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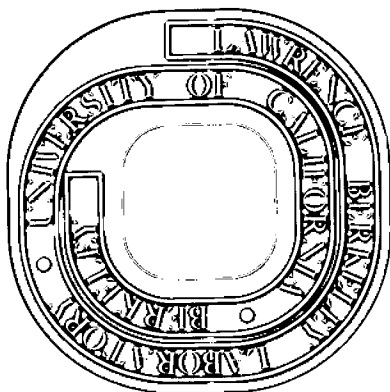
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CALCULATION OF THE CRYSTAL FIELD SPLITTINGS OF
Sm³⁺ LEVELS IN LaCl₃ WITH INCLUSION OF J-MIXING*

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ABSTRACT

A complete diagonalization of the matrices for the electrostatic, spin-orbit, and crystal field interactions for Sm³⁺ in LaCl₃ has been carried out using a truncated set of basis vectors containing 42 of the 73 LS states. This diagonalization allowed many new assignments to be made. Correction of some of the centers of gravity previously used in a fit of free ion parameters was also possible. The newly obtained free ion parameters are more in accord with the trends for the other lanthanide ions in LaCl₃. They reduce the rms deviation from 119 to 54 cm⁻¹. The parameters (in cm⁻¹) used in the final diagonalization are E¹ = 5465.27 ± 17.21, E² = 25.40 ± .39, E³ = 547.62 ± 1.65, ζ = 1153.8 ± 8.9, α = 24.29 ± 1.98, β = -795.72 ± 98.4, γ = 800, B₀² = 161.70, B₀⁴ = -182.00, B₀⁶ = -710.24, B₆⁶ = 448.14.

I. INTRODUCTION

Energy levels of Sm^{3+} in LaCl_3 have been measured by Magno and Dieke¹. A crystal field calculation by Axe and Dieke² (including J-mixing) for the ^6H and ^6F multiplets reproduced 39 observed levels with an rms deviation of $\pm 3.2 \text{ cm}^{-1}$. Further assignments of higher levels and some additional data were included in the book of Dieke³. Some assignments of the centers of gravity (often estimated from one observed crystal field component) were made from a least-squares fitting procedure by Carnall, Fields, and Rajnak⁴ who included the configuration interaction parameters α , β and γ .⁵ The fit was quite unsatisfactory, however. The rms deviation was 119 cm^{-1} (vs. ~ 50 for most other rare earth ions). Two levels whose identification was quite certain had deviations of $\sim 200 \text{ cm}^{-1}$. Furthermore α was determined to be 16 cm^{-1} whereas it was 22 cm^{-1} for Sm^{3+} in solution. It was impossible to determine a value for γ . Any attempt to include γ , even if it were not allowed to vary, immediately led to $\alpha \sim 10 \text{ cm}^{-1}$ and large errors in all the parameters. This difficulty arose because γ is essentially dependent on seniority number. Low lying states all tend to have the same seniority. Consequently assignment of rather high levels is required before γ can be determined.

