

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

AD-A 200 108

REPORT DOCUMENTATION PAGE				Form Approved OMB No 0704-0188 Exp Date Jun 30, 1986	
1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKINGS			
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited			
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S) HDL-TR-2150		5. MONITORING ORGANIZATION REPORT NUMBER(S)			
6a. NAME OF PERFORMING ORGANIZATION Harry Diamond Laboratories	6b. OFFICE SYMBOL (if applicable) SLCHD-ST-AP	7a. NAME OF MONITORING ORGANIZATION			
6c. ADDRESS (City, State, and ZIP Code) 2800 Powder Mill Road Adelphi, MD 20783-1197		7b. ADDRESS (City, State, and ZIP Code)			
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Center for Night Vision and Electro-Optics	8b. OFFICE SYMBOL (if applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER			
8c. ADDRESS (City, State, and ZIP Code) Ft. Belvoir, VA 22060		10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. 612120.H25	PROJECT NO. AH25	TASK NO.	WORK UNIT ACCESSION NO.
11. TITLE (Include Security Classification) Analysis of the Optical Spectra of Triply Ionized Transition Metal Ions in Yttrium Aluminum Garnet (YAG)					
12. PERSONAL AUTHOR(S) Clyde A. Morrison and Gregory A. Turner					
13a. TYPE OF REPORT Final	13b. TIME COVERED FROM 2/87 TO 10/87	14. DATE OF REPORT (Year, Month, Day) October 1988	15. PAGE COUNT 42		
16. SUPPLEMENTARY NOTATION HDL project: 520851, AMS code: 612120.H250011					
17. COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)			
FIELD	GROUP	SUB-GROUP	YAG, transition metals, optical spectra, Ti ³⁺ , V ³⁺ , Cr ³⁺ , Mn ³⁺ , Fe ³⁺ , Co ³⁺ , Ni ³⁺		
20	02		Cu ³⁺ , Zn ³⁺ , crystal field		
20	05		Yttrium, Aluminum, Garnet		
19. ABSTRACT (Continue on reverse if necessary and identify by block number) An analysis of the reported spectra of five transition metal ions in yttrium aluminum garnet (YAG) is given. The reported data assumed that the ions occupied the C _{3i} site in YAG, and this was also assumed in the analysis. The point charge lattice sums, A _{nm} , were calculated for the the C _{3i} site, and the concept of rotational invariance was used to obtain a set of crystal field parameters, B _{nm} ⁿ , for the triply ionized 3d ^N electronic series. The energy levels for the entire (Ti ³⁺ —Zn ³⁺) series of transition metal ions was calculated using the B _{nm} ⁿ for the C _{3i} site. The spin-orbit interaction was included in the calculation.					
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED		
22a. NAME OF RESPONSIBLE INDIVIDUAL Clyde A. Morrison		22b. TELEPHONE (Include Area Code) (202) 394-2042	22c. OFFICE SYMBOL SLCHD-ST-AP		

DD FORM 1473, 84 MAR

83 APR edition may be used until exhausted
All other editions are obsolete

SECURITY CLASSIFICATION OF THIS PAGE

UNCLASSIFIED

Contents

	Page
1. Introduction	5
2. Free Ion and Crystal Field Interactions	6
3. Analysis in the Cubic Approximation for the C_{3i} Site	7
4. Theoretical Crystal Field Parameters	20
4.1 Point Charge Crystal Field	20
4.2 Discussion of Results	33
References	36
Distribution	39

Tables

1. Experimental Values of $F^{(2)}$, $F^{(4)}$, α , and B_{40} for Triply Ionized Transition Metal Ions, X^{3+} , in $Y_3Al_5O_{12}$	7
2. Energy Levels of Ti^{3+} in $Y_3Al_5O_{12}$	8
3. Energy Levels of V^{3+} in $Y_3Al_5O_{12}$	8
4 - 8. Energy Levels of Cr^{3+} in $Y_3Al_5O_{12}$	9-13
9. Energy Levels of Mn^{3+} in $Y_3Al_5O_{12}$	14
10. Energy Levels of Fe^{3+} in $Y_3Al_5O_{12}$	15
11. Energy Levels of Fe^{3+} in $Y_3Al_5O_{12}$	17
12. Energy Levels of Co^{3+} in $Y_3Al_5O_{12}$	18
13. Crystallographic Data on $Y_3Al_5O_{12}$	22
14. Lattice Sum, A_{nm} , for Al_2 Ion in $24(d)$ (S_4) Site in $Y_3Al_5O_{12}$	23

Tables (cont'd)

15. Lattice Sum, A_{nm} , for Al Ion in 16(a) (C_{3i}) Site in $Y_3Al_5O_{12}$	23
16. Linear Least-Squares Best Fit Values of ρ_2 and ρ_4 for Triply Ionized Transition Metal Ions in Octahedral (C_{3i}) Site in YAG	23
17. Linear Least-Squares Best Fit $F^{(k)}$ and B_{nm} for Triply Ionized Transition Metal Ions in Octahedral Site (C_{3i}) in YAG	23
18. Racah Parameters, B and C ; Macfarlane's parameters, Dq , v , and v' ; and Ballhausen's parameters, Dq , $D\sigma$, and $D\tau$, for Triply Ionized Transition Metal Ions in Octahedral (C_{3i}) Site in YAG.	23
19. Energy Levels of Ti^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 122.24$	24
20. Energy Levels of V^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 164.80$	24
21. Energy Levels of Cr^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 220.00$	25
22. Energy Levels of Mn^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 289.44$	26
23. Energy Levels of Fe^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 370.40$	28
24. Energy Levels of Co^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 484.80$	29
25. Energy Levels of Ni^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 599.20$	31
26. Energy Levels of Cu^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 728.80$	32
27. Energy Levels of Zn^{3+} in $Y_3Al_5O_{12}$ Using Parameters of Table 17 with $\alpha = 30$ and $\zeta = 923.88$	33

1. Introduction

We report here on the analysis of the spectra of triply ionized transition metal ions, X^{3+} , with the electronic configuration $3d^N$ in the host lattice $Y_3Al_5O_{12}$ (YAG). The analysis is restricted predominantly to ions assumed to occupy the octahedral site (C_{3i}). Most of the experimental data on the $3d^N$ electronic configuration are for $N < 5$, with a large number of results for the $3d^3$ configuration, Cr^{3+} . The possibility that the X^{3+} ions may occupy sites other than the C_{3i} site (dodecahedral, D_2 , or tetragonal, S_4) further complicates the analysis [1].* Further, much of the experimental data used in the analysis has been taken at room temperature, and any possibility of observing detailed electronic line structure is lost. Despite these shortcomings in the reported data, we analyze the existing data and formulate a method of calculating a set of parameters which can be used as first approximates to experimental energy levels. These parameters are used to calculate the energy levels of the entire $3d^N$ triply ionized transition elements. This latter calculation includes the full C_{3i} symmetry as well as spin-orbit coupling.



Assignment for	
1. [unclear]	<input checked="" type="checkbox"/>
2. [unclear]	<input type="checkbox"/>
3. [unclear]	<input type="checkbox"/>
4. [unclear]	<input type="checkbox"/>
5. [unclear]	<input type="checkbox"/>
6. [unclear]	<input type="checkbox"/>
7. [unclear]	<input type="checkbox"/>
8. [unclear]	<input type="checkbox"/>
9. [unclear]	<input type="checkbox"/>
10. [unclear]	<input type="checkbox"/>
11. [unclear]	<input type="checkbox"/>
12. [unclear]	<input type="checkbox"/>
13. [unclear]	<input type="checkbox"/>
14. [unclear]	<input type="checkbox"/>
15. [unclear]	<input type="checkbox"/>
16. [unclear]	<input type="checkbox"/>
17. [unclear]	<input type="checkbox"/>
18. [unclear]	<input type="checkbox"/>
19. [unclear]	<input type="checkbox"/>
20. [unclear]	<input type="checkbox"/>
21. [unclear]	<input type="checkbox"/>
22. [unclear]	<input type="checkbox"/>
23. [unclear]	<input type="checkbox"/>
24. [unclear]	<input type="checkbox"/>
25. [unclear]	<input type="checkbox"/>
26. [unclear]	<input type="checkbox"/>
27. [unclear]	<input type="checkbox"/>
28. [unclear]	<input type="checkbox"/>
29. [unclear]	<input type="checkbox"/>
30. [unclear]	<input type="checkbox"/>
31. [unclear]	<input type="checkbox"/>
32. [unclear]	<input type="checkbox"/>
33. [unclear]	<input type="checkbox"/>
34. [unclear]	<input type="checkbox"/>
35. [unclear]	<input type="checkbox"/>
36. [unclear]	<input type="checkbox"/>
37. [unclear]	<input type="checkbox"/>
38. [unclear]	<input type="checkbox"/>
39. [unclear]	<input type="checkbox"/>
40. [unclear]	<input type="checkbox"/>
41. [unclear]	<input type="checkbox"/>
42. [unclear]	<input type="checkbox"/>
43. [unclear]	<input type="checkbox"/>
44. [unclear]	<input type="checkbox"/>
45. [unclear]	<input type="checkbox"/>
46. [unclear]	<input type="checkbox"/>
47. [unclear]	<input type="checkbox"/>
48. [unclear]	<input type="checkbox"/>
49. [unclear]	<input type="checkbox"/>
50. [unclear]	<input type="checkbox"/>
51. [unclear]	<input type="checkbox"/>
52. [unclear]	<input type="checkbox"/>
53. [unclear]	<input type="checkbox"/>
54. [unclear]	<input type="checkbox"/>
55. [unclear]	<input type="checkbox"/>
56. [unclear]	<input type="checkbox"/>
57. [unclear]	<input type="checkbox"/>
58. [unclear]	<input type="checkbox"/>
59. [unclear]	<input type="checkbox"/>
60. [unclear]	<input type="checkbox"/>
61. [unclear]	<input type="checkbox"/>
62. [unclear]	<input type="checkbox"/>
63. [unclear]	<input type="checkbox"/>
64. [unclear]	<input type="checkbox"/>
65. [unclear]	<input type="checkbox"/>
66. [unclear]	<input type="checkbox"/>
67. [unclear]	<input type="checkbox"/>
68. [unclear]	<input type="checkbox"/>
69. [unclear]	<input type="checkbox"/>
70. [unclear]	<input type="checkbox"/>
71. [unclear]	<input type="checkbox"/>
72. [unclear]	<input type="checkbox"/>
73. [unclear]	<input type="checkbox"/>
74. [unclear]	<input type="checkbox"/>
75. [unclear]	<input type="checkbox"/>
76. [unclear]	<input type="checkbox"/>
77. [unclear]	<input type="checkbox"/>
78. [unclear]	<input type="checkbox"/>
79. [unclear]	<input type="checkbox"/>
80. [unclear]	<input type="checkbox"/>
81. [unclear]	<input type="checkbox"/>
82. [unclear]	<input type="checkbox"/>
83. [unclear]	<input type="checkbox"/>
84. [unclear]	<input type="checkbox"/>
85. [unclear]	<input type="checkbox"/>
86. [unclear]	<input type="checkbox"/>
87. [unclear]	<input type="checkbox"/>
88. [unclear]	<input type="checkbox"/>
89. [unclear]	<input type="checkbox"/>
90. [unclear]	<input type="checkbox"/>
91. [unclear]	<input type="checkbox"/>
92. [unclear]	<input type="checkbox"/>
93. [unclear]	<input type="checkbox"/>
94. [unclear]	<input type="checkbox"/>
95. [unclear]	<input type="checkbox"/>
96. [unclear]	<input type="checkbox"/>
97. [unclear]	<input type="checkbox"/>
98. [unclear]	<input type="checkbox"/>
99. [unclear]	<input type="checkbox"/>
100. [unclear]	<input type="checkbox"/>

