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Supplementary Tables for

A Systematic Analysis of the Spectra of the Lanthanides Doped into Single Crystal LaF3

by

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Supplementary tables to which we refer in our article of the same title in the Journal of Chemical Physics are reproduced here. These tables along with certain supplementary figures and an expanded discussion of the experimental data are also contained in an unpublished report, ANL-88-8. This report is available from the NTIS Distribution Service, P. O. Box 1300, Oak Ridge, TN 37831 (telephone number: (615) 576-1301).

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				Caspers	Wong	Voron'ko
SLJa	Obsd.b	Calc.c		et al. ^d	et al.e	et al.f
State	(cm^{-1})	(cm^{-1})	0 - C	(cm^{-1})	(cm^{-1})	(cm^{-1})
⁴ I _{9/2}	0	5	- 5	0		0
-9/2	45	48	-3	45		44
	136	153	-17	136		140
	296	304	-8	296		297
	500	513	-13	500		502
⁴ I _{11/2}	1978	1965	13	1978		1980
11/2	2037	2027	10	2037		2039
	2068	2070	-2	2068		2069
	2091	2089	2	2091		2093
	2187	2193	-6	2187		2190
	2223	2226	-3	2223		2225
					•	
⁴ I _{13/2}	3918	3902	16	3919		3919
137 -	3978	3970	8	3979		3973
	4038	4033	5	4039		4039
	4076	4087	-11	4078		4077
	4118	4115	3	4120		4119
	4208	4 2 0 5	3	4213		4213
	4278	4267	11	4278		4277
					∳ *	
⁴ I _{15/2}	5816	5804	12	5815		5817
13/ 2	5874	5871	3	5877		5876
	5986	5999	-13	5988		5989
	6141	6163	-22			6142
	6167	6185	-18			6173

Appendix I. (cont.)

				Caspers	Wong	Voron'ko
SLJa	Obsd.b	Calc.c		$et \ al.^d$	et al. ^e	et al. $^{ m f}$
State	(cm^{-1})	(cm^{-1})	<u>0-C</u>	(cm^{-1})	(cm^{-1})	(cm^{-1})
⁴ I _{15/2}	6323	6113	10			6320
13/2	6454	6445	9			6448
	6556	6538	18	•		6551
⁴ F _{3/2}	11592	11596	-4	11592	11591.6	11594
3/ 2	634	638	-4	634	633.6	637
2 _{Ho/2} ,	12596	12576	20	12596	12595.6	
² H _{9/2} , ⁴ F _{5/2}	614	595	19	613	612.9	
5/2	622	633	-11	621	620.7	
	676	680	-4	675	674.6	
	694	704	-10	693	692.6	
	754	761	-7	755	755.3	
	843	847	-4	-	-	
	902	874	27	-	-	
⁴ F _{7/2}	13514	13521	-7	13515	13514.8	
,,_	590	591	-1	591	590.8	
⁴ S _{3/2}	671	670	1	671	670.9	
3/ 2	676	678	-2	677	676.7	
⁴ F _{7/2}	711	690	21	710	710.1	
// 2	715	7 25	-10	714	714.2	
	x					
⁴ F _{9/2}	14834	14840	-6	14835	14834.7	
) L	861	860	1	860	861.8	
	892	891	1	891	890.6	

Appendix I. (cont.)

				Caspers	Wong
SLJ ^a	Obsd.b	Calc.c		et al. $^{ m d}$	et al. ^e
State	(cm^{-1})	(cm^{-1})	0-C	(cm^{-1})	(cm^{-1})
State	<u>/cm /</u>	<u> </u>			
⁴ F9/2	14926	14925	1	14927	
- 9/2	959	955	4	958	14959.4
2,,	15997	16025	-28	15998	15998.1
² H _{11/2}	16033	043	-10	16033	-
	046	049	- 3	045	16046.4
	060	067	- 7	059	-
	100	093	7	103	-
	165	136	29	_	-
	103				
4G5 / 20	17306	17301	5	17304	17304.6
⁴ G _{5/2} , ⁴ G _{7/2}	316	318	-2	315	316.0
-//2	363	360	3	364	362.9
	511	492	19	. 512	509.2
	518	512	6	5 20	520.3
	571	567	4	570	
	605	607	-2	601	603.2
4 _C	19147	19134	13	19147	19147.4
⁴ G _{7/2}	235	243	-8	235	236.2
	252	266	-14	251	252.1
	324	322	2	3 23	325.4
2			2	10549	19568.2
2 K _{13/2} ,	19567	19570	-3 -	19568	17300.2
² K _{13/2} , ⁴ G _{9/2}	615	622	-7	617	450 O
	651	638	13	651	650.9
	686	681	5	685	686.2

Appendix I. (cont.)

				Caspers	Wong
SLJa	Obsd.b	Calc.c		$et \ al.^d$	et al.e
State	(cm ⁻¹)	(cm ⁻¹)	<u>0-C</u>	(cm ⁻¹)	(cm ⁻¹)
² K _{13/2} ,	19704	19696	8	19702	19704.0
4 _{G9/2}	-	7 27		-	-
., =	741	741	0	739	739.4
	799	786	13	801	
	835	834	1	839	
	-	892		-	
	-	946		_	
	960	970	-10	-	
² G _{9/2}	21155	21151	4	21158	
<i>5</i> / 2	176	180	-4	176	
	. 198	202	-4	201	
	232	24 2	-10	234	
	252	271	-19	254	
² D _{3/2}	21338	21337	1	21339	
5, -	353	355	-2	351	
⁴ G _{11/2} ,	21542	21535	7		
2 K _{15/2}	-	618			
	633	630	3		•
	718	704	14		
	-	754			
	768	767	1		
	-	783			
	807	810	-3		
	-	821			
	846	861	-15		
		884			

Appendix I. (cont.)

				Caspers
SLJa	$0bsd.^{b}$	Calc.c		et al. $^{ m d}$
State	(cm^{-1})	(cm^{-1})	<u>0-C</u>	(cm^{-1})
40	_	21929		
$\frac{^{4}G_{11}}{^{2}v}$	_	957		
2 K _{15/2}	21992	989	3	
	21332	707	J	
² P _{1/2}	23473	23463	10	23468
² D _{5/2}	23991	23985	6	23991
·	24033	24035	-2	
	080	075	5	
•				
² P _{3/2}	26378	26389	-11	
	4 26	424	2	
⁴ D _{3/2}	28341	28342	-1	
3/ 2	374	371	3	
,				
⁴ D _{5/2}	28501	28500	1	
	5 2 5	5 2 6	-1	
	676	672	4	
⁴ D _{1/2}	28962	28943	19	
² I _{11/2}	29463	29467	-4	
, -	489	476	13	
	568	558	10	
	644	646	-2	
	-	648		
	773	777	-4	

•

Appendix I. (cont.)

SLJa	Obsd.b	Calc.c		SLJa	Obsd. ^b	Calc.c	
State	(cm^{-1})	(cm^{-1})	<u>0-C</u>		(vac cm ⁻¹)	(cm^{-1})	<u>0-C</u>
² L _{15/2} ,	30275	30270	5	² L _{17/2}	-	31987	
4 _{D7/2}	318	317	1		-	32008	
, -	-	363			-	030	
	-	471			-	074	
	517	523	-6		-	172	
	-	536					
	576	593	-17	² H9/2	33030	33036	-6
		600			107	117	-10
	631	644	-13		181	178	3
	682	691	-9		228	226	2
	719	722	-3		255	255	0
	807	796	11				
				² D _{3/2}	33619	33616	3
² I _{13/2}	-	30860			649	647	2
13, =	30893	898	- 5				
	933	948	-15	² H _{11/2} ,	34 29 2	34 26 4	28
	994	31010	-16	² D _{5/2}	380	368	12
	31030	31029	1	·	419	443	-24
	068	054	14		-	501	
	-	118			521	534	-13
						578	
² L _{17/2}	31781	31768	13		678	659	19
17,2	-	817			706	723	-17
	859	851	8		-	811	
	-	983					

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SLJ ^a State	0bsd. ^b (cm ⁻¹)	Calc. ^c (cm ⁻¹)	<u>o-c</u>	SLJ ^a	Obsd.b (vac cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>
² F _{5/2}	38690	38708	-18	² G _{7/2}	48839	48852	-13
3/2	735	764	-29		908	868	40
	841	811	30		977	979	-2
					49088	49071	17
² F7/2	40103	40104	-1				
1/2	-	120		² F7/2	-	66565	
	155	176	-21			716	
	288	247	41		-	772	
					-	916	
² G _{9/2}	-	47867					
9/2	47894	887	7	² F _{5/2}	-	67856	
	937	954	-17	·	-	900	
	999	48021	-22		-	68126	
•	48043	056	-13				

^aThe principal component of the eigenvector is given.

 $b_{\text{(cm}^{-1} \text{ vac)}}$. Components of ${}^4\text{I}_{9/2}$ and ${}^4\text{I}_{11/2}$ taken from ref. 32.

cEnergy level parameters are given in Table 1.

dRef. 32.

e_{Ref. 6}.

f_{Ref.} 34.