II. PRELIMINARY DISCUSSION

In the present work we took the free ion parameters of Carnall, et al., and the crystal field parameters⁶ of Axe and Dieke and diagonalized the matrices for the electrostatic, spin-orbit, and crystal field interactions simultaneously. Truncation of the basis vectors was necessary, however, since the f^5 configuration contains 73 LS states. We chose to include only 42 states: all the sextets and quartets except the $4S$ and $4I_2$, and the following doublets: $2P_1$, $2P_3$, $2P_4$, $2D_1$, $2D_2$, $2D_4$, $2D_5$, $2F_1$, $2F_2$, $2F_4$, $2F_5$, $2F_6$, $2F_7$, $2H_6$, $2I_4$, $2K_1$, $2K_4$, and $2K_5$.⁷ Limiting the J -values to $J \leq 15/2$ leads to 3 matrices to be diagonalized: $\mu = 1/2$, rank = 184; $\mu = 3/2$, rank = 178; $\mu = 5/2$, rank = 172, where $\mu = J_z \pmod{6}$. Comparison of the results of diagonalization of these matrices with the crystal field parameters set equal to zero and the free ion calculation of Carnall, et al., gave a value for the truncation error of each J -level. For the levels below 20100 cm^{-1} these errors were $\sim 20 \text{ cm}^{-1}$, but were much larger for some higher states. The exclusion of $2L_1$ and $2L_3$ from the basis vectors resulted in a large error for the $J = 15/2$ levels, particularly the one at $\sim 20300 \text{ cm}^{-1}$. Comparison of the calculated centers of gravity from a complete diagonalization including the crystal field matrix elements with those from the truncated eigenvectors with the crystal field parameters equal to zero gave a crystal field shift for each J -level. When a correction was made for the truncation error, crystal field shifts were $< \pm 25 \text{ cm}^{-1}$ except for the $J = 9/2$ at 20500 cm^{-1} . Since this was one of the levels with a very large truncation error, the larger shift (-44 cm^{-1}) may not be meaningful. The $J = 15/2$ and $J = 11/2$ at 20300 and 21000 cm^{-1} are so badly J -mixed that it is impossible to determine a center of gravity for the levels independently. Consequently no crystal field shift could be computed.

Having ascertained that J-mixing does not cause appreciable shifts of the center of gravity of the levels, we then used the results of the crystal field calculation (including splitting factors) to make some additional assignments and corrected a couple of the centers of gravity chosen by Carnall, et al. A new free ion fit to these centers of gravity was carried out, fixing $\gamma = 800 \text{ cm}^{-1}$ (near the value for Sm^{3+} in solution). The rms deviation was reduced to 54 cm^{-1} . A "complete" diagonalization with these new free ion parameters (see Table I) gave considerable improvement for some of the levels and allowed some additional assignments to be made. These new assignments were insufficient to determine γ by fitting, however.

III. DISCUSSION OF RESULTS

The ${}^6\text{H}$ and ${}^6\text{F}$ multiplets are quite well represented by the parameters used (Table II). If the errors in fitting the centers of gravity are removed from Column 6 of Table II, the errors are generally $< 10 \text{ cm}^{-1}$ and the parallel splitting factors are in reasonable agreement. One should note, however, that for ${}^6\text{H}_{7/2}$ (Y_4), Magno and Dieke¹ give $s_{\parallel} = .13$, whereas Dieke³ gives 3.9. The former value is in much better agreement with the calculations. The ${}^6\text{F}_{1/2}$ level was not assigned by Dieke³, but the calculated level is in excellent agreement with the $\mu = 1/2$ level at 6331.5 (T_2) of Magno and Dieke¹. This assignment has been made in Table II. Many of the components of ${}^6\text{F}_{3/2}$ and ${}^6\text{H}_{15/2}$ are highly J-mixed and it is impossible to assign centers of gravity to the levels individually. The ${}^6\text{F}_{5/2}$ components contain up to 3% J = 15/2 which may mean that the good agreement of the calculated and experimental centers of gravity is accidental because of a compensating crystal field shift.

The ${}^4\text{I}_{9/2}$ is the first level to exhibit large truncation effects. Levels D_1 - D_4 have some mixing with ${}^4\text{M}_{15/2}$ where this effect is even larger. This may account for the large variation of the errors for the levels in Column 6 of Table II. For the lower levels the truncation of the basis set has caused a shift of the centers of gravity, but there is little indication that it has greatly distorted the crystal field splittings. This is obviously not true for the ${}^4\text{I}_{9/2}$ where the total splitting is calculated to be $\sim 75 \text{ cm}^{-1}$ and observed to be $\sim 300 \text{ cm}^{-1}$.

The levels H_1 and H_2 have been assigned to the two lowest levels of ${}^4\text{G}_{9/2}$. The total calculated splitting is $\sim 100 \text{ cm}^{-1}$. Therefore, it seems unlikely that H_3 , which is $> 1000 \text{ cm}^{-1}$ above H_1 , is also part of this group.

