Journal of İstanbul Kültür University
2004/1 pp. 19-27

Fine Structure of the Configurations $3d^3$, $3d4s5s$, $3d5s^2$, $3d4s4d$ and $3d^25s$ of Neutral Scandium Atom

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Abstract

Investigation of parametric analysis of the fine structure (fs) for the even parity configurations 3d^3, 3d4s5s, 3d5s^2, 3d4s4d and 3d^{2}5s configurations of atomic Scandium (Sc I) was aimed in this work. Fine structure calculation has been done by using multi-configuration fit method. More precise values for the theoretical g factors are also reported.

Özet

Bu çalışmada, Skandiyum I (Sc I) elementinin çift pariteli 3d^3, 3d4s5s, 3d5s^2, 3d4s4d ve 3d^{2}5s konfigürasyonlarının ince yapısının parametrik analizinin incelenmesi amaçlandı. İnce yapı hesapları çok-konfigürasyonlu fit metodu kullanılarak yapıldı. Aynı zamanda hassas olarak belirlenen teorik g faktörleri verildi.

Key Words: *Fine structure parameters, g-factor, Scandium*

1.Introduction

Hyperfine structure effect of 3d-shell elements became increasingly important in astrophysics, e.g., for the analysis of stellar abundances and for the determination of physical parameters in stellar atmospheres [1-6]. It requires very high accuracy of wave functions in intermediate coupling to interpret accurate experimental hyperfine structure data. So, the interest in the fine structure of the elements has been stimulated [7]. Scandium is the lightest of the 3d elements. It has only one stable isotope which was atomic mass 45 and a nuclear spin of 7/2. Its nuclear magnetic dipole moment and quadrupole moment are $\mu_I = 4.748711(2)\ \mu_N$ [8] and Q = -0.22 b [9], respectively.

In most cases energy levels of different electron configurations of 3d elements are very close in energy and strongly mixed. Therefore fine structure parametric analysis has to be done by using multi-configuration fit method.

2.Fine Structure

Especially for Sc I the two lowest configurations of even parity, $3d4s^2$ *and* $3d^24s$, are energetic well separated whereas the higher configurations are strongly mixed. The fine structure of the two lower configurations of even parity is already discused in [6].

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Here, a multi-configuration fit of five high lying configurations, $3d^3$, $3d4s5s$, $3d5s^2$, $3d4s4d$ and $3d^25s$, of even parity is presented. The parametric analysis of the fine structure has been done using the program code of Cowan in SL-coupling scheme. All of the parameters which are used in this program has been described in reference [10].

The configurations $3d^3$, $3d4s5s$, $3d5s^2$, $3d4s4d$ and $3d^25s$ are comprised of 19, 8, 2, 34 and 16 theoretical fine structure levels, respectively, altogether 79 levels. 65 of them are experimentally known and already identified in the NIST atomic data tables [11]. The $3d5s^2$ configuration has not any experimental energy value. Nevertheless, one have to take into account the unknown $3d5s^2$ configuration due to effect of configuration mixing, which concern levels with J = 3/2 and J = 5/2. $3d5s^2$configuration has energy levels about 35000 cm^{-1}, but these are the not exact values. The positions of these both levels are depend on the initial values of the parameters.

The configuration center of gravity E_{av} , the Slater-integrals F^k and G^k , the spin-orbit parameter ζ_{nl} , the effective parameters α and β and configuration interaction radial integrals R^k are considered as adjustable parameters whose values are to be determined emprically to give the best possible fit between the calculated eigenvalues and observed energy levels.

Besides the usual fine structure parameters effective parameters had to be included to fit the experimental energies with satisfactory accuracy. Fits with different conditions, i.e. choice of the parameters and the coupling ratios, were compared with the following results: No reliable values for the effective parameters T, T^1 and T^2 could be found therefore these parameters were not used for the fit. On the other hand the effective parameters α and β have significant values for the $3d^3$ configuration. So for the calculations 41 parameters were used, compiled in **Table 1**. The parameter values of $3d^24s$ in referens [6] are given in table 1 in last coulomn.