Appendix II. $\label{eq:appendix} \mbox{Experimental and Computed Energy Level Structure for \Pr^{3+}:LaF_3 }$

SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm-1)	Calc. ^c (cm ⁻¹)	o-c	SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm ⁻¹)	Calc. ^c (cm ^{-l})	0-с
3 _{H24}	0	0	0.2	0	3 _{H5}	2281	227 2	2284	-12
	90	57	71	-14	_	2289	2299	2290	9
	95	71	95	-24		2294	2304	2295	9
	124	136	138	-2		2327	2354	2318	36
	144	195	183	12		2363	2412	2399	13
	226	204 ^d	221	-17		2441	2431	2412	19
	305	322 ^d	333	-11		2442	2457	2438	19
	386	• •	444			2538	2567	2540	27
	479	(508) ^e	463						
					3 _{H6}	4220		4179	
3_{H_5}	2160	-	21 26			4230	4223	4200	23
	2184	-	2158			4319	4268	4283	-15
	2188	2179	2191	-12		4381	4305	4321	-16

10

SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm ^{-l})	Calc. ^c (cm ⁻¹)	o-c	SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm ⁻¹)	Calc. ^c (cm ⁻¹)	0-C
3 _{H6}	4414	4388	4384	4	3 _{F2}	5263	5280 ^d	5276	4
	4473	4440 ^d	4467	-27	_				
	4494	-	4478		3 _{F3}	6420	6453	6456	-3
	4507	4508	4496	12		6481	6495	6490	5
	4545	4529	4508	21		6489	6499	6508	-9
	4621	4581	4590	-9		6562	6587	6579	8
	4713	4673	4693	-20		6576	6602	6600	2
	4715	-	4712			6602	6622	66 28	-6
•	4821	- 4785	4814	-29		6701	6722	6740	-18
${}^{3}\mathbf{F}_{2}$	5130	5137	5145	-8	3 _{F4}	6907	6927	6918	9
	5153	5182	5182	0		6920		6936	
	5180	5201	5185	16		6944	6946	6950	-4
	5245	5275	5270	5		6956	-	6952	

. 1	
7/0	
47	
9	
ر م	
0	

SLJ	Model ^a	Expt.b	Calc.c		SIJ	Model ^a	Expt.b	Calc.c	
State	(cm ⁻¹)	(cm^{-1})	(cm ⁻¹)	0-C	State	(cm^{-1})	(cm ⁻¹)	(cm ⁻¹)	0-C
3 _{F4}	6958	6946	6953	-7	1 _{G4}	10477	10/00	1051/	
·	6996	6980	6983	-3	94	104//	10499	10516	-17
	7000	7029	7034	- 5	$^{1}\mathrm{D}_{2}$	16879	16873	16887	-14
	7084	7104	7096	8	_	925	893	895	-2
	7129	7165	7152	13		17072	17083	17082	1
						095	-	117	
$^{1}G_{4}$	9720	9716	9721	- 5		149	183	170	13
	9761	9751	9762	-11					
	9840	1 9876	9860	16	3 _{P0}	20942	20927	20911	16
	9936	9912	9927	-15					
	9937	-	9958		¹ 1 ₆	21 276	21 279	21 284	-5
	9979	10005	9996	9		21313	••••	304	
	10031	042	10030	12		320	331	340	-9
$^{1}G_{4}$	10154	10163	10150	13		398	404	390	14

SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm ⁻¹)	Calc. ^c (cm ⁻¹)	0-с	SLJ State	Model ^a (cm ⁻¹)	Expt.b (cm ⁻¹)	Calc. ^c (cm ^{-l})	0-С
¹ I ₆	21440	21418	21406	12	¹ 1 ₆	21852	21897	21889	8
	447	-	481			905	942	958	-16
3 _{P1}	21472	21475	21487	-12					
	532	522	519	3	3 _{P2}	22607	22691	22668	23
$^{1}I_{6}$	21541	-	21570	,		664	714	704	10
3 _{P1}	21556	21567	21592	-25		673	734	738	-4
¹ I ₆	598	585	588	-3		725	772	787	-15
	619	-	637			767	819	817	2
	650	1 668	666	2					
	738	_	804		¹ S ₀	46961	46965 [£]	46965	0

 $^{^{}a}$ Ref. 13. Values for the 1 I $_{6}$ components (but not the 3 P $_{1}$) were reduced by 100 cm $^{-1}$ to correspond to present assignments. b Ref. 36 and 39 except as indicated; cm $^{-1}$ vac.

Energy level parameters are given in Table 1.

dRef. 38.

^eNot used in fitting parameters.

f_{Ref.} 42.

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Appendix III.

Computed Energy Level Structure for Pm3+:LaF3

SLJ ^a	Calc.b	SLJa	Calc.b	SLJ ^a	Calc.b	SLJa	Calc.b
State	(cm ⁻¹)	State	(cm^{-1})	State	(cm ⁻¹)	State	(cm ⁻¹)
5 ₁₄	0	5 ₁₆	3376	5 ₁₈	6556	5 _{F 2}	13156
~	135	v	3389	ŭ	6605	_	170
	189		3392		6621		
	233		3413		6653	⁵ F3	13853
	266		3413		6672	-	900
	294		3416		6746		918
	332		3439		6763		952
	437		3462		6824		965
	474		3470		6827		998
					6857		14020
⁵ 15	1667	⁵ 1 ₇	5042		6959		
_	1710		5045		6977	⁵ s ₂	14525
	1717		5059		7060	_	5 29
	1769		5060		7063		5 29
	1769		5066		7129		529
	1810		5074		7131		530
	1812		5078		7152		
	1821		5084			⁵ F ₄	14804
	1828		5086	5 _{F1}	1 26 50		837
	1829		5090	_	671	•	892
	1845		5110		684		894
			5114				895
⁵ 16	3285		5116	5 _{F2}	13031		898
ŭ	3322		5143	-	076		9 26
	3326		5149		091		965
	3369						998

Appendix	III.	(cont.)
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SLJa	Calc. b	SLJ ^a	Calc.b	SLJ ^a	Calc.b	SLJa	Calc.b
	(cm^{-1})		(cm^{-1})	State	(cm^{-1})	State	(cm^{-1})
				, in			
5 _{F5}	16145	⁵ G ₄ ,	18045	⁵ G ₃	18679	⁵ ₆₅ ,	20471
,	148	⁵ G ₃ ,	066	· 3 _{K7}	689	⁵ G ₄	492
	149	3 _{K7}	068				532
	151	,	076	³ K ₈	19854		541
	21 2		079		859		579
	226		104		870		592
	249		104		872		611
	250		1 26		885		664
	273		147		890		700
	307		252		928		713
	322		316		951		
			364		973	3 G $_{3}$	21968
3 _{K6}	17071		381		974		974
Ū	088		408		20005		22020
	088				012		040
	091	⁵ G ₃ ,	18426		035		062
	092	3 K ₇	426		036		070
	093		444		107		117
	104		461		111		
	106		500		136	⁵ G ₅ ,	22424
	109		508			5 _G	4 29
	115		510	⁵ G ₅ ,	20243		433
	1 23		535	5 _{G4}	260		461
	123		536		294		469
	137		545		303		480
			557		20361		500
5 G $_{2}$	17904		559		365		503
_	932		611		366	•	512
	949		657		387		539
	18007		665		445		563
	017				463		575

Appendix I	ΞΙ. (cont.	.)
------------	-------	-------	----

SLJa	Calc.b	SLJ ^a	Calc.b	SLJª	Calc. ^b
State	(cm^{-1})	State	(cm^{-1})	State	(cm^{-1})
$^{5}G_{5}$,	22663	3 _{L7}	24028	3 _{H₆} ,	24992
⁵ G ₅ , ⁵ G ₆	683		043	3 _{G4} ,	25014
	696		046	³ _{G4} , ³ L ₈	018
	696				023
	754	$^{3}P_{1}$	24 289		038
	769		299		068
	779		306		071
	8 27				073
	831	3 _{H6} ,	24635		122
	895	3 _{G4} ,	661		136
	909	³ G ₄ , ³ L ₈	664		156
	942		678		157
			695		171
3 _{D2}	23189		708		172
-	253		762		224
	288		772		263
	327		780		
	3 27		785	((25816-50000°)
			810		
3 _{L7}	23699		817		
•	701		834		
	8 28		849		
	840		869		
	841		874		••
	887		893		
	889		24905		
	954		917		
	956		918		
	965		9 24		
	968		945		
	24022		950		

aThe leading component of the state eigenvector is indicated.

bThe energy level parameters (interpolated) used to compute these level energies are given in Table 1.

cSince there are no experimental data available, the tabulation has been arbitrarily stopped at $25263~\rm cm^{-1}$. At higher energies, starting with the next level at $25816~\rm cm^{-1}$, the computed density of states is relatively high. Some additional results are given for $\rm Pm^{3+}$:LaCl $_3$ in Ref. 45. Figure 7 indicates the larger gaps in energy where no crystal-field components are computed to occur.

Appendix IV.

