Application of detailed quantum codes in the evaluation of rare gas ions radiative transition probabilities

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INTRODUCTION

Radiative transition probabilities of rare gas ions

to do spectral analysis of fusion plasmas, especially Ar and Xe

Collection of data available for various ionisation stages of Ar

ArI, ArII, ArIII, ArIV

Recent work: Radiative transition probabilities:

ArII: Multiplet 5s-5p

ArIII: Multiplet 4d-4p

ArIV: Multiplet 4p-4s

DATA and CODES

DATA:

FOR ATOMIC STRUCTURE

Energy levels

Oscillator strengths

Wavelengths

Transition probabilities for ArII, ArIII, ARIV

CODES:

FOR ATOMIC STRUCTURE

Hartree Fock OPM (1)

Dirac Fock SICODIFO (2)

SUPERSTRUCTURE SST (3)

FAC(4)

RESULTS

Ab.Initio Calculation: SUPERSTRUCTURE

Energy levels, line strengths, weighted oscillator strengths and radiative transition probabilities are calculated in LSJ coupling using the SUPERSTRUCTURE code (SST), (3) which is well suited for the computaion of large quantities of atomic data for multiplied ions.

In the first step, wave function are determined by diagonalization of the non-relatisvitic Hamiltonian using orbitals calculated in Thomas-Fermi-Dirac-Amaldi potentiels. The scaling parameters are obtained by a self-consistent minimization procedure.

In the second step RELATIVISTIC corrections (spin-orbit, mass, Darwin and one body) are introduced accordind to the Breight-Pauli approach. The results are obtained in LS and LSJ couplings.

Results for ArII 5s-5p, ArIII 4d-4p, ArIV 4p-4s multiplets in LSJ coupling are presented

[14] $A_{j\to i}$ / Ar II / 5*s* ← 5*p* Transition Probabilities in $10^7 s^{-1}$

5s-5p	CbA														SST				LANL			
	E_i (cm^{-1})	Term	E_j (cm^{-1})	Term	λ[Å]	L_i	J_i	S_i	l_{ci}	L_j	J_j	S_j	$2J_j$+1	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$
5s, 5p $^3P_2$ (+ e^- → doublet, quartet)																						
1	181594.14	$^4P_{5/2}$	188766.21	$^4P_{5/2}$	13942.98	1	2.5	1.5	1	1	2.5	1.5	6	1.13	182459	189384	14438	1.37				
2			189040.93	$^4P_{3/2}$	13428.60	1	2.5	1.5	1	1	1.5	1.5	4	0.81		189655	13895	1.20				
3			189415.03	$^4D_{7/2}$	12786.27	1	2.5	1.5	1	2	3.5	1.5	8	2.06		190129	13037	2.06				
4			189934.63	$^2P_{1/2}$	11989.70	1	2.5	1.5	1	1	0.5	0.5	2			193227						
5			190511.27	$^2D_{5/2}$	11214.37	1	2.5	1.5	1	2	2.5	0.5	6			198267						
6			190592.23	$^2P_{3/2}$	11113.47	1	2.5	1.5	1	1	1.5	0.5	4			192933						
7	183090.89	$^2P_{3/2}$	188766.21	$^4P_{5/2}$	17620.15	1	1.5	0.5	1	1	2.5	1.5	6		184255	189384						
8			189040.93	$^4P_{3/2}$	16806.61	1	1.5	0.5	1	1	1.5	1.5	4			189655						
9			189415.03	$^4D_{7/2}$	15812.43	1	1.5	0.5	1	2	3.5	1.5	8			190129						
10			189934.63	$^2P_{1/2}$	14611.89	1	1.5	0.5	1	1	0.5	0.5	2	0.50		193227	11145	0.21				
11			190511.27	$^2D_{5/2}$	13476.40	1	1.5	0.5	1	2	2.5	0.5	6	1.88		198267						
12			190592.23	$^2P_{3/2}$	13330.95	1	1.5	0.5	1	1	1.5	0.5	4	1.62		192933	11522	1.67				
5s, 5p $^3P_1$ (+ e^- → doublet, quartet)																						
13	182222.12	$^4P_{3/2}$	189437.74	$^4P_{1/2}$	13858.82	1	1.5	1.5	1	1	0.5	1.5	2	1.34	183135	190020	14525	1.36				
14			189654.85	$^4D_{5/2}$	13454.01	1	1.5	1.5	1	2	2.5	1.5	6	1.23		190491	13593	1.47				
15			190942.72	$^2S_{1/2}$	11467.10	1	1.5	1.5	1	0	0.5	0.5	2			191759	11595	0.05				
16			191012.42	$^2D_{3/2}$	11376.18	1	1.5	1.5	1	2	1.5	0.5	4			191766						
17			191169.60	$^4S_{3/2}$	11176.33	1	1.5	1.5	1	0	1.5	1.5	4	0.96		191975	11311	1.06				
18	183914.64	$^2P_{1/2}$	189437.74	$^4P_{1/2}$	18105.77	1	0.5	0.5	1	1	0.5	1.5	2		185102	190020						
19			189654.85	$^4D_{5/2}$	17420.96	1	0.5	0.5	1	2	2.5	1.5	6			190491						
20			190942.72	$^2S_{1/2}$	14228.64	1	0.5	0.5	1	0	0.5	0.5	2	0.53		191759	15022	0.09				
21			191012.42	$^2D_{3/2}$	14088.91	1	0.5	0.5	1	2	1.5	0.5	4	1.37		191766	15007	0.73				
22			191169.60	$^4S_{3/2}$	13783.67	1	0.5	0.5	1	0	1.5	1.5	4			191975	14549	0.02				
5s, 5p $^3P_0$ (+ e^- → quartet)																						
23	182951.26	$^4P_{1/2}$	190106.30	$^4D_{3/2}$	13976.16	1	0.5	1.5	1	2	1.5	1.5	4	0.66	183684	190994	13678	0.83				
24			190733.02	$^4D_{1/2}$	12850.56	1	0.5	1.5	1	2	0.5	1.5	2	1.68		191267	13187	1.85				