A-1

*References are listed at the end of the text (p 36).

2. Free Ion and Crystal Field Interactions

The interaction considered in the analysis given here has been described in detail previously [2] and will be covered only briefly here. The free ion terms in the interaction contain the Slater parameters $F^{(2)}$ and $F^{(4)}$, and the configuration interaction contains the parameters α and γ . In the analysis here we shall assume $\gamma = 0$ throughout. The crystal field of C_{3i} symmetry for the nd^N configuration is

$$H_{CEF} = B_{20} \sum_{i=1}^N C_{20}(i) + B_{40} \sum_{i=1}^N C_{40}(i) + B_{43} \sum_{i=1}^N [C_{43}(i) - C_{4-3}(i)], \quad (1)$$

$$C_{nm}(i) = \sqrt{4\pi/(2n+1)} Y_{nm}(\theta_i, \Phi_i),$$

where the crystal field parameter, B_{43} , is real and, for definiteness, with no loss in generality, we assume B_{43} positive. For the cubic approximation in equation (1), we have

$$B_{20} = 0, \quad (2)$$

$$B_{43} = \sqrt{10/7} |B_{40}|.$$

(The z axis of the crystal field is parallel to the $\langle 111 \rangle$ cubic axis.) The relationship of the crystal field parameters B_{nm} to other notations is given by König and Kremer [3]. For ions in the S_4 site, the crystal field interaction is taken as

$$H_{CEF} = B_{20} \sum_{i=1}^N C_{20}(i) + B_{40} \sum_{i=1}^N C_{40}(i) + B_{44} \sum_{i=1}^N [C_{44}(i) + C_{4-4}(i)], \quad (3)$$

where the crystal field parameter B_{44} is real and assumed positive. In S_4 symmetry, the total crystal field interaction contains terms with B_{32} and B_{52} . Both parameters are generally complex, but since we are considering interactions only in the $3d^N$ configuration, we shall ignore these terms. Further, it should be noted that since the odd terms B_{32} and B_{52} are present, electric dipole transitions can exist, and if they are present, their absorption intensity should be much larger [1] than for ions in the C_{3i} site for which only magnetic dipole or electric quadrupole transitions are allowed. This, of course, has been recognized by others and has been used to identify the site occupancy of the ions, particularly Fe^{3+} in YAG. The cubic approximation (tetrahedral) is obtained by letting

$$B_{20} = 0 \quad (4)$$

$$B_{44} = \sqrt{5/14} |B_{40}|.$$

in equation (3) [3].

3. Analysis in the Cubic Approximation for the C_{3i} Site

The reported parameters for the various ions X^{3+} in YAG were used in a least-squares fit to the experimental data. Most of the data were analyzed in terms of Dq , B , and C . The relation of these parameters to our parameters is

$$F^{(2)} = 7(7B + C)$$

$$F^{(4)} = 63C/5$$

$$B_{40} = -14 Dq ,$$

and B_{43} given by equation (2). This latter relation is for C_{3i} symmetry; however, for S_4 symmetry sites, $B_{40} = -21Dq$ and B_{44} is given by equation (4). Starting with the parameters given in the references in table 1 [4-13] and the experimental data from these references, we obtained a best least-squares fit to the experimental data by varying $F^{(2)}$, $F^{(4)}$, α , and B_{40} . These results are given in table 1. Tables 2 through 12 give the experimental and calculated energy levels from our fitting. In these tables $F^{(2)}$, $F^{(4)}$, α , and B_{40} were, in general, varied to obtain the best fit to the experimental data reported in the given references. For several ions the number of experimental energy levels did not exceed the number of parameters, and in these cases the results should be viewed accordingly. In particular the results obtained for Co^{3+} are very questionable because of the large rms value with only six experimental energy levels.

Table 1. Experimental values of $F^{(2)}$, $F^{(4)}$, α , and B_{40} for triply ionized transition metal ions, X^{3+} , in $Y_3Al_5O_{12}$

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	α	$B_{40}^{(a)}$	Ref No.	Table No.
Ti	$3d^1$	—	—	—	-25928	4	2
V	$3d^2$	52164	38344	70	-24104	5	3
Cr	$3d^3$	60360	40020	0	-22442	6	4
Cr	$3d^3$	54870	36073	97	-23116	7	5
Cr	$3d^3$	56509	34680	110	-22941	8	6
Cr	$3d^3$	58125	44929	0	-23978	9	7
Cr	$3d^3$	54834	35666	122	-22960	10	8
Mn	$3d^4$	61762	41454	0	-29419	11	9
Fe	$3d^5$	49147	36324	23.8	-17580	12	10
Fe	$3d^5$	49280	37297	0	-17703	13	11
Co	$3d^6$	41033	22381	26.8	-23292	11	12

$$^a B_{43} = \sqrt{10/7} |B_{40}|$$

Table 2. Energy levels
(cm^{-1}) of Ti^{3+} in
 $\text{Y}_3\text{Al}_5\text{O}_{12}$

Level No.	IR ^a	Energy ^b (exp)	Energy (theor)	Free-ion state (%)
1	${}^2\text{T}_2$	0	-1	100 2D
2	${}^2\text{E}$	18519	18519	100 2D

[Theoretical levels were calculated with parameters in table 1]

^aIn this and other tables which follow, IR is the irreducible representation of the cubic group.

^bExperimental energy levels are taken from reference 4.

Table 3. Energy levels
(cm^{-1}) of V^{3+} in
 $\text{Y}_3\text{Al}_5\text{O}_{12}$

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^3\text{T}_1$	0	0	91 3F + 9 3P
2	${}^1\text{T}_2$	10256	10256	58 1D + 42 1G
3	${}^1\text{E}$	0	10468	51 1D + 49 1G
4	${}^3\text{T}_2$	16000	16000	100 3F
5	${}^1\text{A}_1$	0	22142	68 1G + 32 1S
6	${}^3\text{T}_1$	23530	23530	91 3P + 9 3F
7	${}^1\text{T}_2$	0	27546	58 1G + 42 1D
8	${}^1\text{T}_1$	0	30204	100 1G
9	${}^3\text{A}_2$	0	33217	100 3F
10	${}^1\text{E}$	0	44552	51 1G + 49 1D
11	${}^1\text{A}_1$	0	58381	68 1S + 32 1G

[Theoretical levels were calculated with parameters in table 1]

^aExperimental energy levels are taken from reference 5.

Table 4. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	$^4\text{A}_2$	0	124	100 4F
2	^2E	14500	15264	63 2G + 19 2H + 17 2D2
3	$^2\text{T}_1$	0	15994	41 2G + 35 2H + 20 2P
4	$^4\text{T}_2$	16700	16154	100 4F
5	$^2\text{T}_2$	0	22621	35 2H + 27 2D1 + 1 2D2
6	$^4\text{T}_1$	23200	23511	58 4F + 42 4P
7	$^2\text{A}_1$	0	28795	100 2G
8	$^2\text{T}_2$	31200	31187	58 2G + 38 2H + 3 2D2
9	$^2\text{T}_1$	31200	31725	54 2H + 25 2G + 21 2P
10	^2E	0	33498	49 2H + 40 2D2 + 10 2D1
11	$^4\text{T}_1$	36300	36498	58 4P + 42 4F
12	$^2\text{T}_1$	37800	36921	37 2H + 35 2P + 25 2F
13	$^2\text{T}_2$	43100	42673	56 2F + 41 2D2 + 2 2G
14	$^2\text{A}_2$	0	44357	100 2F
15	$^2\text{T}_1$	0	47324	68 2H + 32 2G
16	$^2\text{T}_2$	0	49268	26 2G + 25 2F + 22 2H
17	^2E	0	52404	43 2D2 + 24 2G + 17 2D1
18	$^2\text{T}_1$	55000	55274	71 2F + 23 2P + 5 2H
19	$^2\text{T}_2$	0	71313	61 2D1 + 22 2D2 + 13 2F
20	^2E	0	71538	71 2D1 + 16 2H + 13 2G

^aExperimental energy levels are taken from reference 6.