In Büttgenbach [12] it is mentioned that the spin-orbit interaction parameter ζ for 4d and 5d shell atoms the following relation is supplied;

$$\zeta_n\left(d^N\right)-\zeta_n\left(d^{N-1}s\right)=\zeta_n\left(d^{N-1}s\right)-\zeta_n\left(d^{N-2}s^2\right). \tag{1}$$

We have used this relation for our ζ_{3d} parameters. On the other hand, ζ_{3d} parameters of the configurations 3d4s5s and 3d4s4d are held at a constant ratio to corresponding ζ_{3d} parameter of the other configurations according to

$$\frac{\zeta\left(3d^3\right)}{\zeta\left(3d^25s\right)}=\frac{\zeta\left(3d^25s\right)}{\zeta\left(3d4s5s \ or\ 3d4s4d\ resp.\right)} \tag{2}$$

So, the spin-orbit parameters ζ_{3d} belonging the all configurations were held a constant ratio. The Slater parameters F^2(d,d) and F^4(d,d) were held in a constant ratio between the $3d^3$ and $3d^25s$ configurations. The Slater parameters G^2(d,s) were held in a constant ratio between the *3d4s5s* and *3d4s4d* configurations. The Slater parameters G^2(d,d) and G^4(d,d) were held in a constant ratio in the *3d4s4d* configuration. All these interaction parameters are held in the constant ratio of their Hartree-Fock values as calculated by the Cowan programe[10]. These ratios gave the best average deviation. The Slater parameters G^2(d,s), G^0(s,s) and G^2(s,d) were fixed to their Hartree-Fock values.

3. Results

Most levels are more than 80% pure in the configurations. Using 59 experimental energy levels in a least squares fit with 15 free parameters, 7 fix parameters, an avarage deviation of 95 cm^{-1} was achieved. In **Table 1** the fitted parameters are listed.

The best fitted energy values of the least squares fit are listed in **Table 2** together with the experimental values, leading eigenvector components and percentage distributions over the configurations. The comparison between experimental and calculated energies shows good agreement except six levels, $^2D_{5/2}$ at 35745.62 cm^{-1}, $^2D_{3/2}$ at 40257.52 cm^{-1}, $^4S_{3/2}$ at 40282.16 cm^{-1} , $^2D_{5/2}$ at 40334.31 cm^{-1}, $^2G_{7/2}$ at 40418.55 $cm^{-1}$and $^2G_{9/2}$ at 40562.06 cm^{-1} so these levels have been removed from the fit. Two of these six levels have no experimental g-values. In order to emphasize the good fit, the experimental *g* factors are compared with the calculated factors in columns 4 to 6 of **Table 2**. With one exception, 42942.51 cm^{-1} $J = 4.5$, the agreement is also very good. There is no known reason for this discrepancy of *g* factor of this level.

4.Conclusion

With this fs analysis a further contribution to the systematic investigation of the atomic properties of 3d-shell elements has been done. To confirm the quality of the fs calculation the hyperfine structure of the configurations under consideration should be analysed. Therefore more experimental hfs data for high lying levels of Sc I are required.

Acknowledgements

İpek Kanat Ozturk thanks the research fund of the Istanbul University, project number 201/29042004.

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Table 1. Fine structure parameters for the even parity configurations $3d^3$, 3d4s5s, $3d5s^2$, 3d4s4d and $3d^25s$ of Sc I in cm^{-1}. ^{k}: parameter is held in a constant ratio with the same parameter in the all configurations. ^{f}: parameter is held a fixed value. ^{m}: parameter is held in a constant ratio in the same configuration.

