^{-01}$	$\Omega(3s_{1/2})$ $\times 10^{-04}$	$\Omega(3p_{1/2})$ $\times 10^{-03}$	$\Omega(3p_{3/2})$ $\times 10^{-02}$	$\Omega(3d_{3/2})$ $\times 10^{-02}$	$\Omega(3d_{5/2})$ $\times 10^{-02}$
1.90	1.990	3.986	3.621	4.355	1.690	2.124	4.639
1.95	1.981	3.964	4.011	4.632	1.738	2.205	4.701
2.00	1.972	3.942	4.430	4.918	1.787	2.283	4.756
2.10	1.955	3.900	5.366	5.510	1.887	2.425	4.842
2.20	1.940	3.861	6.422	6.117	1.985	2.551	4.901

A full-exchange *LS* coupling calculation is given in *Table 5*.

Table 5*: Effective collision strengths, $\Omega(n_1l_1 \rightarrow n_2l_2)$, a full-exchange LS coupling*

energy	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$	$\Omega \times$
$\times 10^{-01}$	10^{-02}	10^{-03}	10^{-04}	10^{-03}	10^{-04}	10^{-02}	10^{-02}	10^{-01}	10^{-02}
ryd	2s-2p	2s-3s	2s-3p	2s-3d	2p-3s	2p-3p	2p-3d	3s-3p	3s-3d
1.90	6.91	3.05	2.25	2.67	8.10	4.38	2.84	2.94	2.75
1.95	6.84	3.04	2.12	2.63	8.00	4.29	2.83	2.88	2.57
2.00	6.77	3.02	2.01	2.59	7.89	4.19	2.83	2.82	2.39
2.05	6.71	3.01	1.92	2.55	7.77	4.11	2.82	2.76	2.23
2.10	6.64	2.99	1.85	2.50	7.65	4.03	2.79	2.69	2.09

3. Conclusions

The effective collision strengths for electron-impact excitation of the Li-like Al ion have been evaluated using the multichannel R-matrix method. Five LS target eigenstates have been included in the expansion of the total wavefunction, consisting of *n=2* and *n=3* states. The effective collision strengths for all possible forbidden and allowed transitions have been obtained by averaging the electron collision strengths, for a wide range of the incident electron energies, over a Maxwellian distribution of velocities. Results agree well with those calculated on the use of the fitting procedure from Ref.1., for forbidden transitions.

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4. References

[1] Burgess, A., Chidichimo, M.C., Tully, -J.A., *Astron. Astrophys.Suppl. Ser.* **131**(1998)145.

[2] Stancalie, V., Burke, V.M., Sureau, A., *Phys. Scr.* **59**(1999)52.

[3] Stancalie, V., *Phys. Scr.* **61**(2000)459.

[4] Hibbert, A., *Comput. Phys. Comm.* **9**(1975)141.

[5] Eissner, W., Jones, M., Nussbaumer, H., *Comput. Phys. Commun.* **8**(1974)270.

[6] Burke, V.M., Burke, P.G., Scott, N.S., *Comput. Phys. Commun.* **69**(1992)76.

[7] Frose Fisher, C., Saparov, M., Gaigalas, G., Godefroid, M., *At.Data & Nucl.Data Tables,* **70**(1998)119.

[8] Cowan, R. D., "*The Theory of Atomic Structure And Spectra*", University of California Press, Berkley, California, 1981.