Table 5. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^4\text{A}_2$	0	138	100 4F
2	${}^2\text{E}$	14559	14592	62 2G + 20 2D2 + 17 2H
3	${}^2\text{T}_1$	15265	15247	38 2G + 33 2H + 24 2P
4	${}^4\text{T}_2$	16700	16650	100 4F
5	${}^2\text{T}_2$	21281	21278	30 2H + 30 2D1 + 20 2D2
6	${}^4\text{T}_1$	23200	23146	51 4P + 49 4F
7	${}^2\text{A}_1$	0	28858	100 2G
8	${}^2\text{T}_2$	0	31407	57 2G + 40 2H + 3 2D2
9	${}^2\text{T}_1$	0	31551	39 2H + 30 2G + 29 2P
10	${}^2\text{E}$	0	32924	49 2H + 41 2D2 + 10 2D1
11	${}^2\text{T}_1$	0	36171	52 2H + 25 2F + 22 2P
12	${}^4\text{T}_1$	36300	36357	51 4F + 49 4P
13	${}^2\text{T}_2$	0	40606	60 2F + 38 2D2 + 2 2G
14	${}^2\text{A}_2$	0	42298	100 2F
15	${}^2\text{T}_1$	0	48295	69 2H + 31 2G
16	${}^2\text{T}_2$	0	48888	29 2G + 25 2H + 19 2F
17	${}^2\text{E}$	0	50425	39 2D2 + 27 2D1 + 21 2G
18	${}^2\text{T}_1$	0	53834	69 2F + 24 2P + 7 2H
19	${}^2\text{T}_2$	0	68067	59 2D1 + 22 2D2 + 15 2F
20	${}^2\text{E}$	0	70007	61 2D1 + 21 2H + 17 2G

^aExperimental energy levels are taken from reference 7.

Table 6. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^4\text{A}_2$	0	16	100 4F
2	${}^2\text{E}$	14616	14523	62 2G + 20 2D2 + 16 2H
3	${}^2\text{T}_1$	15200	15255	39 2G + 32 2H + 25 2P
4	${}^4\text{T}_2$	16400	16402	100 4F
5	${}^2\text{R}_2$	21100	21110	31 2D1 + 29 2H + 21 2D2
6	${}^4\text{T}_1$	23200	23187	52 4F + 48 4P
7	${}^2\text{A}_1$	0	28579	100 2G
8	${}^2\text{T}_2$	0	31307	57 2G + 40 2H + 3 2D2
9	${}^2\text{T}_1$	0	31432	37 2H + 31 2P + 30 2G
10	${}^2\text{E}$	0	32783	49 2H + 40 2D2 + 11 2D1
11	${}^2\text{T}_1$	0	36300	54 2H + 24 2F + 22 2P
12	${}^4\text{T}_1$	36300	36304	52 4P + 48 4F
13	${}^2\text{T}_2$	0	41060	58 2F + 39 2D2 + 2 2G
14	${}^2\text{A}_2$	0	42900	100 2F
15	${}^2\text{T}_1$	0	48153	70 2H + 30 2G
16	${}^2\text{T}_2$	0	48699	27 2G + 26 2H + 21 2F
17	${}^2\text{E}$	0	50858	40 2D2 + 25 2D1 + 21 2G
18	${}^2\text{T}_1$	0	54084	70 2F + 23 2P + 7 2H
19	${}^2\text{T}_2$	0	68579	58 2D1 + 23 2D2 + 15 2F
20	${}^2\text{E}$	0	69692	62 2D1 + 21 2H + 16 2G

^aExperimental energy levels are taken from reference 8.

Table 7. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^4\text{A}_2$	0	-132	100 4F
2	${}^2\text{E}$	0	15593	61 2G + 19 2H + 18 2D2
3	${}^2\text{T}_1$	0	16164	39 2G + 35 2H + 21 2P
4	${}^4\text{T}_2$	16950	16995	100 4F
5	${}^2\text{T}_2$	0	23329	38 2H + 27 2D1 + 17 2D2
6	${}^4\text{T}_1$	23730	23783	50 4P + 50 4F
7	${}^2\text{A}_1$	0	30400	100 2G
8	${}^2\text{T}_2$	0	32556	58 2G + 37 2H + 4 2D2
9	${}^2\text{T}_1$	0	32946	55 2H + 25 2G + 20 2P
10	${}^2\text{E}$	0	34794	49 2H + 43 2D2 + 9 2D1
11	${}^4\text{T}_1$	37540	37486	50 4F + 50 4P
12	${}^2\text{T}_1$	0	37700	36 2H + 32 2P + 29 2F
13	${}^2\text{T}_2$	0	42524	62 2F + 37 2D2 + 1 2G
14	${}^2\text{A}_2$	0	43936	100 2F
15	${}^2\text{T}_1$	0	49675	67 2H + 33 2G
16	${}^2\text{T}_2$	0	51438	29 2G + 22 2D2 + 21 2H
17	${}^2\text{E}$	0	52976	39 2D2 + 24 2D1 + 23 2G
18	${}^2\text{T}_1$	0	56329	66 2F + 27 2P + 7 2H
19	${}^2\text{T}_2$	0	72119	63 2D1 + 19 2D2 + 14 2F
20	${}^2\text{E}$	0	74668	66 2D1 + 18 2H + 15 2G

^aExperimental energy levels are taken from reference 9.

Table 8. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^4\text{A}_2$	0	1	100 4F
2	${}^2\text{E}$	14542	14541	61 2G + 21 2D2 + 16 2H
3	${}^2\text{T}_1$	15200	15199	38 2G + 32 2H + 25 2P
4	${}^4\text{T}_2$	16400	16401	100 4F
5	${}^2\text{T}_2$	21100	21100	31 2D1 + 29 2H + 21 2D2
6	${}^4\text{T}_1$	0	22789	51 4P + 49 4F
7	${}^2\text{A}_1$	0	28727	100 2G
8	${}^2\text{T}_2$	0	31373	56 2G + 40 2H + 3 2D2
9	${}^2\text{T}_1$	0	31385	35 2H + 32 2P + 31 2G
10	${}^2\text{E}$	0	32741	49 2H + 41 2D2 + 10 2D1
11	${}^2\text{T}_1$	0	35913	51 4F + 49 4P
12	${}^4\text{T}_1$	0	36059	56 2H + 24 2F + 19 2P
13	${}^2\text{T}_2$	0	40290	60 2F + 38 2D2 + 2 2G
14	${}^2\text{A}_2$	0	42045	100 2F
15	${}^2\text{T}_1$	0	48240	69 2H + 30 2G
16	${}^2\text{T}_2$	0	48595	29 2G + 26 2H + 19 2F
17	${}^2\text{E}$	0	50105	38 2D2 + 28 2D1 + 21 2G
18	${}^2\text{T}_1$	0	53436	69 2F + 23 2P + 8 2H
19	${}^2\text{T}_2$	0	67566	58 2D1 + 22 2D2 + 15 2F
20	${}^2\text{E}$	0	69492	60 2D1 + 22 2H + 17 2G

^aExperimental energy levels are taken from reference 10.

Table 9. Energy levels (cm^{-1}) of Mn^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^3\text{T}_1$	0	0	40 3H + 17 3G + 16 3F1
2	${}^5\text{E}$	0	1087	100 5D
3	${}^1\text{T}_2$	0	9356	35 1I + 28 1G2 + 23 1G1
4	${}^1\text{E}$	0	10500	57 1I + 22 1D2 + 11 1G1
5	${}^3\text{E}$	0	18226	84 3H + 15 3G + 1 3D
6	${}^1\text{A}_1$	0	18869	38 1G1 + 24 1I + 20 1S2
7	${}^3\text{T}_1$	0	19072	45 3H + 23 3G + 19 3P2
8	${}^3\text{T}_2$	0	19913	41 3F2 + 32 3H + 13 3F1
9	${}^3\text{A}_1$	0	21361	100 3G
10	${}^5\text{T}_2$	22100	22100	100 5D
11	${}^1\text{T}_2$	0	22154	94 3F2 + 6 3F1
12	${}^3\text{E}$	0	24733	56 3D + 41 3G + 3 3H
13	${}^1\text{A}_2$	0	27162	91 1I + 9 1F
14	${}^1\text{T}_2$	27200	27200	61 1I + 23 1G2 + 7 1G1
15	${}^1\text{T}_1$	0	29443	40 1I + 24 1G2 + 20 1G1
16	${}^1\text{E}$	31500	31500	41 1D2 + 33 1G2 + 20 1I
17	${}^3\text{T}_1$	0	32447	35 3G + 27 3H + 25 3P1
18	${}^3\text{T}_2$	0	34073	39 3D + 32 3F1 + 23 3G
19	${}^3\text{T}_1$	0	39507	52 3H + 32 3F2 + 6 3F1
20	${}^3\text{T}_2$	0	40957	56 3H + 21 3F2 + 11 3D
21	${}^1\text{A}_1$	0	41615	62 1G2 + 18 1S2 + 16 1G1
22	${}^1\text{T}_1$	0	43564	37 1F + 24 1G1 + 22 1G2
23	${}^3\text{T}_2$	0	43717	44 3G + 43 3D + 12 3H
24	${}^1\text{T}_2$	0	44831	62 1F + 19 1D1 + 13 1G1
25	${}^3\text{T}_2$	0	45135	40 3G + 33 3F2 + 24 3D
26	${}^1\text{T}_2$	0	47185	85 1I + 9 1G2 + 3 1G1
27	${}^3\text{T}_1$	0	48161	57 3P2 + 20 3G + 17 3F2
28	${}^1\text{E}$	0	48262	43 1G2 + 26 1G1 + 22 1I
29	${}^1\text{A}_1$	0	49786	41 1I + 29 1S2 + 18 1G2
30	${}^1\text{T}_2$	0	56126	70 1D2 + 11 1I + 9 1G1
31	${}^1\text{A}_2$	0	56846	91 1F + 9 1I
32	${}^1\text{T}_1$	0	57683	53 1G2 + 46 1F + 1 1I
33	${}^3\text{T}_1$	0	59751	71 3F1 + 19 3H + 6 3P2

Table 9. Energy levels (cm⁻¹) of Mn³⁺ in Y₃Al₅O₁₂ (cont'd)

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
34	³ A ₂	0	62517	94 3F1 + 6 3F2
35	¹ E	0	67079	62 1G1 + 23 1G2 + 11 1D2
36	³ T ₁	0	68610	51 3P1 + 27 3F2 + 13 3H
37	¹ T ₁	0	72164	55 1G1 + 43 1I + 1 1F
38	³ T ₂	0	73296	53 3F1 + 19 3G + 19 3D
39	¹ T ₂	0	76810	28 1G1 + 28 1D1 + 22 1D2
40	¹ A ₁	0	84593	27 1S2 + 26 1I + 23 1G1
41	¹ E	0	86023	79 1D1 + 20 1D2 + 1 1I
42	¹ T ₂	0	86877	41 1D1 + 23 1F + 17 1G2
43	¹ A ₁	0	108559	66 1S1 + 23 1G1 + 6 1S2

^aExperimental energy levels are taken from reference 11.