If the crystal field splittings are large, H_3 could belong to either ${}^4M_{17/2}$ or ${}^4M_{19/2}$ which were not calculated.

The experimental levels K_3-K_{10} , closely spaced in the range 24530-24569 cm^{-1} , must belong to ${}^4L_{13/2}$ as indicated by Dieke³. The calculated levels are even more closely packed. There is one extra experimental value for $J = 13/2$ but without g values or a more accurate calculation it is impossible to pick it out. Likewise the calculation is not sufficiently accurate to assign the individual lines.

Dieke assigned the levels L_1-L_5 to a ${}^4F_{9/2}$, but there are three $\mu = 5/2$ levels which is not possible for a $J = 9/2$. There is no $J = 9/2$ level calculated in that region. L_1 and L_2 have been assigned to the two $\mu = 5/2$ levels of ${}^4F_{7/2}$. Their separation of 11 cm^{-1} is in reasonable agreement with the calculated separation of 18 cm^{-1} . The levels L_3-L_5 probably belong to ${}^4K_{11/2}$. In fact, the calculated g_{\parallel} of 2.09 for the lowest level is in excellent agreement with the observed s_{\parallel} of 2.05. In view of the large truncation error, the order of the calculated levels may not be correct and assignment of L_3 and L_5 is impossible.

This leaves the levels M_1-M_5 to be assigned to ${}^4G_{11/2}$ and ${}^4L_{15/2}$. There is significant J-mixing between the two and a calculation with less truncation error will be necessary before individual lines can be assigned.

The levels N_1-N_4 can clearly be assigned to ${}^6P_{7/2}$ as indicated in Table II. The g values and splitting pattern agree well and the truncation error is small. Likewise N_5 is very likely ${}^4D_{1/2}$. The levels N_6-N_9 , three of which probably have $\mu = 5/2$, very likely belong to ${}^4L_{17/2}$ for which the

crystal field splittings weren't calculated. Clearly they can't be the ${}^4K_{11/2}$ as assigned by Dieke since that is calculated to be 1000 cm^{-1} lower in energy.

The $0'$ levels must be assigned to the ${}^4K_{13/2}$ and $({}^4D, {}^6P)_{5/2}$ which are badly J-mixed. The splitting factor of the $0'_4$ level makes its assignment clear but the others can't be assigned because of the large truncation error for the $J = 13/2$ state.

Beyond this point truncation errors are very large and J-mixing is considerable. This makes assignments impossible for the P' levels at the present time.

IV. CONCLUSIONS

The results are remarkably good considering the truncation of the basis states and the fact that no fitting of the crystal field parameters was carried out. J-mixing does occur and makes the interpretation of some levels difficult, but it is considerably less than had been expected. The crystal field parameters determined by Axe and Dieke for the ${}^6\text{H}$ and ${}^6\text{F}$ multiplets seem to represent the higher multiplets reasonably well. Detailed consideration of the crystal field splittings of the higher states is made difficult by the truncation errors, however. Such an approximate calculation did prove valuable in understanding the overall structure of the energy levels and allowed computation of an improved set of free ion parameters. Further progress on the analysis of Sm^{3+} in LaCl_3 must await the ability to carry out least squares fits on large matrices and computations with a larger basis set than that chosen here. One must be very cautious about fitting free ion parameters with a truncated basis set, however. The g values as well as energies should be fit. If such a complete fit is carried out, it should also include the additional 3-body operators of configuration interaction.^{8,9}