Experimental and Computed Energy Level Structure of Sm³⁺:LaF₃

				Rast ^d	
SLJa	Expt.b	Calc.c		et al.	Dieke ^e
State	(cm^{-1})	(cm ⁻¹)	<u>o-c</u>	(cm^{-1})	(cm^{-1})
6 _{H5/2}	0	-6	6	0	0
-, -	44	53	-9	48	44
	159	135	24	115	159
⁶ H _{7/2}	1000	990	10	1000	1003
	1044	1027	17	044	046
	1185	1 205	-20	185	100
	1280	1 26 2	18	280	187
⁶ H _{9/2}	2209	2193	16	2209	2213
	244	233	11	244	247
	342	332	10	342	344
	409	408	1	409	404
•	473	468	5	473	493
	•				
⁶ H _{11/2}	35 20	3510	10	3517	
	568	553	15	567	
	651	628	23	647	
	671	667	4	670	
	7 27	739	-12	7 26	
	791 ^d	793	-2	791	
⁶ H _{13/2}	4972	4947	25	4971	4969
	982	975	7	982	
	5007	5004	3	5007	5005
	046	042	4	047	044
	057	059	-2	057	
	122	114	8	122	
	160	170	-10	160	

Appendia	(co	nt.)		Rast ^d	
SLJ ^a	Expt.b	Calc.c		et al.	Dieke ^e
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	(cm^{-1})	(cm^{-1})
⁶ H _{15/2} ,	6309	6300	9	-	
6 _{F1/2}	341	334	7	6346	
-, -	406	417	-11	408	6404
	460	465	- 5	454	
		472		462	
	-	553		492	
	568	578	-10	538	
	609	605	4	571	
	_	666			
⁶ F _{3/2}	6707	6724	-17	6707	
*3/2	-	738	- ·		
		, 30			
⁶ F _{5/2}	7177	7177	0	7174	7173
- 3/ 2	184	190	- 6	184	180
	223	239	-16	225	
6 _{F7/2}	7992	8008	-16	7993	7987
7 / 2	8041	026	15	8042	8034
	060	059	1	059	054
	092	108	-16	092	086
⁶ F _{9/2}	9170	9173	-3	9170	9162
-, -	178	189	-11	180	173
	228	223	5	231	222
	252	243	9	254	247
	268	281	-13	270	26 2
6 _{F11/2}	10561	10567	- 6	10559	
-11/2	584	583	1	581	
	592	590	2	590	
	603	621	-18	602	
	613	633	-20		
	644	656	-12		
	0				

Appendix IV. (cont.)				Rast ^d
SLJ ^a	Expt.b	Calc.c		et al. Dieke ^e
		(cm^{-1})	<u>o-c</u>	$\frac{(cm^{-1})}{(cm^{-1})}$
4 _{G5/2}	17858	17863	- 5	17858
95/2	949	960	-11	949
	(18045)	18087		18046
⁴ F3/2	18924	18933	-9	18924
•	942	951	-9	942
40	20037	20041	-4	20037
⁴ G _{7/2}	093	094	-1	093
	112	123	-11	111
	164	168	-4	
	101			
⁴ 1 _{9/2}	20416	20406	10	20417
<i>3/2</i>	472	472	0	471
	499	505	- 6	497
	522	531	-9	523
	570	551	19	
⁴ M _{15/2} ,	•	20685		
⁴ I _{11/2}	-	770		
	-	808		
	-	858		
	-	892		
	-	904		•
	-	922		20944
	-	974		
	-	21004		
	-	071		
	-	164		
	-	179		
	-	248		
	-	265		
				•

SLJa	Obsd.b	Calc.c			SLJa				Dieke ^e
State	(cm^{-1})	(cm ⁻¹)	0-C	(cm^{-1})	State	(cm^{-1})	(cm^{-1})	<u>0-C</u>	(cm^{-1})
⁴ I _{13/2}	215 20	21541	-21	21520	4M _{17/2} ,	-	23116		
-13/2	602	602	0		⁶ 9/2,	-	158		
	636	616	20	637	⁴ I _{15/2}				
	665	649	16	647	424	23988	23989	-1	
	_	652			⁴ M _{19/2} ,	23988	24035	-13	
	674	666	8		⁶ P _{5/2}	24022		-37	
	7 06	684	22	709		031	068 080	-37 -16	
						064	101	-17	24084
⁴ F _{3/2}	22164	22178	-14	22164		084		-17 -7	119
- 3/2	207	213	-6	207		119 135	126	1	117
	240	254	-14	241			134	-9	153
						153	162	-,	133
4 _M 17/2,	22501	22500	1	22501			169		
4 _{G9/2} ,	531	539	-8	532		-	181		
4 ₁₁₅ /	2 542	552	-10			-	186		
-15/	_	573				-	207		
	579	581	-2			_	218		
	6 28	630	-2		4	01600	0/616	-8	24607
	695	693	2		⁴ L _{13/2}	24608	24616	-o -3	628
	_	738				629	632	-11	631
	_	770				631	642	-14	643
	808	801	7			644	658	-10	678
	8 2 9	834	-5			679	689	-10	
		867				683	695	-10	
	_	912				710	7 20	-10	709
	942	943	-1		4_		0/ 000	1.1	24911
	_	982			⁴ F7/2	24911	24900	11	
	_	23020				993	987	6 5	
	_	023				25007	25002		
	_	036			6-	064	071	-7 -7	
		054			⁶ P _{3/2}	081	088	-7	
	_	083				-	106		

Appendix	ora b	Calcac		Dieke ^e	SLJ ^a	Obsd.b	Calc.c		Dieke ^e
SLJ"	Obsa.	(cm ⁻¹)	00	(cm^{-1})	State	(cm^{-1})	(cm^{-1})	0-C	(cm^{-1})
State	(cm -)	<u>(Cm)</u>	<u> </u>	<u> </u>					
⁴ G _{11/2} ,	25166	25169	-3		⁴ L _{17/2} ,	26702	26694	8	26699
⁴ M _{21/2} ,		177	5		6 _p 7/2	712	705	7	709
4 _M	204	203	1		• •	717	718	-1	712
⁴ H ₁₁	2, 216	217	-1			743	751	-8	758
"11,	-	220				776	763	13	776
	_	243				792	777	15	791
	248	259	-11			797	800	-3	796
	282	285	-3	•			803		
	_	308				812	812	0	810
	_	343				822	8 26	-4	822
	_	398				859	349	10	857
	_	439				-	862		
	-	476				874	868	6	
	-	543							
	_	565			⁴ K _{13/2}	26942	26931	11	
	611	603	8	25614	13/2	962	955	7	
	636	621	15	632		27003	991	12	
	650	645	5	649		018	27014	4	
	672	654	18	666		031	026	5	
	684	682	2	681		061	073	-12	
	-	698				1 20	109	11	
	711	708	3						
	718	713	5		⁴ F9/2	27417	27381	36	27419
	771	762	9	767	-,-	432	443	-11	434
	789	782	7	787		448	467	-19	448
	801	795	6	798		508	510	-2	
	8 26	8 2 3	3			_	552		
	832	845	-13						
	866	866	0		⁴ D _{3/2}	27648	27646	2	27649
	904	882	22		J, &	658	654	4	659
	-	921							
⁴ D _{1/2} .	26495	26472	23	26495					

SLJª	Obsd.b	Calc.c		Dieke ^e	SLJ ^a	Obsd.b	Calc.c		Dieke ^e
State	(cm^{-1})	(cm^{-1})	<u>0-C</u>	(cm^{-1})	State	(cm ⁻¹)	(cm^{-1})	<u>0-C</u>	(cm^{-1})
4 _{P5/2}	27691	27714	-23	27692	$(^{4}K, ^{4}L)_{1}$	7/2 ²⁹¹⁶⁶	29169	-3	
3/ 2	734	763	-29	735		-	183		
	758	787	-29	759		195	191	4	
						-	219		
4 _{H7/2}	28 247	28242	5	28247		-	238		
7,2	261	25 2	9	26 2	⁴ L _{19/2} ,	29 268	29270	-2	
	344	359	-15		⁴ H _{11/2} ,	304	298	6	
	409	393	16	410	⁴ H _{13/2}	-	315		
					·	-	325		
4 _{K15/2}	287 22	28735	-13			-	335		
13/2	732	743	-11	28732		-	347		
	760	757	3			-	356		
		770					363		
	784	783	1			-	397		
	797	793	4			-	416		
	_	804				_	457		
	817	823	-6			-	478		
						_	505		
4 _{H9/2}	28938	28925	13	28938		-	514		
3/2		929				-	555		
	981	989	-8	980		-	558		
	29035	29045	-10	036		-	562		
	055	070	-15	052		-	607		
						-	615		
⁴ D _{7/2}	29086	29098	-12	29083		- "	650		
1/2	094	108	-14	092		709	681	28	
	112	115	-3	111		7 23	693	30	
	_	122		•		738	738	0	
$(^4K, ^4L)$	17/2	137							
, .,	-	140			4 _{G7/2} ,	30027	30031	-4	30028
	29154	154	0	29154	4 _{G9/2}	120	118	2	120
	_	156) / L	136	159	-23	136