Table 10. Energy levels (cm⁻¹) of Fe³⁺ in Y₃Al₅O₁₂

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	⁶ A ₁	0	-2	100 6S
2	⁴ T ₁	10400	10400	59 4G + 38 4P + 3 4F
3	² T ₂	0	10827	30 2I + 26 2H + 19 2F1
4	⁴ T ₂	14300	14309	46 4G + 29 4F + 25 4D
5	² A ₂	0	20610	54 2I + 42 2F1 + 4 2F2
6	⁴ (A ₁ ,E)	20717	20800	100 4G
7	² T ₁	0	20931	58 2I + 24 2H + 14 2F1
8	² T ₂	0	22075	48 2I + 24 2F1 + 12 2H
9	⁴ T ₂	22880	22679	55 4D + 43 4G + 2 4F
10	² E	0	23473	33 2I + 31 2H + 15 2D3
11	⁴ E	24440	24605	100 4D
12	² T ₁	0	26897	32 2G2 + 21 2F1 + 20 2H
13	² T ₂	0	28889	30 2G2 + 25 2F2 + 14 2I
14	² A ₁	0	29251	62 2I + 19 2G2 + 13 2G1
15	⁴ T ₁	0	30530	46 4F + 42 4P + 13 4G

Table 10. Energy levels (cm^{-1}) of Fe^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ (cont'd)

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
16	${}^2\text{E}$	0	30665	47 2I + 26 2D3 + 13 2D1
17	${}^2\text{T}_2$	0	32011	51 2I + 36 2D3 + 8 2D1
18	${}^2\text{A}_1$	0	32131	44 2G2 + 37 2I + 11 2G1
19	${}^4\text{A}_2$	0	33470	100 4F
20	${}^2\text{E}$	0	34902	74 2G2 + 11 2I + 5 2D3
21	${}^2\text{T}_2$	0	36135	45 2F2 + 26 2G2 + 16 2I
22	${}^2\text{T}_1$	0	36592	68 2H + 30 2F1 + 1 2G2
23	${}^2\text{A}_2$	0	36949	71 2F2 + 22 2I + 7 2F1
24	${}^2\text{T}_1$	0	37093	48 2F2 + 39 2G2 + 9 2I
25	${}^4\text{T}_1$	0	37704	51 4F + 29 4G + 20 4P
26	${}^2\text{A}_1$	0	39945	69 2S + 27 2G2 + 4 2G1
27	${}^2\text{E}$	0	40975	41 2H + 33 2D3 + 25 2D2
28	${}^4\text{T}_2$	0	41888	69 4F + 21 4D + 10 4G
29	${}^2\text{T}_1$	0	42283	37 2H + 19 2F2 + 18 2F1
30	${}^2\text{T}_2$	0	43413	31 2F1 + 19 2H + 15 2G2
31	${}^2\text{T}_1$	0	46706	43 2H + 30 2I + 16 2F1
32	${}^2\text{A}_2$	0	46747	51 2F1 + 25 2F2 + 24 2I
33	${}^2\text{E}$	0	49269	72 2G1 + 9 2H + 8 2D1
34	${}^2\text{T}_2$	0	51523	53 2D2 + 13 2G1 + 12 2I
35	${}^2\text{E}$	0	52402	54 2D2 + 11 2G1 + 11 2G2
36	${}^2\text{T}_2$	0	53835	25 2D3 + 25 2H + 16 2I
37	${}^2\text{T}_1$	0	54302	78 2G1 + 8 2P + 6 2F2
38	${}^2\text{T}_2$	0	57447	47 2G1 + 13 2G2 + 12 2F2
39	${}^2\text{A}_1$	0	59526	72 2G1 + 17 2S + 11 2G2
40	${}^2\text{T}_1$	0	63651	86 2P + 5 2F2 + 5 2G2
41	${}^2\text{T}_2$	0	73086	66 2D1 + 7 2H + 7 2D3
42	${}^2\text{E}$	0	73251	67 2D1 + 13 2D3 + 12 2G1

^aExperimental energy levels are taken from reference 12.

Table 11. Energy levels (cm^{-1}) of Fe^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	${}^6\text{A}_1$	0	-1	100 6S
2	${}^4\text{T}_1$	10360	10377	60 4G + 37 4P + 4 4F
3	${}^2\text{T}_2$	0	10680	32 2I + 27 2H + 18 2F1
4	${}^4\text{T}_2$	14200	14195	48 4G + 29 4F + 24 4D
5	${}^2\text{A}_2$	0	20438	56 2I + 41 2F1 + 4 2F2
6	${}^2\text{T}_1$	0	20610	60 2I + 24 2H + 13 2F1
7	${}^4(\text{A}_1, \text{E})$	20530	20627	100 4G
8	${}^2\text{T}_2$	0	21874	49 2I + 24 2F1 + 11 2H
9	${}^4\text{T}_2$	22940	22659	55 4D + 42 4G + 3 4F
10	${}^2\text{E}$	0	23329	36 2I + 30 2H + 14 2D3
11	${}^4\text{E}$	24450	24707	100 4D
12	${}^2\text{T}_1$	0	26902	33 2G2 + 21 2F1 + 20 2H
13	${}^2\text{T}_2$	0	28814	30 2G2 + 24 2F2 + 17 2I
14	${}^2\text{A}_1$	0	28912	68 2I + 16 2G2 + 11 2G1
15	${}^2\text{E}$	0	30639	47 2I + 25 2D3 + 13 2D1
16	${}^4\text{T}_1$	0	30741	47 4F + 42 4P + 11 4G
17	${}^2\text{T}_1$	0	31947	48 2G2 + 31 2I + 13 2G1
18	${}^2\text{T}_2$	0	31985	48 2I + 37 2D3 + 8 2D1
19	${}^4\text{A}_2$	0	33542	100 4F
20	${}^2\text{E}$	0	34885	74 2G2 + 9 2I + 6 2D3
21	${}^2\text{T}_2$	0	36158	45 2F2 + 25 2G2 + 15 2I
22	${}^2\text{T}_1$	0	36678	69 2H + 30 2F1 + 1 2G2
23	${}^2\text{A}_2$	0	36961	71 2F2 + 21 2I + 8 2F1
24	${}^2\text{T}_1$	0	37090	48 2F2 + 39 2G2 + 9 2I
25	${}^4\text{T}_1$	0	37850	50 4F + 29 4G + 22 4P
26	${}^2\text{A}_1$	0	40168	69 2S + 26 2G2 + 4 2G1
27	${}^2\text{E}$	0	41121	40 2H + 35 2D3 + 25 2D2
28	${}^4\text{T}_2$	0	42022	69 4F + 21 4D + 10 4G
29	${}^2\text{T}_1$	0	42379	36 2H + 20 2F2 + 18 2F1
30	${}^2\text{T}_2$	0	43560	31 2F1 + 20 2H + 15 2G2
31	${}^2\text{T}_1$	0	46693	42 2H + 29 2I + 17 2F1
32	${}^2\text{A}_2$	0	46953	52 2F1 + 25 2F2 + 23 2I
33	${}^2\text{E}$	0	49272	73 2G1 + 9 2H + 8 2D1

Table 11. Energy levels (cm^{-1}) of Fe^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ (cont'd)

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
34	2T_2	0	51725	50 2D2 + 16 2G1 + 13 2I
35	2E	0	52668	56 2D2 + 11 2G2 + 10 2H
36	2T_2	0	54029	26 2D3 + 23 2H + 16 2F1
37	2T_1	0	54335	78 2G1 + 8 2P + 7 2F2
38	2T_2	0	57575	47 2G1 + 13 2G2 + 12 2F2
39	2A_1	0	59643	71 2G1 + 17 2S + 10 2G2
40	2T_1	0	63922	86 2P + 5 2F2 + 5 2G2
41	2T_2	0	73556	67 2D1 + 7 2H + 7 2D3
42	2E	0	73691	68 2D1 + 13 2D3 + 12 2G1

^aExperimental energy levels are taken from reference 13.

Table 12. Energy levels (cm^{-1}) of Co^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
1	1A_1	0	-232	35 1G1 + 33 1I + 20 1G2
2	3T_1	0	11110	41 3H + 25 3F2 + 20 3P1
3	3T_2	14900	14919	38 3G + 24 3H + 23 3F1
4	1T_1	15600	15464	55 1I + 28 1G1 + 18 1G2
5	5T_2	0	16390	100 5D
6	1T_2	22400	22672	27 1I + 21 1D2 + 20 1F
7	3T_1	26600	26802	64 3H + 26 3F2 + 7 3F1
8	3T_2	0	27829	53 3H + 42 3G + 5 3F2
9	3E	29700	29359	52 3G + 29 3H + 19 3D
10	3T_1	0	29359	48 3G + 32 3P2 + 11 3H
11	1E	0	31597	45 1G2 + 30 1G1 + 22 1I
12	3T_2	0	31673	54 3D + 43 3F2 + 4 3G
13	1T_2	0	32124	69 1I + 12 1G2 + 10 1D2
14	1A_1	0	32352	52 1I + 28 1S2 + 10 1S1
15	5E	0	33027	100 5D
16	3A_2	0	35959	74 3F1 + 26 3F2

Table 12. Energy levels (cm^{-1}) of Co^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ (cont'd)

[Theoretical levels were calculated with parameters in table 1]

Level No.	IR	Energy ^a (exp)	Energy (theor)	Free-ion state (%)
17	1T_1	0	36366	39 1G2 + 32 1F + 25 1I
18	1A_2	0	37076	58 1F + 42 1I
19	1T_2	0	37610	27 1D2 + 27 1F + 23 1I
20	3T_1	0	40727	32 3H + 29 3F2 + 17 3F1
21	1E	0	41617	38 1D2 + 36 1G1 + 19 1D1
22	3E	0	43870	69 3H + 29 3G + 2 3D
23	3T_1	0	44577	33 3G + 29 3P2 + 22 3H
24	3T_2	0	44791	31 3F2 + 23 3H + 19 3D
25	1T_2	0	44988	43 1G1 + 30 1I + 15 1D2
26	3A_1	0	45760	100 3G
27	3E	0	48475	79 3D + 19 3G + 2 3H
28	1E	0	48642	48 1I + 37 1G2 + 9 1D1
29	1A_1	0	50412	57 1G2 + 21 1S2 + 18 1S1
30	1A_2	0	50540	58 1I + 42 1F
31	1T_2	0	51406	43 1G2 + 22 1I + 18 1F
32	1T_2	0	51995	74 3F2 + 26 3F1
33	1T_1	0	52204	61 1F + 17 1I + 15 1G1
34	3T_1	0	57039	57 3P1 + 19 3F2 + 12 3P2
35	3T_2	0	57173	61 3F1 + 18 3F2 + 15 3D
36	1T_2	0	60211	40 1G1 + 25 1I + 15 1D2
37	1A_1	0	60860	37 1S2 + 37 1G1 + 10 1S1
38	1E	0	61751	54 1D1 + 34 1D2 + 7 1G2
39	1T_1	0	62434	54 1G1 + 36 1G2 + 7 1F
40	3T_1	0	64466	53 3F1 + 19 3H + 18 3G
41	1E	0	71113	30 1G1 + 23 1D2 + 20 1I
42	1T_2	0	76690	59 1D1 + 19 1F + 10 1D2
43	1A_1	0	87780	57 1S1 + 26 1G1 + 8 1S2

^aExperimental energy levels are taken from reference 11.