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FOOTNOTES AND REFERENCES

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6. The values used here correspond to the definitions of Wybourne, not those originally used by Axe and Dieke.
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Table I. Parameters for Sm^{3+} in LaCl_3 (cm^{-1})

$$E^1 = 5465.27 \pm 17.21$$

$$E^2 = 25.40 \pm .39$$

$$E^3 = 547.62 \pm 1.65$$

$$\zeta = 1153.8 \pm 8.9$$

$$\alpha = 24.29 \pm 1.98$$

$$\beta = -795.72 \pm 98.4$$

$$\gamma = 800$$

$$B_0^2 = 161.70$$

$$B_0^4 = -182.00$$

$$B_0^6 = -710.24$$

$$B_6^6 = 448.14$$

Table II. Energy Levels of Sm^{3+} in LaCl_3

S'L'J ^a	Level	2μ	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	g (calc.)	s (obs.)	Centers of Gravity		Truncation Error (cm ⁻¹)
								(calc.) ^c (cm ⁻¹)	(obs.) ^d (cm ⁻¹)	
$6H_{5/2}$	Z ₁	1	0.0	0.0	0.0	.598	.58			
	Z ₂	3	36.0	40.7	-4.7	.909	.89	37.9	35.6	2.3
	Z ₃	5	64.4	66.1	-1.7	1.529	2.0			4.3
$6H_{7/2}$	Y ₁	3	984.5	992.3	-7.8	2.54	2.39			
	Y ₂	5	1045.5	1051.2	-5.7	1.55		1072.3	1080.2	-7.9
	Y ₃	1	1100.0	1104.7	-4.7	.54				5.8
	Y ₄	5	1166.5	1172.6	-6.1	.01	3.9 ^e			
$6H_{9/2}$	X ₁	5	2212.8	2211.7	1.1	3.96	3.81			
	X ₂	3	2227.9	2230.2	-2.3	.98	1.05			
	X ₃	1	2308.2	2308.0	0.2	1.08		2282.9	2290.2	-7.3
	X ₄	3	2320.6	2324.5	-3.9	7.40	7.02			
	X ₅	5	2364.2	2376.9	-12.7	6.23				7.3
$6H_{11/2}$	W ₁	5	3533.2	3522.7	10.5	1.89	1.95			
	W ₂	3	3584.2	3571.1	13.1	2.55	2.52			
	W ₃	1	3610.6	3599.6	11.0	6.64		3617.8	3608.5	9.3
	W ₄	5	3627.8	3614.0	13.8	4.21				7.3
	W ₅	1	3657.3	3646.0	11.3	5.36				
	W ₆	3	3709.1	3697.9	11.2	9.63				

(continued)

Table II. (continued)

S'L'J' ^a	Level	2μ	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	g (calc.)	s (obs.)	Centers of Gravity		Truncation Error (cm ⁻¹)		
								(calc.) ^c (cm ⁻¹)	(obs.) ^d (cm ⁻¹)		ΔE	
⁶ H _{13/2}	V ₁	5	4983.1	4957.4	25.7	1.56						
	V ₂	3	4998.4	4968.1	30.3	1.89	2.35					
	V ₃	1	5022.5	4988.0	34.5	.71	1.35					
	V ₄	5	5026.6	4997.4	29.2	4.10			5036.2	5005.9	30.3	6.6
	V ₅	1	5050.3	5023.1	27.2	16.49						
	V ₆	3	5062.5	5034.0	28.5	9.46						
⁶ F _{1/2}	T ₂	1	6334.2	6331.5	2.7	.90			6319.4			4.3
⁶ H _{15/2} ,		1	6395.2			1.41						
		3	6436.1			2.28			6503.8 ^f			11.6
		5	6481.1			2.04						
		1	6483.1			15.14						
		3	6540.9			11.56			6563.8 ^g			4.4
⁶ F _{3/2}		1	6524.6			11.90						
		3	6571.9			6.80						
		1	6592.0			.20						
		5	6585.2			4.82						
		3	6621.1			7.48						
⁶ F _{5/2}	R ₁	1	7074.8	7046.8	28.0	1.50						
		3	7076.5			4.08			7055.4	7058.0	-2.6	4.4
	R ₂	5	7077.2	7051.9	26.3	6.50						