SLJa	Ohed b	Calc.c		Dieke ^e	SLJ ^a	Obsd.b	Calc.c		Dieke ^e
State	(cm^{-1})	(cm ⁻¹)	o-c	(cm^{-1})	State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	(cm^{-1})
State	<u> </u>								
4 _{G= 40}	_	30193			⁴ P _{5/2}	32800	32797	3	32799
⁴ G _{7/2} , ⁴ G _{9/2}	30216	210	6	213	•, -	8 2 3	824	-1	8 2 3
09/2	235	21 2	23			857	856	1	858
	_	260							
	293	289	4		² F _{5/2} ,	-	33548		
	332	347	-15		$^{2}K_{13/2}$, 33615	642	-27	
					⁴ F9/2	-	708		
⁴ G _{5/2}	-	30438			. ,	777	787	-10	•
3/ 2	-	508					813		
	_	549				-	865		
						-	900		
⁴ P _{1/2}	-	31226					955		
1/2						-	962		
² L _{15/2} ,	-	31337				-	977		
4 _{G11/2}	, -	352				-	34007		
4 _P 3/2	31410	394	16	31412		-	028		
3/ 2	433	445	-12	435			049		
	463	476	-13	465		•••	081		
	488	495	-7	489			095		
	511	504	7	511					
	523	513	10	5 24	² L _{17/2} ,	_	34341		
	532	530	2	533	⁴ 1 _{9/2}		358		
	543	558	-15	538		-	386		
	583	604	-21	582		-	4 26		
	6 24	6 23	1	6 27		- ·	434		
	-	630				34454	467	-13	
	-	682				468	468	0	
	-	707				481	488	-7	34484
	759	734	25			497	495	2	499
						519	536	-17	
						-	552		
						-	590		

SLJa	Obsd.b	Calc.	!	SLJ ^a	Obsd.b	Calc.c	
State	(cm^{-1})	(cm^{-1})	0-C	State	(cm^{-1})	(cm^{-1})	<u>0-C</u>
							
² L _{17/2} ,		34612			(:	38906-417	74) ^{f,g}
	_	654				46 level	s
3/2							
4 _{F7/2} ,	(3	5612-358	323) ^f	² G _{9/2}	-	42039	
2 _{N19/2}				·	42066	072	-6
19/2					124	104	20
² P _{1/2}	_	35846			135	137	-2
1/2					176	183	- 7
⁴ I _{11/2}	35890	35892	-2				
11/2	905	905	0	² 0 _{23/2}	42227	42215	12
	_	932		⁴ G _{5/2}	, 378	400	-22
	954	945	9	4 _{G7/2}	, 378 ₂ -	456	
	996	987	9		462	472	-10
	36007	999	8		486	480	6
	055	36054	1		-	506	
					-	514	
	(3	6315-372	73) ^f		_	546	
		(39 leve	ls)			574	
					-	594	
⁴ H _{9/2}	37623	37607	16		-	612	
3/2		618			616	614	2
	634	638	-4		-	642	
	657	654	3		-	643	
	679	667	12		658	661	-3
					- ;	668	
² F _{7/2} ,	_	38175			-	699	
² P _{3/2}	•••	219			711	720	-9
J, -	-	300			-	744	
	38467	461	6	² 0 _{21/2}	, -	809	
	492	485	7	4K ₁₅ /	2 -	914	
		512			_	951	
					959	963	-4

Appendi	x 14. (co	1111.)					
SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b	Calc.c	
	(cm^{-1})			State	(cm^{-1})	(cm^{-1})	<u>0-C</u>
						J.	
² 0 _{21/2} ,	-	42976			(4	4491-470	29) ^f
	4 29 9 0	996	- 6			54 level	8
13/2		43022					
	43040	041	-1	² H _{11/2}	47336	47306	30
	-	056		•	374	363	11
	074	080	- 6		-	430	
						523	
	(4	¥3088 – 436	58) [£]		-	536	
		27 level	s		-	675	
_						47812-489	oosf
² H _{11/2}	43769		9		(4		
	-	762				45 level	.s
	-	808					:
	844	855	-11	±/ =	(4958)	1-49865) ^f	
	-	869		² H _{9/2} ,			
		921		² F _{5/2}			
2							
$^{2}G_{7/2}$	43991		16				
	-	44005					
	-	033					
	-	041					

^aLargest or two largest eigenvector components are indicated.

^bExperimental results for the $^{6}\mathrm{H}_{5/2}$ state taken from Ref. 1 based on correlation with model calculation. Observed data for the $^{6}\mathrm{H}_{9/12}$ and $^{6}\mathrm{H}_{9/2}$ states in the ground multiplet from Ref. 46. Values in parentheses were not included in the parameter fitting process. All entries in cm⁻¹ vac.

^CEnergy level parameters are given in Table 1.

dRef. 46.

e_{Ref. 1}.

fin certain regions of the spectrum where no structure was observed and computations indicated a high density of levels, only the initial and final energies of the group are indicated. In some cases one or two very weak bands were observed consistent with calculation, but not included.

gThere is an energy gap, 39500-40340 cm⁻¹, in which no levels are computed to occur.

Experimental and Computed Energy Level Structure for Er³⁺:LaF₃

SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b	Calc.c	
State	(cm^{-1})	(cm ⁻¹)	<u>0-C</u>	State	(cm ⁻¹)	(cm^{-1})	<u>0−C</u>
4.	0	-22	22	⁴ F9/2	15391	15406	-15
⁴ I _{15/2}	51.2	27	24	- 9/2	432	443	-11
	121.2	92	30		443	462	-19
	199.7	176	24		474	488	-14
	219.4	193	26		527	538	-11
	313.8	289	25		32,	340	
	400.3	375	25	⁴ S _{3/2}	18557	18577	-20
	442.9	420	23	3/2	588	610	
			_	2			22
⁴ I _{13/2}	6604	6612	- 8	² H _{11/2}	19266	19299	-33
	630	637	-7		307	324	-17
	670	686	-16		314	344	-30
	700	699	1		363	371	-8
	7 23	732	- 9		367	379	-12
	754	771	-17		419	430	-11
	8 2 3	830	-7	,			
				⁴ F _{7/2}	20656	20654	2
⁴ I _{11/2}	10301	10300	1		703	697	6
	311	314	- 3		734	735	-1
	330	336	- 6		786	790	-4
	344	351	- 7		•*•		
	358	364	-6	⁴ F5/2	22370	22380	-10
	395	405	-10		374	389	-15
					407	414	-7
⁴ 1 _{9/2}	12419	12392	27				
- , -	518	512	6	⁴ F _{3/2}	22684	22692	-8
	615	596	19	-, -	751	748	3
	701	681	20				
	730	720	10				

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Appendi	k V. (con	t.)					
SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b		
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	State	(cm^{-1})	(cm ⁻¹)	<u>o-c</u>
2-	24602	24587	15	² G _{7/2}	28 23 9	28 23 3	16
² G ₉ /2		698	-18	7/2	255	237	18
	680	755	-1		-	246	
	754		9		264	250	14
	840	831	-2				
	862	864	-2	² P3/2	31695	31723	-28
⁴ G _{11/2}	26526	26534	-8		752	786	-34
-11/2	554	559	- 5				
	582	586	-4	² K _{13/2}	33107	33086	21
	(621) ^d	637			116	106	10
	647	640	7		141	154	-13
	707	700	7		163	161	2
			•		186	196	-10
⁴ G _{9/2}	27602	27608	-6		-	228	
<i>5 L</i>	616	615	1				
	6 28	6 25	3	² P _{1/2}	33346	33350	-4
	641	637	4.				
	668	660	8	² K _{13/2}	397	405	-8
² K _{15/2}	27817	27826	-9	⁴ G ₅ /2	-	33510	
*15/2	8 27	838	-11		-	522	
	872	877	- 5		4	628	
	898	893	5			•	
	933	932	1	⁴ G _{7/2}	34159	34154	5
	-	978		1 / 2	197	182	15
	_	28014	,		222	215	7
	28125	132	- 7		280	27 1	9
	20123	132	•				

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Appendix	V.	(cont.))
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Appendix	v. (com	-•)			_		
SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b	_	
State	(cm^{-1})	(cm^{-1})	<u>0-C</u>	State	(cm^{-1})	(cm ⁻¹)	<u>o-c</u>
				_			
² D _{5/2}	35026	35043	-17	² L _{17/2}	41802	41832	-30
-5/2	052	052	0		_	861	
	085	091	-6		-	922	
					934	957	-23
² H _{9/2}	36520	36526	-6		42002	42045	-43
-, -	556	549	7		-	054	
	6 23	637	-14				
	7 20	7 29	-9	⁴ D3/2	42499	42484	15
	804	796	8	·	5 29	517	12
⁴ D _{5/2}	38807	38815	-8	² D3/2	43090	43108	-18
3/ =	837	858	-21		1 27	138	-11
	844	863	-19				
				² 1 _{13/2}	43686	43672	14
⁴ F _{7/2}	39454	39460	-6		742	7 25	17
., -	537	540	-3		759	750	9
	603	605	-2		770	769	1
	634	630	4		833	815	18
					914	898	16
² I _{11/2}	41237	41211	26		-	956	
11, 2	294	269	25				
	313	304	9 .	⁴ D _{1/2}		47347	
	380	352	28				
	395	375	20	² L _{15/2}	47891	47891	0
	493	466	27		951	922	29
					_	990	
² L _{17/2}	41680	41720	-40			48007	
,-	-	801			48071	066	5
	783	822	-39			083	

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SLJ ^a State	Obsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>
² L _{15/2}	-	48168	
	-	199	
² H _{9/2}	-	48306	
<i>></i> / -		349	
	-	394	
	-	438	
	-	461	
2			
² D _{5/2}	49223	49178	45
	27 2	248	24
	357	321	36

^aThe principal SLJ-component of the state is indicated.