[14] $A_{j\to i}$ / Ar II / 5*s* ← 5*p* Transition Probabilities in $10^7 s^{-1}$

5*s*-5*p*	CbA														SST				LANL			
	E_i (cm^{-1})	Term	E_j (cm^{-1})	Term	λ[Å]	L_i	J_i	S_i	l_{ci}	L_j	J_j	S_j	$2J_j+1$	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$
5*s*, 5*p* $^1D_2$ (+ e^- → doublet)																						
25	195864.73	$^2D_{5/2}$	203007.81	$^2P_{3/2}$	13999.56	2	2.5	0.5	2	1	1.5	0.5	4	1.45	198267	206481	12174	2.43				
26			203151.26	$^2F_{5/2}$	13723.95	2	2.5	0.5	2	3	2.5	0.5	6	0.11		205263	14293	0.13				
27			203197.57	$^2F_{7/2}$	13637.28	2	2.5	0.5	2	3	3.5	0.5	8	1.74		205310	14187	1.59				
28			203594.35	$^2P_{1/2}$	12937.25	2	2.5	0.5	2	1	0.5	0.5	2			206668						
29			204113.76	$^2D_{3/2}$	12122.64	2	2.5	0.5	2	2	1.5	0.5	4	0.24		206308	12435	0.03				
30			204134.07	$^2D_{5/2}$	12092.86	2	2.5	0.5	2	2	2.5	0.5	6	2.25		206364	12349	2.22				
31	195866.84	$^2D_{3/2}$	203007.81	$^2P_{3/2}$	14003.70	2	1.5	0.5	2	1	1.5	0.5	4	0.16	198269	206481	12178	0.04				
32			203151.26	$^2F_{5/2}$	13727.93	2	1.5	0.5	2	3	2.5	0.5	6	1.59		205263	14298	1.43				
33			203197.57	$^2F_{7/2}$	13641.21	2	1.5	0.5	2	3	3.5	0.5	8			205310						
34			203594.35	$^2P_{1/2}$	12940.78	2	1.5	0.5	2	1	0.5	0.5	2	2.01		206668	11908	0.26				
35			204113.76	$^2D_{3/2}$	12125.74	2	1.5	0.5	2	2	1.5	0.5	4	2.15		206308	12438	2.33				
36			204134.07	$^2D_{5/2}$	12095.95	2	1.5	0.5	2	2	2.5	0.5	6	0.16		206364	12353	0.20				
5*s*, 5*p* $^1S_0$ (+ e^- → doublet)																						
37	**220456.00**	$^2S_{1/2}$	**228046.00**	$^2P_{3/2}$	**13175.23**	0	0.5	0.5	0	1	1.5	0.5	4	**2.28**	220456	228046	13175	1.99				
38			**228035.00**	$^2P_{1/2}$	**13194.35**	0	0.5	0.5	0	1	0.5	0.5	2	**2.27**		228035	13194	1.98				