(continued)

Table II. (continued)

S'L'J ^a	Level	2J	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	g (calc.)	s (obs.)	Centers of Gravity		Truncation Error (cm ⁻¹)	
								(calc.) ^c (cm ⁻¹)	(obs.) ^d (cm ⁻¹)		ΔE
⁶ F _{7/2}	Q ₁	5	7884.2	7871.1	7.1	2.77					
	Q ₂	1	7912.6	7900.9	11.7	1.30	1.49	7901.2	7920.2	-19.0	8.0
	Q ₃	5	7936.0	7931.3	4.7	5.42					
	Q ₄	3	7940.7	7937.1	3.6	4.20					
⁶ F _{9/2}	F ₁	5	9049.2	9047.6	1.6	4.08	3.84				
	F ₂	3	9058.0	9052.8	5.2	5.12					
	F ₃	3	9088.5	9088.5	0.0	3.32		9057.9	9082.3	-24.4	17.9
		1	9108.5			1.53					
	P ₄	5	9109.8	9114.2	-4.4	7.02	6.65				
⁶ F _{11/2}		1	10435.8			15.76					
	O ₁	3	10444.9	10449.2	-4.3	12.29					
		1	10457.8			1.24		10436.1	10457.3	-21.2	14.1
	O ₂	5	10459.3	10468.2	-8.9	5.54					
	O ₃	3	10463.6	10478.8	-15.2	3.54					
	5	10469.7	10480.2	-10.5	2.60						
(⁴F, ⁴G) _{5/2}	A ₁	3	17877.0	17849.6	27.4	2.14	2.02	17890.9	17874.	17	23.4
	A ₂	1	17886.6	17870.8	15.8	.94	.86				
		5	17937.5			3.78					
⁴ F _{3/2}		1	18841.2			.42					
	B ₁	3	18843.3	18857.2	-7.9	1.33	1.07	18830.6	18856.	-26	23.7

(continued)

Table II. (continued)

S'L'J' ^a	Level	2u	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	ε (calc.)	s (obs.)	Centers of Gravity (calc.) ^c (obs.) ^d ΔE (cm ⁻¹) (cm ⁻¹) (cm ⁻¹)	Truncation Error (cm ⁻¹)	
⁴ G, ⁴ F) _{7/2}	C ₁	3	19970.2	20003.3	-32.9	3.32	3.25	19986.5	20025. -39	75.2
		1	19981.6			.94				
	C ₂	5	19983.3	20014.0	-30.7	5.12	5.01			
		5	20031.7			7.34				
⁴ I _{9/2}	D ₁	3	20925.0	20454.4	470.6	2.05				
	D ₂	1	20931.2	20518.0	413.2	.66		20519.6	20599.5	-79.9
	D ₃	5	20945.9	20565.1	380.8	3.01				461.3
	D ₄	3	20959.5	20707.9	251.6	6.42				
	D ₅ ^h	5	21001.1	20752.2	248.9	4.62				
⁴ M _{15/2}								20685.5		276
								21089.0		1120
								21640.4	~21560. 80	339
⁴ F, ⁴ G) _{5/2}	G ₁	5	22085.8	22115.7	-29.9	4.20	5.30			
	G ₂	3	22087.7	22134.7	-47.0	2.54	2.77	22062.6	22129.1	-66.5
	G ₃	1	22092.6	22137.0	-34.4	1.10				13.0
⁴ M _{17/2}								22431.6		

(continued)

Table II. (continued)