Parameters	**$3d^3$**	**3d4s5s**	**$3d5s^2$**	**3d4s4d**	**$3d^25s$**	**$3d^24s$**
E_{AV}	37594 (41)	35659 (64)	35535^f	40975 (28)	44606 (79)	16166 (4)
F^2(3d, 3d)	13091^k	-	-	-	19248^k	26185 (33)
F^4(3d, 3d)	3759^k	-	-	-	5696^k	11974 (35)
F^2(3d, 4d)	-	-	-	5222 (198)	-	-
F^4(3d, 4d)	-	-	-	3867 (236)	-	-
ζ_{3d}	44^k	68^k	70^f	68^k	56^k	45 (5)
ζ_{4d}	-	-	-	3^f	-	-
G^2(3d, 4s)	-	4880^k	-	4768^k	-	5682 (17)
G^2(3d,5s)	-	417^f	-	-	641	
G^0(4s,5s)	-	1294^f	-	-	-	
G^0(3d,4d)	-	-	-	977 (36)	-	
G^2(3d,4d)	-	-	-	784^m	-	
G^4(3d,4d)	-	-	-	516^m	-	
G^2(4s,4d)	-	-	-	121^f	-	
α	67 (6)	-	-	-	-	30 (1)
β	1069 (110)	-	-	-	-	863 (12)
$3d^3$ -3d4s5s						
$R^2(d^2,s^2)$	1377^k					
$3d^3$ -$3d5s^2$						
$R^2(d^2,s^2)$	939^k					
$3d^3$ -3d4s4d						
$R^2(d^2,sd)$	-110^k					
$3d^3$ -$3d^25s$						
$R^2(d^2,ds)$	-2553^k					
3d4s5s -$3d5s^2$						
$R^0(ds,ds)$	190^k					
3d4s5s -$3d5s^2$						
$R^0(s^2,s^2)$	1879^k					
3d4s5s -$3d5s^2$						
$R^2(ds,d^2)$	208^k					
3d4s5s -3d4s4d						
$R^2(ds,d^2)$	-321^k					
3d4s5s -3d4s4d						
$R^2(ds,d^2)$	-111^k					
3d4s5s -$3d^25s$						
$R^2(ds,d^2)$	-7112^k					
$3d5s^2$-$3d^25s$						
$R^2(ds,d^2)$	-1299^k					
3d4s4d -$3d^25s$						
$R^2(sd,ds)$	47^k					
3d4s4d -$3d^25s$						
$R^0(sd,ds)$	68^k					
Number of free parameters	15					7
Number of fitted levels	59					16
Average deviation	95 cm^{-1}					12 cm^{-1}

Table 2. List of levels of the even parity configurations $3d^3$, 3d4s5s, $3d5s^2$, 3d4s4d and $3d^25s$ of Sc I with experimental values E_{exp} and g_{exp} according to [11], calculated values E_{calc} and g_{calc}, the respective deviations, leading eigenvector components, percentage distributions over the configurations.