 $^{^{}b}$ All energies are corrected to vacuum cm $^{-1}$. The energies of the ground 4 I $_{15/2}$ state are taken from Ref. 47.

CEnergy level parameters are given in Table 1.

 $d_{\mbox{Not}}$ included in the energy level parameter fitting.

Appendix VI.

Experimental and Computed Energy Level Structure for Im3+;LaR3

SLJ	SLJ Model ^a Expt. ^b	Expt.b	Calc.c		SLJ	Model ^a	Expt.b	Calc.c	
State	(GM ⁻¹)	(cm^{-1})	(cm^{-1})	ያ	State	(\mathbb{G}^{-1})	(cm ⁻¹)	(cm^{-1})	3
$^{3}_{\rm Hc}$	0	0	4	4	$^{3}F_{4}$	5585	5615	5613	2
	19	<i>L</i> 9	%	н		5689	5706	5703	3
	74	ı	76			5790	5814	5820	φ
	156	118	131	-13		5813	5826	5838	-12
	204	i	197			5836	5829	2857	2
	235	ŧ	198			5851	2866	5863	ĸ
	272	ŧ	**			5903	ı	5905	
	274	Į.I	73			5916	5918	5924	٩
	349	ı	339			5929	5958	5941	17
	354	i	346						
	400	i	386		345	8306	8305	8293	12
	418	f	399			8354	8332	8331	
	441	i	420						

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ζ		9		۲			-14		1	-2	0	က		
Calc. ^c	12770	819	824	863	890		14522	537	538	556	288	593	<i>I</i> 29	
Expt.b (cm ⁻¹)	1	12825	ı	898	ı		14508	i	539	554	288	2%	ı	
Model ^a	12784	828	832	880	606		14514	530	534	550	582	290	622	÷
State	3H,						3 _F 3							
ğ		7	-15					-12			∞	۴	10	œ
Calc. ^c (cm ⁻¹)	8337	8368	8415	8442	8446	7978	8499	8562	8568		1253	578	069	719
Expt.b (cm ⁻¹)	8338	8366	8400	1	i .	ı	ı	8550	ŀ		12561	570	700	127
Model ^a (cm ⁻¹)	8365	8395	8451	8460	8470	8481	8522	8581	8589		12547	597	8/9	734
SLJ	3 _{H5}										3 H $_{4}$			

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Calc. ^c (cm ⁻¹)	21512	28024	470	640	880	114		34772	795	906	766	35015	106
Expt.b (cm-1)	21519	28021	750	290	880	106	٠	34769	1	968	ı	ı	1
Model ^a	21511	28022	023	041	9/20	100		34781	808	906	35000	022	870
State	1 _G	$^{1}D_{2}$						$^{1}I_{6}$					
ç	φ ?	14	0			7	-2	-10	10	ዋ	-5		
Calc. ^c (cm ⁻¹)	15144	193	240	\$		21041	198	319	339	372	382	904	511
Expt.b (cm ⁻¹)	15138	207	240	1		21037	1%	306	349	366	380	ı	ı
Model ^a (cm ⁻¹)	15153	300	7	3 99		21016	193	300	335	362	364	425	208
SLJ	³ F ₂				•	1 _G ,							

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ζ	12			9	-	10	-13	-13		
Calc. ^c (cm ⁻¹)	36575	% 29		38.244	280	326	427	797		75025
Expt.b (cm ⁻¹)	36587	1		38250	162	336	414	451		1
Model ^a (cm ⁻¹)	36549	288		38225	399	38	415	426		75158
State	3 _P 1			3 ₂ 2						$0_{\rm S_I}$
	-5	17							-30	9
Calc. ^c (cm ⁻¹)	35109	143	184	23%	234	253	270		35624	36525
Expt.b (cm-1)	35107	160	1	ı	t	ı	ľ		35604	36531
Model ^a (cm ⁻¹)	35079	149	201	216	217	257	272		35588	36502
SLJ State	1								³ -0	3

Ref. 13.

bRef. 49 (cm⁻¹ vac).

Genergy level parameters are given in Table 1.

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Appendix VII.

Experimental and Computed Energy Level Structure for Ho³⁺:LaF₃

SLJª	Obsd.b	Calc.c		SLJa	Obsd.b	Calc.c	
State	(cm ⁻¹)	(cm^{-1})	<u>o-c</u>	State	(cm ⁻¹)	(cm^{-1})	<u>o-c</u>
5-	0	-2	2	5 ₁₇	5287	5291	-4
⁵ 18				- 7	296	293	3
	4.5	3	1		309		9
	42	29	13		314	300 303	11
	50	54	-4		314	303	11
	69	67	2	⁵ 16	07.16	0700	
	122	130	-8	516	87 26	8722	4
	145	151	-6 20		730	723	7
	201	221	-20 -		733	732	1
	215	222	- 7		735	735	0
	227	23 2	- 5		747	740	7
	(261) ^d	298	•		753	754	-1
	307	307	-0		761	767	-6
	322	324	-2		773	776	- 3
	349	339	10		783	778	5
	387	388	-1		786	791	-5
	398	391	7		814	812	2
	409	410	-1		-	817	
_					834	839	- 5
⁵ 1 ₇	-	5182		"			
	5192	182	10	⁵ 1 ₅	11304	11298	6
	-	24 2			306	303	3
	-	243			308	303	5
	-	244			311	314	-3
	246	248	-2		-	315	
	250	250	0		321	319	2
	-	256			332	333	-1
	264	268	-4		-	338	
	273	276	-3		363	360	3
	280	276	4				

Appendix V	ZII.	(cont	.)
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SLJ ^a State	0bsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>	SLJ ^a State	0bsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>
⁵ 15		11369		⁵ s ₂	18603	18602	1
	11386	392	-6		6 20	6 20	0
5-		12260		5 _{F4}	18677	18677	0
⁵ 1 ₄	12006	13260	1	^F 4	688	683	5
	13286	285	-20		709	719	-10
	362	382	-20 -8		709	7 28	-10 -8
	380	388 394	-6		720	749	-12
		419			757	760	-7
	_	455				767	•
	_	477			776	793	-17
	_	607			814	812	2
		007			011	012	_
5 _{F5}	15576	15587	-11	5 _{F3}	20744	207 25	19
•	593	603	-10		754	750	4
	608	615	-7		796	789	7
	6 2 5	629	-4		799	791	8
	641	637	4		8 26	821	5
	659	661	-2		832	823	9
		681			866	861	5
		712					
	-	714		⁵ F 2	21 238	21 228	10
	708	717	-9		249	232	17
	730	734	-4		265	260	5
					275	281	-6
⁵ s ₂	18590	18597	-7		286	287	-1
•	600	598	2				
	603	601	2	3 _{K8}	21411	21405	6
				-	419	424	- 5

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SLJa	$0bsd.^{b}$	Calc.c		SLJ ^a	Obsd. ^b	Calc.c	
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	State	(cm^{-1})	(cm^{-1})	<u>o-c</u>
						•	
3 _{K8}	21423	21427	-4	5 _{F1}	-	22504	
·	432	4 26	6		22508	504	4
	440	449	-9		-	535	
	451	457	-6				
	461	458	3	⁵ G ₅	24112	24123	-11
	-	468		-	116	130	-14
	481	479	2		1 25	136	-11
	495	480	15		146	165	-19
	514	507	7		-	167	
	5 27	514	13		170	173	-3
	532	546	-14		182	180	2
	550	552	-2		-	185	
	566	564	2		196	194	2
	-	573			-	222	
	579	574	5		247	222	25
⁵ G ₆	22220	22238	-18	⁵ G ₄	25985	25982	3
-	235	250	-15		26008	980	28
	263	260	3		037	26051	-14
	283	303	-20		054	057	-3
	3 28	331	-3		-	058	
	346	342	4		• 084	059	25
	361	348	13		096	096	0
	374	360	14		-	155	
	389	380	9		161	169	-8
	407	395	12				
	4 24	4 23	1	3 _{K7}	26 25 5	26 26 1	-6
	438	429	9	,		26 2	
	454	479			_	266	