S'L'J' ^a	Level	2μ	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	ε (calc.)	s (obs.)	Centers of Gravity (calc.) ^c (obs.) ^d ΔE (cm ⁻¹) (cm ⁻¹)	Truncation Error (cm ⁻¹)
⁴ G _{9/2}	H ₁	5	22697.6	22515.9	181.7	6.10			
	H ₂	1	22700.0	22518.1	181.9	1.14			
		3	22738.3			.31		22680.0	70.8
		5	22800.0			3.76			
		3	22809.4			7.45			
⁴ I _{15/2}							k		
		1	23777.0			1.72		22977.6	380
⁶ P _{5/2}	I ₁	3	23800.9	23774.3	26.6	5.09	4.62	23783.0	7
	I ₂	5	23827.4	23803.3	24.1	8.19	7.58		13.0
⁴ M _{19/2}									j
								23966.	
⁶ P _{3/2}	K ₁	3	24588.4	24519.9	68.5	6.55		24566.4	46.2
	K ₂	1	24598.5	24520.3	78.2	2.16			27.6
⁴ L _{13/2}		3	24694.4			2.50			
		1	24694.5			4.02			
		5	24695.5			6.20		24530.9	182
		5	24714.0			4.36			
		1	24714.7			2.45			
	3	24716.0			2.62				
	1	24723.5			9.15				

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(continued)

Table II. (continued)

S'L'J' ^a	Level	2J	E(calc.) (cm ⁻¹)	E(obs.) ^b (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	g (calc.)	s (obs.)	Centers of Gravity		Truncation Error (cm ⁻¹)
								(calc.) ^c	(obs.) ^d ΔE	
⁴ F _{7/2}	I ₁	5	24846.7	24825.0	78.3	.02				
		1	24857.0			1.24		24742.4		120
	L ₂	5	24865.1	24836.1	29.0	2.28				
		3	24890.8			3.18				
⁴ K _{11/2}	I ₄	5	25483.6	25072.5	411.1	2.09	2.05			
		3	25488.1			2.03				
		1	25497.2			.42				
		5	25507.1			3.70		25168.1		338
		1	25521.9			8.93				
		3	25531.2			6.90				
⁴ L _{15/2} } ⁴ G _{11/2} } M ₁ -M ₅										
⁶ P _{7/2}	N ₁	5	26297.4	26300.1	-2.7	10.45	10.3			
		5	26317.6	26328.8	-11.2	7.27	7.28	25290.5	25332.9	-42.4
	N ₃	3	26334.5	26350.3	-15.8	4.82				
	N ₄	1	26336.8	26352.4	-15.6	1.56				
⁴ D _{1/2}	N ₅	1	26506.4	26502.2	4.2	.08				

(continued)

Table II. (continued)

S ¹ L ¹ J ¹ ^a	Level	2μ	E(calc.) (cm ⁻¹)	E(obs.) (cm ⁻¹)	E(calc.) - E(obs.) (cm ⁻¹)	g (calc.)	s (obs.)	Centers of Gravity (calc.) ^c (obs.) ^d ΔE (cm ⁻¹) (cm ⁻¹)	Truncation Error (cm ⁻¹)
(⁴ D, P) _{5/2}		5	27451.6			.71		27460.1	13.0
		1	27456.5 ^h			1.44			
⁴ K _{13/2}		3	27462.8 ^h			3.84		26953.1	541
		3	27465.3			.28			
		5	27482.1			2.38			
		1	27485.7			2.29			
		1	27496.2			8.59			
	0 ₄ ⁱ	5	27498.7 ^h	27402.0	96.7	7.48	7.00		
		3	27500.4			4.89			

^gMajor component(s).

^bEnergy and assignment of Dieke unless noted in text.

^cCalculated in fit to "free ion" levels.

^dCalculated components used to estimate center where all components are not observed.

^eMagno and Dieke give .13.

^fJ = 15/2.

^gJ = 3/2.

^hDieke calls this ⁴M_{15/2} but the coefficient of ⁴M in the eigenvector < .05.

ⁱCalculated levels are not included because of the large truncation errors and strong J-mixing. Observed levels are E₁ = 20977.68, F₁ = 21519.8, F₂ = 21545.5, F₃ = 21594.1.

^jNo calculation for J > 15/2.

^kNot included because of large truncation error.

^lMostly J = 5/2.

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