E_{exp}/(cm^{-1})	E_{calc}/(cm^{-1})	ΔE/(cm^{-1})	g_{exp}	g_{calc}	Δg	Leading component		Percentage distribution					
						Config.	Term	%	$3d^3$	3d4s5s	$3d5s^2$	3d4s4d	$3d^25s$
J=0.5													
34390.25	34380	10	0.000	-0.002	-0.002	3d4s5s	$^3D\,^4D\,^4D$	100	.00	99.99	.00	.01	.00
36492.64	36500	-7	2.634	2.643	-0.009	$3d^3$	^4P	99	99.98	.00	.00	.00	.02
37085.84	36974	112	0.682	0.693	-0.011	$3d^3$	^2P	97	98.46	.00	.00	.01	1.53
39701.44	39583	119	0.008	0.017	-0.009	3d4s4d	$^3D\,^3D\,^4D$	97	.00	.01	.00	99.99	.00
40070.30	39922	148	0.660	0.648	0.012	3d4s4d	$^3D\,^3D\,^2P$	90	.01	.00	.00	99.99	.00
41446.85	41589	-142	2.659	2.670	-0.011	3d4s4d	$^3D\,^3D\,^4P$	100	.00	.00	.00	99.98	.02
42877.65	43009	-131	1.991	1.951	0.040	3d4s4d	$^3D\,^3D\,^2S$	59	.00	.00	.00	100.00	.00
43429.68	43288	142	0.680	0.717	-0.037	3d4s4d	$^1D\,^1D\,^2P$	89	.00	.00	.00	99.94	.06
45514.98	45375	140	2.000	2.002	-0.002	3d4s4d	$^1D\,^1D\,^2S$	61	.00	.00	.00	99.99	.01
	46886			2.669		$3d^25s$	$^3P\,^4P$	100	.00	.00	.00	.02	99.97
	47446			0.668		$3d^25s$	$^3P\,^2P$	98	1.55	.00	.00	.06	98.39
	52529			2.002		$3d^25s$	$^1S\,^2S$	100	.00	.00	.00	.01	99.98
J=1.5													
33763.30	33756	7	0.395	0.399	-0.004	$3d^3$	^4F	100	99.99	.00	.00	.00	.00
34422.83	34409	13	1.192	1.198	-0.006	3d4s5s	$^3D\,^3D\,^4D$	99	.00	99.92	.06	.01	.01
	35094		0.801			$3d5s^2$	^2D	61	1.66	36.51	61.10	.01	.73
35671.04	35726	-55	-	0.800		3d4s5s	$^3D\,^2D\,^2D$	36	1.61	61.06	34.63	.02	2.68
36276.63	36230	46	-	0.812		$3d^3$	^2D	36	72.96	23.60	1.19	.02	2.23
36515.76	36516	0	1.712	1.715	-0.003	$3d^3$	^4P	96	99.58	.35	.00	.00	.07
37148.22	37031	117	1.328	1.339	-0.011	$3d^3$	^2P	95	97.64	.80	.01	.01	1.54
37780.87	37776	5	0.800	0.801	-0.001	3d4s5s	$^1D\,^2D\,^2D$	35	25.73	68.92	2.69	.00	2.65