4. Theoretical Crystal Field Parameters

4.1 Point Charge Crystal Field

The crystallographic data of Euler and Bruce [14] on YAG are given in table 13. The yttrium site (24c) and the Al₂ site (24d) have been chosen to have the principal axis of each site along the crystallographic *c*-axis. The crystal field components, A_{nm} , for the Al₂ site are given in table 14. The various contributions to the A_{nm} are individually given, but most of our analysis will center about the point charge values of A_{nm} (for the dipole contribution, the polarizabilities of Schmidt et al [15] are used). In tetrahedral coordination (Al₂), the lattice sum components should be such that $|A_{44}/A_{40}| = (5/14)^{1/2}$, which for the point charge given in table 14, $|A_{44}/A_{40}| = 0.3928$, which is considerably less than the true tetrahedral value. From these results one would expect that a tetrahedral approximation to the analysis of ions occupying the Al₂ site would be a rather poor one. The corresponding A_{nm} for the Al₁ site (16a) are given in table 15. In this table the crystal field components were first computed in the crystallographic coordinates and then rotated so that the principal axis of C_{3i} was parallel to the (111) crystallographic axis. If the site were pure octahedral, we would have $|A_{43}/A_{40}| = (10/7)^{1/2} = 1.1952$, and for the point charge values of A_{40} and A_{43} of table 15, $|A_{43}/A_{40}| = 1.1243$, which is quite close to the octahedral value. Of course the A_{20} value is significantly different from the octahedral value of zero.

In the point charge or point multipole theory of the crystal field interaction, the theoretical crystal field parameters are given by

$$B_{nm} = \rho_n A_{nm} \quad , \quad (6)$$

where the A_{nm} are the crystal field components given in tables 14 and 15 and ρ_n is an effective radial expectation value. To relate the theoretical B_{nm} with those obtained by fitting the experimental data, we use the concept of a rotational invariant [16,17], which we define as

$$S_n(B) = \left(\sum_{m=-n}^n B_{nm}^* B_{nm} \right)^{1/2} \quad . \quad (7)$$

For $n = 4$ and C_{3i} symmetry, we have

$$S_4(B) = (B_{40}^2 + 2B_{43}^2)^{1/2}, \quad (8)$$

and from equation (6) we obtain

$$S_4(B) = \rho_4 S_4(A), \quad (9)$$

where

$$S_4(A) = (A_{40}^2 + 2A_{43}^2)^{1/2}.$$

For cubic symmetry and using equation (2), we obtain

$$S_4(B) = \sqrt{27/7} |B_{40}^e|, \quad (10)$$

where the B_{40}^e are the experimental values given in table 1. The results of table 15 for the point charge A_{4m} along with the B_{40}^e given in table 1 were used to obtain ρ_4 with

$$\rho_4 = \frac{\sqrt{27/7} |B_{40}^e|}{S_4(A)}. \quad (11)$$

In ions for which we have more than one set of data, we selectively average the ρ_4 obtained from equation (11). If we assume that the wavefunctions expand from the Hartree-Fock value, then we assume that

$$\rho_n = \langle r^n \rangle_{HF} \tau^n, \quad (12)$$

where this result is obtained by assuming the radial wavefunction $R(r) = R_{HF}(\tau r)$. Using equation (12) we have

$$\frac{1}{\tau^2} = (\rho_4 / \langle r^4 \rangle_{HF})^{1/2}, \quad (13)$$

and from equation (12) for $n = 2$, we obtain

$$\rho_2 = \langle r^2 \rangle_{HF} (\rho_4 / \langle r^4 \rangle_{HF})^{1/2}, \quad (14)$$

which can be used to obtain theoretical values of B_{2m} by equation (6). The ρ_2 and ρ_4 determined by equations (14) and (11) were used in equation (6) to determine values of the crystal field parameter for Cr^{3+} . These values of B_{nm} along with the $F^{(k)}$ of table 8 and with $\zeta = 220 \text{ cm}^{-1}$ (80 percent of the free ion value) were used to calculate the ground-state splitting (0.53 cm^{-1}) and the splitting of the 2E level (19.6 cm^{-1}). Both of these calculated splittings were much too large. Consequently, the value of B_{20} was varied to obtain a best fit to these splittings, and a value of $B_{20} = 2832 \text{ cm}^{-1}$ was found, which is approximately 0.5301 times the value given by equation (14). Thus all the values of ρ_2 given by equation (14) were multiplied by 0.5301. The values of ρ_4 were obtained from equation (11) and these values are given in table 16 for the triply ionized $3d^N$ transition metal ion series. In obtaining these results, we used the Hartree-Fock values of $\langle r^n \rangle$ given by Fraga et al [18]. Further, the results obtained from the experimental values of ρ_4 were linear least-squares fit to obtain values of ρ_2 and ρ_4 for ions not reported.

The values of ρ_2 and ρ_4 given in table 16 were used in equation (6) to obtain crystal field parameters B_{nm} which were used (fixed) to fit the experimental data given in tables 2 through 12 with $F^{(2)}$ and $F^{(4)}$ varying. The resulting $F^{(2)}$ and $F^{(4)}$ were linear least-squares fit, and the final $F^{(k)}$ and B_{nm} are given in table 17. Since most of the experimental data are analyzed in terms of Racah parameters B and C , as well as various crystal field parameters, two sets of these parameters (Macfarlane's [19] and Bellhauser's [20]) are given in table 18.

The set of parameters given in table 17, along with the spin-orbit coupling set at 80 percent of the free ion value [21] and $\alpha = 30 \text{ cm}^{-1}$, was used to calculate the energy levels for the $3d^1$ through the $3d^9$ ions. The results are given in tables 19 through 27.

Table 13. Crystallographic data on $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Cubic O_h^{10} ($Ia3d$) No. 230, $z = 8$]

Ion	Site	Symm	x^a	y	z	q	$\alpha(\text{\AA}^3)^{(b)}$
Al_1	16(a)	C_{3i}	0	0	0	3	0.0530
Al_2	24(d)	S_4	0	1/4	3/8	3	0.0530
Y	24(c)	D_2	0	1/4	1/8	3	0.870
O	96(h)	C_1	-0.0306	-0.0512	0.1500	-2	1.349

^aX-ray data, $a = 12.000 \text{ \AA}$, reference 14.

^bTaken from reference 15.

Table 14. Lattice sum, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Al_2 ion in $24(d)$ (S_4) site in $\text{Y}_3\text{Al}_5\text{O}_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,355	-2,604	14,013	17,765
$\text{Re}A_{32}$	-27,522	8,609	-11,957	-30,870
$\text{Im}A_{32}$	37,839	-11,913	6,332	32,258
A_{40}	-25,089	11,879	-8,516	-21,726
$\text{Re}A_{44}$	-3,763	1,614	1,964	-185.1
$\text{Im}A_{44}$	-9,108	4,740	-2,875	-7,243
$\text{Re}A_{52}$	-2,931	2,287	-3,498	-4,142
$\text{Im}A_{52}$	4,328	-3,207	3,640	4,762
$ \text{A}_{44} $	9,855	—	—	7,245

Table 16. Linear least-squares best fit values of ρ_2 and ρ_4 for triply ionized transition metal ions in octahedral (C_{3i}) site in YAG

Ion	$3d^N$	$\rho_2(\text{\AA}^2)$	$\rho_4(\text{\AA}^4)$
Ti	d^1	0.4301	1.3431
V	d^2	0.4234	1.3039
Cr	d^3	0.4142	1.2647
Mn	d^4	0.4050	1.2255
Fe	d^5	0.3963	1.1864
Co	d^6	0.3855	1.1472
Ni	d^7	0.3756	1.1080
Cu	d^8	0.3660	1.0689
Zn	d^9	0.3567	1.0297

Table 18. Racah parameters, B and C ; Macfarlane's parameters, Dq , v , and v' ; and Ballhausen's parameters, Dq , $D\sigma$, and $D\tau$, for triply ionized transition metal ions in octahedral (C_{3i}) site in YAG.

Ion	$3d^N$	B	C	$Dq^{(a)}$	v	v'	$Dq^{(b)}$	$D\sigma$	$D\tau$
Ti	d^1	—	—	1839	758.0	-776.1	1810	-421.9	76.15
V	d^2	748.1	2868	1786	747.7	-759.0	1757	-413.5	73.93
Cr	d^3	783.0	3088	1732	735.5	-741.1	1704	-404.5	71.71
Mn	d^4	817.8	3309	1678	723.3	-723.3	1651	-395.5	69.49
Fe	d^5	852.7	3529	1625	712.7	-705.9	1599	-387.0	67.27
Co	d^6	887.6	3749	1571	695.8	-685.7	1546	-376.5	65.04
Ni	d^7	922.5	3969	1517	681.6	-666.8	1493	-366.8	62.82
Cu	d^8	957.3	4190	1464	668.3	-648.3	1441	-357.4	60.60
Zn	d^9	—	—	1410	655.8	-630.2	1387	-348.3	58.38

^aReference 19. ^bReference 20.