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Appendi	k VII. (c	ont.)					
SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b	Calc.c	
State	(cm ⁻¹)		<u>0-C</u>	State	(cm ⁻¹)	(cm ⁻¹)	<u>0-C</u>
³ K ₇	26 26 6	26 26 7	-1	⁵ G ₅ , ³ H ₆	27945	27948	-3
,	277	282	- 5	-	-	973	
	_	287			-	984	
	288	287	1		-	991	
	293	298	- 5		997	28000	-3
	-	299			-	020	
	298	299	-1		_	076	
	312	312	0		28092	077	15
	320	314	6				
		324		⁵ F 2	284 26	28433	-7
	328	331	-3		-	450	
	328	332	-4		-	479	
					-	492	
$^{5}G_{5}, ^{3}H_{6}$	27749	27746	3		-	506	
, ,	758	751	7				
	804	788	16	⁵ G ₃ , ³ L ₉	-	28956	
	-	814			28981	996	-15
	815	814	1		29011	29017	-6
	-	819			020	019	1
		820			032	020	12
	8 2 5	826	-1		035	028	7
	839	840	-1		039	036	3
	-	846			-	049	
	854	851	3		_	051	
	869	859	10		068	052	16
	879	882	-3		-	094	
		926			-	094	4
	-	927			-	095	
	932	9 28	4		102	100	2

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Appendix	VII. (co	ont.)					
SLJa	Obsd.b	Calc.c		SLJª	Obsd.b	Calc.c	
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	State	(cm ⁻¹)	(cm ⁻¹)	<u>0-C</u>
⁵ G ₃ , ³ L ₉	29122	29125	-3	3 _{F4} ,3 _{K6}		30 26 7	
	****	127			-	288	
		128			30292	306	-14
	-	146			•••	322	
	161	160	1		-	325	•
	-	164			330	331	-1
	-	166					
	187	174	13	5 G $_{2}$	-	30997	
	-	220			31002	31006	-4
	230	220	10		020	800	12
	_	303			-	026	
	292	303	-11		06 2	072	-10
3 _{F4} ,3 _{K6}	-	30023		3 _{D3}	****	33313	
4,	_	027		•	-	330	
	30058	058	0			346	
	078	072	6		-	360	
	094	101	- 7		-	382	
•	101	105	-4		-	412	
	-	114			-	437	
	116	122	-6				
	-	140		3 _P 1	÷	33554	
	157	155	2	-	-	560	
	186	187	-1		-	564	
	_	197					
	197	198	-1	$_{M_{10}}^{3},_{L_{8}}^{3}$	34022	34033	-11
			_				

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Appendix	VII. (c	ont.)			J 97 .		- () -
SLJ ^a	Obsd.b	Calc.c		SLJ ^a	Obsd.b	Calc.c	
State	(cm^{-1})	(cm ⁻¹)	<u>o-c</u>	State	(cm ⁻¹)	(cm^{-1})	<u>0-C</u>
3 _{M10} ,3 _{L8}	<u> </u>	34105		5 _{D4}	36058	3 6040	18
10, 0	34116	122	-6	/ ·· ···· ·	070	071	-1
		138			086	085	1
		166			100	090	10
	_	191			111	140	-29
	205	205	0		-	221	
	_	212			-	251	
	-	221			244	252	-8
	((34234-3454	2) ^e		-	270	
5 _{G4}	-	34967		3 _{P0}	-	36318	
•	-	978					
	-	978			(36450-3670	3) [£]
	34994	984	10				
	****	998		³ H ₅	36852	36868	-16
	35003	35002	1		869	875	-6
	023	024	-1		894	909	-15
		024			-	935	
	049	032	17		-	965	
					37001	990	11
³ F ₃	35335	35327	8		-	37021	
-	-	343			034	032	2
	369	368	1		-	032	
	424	415	9		<u> </u>	045	
	-	435			-	066	
	489	491	-2				•
	-	530				(37975-382	37) ^g

SLJa	Obsd.b	Calc.c	
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>
3 ₁₇	-	38560	
	-	568	
	38570	571	-1
		585	
	-	590	
	-	590	
	599	597	2
	-	612	
	-	614	
	-	6 20	
	-	621	
	-	6 24	
	38638 ^h	646	
	-	647	
	-	652	

^aThe principal SLJ-component of the state is given.

bThe energies quoted as observed are primarily from ref. 52 as confirmed in the present study. In some instances the band energies reported are those found in the present work where no corresponding observations were quoted in (52); there were also cases in which more crystal-field components than would be allowed for a given J-value were quoted in (52). The present model crystal-field calculations were used as the basis for excluding the extra levels. Units of cm⁻¹ vac.

CEnergy level parameters are given in Table 1.

 $d_{\mbox{Not}}$ included in the energy level parameter fitting.

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eThere are 24 crystal-field components belonging principally to the $^3\mathrm{M}_{10}$ and $^3\mathrm{L}_8$ states computed in the energy range between 34234 and 34542 cm $^{-1}$. No structure was observed in this range.

 $^{\rm f}$ There are 22 crystal-field components belonging principally to the $^{\rm 3}$ F $_2$ and $^{\rm 1}$ L $_8$ states computed in the energy range 36450-36703 cm $^{-1}$. No structure was observed.

gThere are 20 crystal-field components belonging principally to the $^{3}P_{2}$ and $^{3}L_{7}$ states computed in the energy range 37975-38237 cm⁻¹. No structure was observed.

 $^{\rm h}{\rm No}$ structure attributable to f*f transitions was observed at energies $> 36638~{\rm cm}^{-1}$.

Appendix VIII.

Experimental and Computed Energy Level Structure of Dy^{3+} :LaF $_4$

SLJa	q*psqo	Calc.c		Fry et al.d	SLJ ⁸	q*psqo	Calc.c		Fry et al.d
State	(cm ⁻¹)	(cm ⁻¹)	ያ	Obs. (cm ⁻¹)	State	(cm^{-1})	(Fg-1)	9	Obs. (cm ⁻¹)
6 _{H15/2}	0	0	0	0	6H ₁₃ /2	3645	3639	9	3645
	17	88	7	17	Ì	1	8/9		! 1
	69	9/	7-	69		701	681	8	695
	124	136	-5	124					
	184	188	7	184	6 _{H11/2}	5883	5875	80	5882
	208	209	7	308		906	912	7	606
	į	%				776	918	9	925
	307	316	ዋ	307		945	934	11	576
						976	973	e	7.16
6 _{H13/2}	3503	3502	-	3502		6021	6024	ጥ	6024
	575	268	7	576					
	621	602	19	618	6 _{H9/2} ,	7632	7630	2	7633
	979	624	4	630	$^{6\mathrm{F}_{11/2}}$	799	673	ዋ	999

(cont.)
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Appendix

SLJ ^a	q.bsd0	Calc. ^c		Fry et al. ^d	SLJª	q.bado	Calc. ^c		Fry et al.d
State	(cm ⁻¹)	(L-m)	វ	Obs. (cm^{-1})	State	(cm^{-1})	(cm^{-1})	g	Obs. (cm ⁻¹)
6 _{H9/2} ,	77.26	77.28	-2	<u> 277</u>	6 _H _{7/2} ,	9181	9185	7	9179
$^{6\mathrm{F}}_{11/2}$	756	776	-30	758	6F9/2	75.	238	7	235
	812	828	-16	803		282	3%5	17	779
	837	832	S	813		343	330	13	343
	840	841	7	842		435	435	0	438
	854	862	99	887					
	930	126	က	933	6 _{H5/2}	10222	10220	2	10222
	966	866	-5	8019		285	幫	7	**************************************
	8075	\$000	10	075		345	346	7	344
⁶ H _{7/2} ,	8992	9668	7	0668	$^{6}\mathrm{F}_{7/2}$	11037	11038	7	11044
$^{6F_{9/2}}$	9074	5806	7	1/06		108	660	6 5	911
	087	160	7	085		138	138	0	159
	144	139	2	141		152	142	10	206

(cont.)
VIII.
Appendix

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SLJª	oped.b	Calc.c		Fry et al.d	SLJª	oped.	Calc.c		Fry et al. ^d	
State	(cm^{-1})	(cm ⁻¹)	ğ	0bs. (cm ⁻¹)	State	(cm^{-1})	(cm ⁻¹)	ၓၟ	Obs. (cm^{-1})	
										1
6F5/2	12456	12466	-10	12456	⁴ I _{15/2}	22022	21996	8	22020	
	502	501	-	501		132	121	11	136	
	514	517	ሞ	520		175	168	7	169	
						189	185	4	190	
⁶ F _{3/2}	13271	13288	-17	13271		213	211	2	214	
	285	3 82	7	茗		292	297	-	250	
						342	328	14	342	
6 F $_{1/2}$	t	13839		i		379	352	\boldsymbol{z}	380	
		•••								
4 F $_{9/2}$	21057	21058	7	21059	⁴ G _{11/2}	23468	23460	∞	23468	
	142	131	11	141		497	504	1-	501	
	159	147	12	159		513	525	-12	513	
	205	190	15	175		537	\$42	ጥ	534	
	ı	358		218		551	555	7	550	