Table 2. Continued

E_{exp}/(cm^{-1})	E_{calc}/(cm^{-1})	ΔE/(cm^{-1})	g_{exp}	g_{calc}	Δg	Leading component		Percentage distribution					
						Config.	Term	%	$3d^3$	3d4s5s	$3d5s^2$	3d4s4d	$3d^25s$
39721.79	39603	118	1.203	1.202	0.001	3d4s4d	^{3}D ^{3}D ^{4}D	98	.00	.01	.00	99.99	.00
40063.38	39928	134	1.295	1.329	-0.034	3d4s4d	^{3}D ^{3}D ^{2}P	91	.01	.00	.00	99.99	.00
40521.27	40451	70	0.401	0.400	0.001	3d4s4d	^{3}D ^{3}D ^{4}F	99	.00	.00	.00	99.67	.33
	40610			0.803		3d4s4d	^{3}D ^{3}D ^{2}D	74	.01	.02	.00	99.96	.02
41474.87	41596	-120	1.725	1.746	-0.021	3d4s4d	^{3}D ^{3}D ^{4}P	95	.00	.00	.00	99.98	.02
	41882			1.990		3d4s4d	^{3}D ^{3}D ^{4}S	95	.00	.00	.00	100.00	.00
41921.89	41901	20	0.395	0.399	-0.004	$3d^25s$	^{3}F ^{4}F	100	.01	.01	.00	.33	99.65
42466.39	42551	-85	0.802	0.800	0.002	3d4s4d	^{1}D ^{1}D ^{2}D	74	.01	.04	.00	99.93	.02
42937.50	42959	-22	0.780	0.800	-0.020	$3d^3$	^{2}D	56	97.71	.67	.11	.01	1.49
43435.40	43300	135	1.336	1.334	0.002	3d4s4d	^{1}D ^{1}D ^{2}P	92	.00	.00	.00	99.94	.06
	45475			0.800		$3d^25s$	^{1}D ^{2}D	90	1.53	8.07	.21	.05	90.14
	46917			1.734		$3d^25s$	^{3}P ^{4}P	100	.00	.00	.00	.02	99.97
	47506			1.334		$3d^25s$	^{3}P ^{2}P	98	1.55	.01	.00	.06	98.39
J=2.5													
33798.64	33795	3	1.026	1.029	-0.003	$3d^3$	^{4}F	100	100.00	.00	.00	.00	.00
34480.00	34463	17	1.370	1.371	-0.001	3d4s5s	^{3}D ^{4}D ^{4}D	99	.00	99.88	.08	.01	.02
	35168			1.202		3d4s5s	^{1}D ^{2}D ^{2}D	45	1.12	52.67	44.92	.01	1.28
	35788			1.201		$3d5s^2$	^{2}D	50	3.10	44.33	50.17	.02	2.39
36330.59	36347	-16	1.196	1.214	-0.018	$3d^3$	^{2}D	36	73.53	22.68	1.82	.02	1.95
36572.77	36573	0	1.590	1.588	0.002	$3d^3$	^{4}P	97	98.92	.98	.01	.00	.09
37855.61	37906	-50	1.180	1.201	-0.021	3d4s5s	^{3}D ^{2}D ^{2}D	37	24.17	70.50	2.64	.00	2.69
38871.65	39087	-215	0.855	0.857	-0.002	3d4s4d	^{3}D ^{3}D ^{2}F	94	.00	.00	.00	99.98	.01
39755.02	39637	118	1.364	1.371	-0.007	3d4s4d	^{3}D ^{3}D ^{4}D	100	.00	.01	.00	99.99	.00
39861.37	39925	-63	0.555	0.572	-0.017	3d4s4d	^{3}D ^{3}D ^{4}G	100	.00	.00	.00	100.00	.00
40554.99	40484	71	1.035	1.029	0.006	3d4s4d	^{3}D ^{3}D ^{4}F	99	.00	.00	.00	99.68	.32
	40691			1.200		3d4s4d	^{3}D ^{3}D ^{2}D	74	.01	.02	.00	99.95	.02
40802.76	40881	-78	0.843	0.857	-0.014	$3d^3$	^{2}F	81	81.04	.00	.00	.05	18.90