Table 15. Lattice sum, A_{nm} ($\text{cm}^{-1}/\text{\AA}^n$), for Al_1 ion in $16(a)$ (C_{3i}) site in $\text{Y}_3\text{Al}_5\text{O}_{12}$

[Rotated so that the z-axis is parallel to the (111) crystallographic axis]

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,836	-1,107	-13,553	-7,823
A_{40}	-20,054	8,166	3,273	-8,615
$\text{Re}A_{43}$	2,813	-1,422	6,253	7,644
$\text{Im}A_{43}$	-22,370	8,639	2,348	-11,383
$ \text{A}_{43} $	22,546	—	—	13,711

Table 17. Linear least-squares best fit values of $F^{(k)}$ (cm^{-1}) and B_{nm} (cm^{-1}) for triply ionized transition metal ions in the octahedral site (C_{3i}) in YAG

Ion	$3d^N$	$F^{(2)}$	$F^{(4)}$	B_{20}	B_{40}	B_{43}
Ti	d^1	—	—	2953	-26934	30280
V	d^2	56732	36132	2895	-26148	29397
Cr	d^3	59983	38912	2832	-25363	28514
Mn	d^4	63234	41688	2769	-24577	27631
Fe	d^5	66485	44463	2709	-23792	26748
Co	d^6	69736	47239	2635	-23006	25865
Ni	d^7	72987	50015	2568	-22221	24982
Cu	d^8	76238	52790	2502	-21435	24099
Zn	d^9	—	—	2438	-20650	23216

Table 19. Energy levels (cm^{-1}) of Ti^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 122.24$ (cm^{-1})

Level No.	IR ^a	Energy	Free-ion state (%)
1	6	0	100 2D
2	4,5	128	100 2D
3	4,5	868	100 2D
4	4,5	18773	100 2D
5	6	18787	100 2D

^a4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and Γ_6 irreducible representations of the C_{3i} double group. Levels labeled 6 are also doublets.

Table 20. Energy levels (cm^{-1}) of V^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 164.80$ (cm^{-1})

Level No.	IR ^a	Energy	Free-ion state (%)
1	1	0	90 3F + 10 3P
2	2,3	13	90 3F + 10 3P
3	2,3	156	93 3F + 7 3P
4	2,3	313	92 3F + 8 3P
5	1	386	93 3F + 7 3P
6	1	441	92 3F + 8 3P
7	2,3	10582	54 1D + 46 1G
8	1	11086	62 1D + 37 1G
9	2,3	11181	54 1D + 46 1G
10	1	16405	100 3F
11	2,3	16413	100 3F
12	1	16734	100 3F
13	1	16737	100 3F
14	2,3	16783	100 3F
15	2,3	16826	100 3F
16	1	23377	68 1G + 31 1S
17	1	25453	88 3P + 12 3F
18	2,3	25456	88 3P + 12 3F
19	1	26436	92 3P + 8 3F
20	1	26447	92 3P + 7 3F
21	2,3	26504	93 3P + 7 3F
22	2,3	26565	93 3P + 7 3F
23	2,3	28764	57 1G + 43 1D
24	1	28805	62 1G + 37 1D
25	1	31367	100 1G
26	2,3	31837	99 1G + 1 1D
27	1	34650	99 3F + 1 3P
28	2,3	34651	99 3F + 1 3P
29	1	46539	51 1G + 49 1D
30	2,3	61136	69 1S + 31 1G

^aLabels 1 and 2,3 are abbreviations for the Γ_1 and $\Gamma_{2,3}$ irreducible representations of the C_{3i} group.

Table 21. Energy levels (cm^{-1}) of Cr^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and

$\zeta = 220.00$ (cm^{-1})

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	4,5	0	100 4F	31	4,5	34715	50 2H + 38 2D2 + 10 2D1
2	6	0	100 4F	32	4,5	37935	29 2H + 20 4F + 20 4P
3	4,5	15099	61 2G + 19 2H + 17 2D2	33	6	38024	28 4P + 27 4F + 19 2H
4	6	15119	61 2G + 19 2H + 17 2D2	34	4,5	38036	23 2H + 22 4F + 22 4P
5	6	15788	41 2G + 34 2H + 20 2P	35	4,5	38130	52 4P + 48 4F
6	4,5	15816	40 2G + 34 2H + 21 2P	36	4,5	38273	32 4P + 32 4F + 14 2H
7	4,5	16062	38 2G + 32 2H + 23 2P	37	6	38311	24 4P + 22 4F + 21 2H
8	4,5	17163	100 4F	38	4,5	38381	27 4P + 26 4F + 18 2H
9	4,5	17205	99 4F + 1 2G	39	4,5	39898	58 4P + 41 4F
10	6	17250	99 4F + 1 2G	40	6	39916	58 4P + 41 4F + 1 2P
11	4,5	17307	98 4F + 1 2G	41	4,5	43545	56 2F + 40 2D2 + 2 2G
12	6	17630	99 4F + 1 2G	42	6	43586	56 2F + 40 2D2 + 2 2G
13	4,5	17637	99 4F + 1 2G	43	4,5	43768	63 2F + 35 2D2 + 1 2G
14	4,5	22114	30 2H + 29 2D1 + 20 2D2	44	4,5	45378	99 2F
15	6	22750	35 2H + 28 2D1 + 18 2D2	45	4,5	49752	65 2H + 33 2G + 2 2D2
16	4,5	22846	35 2H + 28 2D1 + 18 2D2	46	6	49843	64 2H + 33 2G + 1 2D2
17	4,5	24405	58 4F + 41 4P	47	4,5	50494	69 2H + 29 2G + 1 2P
18	6	24408	58 4F + 41 4P	48	4,5	51132	30 2G + 22 2H + 19 2F
19	4,5	24999	52 4F + 47 4P	49	4,5	51728	27 2H + 26 2G + 21 2F
20	6	25012	51 4F + 48 4P	50	6	51817	26 2G + 26 2H + 22 2F
21	4,5	25025	51 4F + 49 4P	51	4,5	54078	41 2D2 + 22 2D1 + 22 2G
22	4,5	25036	50 4F + 50 4P	52	6	54090	41 2D2 + 22 2D1 + 22 2G
23	4,5	29991	100 2G	53	4,5	57404	69 2F + 23 2P + 7 2H
24	4,5	32345	57 2G + 37 2H + 4 2D2	54	6	57410	68 2F + 24 2P + 7 2H
25	6	32378	58 2G + 36 2H + 4 2D2	55	4,5	57542	69 2F + 24 2P + 6 2H
26	4,5	32662	46 2H + 30 2G + 23 2P	56	6	72614	60 2D1 + 19 2D2 + 14 2F
27	4,5	32823	52 2G + 44 2H + 3 2D2	57	4,5	72734	60 2D1 + 19 2D2 + 14 2F
28	4,5	32975	50 2H + 28 2G + 19 2P	58	4,5	73980	60 2D1 + 23 2D2 + 13 2F
29	6	33077	50 2H + 25 2G + 21 2P	59	6	74606	64 2D1 + 17 2H + 14 2G
30	6	34709	49 2H + 38 2D2 + 10 2D1	60	4,5	74642	64 2D1 + 17 2H + 14 2G

^aLabels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and Γ_6 irreducible representations of the C_{3i} double group. Levels labeled 6 are also doublets.

Table 22. Energy levels (cm^{-1}) of Mn^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 289.44$ (cm^{-1})

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	1	0	99 5D	44	1	21137	95 3G + 3 3F2 + 1 3H
2	2,3	12	99 5D	45	1	21140	33 1G1 + 23 1I + 23 1S2
3	1	24	99 5D	46	1	21370	91 3F2 + 7 3F1 + 1 5D
4	2,3	35	99 5D	47	2,3	21376	90 3F2 + 7 3F1 + 1 3G
5	2,3	50	100 5D	48	1	24200	52 3D + 44 3G + 4 3H
6	1	60	100 5D	49	2,3	24201	52 3D + 44 3G + 4 3H
7	1	66	100 5D	50	1	24202	52 3D + 44 3G + 4 3H
8	1	3295	38 3H + 18 3G + 15 3F1	51	2,3	24204	52 3D + 44 3G + 4 3H
9	1	3354	39 3H + 18 3G + 15 3F1	52	2,3	27088	60 1I + 23 1G2 + 8 1G1
10	2,3	3455	39 3H + 17 3G + 15 3F1	53	1	27310	64 1I + 21 1G2 + 7 1G1
11	2,3	3614	41 3H + 17 3G + 15 3F1	54	1	27328	92 1I + 8 1F
12	2,3	3918	41 3H + 15 3G + 14 3F1	55	1	28890	40 1I + 24 1G2 + 20 1G1
13	1	3921	41 3H + 15 3G + 14 3F1	56	2,3	29238	39 1I + 26 1G2 + 20 1G1
14	1	12948	32 1I + 30 1G2 + 23 1G1	57	2,3	30403	39 3G + 30 3H + 19 3P1
15	2,3	13108	35 1I + 28 1G2 + 23 1G1	58	2,3	30440	39 3G + 29 3H + 19 3P1
16	2,3	14297	59 1I + 20 1D2 + 10 1G1	59	1	30467	40 3G + 29 3H + 18 3P1
17	1	16316	98 5D + 1 3H	60	1	30477	41 3G + 28 3H + 18 3P1
18	2,3	16324	98 5D + 1 3H	61	2,3	30797	43 3G + 27 3H + 19 3P1
19	2,3	16347	99 5D	62	1	30799	44 3G + 28 3H + 19 3P1
20	1	16936	97 5D + 1 3H + 1 3P2	63	2,3	31190	41 1D2 + 32 1G2 + 16 1I
21	1	16936	97 5D + 1 3H + 1 3P2	64	1	32618	33 3D + 26 3G + 24 3F1
22	2,3	17031	97 5D + 1 3H + 1 3F2	65	1	32645	32 3D + 26 3G + 24 3F1
23	2,3	17114	97 5D + 1 3H + 1 3F2	66	2,3	32656	31 3D + 27 3G + 23 3F1
24	1	17173	97 5D + 1 3F2 + 1 3H	67	2,3	32682	29 3D + 28 3G + 23 3F1
25	1	17205	97 5D + 1 3F2 + 1 3H	68	2,3	32819	33 3G + 31 3D + 24 3F1
26	2,3	17260	97 5D + 1 3F2 + 1 3H	69	1	32821	33 3G + 31 3D + 24 3F1
27	2,3	18031	84 3H + 14 3G + 1 3D	70	1	34849	48 3H + 32 3F2 + 6 3G
28	2,3	18049	84 3H + 14 3G + 1 3D	71	1	34873	48 3H + 33 3F2 + 5 3G
29	1	18051	84 3H + 14 3G + 1 3D	72	2,3	34905	47 3H + 33 3F2 + 6 3F1
30	1	18061	84 3H + 14 3G + 1 3D	73	2,3	34944	47 3H + 33 3F2 + 6 3F1
31	1	18344	46 3H + 20 3G + 17 3P2	74	1	35176	51 3H + 30 3F2 + 6 3F1
32	2,3	18402	45 3H + 22 3G + 17 3P2	75	2,3	35182	50 3H + 29 3F2 + 6 3F1
33	1	18640	46 3H + 19 3P2 + 18 3G	76	1	36670	49 3H + 25 3F2 + 18 3D
34	1	18742	45 3H + 21 3G + 19 3P2	77	2,3	36670	49 3H + 26 3F2 + 18 3D
35	2,3	18799	45 3H + 20 3G + 19 3P2	78	1	37256	46 3H + 28 3D + 16 3F2
36	2,3	18879	44 3H + 20 3G + 19 3P2	79	1	37264	45 3H + 28 3D + 16 3F2
37	2,3	19273	38 3F2 + 32 3H + 13 3F1	80	2,3	37274	45 3H + 29 3D + 17 3F2
38	2,3	19333	40 3F2 + 31 3H + 13 3F1	81	2,3	37297	44 3H + 30 3D + 17 3F2
39	1	19379	40 3F2 + 32 3H + 13 3F1	82	2,3	39307	45 3D + 41 3G + 11 3H
40	1	19424	41 3F2 + 32 3H + 13 3F1	83	1	39310	46 3D + 41 3G + 11 3H
41	2,3	19650	40 3F2 + 32 3H + 12 3F1	84	2,3	39313	46 3D + 41 3G + 11 3H
42	1	19662	41 3F2 + 32 3H + 12 3F1	85	1	39316	46 3D + 41 3G + 11 3H
43	2,3	21132	93 3G + 4 3F2 + 1 3H	86	1	40104	47 3G + 34 3F2 + 15 3D