En épais → énergie provenant des calculs de SST.

[3] / $A_{j\to i}$ / Ar IV / 4s ← 4p Transition Probabilities in $10^7 s^{-1}$

	CbA													SST				LANL			
4s-4p	E_i (cm^{-1})	Term	E_j (cm^{-1})	Term	λ[Å]	L_i	J_i	S_i	l_{ci}	L_j	J_j	S_j	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$
4s, 4p $^3P_2$ (+e$^-$ → doublet, quartet)																					
1	251966.5	$^4P_{5/2}$	289829.8	$^4P_{5/2}$	2641.08	1	2.5	1.5	1	1	2.5	1.5	21.97	261981	299517	2664	27.85				
2			289233.2	$^4P_{3/2}$	2683.36	1	2.5	1.5	1	1	1.5	1.5	13.46		299005	2700	15.07				
3			287550.3	$^4D_{7/2}$	2810.27	1	2.5	1.5	1	2	3.5	1.5	25.98		296895	2864	29.67				
4			291662.1	$^2D_{5/2}$	2519.17	1	2.5	1.5	1	2	2.5	0.5			302983	2438	0.94				
5			295667.8	$^2P_{1/2}$	2288.26	1	2.5	1.5	1	1	0.5	0.5			328498						
6			295800.4	$^2P_{3/2}$	2281.34	1	2.5	1.5	1	1	1.5	0.5			329210						
7	257342.3	$^2P_{3/2}$	289829.8	$^4P_{5/2}$	3078.11	1	1.5	0.5	1	1	2.5	1.5		270381	299517	3432	0.27				
8			289233.2	$^4P_{3/2}$	3135.69	1	1.5	0.5	1	1	1.5	1.5			299005	3493	0.02				
9			287550.3	$^4D_{7/2}$	3310.38	1	1.5	0.5	1	2	3.5	1.5			296895						
10			291662.1	$^2D_{5/2}$	2913.77	1	1.5	0.5	1	2	2.5	0.5	24.41		302983	3067	16.89				
11			295667.8	$^2P_{1/2}$	2609.23	1	1.5	0.5	1	1	0.5	0.5	11.36		328498	1720	15.16				
12			295800.4	$^2P_{3/2}$	2600.23	1	1.5	0.5	1	1	1.5	0.5	28.71		329210	1699	30.68				
4s, 4p $^3P_1$ (+e$^-$ → doublet, quartet)																					
13	250901.4	$^4P_{3/2}$	289121.4	$^4P_{1/2}$	2616.43	1	1.5	1.5	1	1	0.5	1.5	26.95	261098	298754	2655	31.75				
14			286747.4	$^4D_{5/2}$	2789.71	1	1.5	1.5	1	2	2.5	1.5	18.63		296104	2856	23.15				
15			290250.4	$^2D_{3/2}$	2541.36	1	1.5	1.5	1	2	1.5	0.5			325128	1561	0.02				
16			291742.8	$^4S_{3/2}$	2448.50	1	1.5	1.5	1	0	1.5	1.5	13.16		310391	2028	28.69				
17			**282616.0**	$^2S_{1/2}$	3153.12	1	1.5	1.5	1	0	0.5	0.5			291626	3216	0.18				
18	256086.4	$^2P_{1/2}$	289121.4	$^4P_{1/2}$	3027.09	1	0.5	0.5	1	1	0.5	1.5		269329	298754	3398	0.08				
19			286747.4	$^4D_{5/2}$	3261.47	1	0.5	0.5	1	2	2.5	1.5			296104						
20			290250.4	$^2D_{3/2}$	2927.06	1	0.5	0.5	1	2	1.5	0.5	20.06		325128	1792	30.12				
21			291742.8	$^4S_{3/2}$	2804.55	1	0.5	0.5	1	0	1.5	1.5			310391						
22			**282616.0**	$^2S_{1/2}$	3769.38	1	0.5	0.5	1	0	0.5	0.5	3.69		291626	4484	2.89				
4s, 4p $^3P_0$ (+e$^-$ → quartet)																					
23	250214.6	$^4P_{1/2}$	286224.2	$^4D_{3/2}$	2777.04	1	0.5	1.5	1	2	1.5	1.5	11.25	260540	295530	2857	14.40				
24			285956.2	$^4D_{1/2}$	2797.86	1	0.5	1.5	1	2	0.5	1.5	22		295185	2886	24.97				