Table 2. Continued

E_{exp}/(cm^{-1})	E_{calc}/(cm^{-1})	ΔE/(cm^{-1})	g_{exp}	g_{calc}	Δg	Leading component		Percentage distribution					
						Config.	Term	%	$3d^3$	3d4s5s	$3d5s^2$	3d4s4d	$3d^25s$
41505.60	41635	-129	1.600	1.600	0	3d4s4d	$^3D\,^3D\,^4P$	99	.00	.00	.00	99.97	.02
41960.97	41947	14	1.021	1.028	-0.007	$3d^25s$	$^3F\,^4F$	99	.16	.01	.00	.34	99.50
42149.66	42179	-30	-	0.858		3d4s4d	$^1D\,^1D\,^2F$	91	1.02	.00	.00	96.23	2.75
42445.55	42530	-84	-	1.201		3d4s4d	$^1D\,^1D\,^2D$	74	.02	.03	.00	99.87	.08
	42669			0.864		$3d^25s$	$^3F\,^2F$	77	18.93	.01	.00	3.77	77.29
42917.83	42908	10	1.190	1.194	-0.004	$3d^3$	^2D	55	96.50	.73	.12	.04	2.59
	45476			1.201		$3d^25s$	$^1D\,^2D$	90	1.47	8.13	.22	.05	90.13
	46967			1.600		$3d^25s$	$^3P\,^4P$	100	.00	.02	.00	.02	99.96
J=3.5													
33846.59	33848	-1	1.230	1.239	-0.009	$3d^3$	^4F	100	100.00	.00	.00	.00	.00
34567.19	34550	17	1.430	1.430	0	3d4s5s	$^3D\,^4D\,^4D$	100	.00	99.99	.00	.01	.00
36977.51	37189	-211	0.890	0.889	0.001	$3d^3$	^2G	100	99.72	.00	.00	.01	.28
38959.16	39126	-167	1.140	1.145	-0.005	3d4s4d	$^3D\,^3D\,^2F$	93	.00	.00	.00	99.99	.01
39799.99	39683	117	1.439	1.427	0.012	3d4s4d	$^3D\,^3D\,^4D$	99	.00	.01	.00	99.99	.00
39902.75	39964	-60	0.968	0.985	-0.017	3d4s4d	$^3D\,^3D\,^4G$	100	.00	.00	.00	100.00	.00
40603.95	40527	77	1.235	1.238	-0.003	3d4s4d	$^3D\,^3D\,^4F$	99	.00	.00	.00	99.68	.31
40825.78	40885	-58	1.140	1.143	-0.003	$3d^3$	^2F	83	83.51	.00	.00	.04	16.46
	40972		-	0.889		3d4s4d	$^3D\,^3D\,^2G$	72	.01	.00	.00	99.98	.01
42015.58	42012	3	1.237	1.238	-0.001	$3d^25s$	$^3F\,^4F$	99	.16	.00	.00	.33	99.50
42198.84	42224	-25	-	1.143		3d4s4d	$^1D\,^1D\,^2F$	90	.73	.00	.00	96.89	2.38
	42776			1.143		$3d^25s$	$^3F\,^2F$	81	15.59	.00	.00	3.07	81.34
42969.78	43037	-67	0.930	0.889	0.041	3d4s4d	$^1D\,^1D\,^2G$	72	.00	.00	.00	99.97	.04
	47011			0.889		$3d^25s$	$^1G\,^2G$	100	.28	.00	.00	.04	99.68
J=4.5													
33906.38	33914	-7	1.330	1.334	-0.004	$3d^3$	^4F	100	100.00	.00	.00	.00	.00
37054.51	37247	-192	1.110	1.111	-0.001	$3d^3$	^2G	99	99.72	.00	.00	.01	.28
39164.11	39022	142	-	0.909		$3d^3$	^2H	100	100.00	.00	.00	.00	.00

Table 2. Continued

$E_{exp}/(cm^{-1})$	$E_{calc}(cm^{-1})$	$\Delta E/(cm^{-1})$	g_{exp}	g_{calc}	Δg	Leading component		Percentage distribution					
						Config.	Term	%	$3d^3$	3d4s5s	$3d5s^2$	3d4s4d	$3d^25s$
39957.79	40016	-59	1.170	1.173	-0.003	3d4s4d	$^3D\ ^3D\ ^4G$	100	.00	.00	.00	100.00	.00
40670.87	40578	92	1.336	1.334	0.002	3d4s4d	$^3D\ ^3D\ ^4F$	99	.00	.00	.00	99.70	.30
	41125		-	1.111		3d4s4d	$^3D\ ^3D\ ^2G$	71	.00	.00	.00	99.99	.01
42085.18	42098	-13	1.320	1.334	-0.014	$3d^25s$	$^3F\ ^4F$	100	.00	.00	.00	.30	99.70
42942.51	42991	-48	1.010	1.111	-0.101	3d4s4d	$^1D\ ^1D\ ^2G$	71	.00	.00	.00	99.97	.03
	47011			1.111		$3d^25s$	$^1G\ ^2G$	100	.28	.00	.00	.04	99.68
J=5.5													
39225.33	39068	157	-	1.091		$3d^3$	^2H	100	100.00	.00	.00	.00	.00
40028.38	40086	-57	1.260	1.273	-0.013	3d4s4d	$^3D\ ^3D\ ^4G$	100	.00	.00	.00	100.00	.00