Table 22. Energy levels (cm^{-1}) of Mn^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 289.44$ (cm^{-1}) (cont'd)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
87	1	40146	46 3G + 34 3F2 + 15 3D	115	1	54639	68 3F1 + 18 3H + 9 3P1
88	2,3	40226	46 3G + 33 3F2 + 16 3D	116	2,3	55026	72 3F1 + 18 3H + 5 3P1
89	2,3	40378	46 3G + 33 3F2 + 17 3D	117	1	55055	72 3F1 + 17 3H + 5 3P1
90	2,3	40681	44 3G + 27 3D + 26 3F2	118	1	58711	91 3F1 + 8 3F2
91	1	40701	44 3G + 28 3D + 26 3F2	119	2,3	58711	91 3F1 + 8 3F2
92	1	41720	38 1G2 + 23 1S2 + 19 1I	120	1	61623	50 3P1 + 22 3F2 + 16 3P2
93	2,3	42473	41 1F + 23 1I + 17 1G1	121	2,3	61627	50 3P1 + 22 3F2 + 16 3P2
94	1	42813	83 1I + 6 1G2 + 3 1D1	122	2,3	62141	44 3P1 + 24 3F2 + 12 3F1
95	2,3	43437	78 1I + 8 1G2 + 5 1F	123	2,3	62260	44 3P1 + 23 3F2 + 12 3P2
96	1	43446	40 1F + 19 1I + 18 1G2	124	1	62342	44 3P1 + 23 3F2 + 12 3P2
97	1	43537	51 3P2 + 22 3F2 + 12 3G	125	1	62385	44 3P1 + 22 3F2 + 13 3P2
98	1	43565	49 3P2 + 20 3F2 + 12 3G	126	2,3	63350	62 1G1 + 24 1G2 + 8 1D2
99	2,3	43603	46 3P2 + 19 3F2 + 11 3G	127	1	64278	63 1G1 + 36 1I + 1 1F
100	2,3	43706	45 3P2 + 17 3F2 + 11 3G	128	1	64891	59 3F1 + 16 3D + 15 3G
101	2,3	43867	22 1F + 19 3P2 + 14 1G2	129	2,3	64892	58 3F1 + 16 3D + 14 3G
102	2,3	43905	40 1F + 11 1G1 + 10 3P2	130	2,3	65357	60 1G1 + 34 1I + 2 1F
103	1	43983	49 1F + 12 3P2 + 10 1G1	131	2,3	66284	54 3F1 + 15 3D + 15 3G
104	1	44088	42 3P2 + 20 3F2 + 13 1F	132	2,3	66292	54 3F1 + 15 3D + 14 3G
105	2,3	44116	40 3P2 + 19 3F2 + 10 1G2	133	1	66299	53 3F1 + 16 3D + 14 3G
106	1	46037	41 1G2 + 27 1I + 18 1S2	134	1	66306	54 3F1 + 16 3D + 14 3G
107	2,3	51578	61 1D2 + 10 1I + 9 1G1	135	2,3	72473	37 1G1 + 27 1G2 + 19 1D2
108	1	51653	71 1D2 + 9 1I + 9 1G1	136	1	73177	37 1G1 + 24 1G2 + 15 1D2
109	1	52486	81 1F + 11 1G2 + 7 1I	137	1	75774	34 1G1 + 24 1I + 18 1S2
110	2,3	53409	49 1G2 + 38 1F + 6 1D2	138	1	78667	54 1D1 + 18 1F + 12 1G1
111	1	53533	52 1F + 45 1G2 + 3 1I	139	2,3	81044	57 1D1 + 18 1F + 10 1G2
112	2,3	54472	68 3F1 + 18 3H + 10 3P1	140	2,3	82543	77 1D1 + 20 1D2 + 1 1G2
113	2,3	54537	68 3F1 + 18 3H + 9 3P1	141	1	102454	73 1S1 + 13 1G1 + 11 1S2
114	1	54606	68 3F1 + 18 3H + 9 3P1				

^aLabels 1 and 2,3 are abbreviations for the Γ_1 and $\Gamma_{2,3}$ irreducible representations of the C_{3i} group.

Table 23. Energy levels (cm^{-1}) of Fe^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 370.40$ (cm^{-1})

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	4,5	0.00	100 6S	44	6	34446	30 2G2 + 24 2F1 + 21 2H
2	6	0.187	100 6S	45	4,5	34478	29 2G2 + 23 2F1 + 21 2H
3	4,5	0.262	100 6S	46	4,5	34972	30 2G2 + 23 2F1 + 20 2H
4	4,5	12196	21 4G + 18 2I + 16 2H	47	4,5	37052	35 2I + 23 2G2 + 14 2F2
5	4,5	12725	38 4G + 26 4P + 9 2I	48	4,5	37848	49 2I + 20 2G2 + 10 2F2
6	6	12729	38 4G + 26 4P + 10 2I	49	6	37898	29 2G2 + 23 2F2 + 19 2I
7	6	13046	57 4G + 38 4P + 4 4F	50	4,5	37950	30 2I + 28 2G2 + 17 2F2
8	4,5	13105	57 4G + 39 4P + 3 4F	51	6	38553	28 4P + 24 4F + 19 2I
9	4,5	13156	57 4G + 39 4P + 3 4F	52	4,5	38634	33 4P + 28 4F + 14 2I
10	4,5	13480	37 4G + 25 4P + 11 2I	53	4,5	38949	30 2I + 18 4P + 16 4F
11	6	13608	20 2I + 20 4G + 18 2H	54	6	39088	25 2I + 22 4P + 19 4F
12	4,5	13618	20 4G + 20 2I + 17 2H	55	4,5	39657	39 4P + 38 4F + 14 4G
13	4,5	18323	50 4G + 28 4F + 21 4D	56	6	39802	37 4P + 36 4F + 14 4G
14	6	18336	50 4G + 28 4F + 21 4D	57	4,5	39848	39 4P + 39 4F + 15 4G
15	4,5	18861	47 4G + 28 4F + 25 4D	58	4,5	39900	38 4P + 37 4F + 14 4G
16	6	18871	48 4G + 28 4F + 24 4D	59	4,5	40763	47 2I + 35 2D3 + 9 2D1
17	4,5	18872	49 4G + 28 4F + 23 4D	60	6	40814	45 2I + 35 2D3 + 9 2D1
18	4,5	18884	49 4G + 28 4F + 23 4D	61	4,5	40869	41 2I + 34 2D3 + 9 2D1
19	4,5	25784	52 2I + 39 2F1 + 3 2F2	62	4,5	41825	52 2G2 + 22 2I + 14 2G1
20	4,5	25958	46 2I + 18 2H + 17 4G	63	4,5	43883	99 4F
21	6	25990	45 2I + 22 4G + 19 2H	64	6	43887	99 4F
22	4,5	26314	40 2I + 29 4G + 17 2H	65	6	45110	68 2G2 + 10 2I + 5 2H
23	4,5	26633	89 4G + 5 2I + 3 2F1	66	4,5	45176	70 2G2 + 10 2I + 5 2D3
24	4,5	26723	95 4G + 2 2I + 1 2F1	67	4,5	46241	60 2H + 28 2F1 + 5 2G2
25	6	26737	95 4G + 2 2I + 1 2F1	68	4,5	46325	55 2H + 22 2F1 + 11 2F2
26	4,5	26956	78 4G + 13 2I + 5 2H	69	6	46373	42 2H + 18 2F2 + 17 2F1
27	4,5	26982	73 4G + 17 2I + 6 2H	70	6	46735	26 2F2 + 22 2H + 18 2G2
28	6	26986	78 4G + 14 2I + 5 2H	71	4,5	46883	34 2F2 + 20 2G2 + 14 2H
29	4,5	27891	46 2I + 23 2F1 + 11 2H	72	4,5	47324	48 2F2 + 22 2G2 + 15 2I
30	6	28000	45 2I + 23 2F1 + 12 2H	73	4,5	47617	51 2F2 + 20 2I + 19 2G2
31	4,5	28003	43 2I + 21 2F1 + 12 2H	74	4,5	48403	33 2F2 + 28 2G2 + 16 4F
32	4,5	29247	43 4D + 35 4G + 6 2H	75	4,5	48445	40 4F + 19 4G + 13 4P
33	6	29289	43 4D + 34 4G + 7 2H	76	6	48533	40 2F2 + 37 2G2 + 7 2I
34	4,5	29418	52 4D + 41 4G + 3 4F	77	4,5	48542	37 2F2 + 19 4F + 14 2G2
35	4,5	29554	56 4D + 41 4G + 3 4F	78	4,5	48565	34 4F + 19 2F2 + 17 4G
36	6	29686	40 4D + 27 4G + 10 2I	79	6	48674	49 4F + 24 4G + 16 4P
37	4,5	29829	38 4D + 25 4G + 11 2I	80	4,5	48813	53 4F + 26 4G + 17 4P
38	4,5	29912	33 4D + 22 4G + 14 2I	81	6	49682	56 4F + 27 4G + 15 4P
39	6	29935	29 4D + 20 4G + 16 2I	82	4,5	49730	55 4F + 26 4G + 15 4P
40	4,5	32302	99 4D	83	4,5	52620	69 2S + 24 2G2 + 5 2G1
41	6	32303	99 4D	84	6	53040	42 2H + 30 2D3 + 22 2D2
42	4,5	32307	99 4D	85	4,5	53069	42 2H + 30 2D3 + 22 2D2
43	4,5	32313	99 4D	86	4,5	54048	31 2H + 22 2F2 + 18 2F1