(cont.)
WIII.
Appendix

SLJ ^a	Obsd. ^b Calc. ^c	Calc.		SLJ ⁸	q.bado	Calc. ^c	
State	(cm ⁻¹)	(cm^{-1})	ý	State	(cm^{-1})	(cm^{-1})	၁
⁴ G _{11/2}	ı	23611		⁴ 1 _{13/2} ,	ı	25636	
				⁴ F7/23	25661	674	-13
⁴ M _{21/2}	24984	24971	13	⁴ K _{17/2}	169	722	-31
	25001	866	9		740	742	2
	290	25070	ę,		748	759	-11
	060	092	-2		778	814	-36
	f	172			ı	829	
	187	185	2		824	837	-13
٠	ŧ	186			ı	845	
	236	223	3		67/8	861	-12
	ı	773			298	892	-25
	303	307	7		ı	768	
	341	333	8		ı	912	
					903	616	-16

(cont.)
VIII.
Appendix

SLJ ^a	q*psq0	Calc.		SLJ ^a	q*psq0	Calc. ^c		1
State	(cm ⁻¹)	(cm^{-1}) (cm^{-1})	ያ	State	(g-1)	(cm^{-1})	ሂ	
⁴ 1 _{13/2} ,	25918	25929	-11	⁴ M _{19/2}	26509	26528	-19	
⁴ F7/2°	ı	935			571	552	19	
⁴ K ₁ 7/2	940	952	-12		583	263	83	
	953	962	ዋ					
	ı	981		6 _{P3/2}	27476	27493	-17	
	066	982	8		529	545	-16	
⁴ M19/2	i	26242		⁶ P _{5/2}	27574	27580	φ	
	ı	. 21			616	611	٧.	
	26.260	257	က		658	099	-5	<i>J</i> (
	i	391						- / -
	i	397		⁴ 1 _{11/2}	27912	27903	6	,
	8448	445	က		ı	786		
	ı	475			982	991	9	

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Ϋ́	17	16		14	-14	1	20	7	-19	7	ጥ	7		
Calc. ^C	30862	888		31105	148	169	190	218	245	998	282	867	316	350
Obsd.b (cm ⁻¹)	30879	914		31119	134	170	195	214	236	262	282	Ŕ	ı	ſ
SLJ ^a State	⁶ P _{3/2}			⁴ K _{15/2} ,	4 L _{19/2}									
· Υ					φ			-12		17		īU		
SLJ^a $\operatorname{Obsd}_\bullet^b$ $\operatorname{Calc}_\bullet^c$ cm^{-1})	76682	30020	025	041	180	092	106	151	194	72/4	263	962		
Obsd.b (cm ⁻¹)	ı	1	ı	i	30073	1	1	139	ı	241	ı	301		
SLJ ^a tate	¹ G _{9/2} ,	M _{17/2}												

ន 0 Calc.^C -31565 8 Obsd.b

(cont.)
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Appendix

SLJ ^a	SLJ ^a Obsd. ^b Calc. ^c	Calc.c		SLJ ^a	q*psq0	Calc.	
State	(m-1)	(ca^{-1})	Ş	State	(cm^{-1})	(cm ⁻¹)	ပ္
4 _{H13/2}	1	33497		⁴ H _{11/2} ,	34227	34237	-10
	33500	200	.0	4 _{L17/2} ,	240	241	7
	208	206	2	⁴ F _{5/2} ,	1	280	
	537	518	19	⁴ H _{9/2}	278	274	4
	552	553	7		293	285	8
	009	995	**		t	292	
					ı	298	
⁴ F3/2	33628	33632	7		1	324	
	642	• 639	m		ı	338	
					346	348	-5
⁴ D _{7/2}	34009	34021	-12		ı	355	
	020	030	-10		1	358	
	031	041	-10		t	370	
	070	690			373	381	ዋ

The writing date.	(cure)						
SLJ ^a	q•psqo	Calc. ^C		SI.J ⁸	q•psq0	Calc. ^c	
State	(cm ⁻¹)	(\mathbb{G}^{-1})	ğ	State	(cm^{-1})	(cm ⁻¹)	ç
⁴ H _{11/2} ,	34398	34383	15		34933	34934	7
⁴ L _{17/2} ,	904	007	9		696	066	-21
4F5/23	i	420					
⁴ H ₉ /2	430	436	ዯ	⁴ K _{11/2} ,	ı	35776	
	445	8448	ጥ	⁴ G _{7/2}	1	818	
	į	457			t	905	
	ı	470			35936	876	-12
	i	472			961	971	-10
	505	. 493	12		36002	36005	ŗ
					022	710	æ
⁴ H _{11/2}	34847	34846	1		051	950	٢
	698	874	ኍ		7.20	100	- 23
	905	891	11		1	153	
	910	910	0				

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Appendix VIII. (cont.)

SLJª	obsd.b	Calc.c		SLJ ⁸	q.bado	Calc.c	
State	(cm ⁻¹)	(cm^{-1})	¥	State	(sm ⁻¹)	(cm ⁻¹)	પ્ર
⁴ G _{7/2}	ſ	37775		² h _{15/2}	1	38366	
	ı	789			ſ	451	
					ı	502	
⁴ F _{3/2}	37933	37921	12				
	962	952	10	⁴ P _{5/2}	38926	38911	15
					766	686	8
² L _{15/2}	ı	38047			39085	39077	æ
	ı	75 0					
	ı	170		⁴ P _{3/2}	39159	39163	7
	í	.¥ 			182	185	e
	ı	274				(39185–50000) ^e	(0000) _e

althe leading component of the eigenvector is given.

^bThe components of the ground state are from Ref. 54. All values in cm⁻¹ vac.

Gnergy level parameters are given in Table 1.

d_{Ref.} 54.

eAt >39185 cm⁻¹, a large number of crystal-field components is computed over the energy range to 50000 cm⁻¹; however, there are five intervals of > 650 cm⁻¹ in which no energy levels are computed. These are 39185-40531 ($\Delta = 1346$) cm⁻¹, 43977-44798 ($\Delta = 821$) cm⁻¹, 45073-46225 ($\Delta = 1152$) cm⁻¹, 46471-47462 ($\Delta = 991$) cm⁻¹, and 48618-49406 ($\Delta = 788$) cm⁻¹.

SLJa	Obsd.b	Calc. ^c		SLJ ^a	Obsd.b	Calc.c	
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	State	(cm^{-1})	(cm^{-1})	<u>0-c</u>
				7			
⁷ F6	0	-6	6	7 _{F4}	-	3281	
	6	0	-6		-	293	
	-	13			-	383	
	_	20			-	396	
	44	26	18		-	397	
	49	58	-9		-	441	
	80	86	-6		-	446	
	-	88			-	506	
		108			-	506	
	-	119			•••	685	
	-	162		_			
	-	233		⁷ _{F3}	4329	4331	-2
	-	244			413	407	6
					4 21	415	6
⁷ F ₅	_	2035			4 29	425	4
	•••	043			440	442	-2
		063			461	448	13
	-	076			487	473	14
	-	082					
	-	131		7 _{F2}	5016	5041	` -25
	_	133			038	045	-7
	-	167			**	161	
	-	261			166	164	2
	_	263			197	200	-3
	-	313					
				⁷ F ₁	5502	5522	-20
				_	568	586	-18
					617	632	-15

Appendix 1	[X. (cont	.)
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SLJa	Obsd.b			SLJ ^a	Obsd.b		
State	(cm^{-1})	(cm^{-1})	<u>o-c</u>	State	(cm^{-1})	(cm^{-1})	<u>0-c</u>
		•					
⁷ F ₀	5819	5806	13	⁵ G ₆	-	26578	
					-	609	
⁵ D ₄	-	20504			26631	634	-3
	20507	506	1		-	680	
	534	533	1				
	534	534	0	⁵ L ₁₀	-	26946	
	-	539			26962	949	13
	-	548				966	
	555	560	- 5			966	
	569	568	1		981	972	9
	580	588	-8		994	981	13
					***	27012	
⁵ D ₃	26 27 0	26 26 3	7		27029	015	14
•	274	266	8		048	041	7
		281			078	075	3
	-	285			142	152	-10
	296	302	-6		161	154	7
	325	318	7		183	166	17
	346	344	2		-	201	
					225	215	10
⁵ G ₆	26405	26410	- 5		-	234	
Ū	415	423	-8		• 251	249	2
	454	462	-8		-	274	
	482	494	-12		-	278	
	493	503	-10		_	286	
	-	536			322	306	16
	532	537	- 5				
	549	556	- 7	⁵ G ₅	_	27829	
	-	564		,	-	833	

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SLJ ^a State	Obsd.b (cm ⁻¹)		<u>0-C</u>	SLJ ^a State	0bsd. ^b (cm ⁻¹)	Calc. ^c (cm ⁻¹)	<u>o-c</u>
⁵ G ₅	27833	27833	0	5 _{G4} ,	28480	28483	-3
-5	839	837	2	5 _{L9}	491	496	-5
	856	872	-16	,	514	510	4
	882	883	-1		540	542	-2
	-	891			-	552	
	903	905	-2		-	563	
	910	916	-6		-	581	
	930	9 26	4		604	598	6
	989	972	17		618	614	4
					-	6 2 6	
⁵ D ₂	28197	28215	-18		_	633	
2	206	222	-16		-	663	
	_	240			-	665	
	233	241	-8		-	671	
	262	260	2		-	678	
⁵ G ₄ , ⁵ L ₉	-	28316		5 _{G3}	29030	29019	11
5 _{L9}	28336	344	-8		032	029	3
-	- .	345			037	038	-1
	-	350			` 045	039	6
	348	351	-3		-	050	
	364	367	-3		068	051	17
		375			090	087	3
	378	376	2				
	392	392	0	⁵ L ₈ ,	-	29183	
	4 28	411	17	⁵ L ₇ ,	29216	220	-4
	-	459		⁵ G ₂ ,	234	230	4
	460	460	0	⁵ L ₆	-	246	
	· -	479			_	249	