[3] / $A_{j\to i}$ / Ar IV / 4*s* ← 4*p* Transition Probabilities in $10^7 s^{-1}$

	CbA													SST				LANL			
4s-4p	E_i (cm^{-1})	**Term**	E_j (cm^{-1})	**Term**	λ[Å]	L_i	J_i	S_i	l_{ci}	L_j	J_j	S_j	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$	E_i (cm^{-1})	E_j (cm^{-1})	λ[Å]	$A_{j\to i}$
4s, 4p $^1D_2$ (+e⁻ → doubltet)																					
25	267760.9	$^2D_{3/2}$	303664.5	$^2F_{5/2}$	2785.24	2	1.5	0.5	2	3	2.5	0.5	25.26	280500	315486	2858	28.15				
26			303989.2	$^2F_{7/2}$	2760.27	2	1.5	0.5	2	3	3.5	0.5			315801						
27			**311272.0**	$^2P_{3/2}$	2298.26	2	1.5	0.5	2	1	1.5	0.5	4.81		329210	2052	12.77				
28			**310982.0**	$^2P_{1/2}$	2313.69	2	1.5	0.5	2	1	0.5	0.5	47.21		328498	2083	58.60				
29			305898.6	$^2D_{3/2}$	2622.08	2	1.5	0.5	2	2	1.5	0.5	29.25		325126	2240	40.36				
30			305826.6	$^2D_{5/2}$	2627.04	2	1.5	0.5	2	2	2.5	0.5	2.15		325067	2243	1.61				
31	267740.7	$^2D_{5/2}$	303664.5	$^2F_{5/2}$	2783.67	2	2.5	0.5	2	3	2.5	0.5	1.81	280478	315486	2856	2.30				
32			303989.2	$^2F_{7/2}$	2758.74	2	2.5	0.5	2	3	3.5	0.5	27.86		315801	2831	30.72				
33			**311272.0**	$^2P_{3/2}$	2297.20	2	2.5	0.5	2	1	1.5	0.5	43.39		329210	2052	50.98				
34			**310982.0**	$^2P_{1/2}$	2312.60	2	2.5	0.5	2	1	0.5	0.5			328498						
35			305898.6	$^2D_{3/2}$	2620.69	2	2.5	0.5	2	2	1.5	0.5	3.25		325126	2239	8.92				
36			305826.6	$^2D_{5/2}$	2625.64	2	2.5	0.5	2	2	2.5	0.5	30.2		325067	2242	45.07				
4s, 4p $^1S_0$ (+e⁻ → doubltet)																					
37	288903.0	$^2S_{1/2}$	**327311.0**	$^2P_{3/2}$	2603.62	0	0.5	0.5	0	1	1.5	0.5	33.06	304670	343810	2394	41.16				
38			**327147.0**	$^2P_{1/2}$	2614.79	0	0.5	0.5	0	1	0.5	0.5	32.64		343870	2551	41.39				

4*s* – 4*p* → F. Bredice, M. Gallardo,and J. G. Reyna Almandos, *"Revised Analysis of Triply Ionized Argon (Ar IV)", Phys. Scr.* ***51****, 446 (1995).*