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Electric dipole transition probabilities in Al IV and Al V ions

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Abstract. Electric dipole transition probabilities in triply and four times ionized aluminum have been calculated in intermediate coupling. The present calculations were carried out with the general purpose atomic-structure program SUPERSTRUCTURE (Eissner, Jones, & Naussbaumer 1974), as modified by Naussbaumer & Storey (1978). The relativistic corrections to the non-relativistic Hamiltonian are taken into account through the Breit-Pauli approximation. We have also introduced a semi-empirical correction (TEC) for the calculation of the energy-levels.

Key words. atomic data – Al IV – Al V – transition probabilities

1. Introduction

Transition probability of spontaneous emission plays an important role in plasma and laser investigation and, also, in astrophysics. Namely, various Kinetic processes appearing in plasma modeling need reliable knowledge of A values. The classification of transitions and determination of energy levels are essential parts of the study of a laboratory spectrum. Neon and fluorine like ions are important in plasma research and theirs corresponding emission lines are essential for diagnostics over a wide range of plasma parameters.

2. The method

In this work, the calculations were carried out with the general purpose atomic-structure program SUPERSTRUCTURE (Eissner, Jones, & Naussbaumer 1974), as modified by Naussbaumer & Storey (1978).The adopted atomic model for Al IV includes 13 configurations corresponding to 115 fine structure levels. For Al V the model includes 25 configurations corresponding to 434 fine structure levels. Wavefunctions are of the type $\Psi = \sum_i \phi_i C_i$, where the basis functions ϕ_i are constructed using one-electron orbitals ψ. The latter are calculated with a scaled Thomas-Fermi statistical model (SM) potential (Eissner & Naussbaumer 1969) or obtained from the Coulomb potential (Naussbaumer & Storey 1978). For each radial orbital $P_{nl}(r)$, the potential can be adjusted using a parameter called λ. In the present case, those n and l-dependent scaling parameters λ_{nl} were determined variationally by primarily minimizing the sum of the non-relativistic term energies. For details on the difference between the λ obtained in SM potential and those calculated in the Coulomb potential , see Naussbaumer & Storey (1978). Relativistic corrections are introduced by means of Breit-

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Table 1. Transition probabilities for Al IV, A_{cal} : our values, A_{MCHF} : Froese Fischer values, A_{Ku} : Kurucz values, A_{NIST} : NIST values. $A(B)$ stands for $A.10^{B}$

Transition	A_{cal}	A_{MCHF}	A_{Ku}	A_{NIST}
$2s^2 2p^6\ ^1S_0 - 2s^2 2p^5(^2P^0)3s\ ^1P_1{}^\circ$	2.715(10)	1.938(10)	1.731(10)	1.70(10)
$2s^2 2p^6\ ^1S_0 - 2s^2 2p^5(^2P^0)3d\ ^3P_1{}^\circ$	3.752(8)	3.740(8)	4.766(8)	4.7(8)
$2s^2 2p^6\ ^1S_0 - 2s^2 2p^5(^2P^0)3d\ ^3D_1{}^\circ$	1.403(9)	1.765(10)	6.258(10)	6.30(10)
$2s^2 2p^6\ ^1S_0 - 2s^2 2p^5(^2P^0)3d\ ^1P_1{}^\circ$	1.334(11)	8.997(10)	3.396(10)	3.40(10)
$2p^5(^2P^\circ)3s\ ^3P_2{}^\circ - 2p^5(^2P^\circ)3p\ ^3S_1$	2.857(8)	2.607(8)	3.610(8)	
$2p^5(^2P^\circ)3s\ ^3P_2{}^\circ - 2p^5(^2P^\circ)3p\ ^3D_3$	7.209(8)	6.699(8)	7.150(8)	

Table 2. Transition probabilities for Al V, A_{cal} : our values, A_{MCHF} : Froese Fischer values, A_V : Verner values, A_{NIST} : NIST values. $A(B)$ stands for $A.10^{B}$

Transition	A_{cal}	A_{MCHF}	A_V	A_{NIST}
$2s^2 2p^5\ ^2P^\circ{}_{1/2} - 2s2p^6\ ^2S_{1/2}$	7.867(9)	7.020(9)	7.00(9)	1.00(10)
$2s^2 2p^5\ ^2P^\circ{}_{3/2} - 2s2p^6\ ^2S_{1/2}$	1.589(10)	1.451(10)	1.44(10)	2.10(10)
$2s^2 2p^5\ ^2P^\circ{}_{1/2} - 2p^4(^3P)3s\ ^2P_{3/2}$	8.109(9)	6.768(9)	7.61(9)	
$2s^2 2p^5\ ^2P^\circ{}_{1/2} - 2p^4(^3P)3s\ ^2P_{1/2}$	3.152(10)	3.051(10)	3.07(10)	
$2s^2 2p^5\ ^2P^\circ{}_{3/2} - 2p^4(^3P)3s\ ^2P_{3/2}$	4.140(10)	3.961(10)	3.86(10)	
$2s^2 2p^5\ ^2P^\circ{}_{3/2} - 2p^4(^3P)3s\ ^2P_{1/2}$	1.581(10)	1.631(10)	1.56(10)	

Pauli approximation. In particular spin-orbit, spin-spin and spin-other orbit interactions are included. This procedure can be improved by means of semi-empirical corrections (TECs) to the term energies (Zeippen et al. 1977). In practice, the TEC for a given term is the difference between the measured and calculated energy of the lowest level in the multiplet. Our transition probabilities are compared with NIST values and other theoretical results (see Table.1 and Table.2). Our results are in good agreement with other calculations, particulary for Al V.

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