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Appendix IX	. (cont.)
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SLJ ^a State	0bsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>	SLJ ^a State	Obsd.b	Calc. ^c (cm ⁻¹)	<u>o-c</u>
⁵ L ₈ ,	29 27 4	29 27 9	-5	⁵ 00	-	31391	
⁵ L ₇ , ⁵ G ₂ ,	•••	284		5 ₁₁₇	_	31399	
⁵ G ₂ ,	-	291	0	,	31402	402	o
⁵ L ₆	295	295	0		_	403	
	336	329	7		-	452	
	-	348	4		_	459	
	360	354	6		494	496	-2
	-	370	- 7		-	506	
	392	. 399	-/		509	506	3
	_	406			_	522	-
	-	412			-	528	
	- (20	413	4		533	535	-2
	430	4 26	4		-	545	_
		434	10		-	592	
	465	447	18		613	608	5
	-	481	1		637	628	9
	503	502	1		037	020	,
	-	504		5 _{H6}	32889	32894	-5
	520	521	-1	ⁿ 6	918	929	-11
	552	542	10		941	942	-1
	-	565				992	-10
	-	57 2			982	998	-10
	-	592	a		-		0
	(29	9598-30057)	<u>u</u>		999	999	U
r					-	33025	1
⁵ D ₁	30765	30755	10		33027	028	-1
	774	770	4			031	•
	800	788	12		047	038	9
					-	102	

Ubbengty Tite ()	Appendix	IX.	(cont.)
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SLJ ^a State	0bsd.b (cm ⁻¹)		0 - C	SLJ ^a State	Obsd.b	Calc.c (cm ⁻¹)	0 - C
State	<u>(Cm /</u>	<u> </u>					
⁵ H ₅	33114	33104	10	5 _F 5,	35021	35030	- 9
2	146	119	27	⁵ н ₂ ,	044	053	-9
	-	817		5 ₁₈	•••	060	
	-	838		J	072	062	10
	_	850			-	068	
	-	878			-	085	
	-	882			-	090	
	887	885	2		_	094	
	909	919	-10		-	102	
	-	9 2 3			-	117	
	-	924			139	137	2
	-	927			167	168	-1
	939	937	2		-	176	
					179	178	1
5 _{H4}	-	34435				183	
·	_	442			203	214	-11
	-	452			211	228	-17
	34452	455	- 3		-	229	
	-	461			237	235	2
	-	462	•		-	243	
		482			-	246	
	-	485			256	250	6
	488	489	-1		274	261	13
					-	309	
⁵ F ₅ ,	-	34958			-	313	
5 _{H3} ,		960			-	315	
5 _{H3} , 5 _{I8}	-	986			316	316	0
-	34980	987	-7		-	323	
	35005	990	15		-	327	
					348	330	18

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Appendix IX. (cont.)

SLJ ^a State	0bsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>0-C</u>	SLJ ^a State		Calc. ^c (cm ⁻¹)	<u>0-C</u>
5 _{F4}	35479	35474	5	⁵ F ₃ ,	-	36737	
7	-	505		5 ₁₇	-	739	
	-	510		•	36741	748	-7
	-	510			_	750	
	-	523				764	
	-	533			-	766	
	555	546	9		•••	766	
	-	581			773	774	-1
	588	588	0		_	783	
					786	787	-1
5 _{F3} ,	-	36587			-	796	
5 _{F3} , 5 _{I7}	-	588		•			
•	36619	599	20	5 _{F2}	-	37 2 2 6	
	-	635			-	230	
	-	663			_	256	
	-	670				278	
	679	682	-3		-	280	
	-	723					
	-	729		5 _{F1}		37527	
	731	735	-4	_		555	
	731	736	- 5		_	579	
	348	330	18		ý.		

(37652-38193)^e

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SLJ ^a State	0bsd.b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>o-c</u>	SLJ ^a State	0bsd. ^b (cm ⁻¹)	Calc.c (cm ⁻¹)	<u>0-C</u>
5 _{Ka} ,	39210	39221	-11		-	410	
⁵ K ₉ , ⁵ D ₂	***	224				450	
2	-	226	11		-	454	
	_	233			-	475	
	-	246			_	480	
	-	269			-	489	
	265	280	-15		-	502	
		303			-	503	
	_	305			_	513	
	356	374	-18		-	521	
	-	378				521	
	383	399	-16				
	- .	405				(39522-50	000) ^f

aThe leading component of the eigenvector is given.

bunits of cm⁻¹ vac.

^CThe energy level parameters are given in Table 1.

 $^{^{}d}$ There are 22 levels belonging principally to the $^{5}L_{7}$, $^{5}D_{2}$, and $^{5}L_{6}$ states in the interval 29598-30059 cm $^{-1}$.

^eThere are 33 levels belonging principally to the 5I_6 , 5I_4 , and 5I_5 states in the interval 37657-38193 cm⁻¹. No structure was observed.

 f_{At} >39521 cm⁻¹ the density of computed levels is high. Energy gaps in the range 39522-50000 cm⁻¹, i.e., regions of >650 cm⁻¹ where no crystal-field components are computed, are as follows: 39522-40253 (Δ =731) cm⁻¹, 43645-44415 (Δ =770) cm⁻¹, 44568-45281 (Δ =713) cm⁻¹, and 48392-49112 (Δ =720) cm⁻¹.

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 $\label{eq:Appendix X.} \textbf{Experimental and Computed Energy Level Structure for $\operatorname{Gd}^{3+}:\operatorname{LaF}_3$}$

SLJ	Expt. ^a	Calc.b		SLJ	Expt.ª	Calc.b	
State	(cm ⁻¹)	(cm^{-1})	<u>o-c</u>	State	(cm^{-1})	(cm^{-1})	0-C
	- /						
8 _{57/2}	0	19.6	-20	6 _{117/2}	36340	36351	-11
-//2		19.7		<i>,</i> –	342	351	-9
		19.8			346	352	-6
		19.9			351	354	-3
					354	355	-1
⁶ P _{7/2}	32176	32169	7		363	357	6
•	185	177	8		370	360	10
	199	194	5		377	362	15
	226	224	2		384	364	20
⁶ P _{5/2}	32771	32774	-3	6 _{111/2}	36549	36554	- 5
•	791	780	11		561	563	-2
	808	802	6		571	572	-1
					584	585	-1
⁶ P _{3/2}	33352	33368	-16		592	590	2
·	370	386	-16		611	606	5
⁶ 1 _{7/2}	35923	35934	, –11	⁶ I _{15/2} ,	36659	36671	-12
	945	945	0	⁶ 1 _{13/2}	668	680	-12
	968	964	4		677	683	-6
	996	979	.17		687	696	-9
					698	699	-1
⁶ 1 _{9/2}	36 27 4	36 27 7	-3		701	707	-6
•	285	286	-1		710	713	-3
	305	303	2		712	714	-2
	313	311	2		717	715	2
	332	323	9		722	7 24	-2

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Appendix X. (cont.)

SLJ	Expt.a	Calc.b		SLJ	Expt.a	Calc.b	
	(cm ⁻¹)		0-C	State	(cm^{-1})	(cm^{-1})	<u>o-c</u>
	36731	367 25	6	⁶ G _{7/2}	240	243	3
6 _{115/2} ,	736	7 29	7	1/2	298	284	14
⁶ I _{13/2}	730	747	2				
	760	753	7	⁶ G _{11/2} ,	49533	49545	-12
	769	760	, 9	6 _{G9/2} ,	560	556	4
	709	700	,	6 _{G5/2}	604	623	-19
6-	20667	39647	20	3/2	638	654	-16
⁶ D ₉ /2	39667	681	5		651	661	-10
	686	709	10		680	688	-8
	719	709	11		_	696	
	742	731	11			711	
	758	/4/	11		-	731	
6		40620			740	741	-1
⁶ D _{1/2}	-	406 20				757	
6	10701	10721	0			810	
⁶ D _{7/2}	40734	40734	0		8 24	823	1
	740	737	3		-	860	_
	.744	741	3			000	
	751	753	-2	60		50486	
,				⁶ G _{3/2}	_	568	
⁶ D _{3/2}	-	40876			_	300	
	-	905		6.		E 1 2 1 0	
•				⁶ G _{13/2}	-	51310	
6 _{D5/2}	-	41003	ч		•	357	
		045			_	382	
	-	059			-	402	
					-	414	
⁶ G _{7/2}	49170	49160	10		-	436	
-	49221	49225	-4		-	483	

 $^{^{}a}$ Experimental results from Refs. 68 and 69, cm $^{-1}$ vac. b The parameter values used in this calculation are given in Table 1.