Table 23. Energy levels (cm^{-1}) of Fe^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 370.40$ (cm^{-1}) (cont'd)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
87	4,5	54476	65 4F + 19 4D + 10 4G	107	4,5	68429	51 2D2 + 16 2G1 + 9 2G2
88	4,5	54514	63 4F + 19 4D + 9 4G	108	6	68481	47 2D2 + 16 2G1 + 11 2H
89	6	54575	61 4F + 18 4D + 9 4G	109	4,5	69067	31 2H + 22 2D3 + 18 2I
90	4,5	54731	49 4F + 16 4D + 10 2H	110	6	69666	21 2D3 + 20 2H + 16 2D2
91	6	54923	59 4F + 18 4D + 9 4G	111	4,5	69869	22 2D3 + 21 2H + 15 2F1
92	4,5	54981	65 4F + 20 4D + 10 4G	112	6	71446	77 2G1 + 6 2F2 + 5 2P
93	6	55138	29 2H + 21 2F2 + 14 2F1	113	4,5	71597	76 2G1 + 6 2F2 + 5 2P
94	4,5	55154	25 2H + 20 4F + 18 2F2	114	4,5	72031	79 2G1 + 8 2F2 + 7 2P
95	4,5	55831	28 2F1 + 19 2H + 17 2G2	115	4,5	75303	44 2G1 + 13 2D1 + 13 2G2
96	6	55938	27 2F1 + 18 2G2 + 17 2H	116	6	75729	53 2G1 + 13 2F2 + 12 2G2
97	4,5	56215	29 2F1 + 18 2H + 17 2G2	117	4,5	75826	52 2G1 + 13 2G2 + 11 2F2
98	4,5	59435	41 2H + 30 2I + 17 2F1	118	4,5	78268	72 2G1 + 17 2S + 10 2G2
99	6	59620	42 2H + 30 2I + 16 2F1	119	4,5	84683	89 2P + 4 2G2 + 4 2F2
100	4,5	59912	41 2F1 + 25 2I + 24 2F2	120	4,5	84860	86 2P + 4 2F2 + 4 2G2
101	4,5	60505	34 2H + 25 2I + 20 2F1	121	6	84892	87 2P + 4 2F2 + 4 2G2
102	4,5	64728	60 2G1 + 10 2H + 9 2D1	122	6	95434	67 2D1 + 10 2D3 + 6 2H
103	6	64792	60 2G1 + 10 2H + 9 2D1	123	4,5	95438	67 2D1 + 10 2D3 + 6 2H
104	4,5	66844	62 2D2 + 12 2G1 + 9 2F2	124	6	96691	65 2D1 + 15 2D3 + 12 2G1
105	6	67257	51 2D2 + 22 2G1 + 10 2I	125	4,5	96724	65 2D1 + 15 2D3 + 11 2G1
106	4,5	67316	51 2D2 + 22 2G1 + 10 2I	126	4,5	97034	63 2D1 + 10 2D3 + 9 2G1

^aLabels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and Γ_6 irreducible representations of the C_{3i} double group. Levels labeled 6 are also doublets.

Table 24. Energy levels (cm^{-1}) of Co^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ (cm^{-1})

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	2,3	0	100 5D	14	1	6537	45 3H + 23 3F2 + 16 3P1
2	1	8	100 5D	15	1	6825	44 3H + 25 3F2 + 15 3P1
3	1	165	100 5D	16	2,3	6940	46 3H + 24 3F2 + 14 3P1
4	2,3	250	100 5D	17	1	7272	44 3H + 24 3F2 + 14 3P1
5	2,3	373	99 5D	18	1	11037	34 3H + 33 3G + 16 3F1
6	1	512	97 5D + 1 1I	19	2,3	11108	34 3H + 34 3G + 16 3F1
7	1	528	99 5D	20	2,3	11349	39 3G + 29 3H + 16 3F1
8	1	1023	87 5D + 4 1I + 3 1G1	21	2,3	11622	36 3G + 32 3H + 16 3F1
9	2,3	1057	99 5D	22	1	11741	36 3G + 32 3H + 16 3F1
10	2,3	1061	99 5D	23	1	11808	34 3H + 33 3G + 16 3F1
11	1	128	31 1I + 26 1G1 + 19 1G2	24	2,3	15231	57 1I + 22 1G1 + 18 1G2
12	2,3	6378	44 3H + 23 3F2 + 16 3P1	25	1	15438	53 1I + 23 1G1 + 20 1G2
13	2,3	6465	44 3H + 23 3F2 + 16 3P1	26	1	16256	99 5D

Table 24. Energy levels (cm^{-1}) of Co^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ (cm^{-1}) (cont'd)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
27	1	16261	99 5D	71	2,3	36321	55 3H + 18 3G + 13 3F2
28	2,3	16273	99 5D	72	1	36445	58 3H + 15 3G + 14 3F2
29	2,3	16289	99 5D	73	2,3	36471	51 3H + 17 3G + 12 3F2
30	1	16296	99 5D	74	1	36563	52 3H + 16 3G + 9 3F2
31	1	16316	99 5D	75	2,3	36813	60 3H + 27 3G + 7 3F2
32	2,3	16317	99 5D	76	1	36823	57 3H + 21 3G + 13 3F2
33	1	20401	66 3H + 27 3F2 + 5 3F1	77	2,3	36872	59 3H + 32 3G + 2 3D
34	2,3	20404	65 3H + 26 3F2 + 5 3F1	78	1	36961	58 3H + 31 3G + 6 3F2
35	2,3	20643	65 3H + 25 3F2 + 6 3F1	79	1	37021	52 1I + 33 1F + 7 3H
36	2,3	20749	65 3H + 25 3F2 + 6 3F1	80	1	37050	46 3H + 23 3G + 8 1I
37	1	20828	67 3H + 25 3F2 + 6 3F1	81	2,3	37098	47 3H + 20 3G + 8 3F2
38	1	20854	66 3H + 25 3F2 + 6 3F1	82	2,3	38359	15 3D + 14 1F + 14 3F2
39	1	21777	48 3G + 47 3H + 4 3F2	83	1	38614	26 3D + 25 3F2 + 19 3H
40	1	21795	48 3G + 48 3H + 3 3F2	84	1	38801	17 1F + 17 3D + 13 1G2
41	2,3	21832	51 3H + 44 3G + 4 3F2	85	2,3	38868	16 1F + 14 3F2 + 14 1I
42	2,3	21898	53 3H + 41 3G + 5 3F2	86	1	39292	30 3D + 26 3F2 + 18 3H
43	2,3	22466	54 3G + 43 3H + 2 3F2	87	2,3	39475	30 3D + 26 3F2 + 18 3H
44	1	22469	54 3G + 43 3H + 1 3F2	88	1	39564	19 1F + 15 3D + 13 3F2
45	1	23628	26 1I + 21 3G + 16 3H	89	2,3	39653	31 3D + 26 3F2 + 18 3H
46	1	23832	45 3G + 30 3P2 + 13 3H	90	2,3	39784	97 3G + 1 3F2 + 1 3H
47	2,3	23863	44 3G + 33 3P2 + 11 3H	91	1	39787	96 3G + 1 3F2 + 1 3H
48	2,3	23877	40 3G + 27 3H + 12 3D	92	2,3	41737	29 3P2 + 26 3G + 23 3F2
49	1	24045	49 3G + 32 3H + 13 3D	93	2,3	41828	31 3P2 + 25 3G + 23 3F2
50	2,3	24059	48 3G + 28 3H + 12 3D	94	1	41919	32 3P2 + 25 3G + 22 3F2
51	2,3	24265	46 3G + 22 3P2 + 18 3H	95	1	41952	34 3P2 + 25 3G + 22 3F2
52	1	24362	40 3G + 21 3P2 + 10 1I	96	2,3	42600	33 3P2 + 28 3G + 20 3F2
53	2,3	24365	46 3G + 30 3P2 + 9 3H	97	1	42613	34 3P2 + 28 3G + 20 3F2
54	1	24504	49 3G + 27 3P2 + 12 3H	98	2,3	43976	33 1D2 + 23 1I + 23 1G1
55	1	24626	37 3G + 15 3H + 14 3P2	99	1	44046	80 3D + 15 3G + 2 1I
56	2,3	24957	37 1I + 14 1D2 + 11 1F	100	1	44061	82 3D + 15 3G + 2 3H
57	2,3	27783	49 3D + 47 3F2 + 1 3G	101	2,3	44067	81 3D + 15 3G + 2 3H
58	2,3	27830	49 3D + 47 3F2 + 1 3G	102	2,3	44097	82 3D + 15 3G + 2 3H
59	1	27868	49 3D + 47 3F2 + 2 3G	103	1	45367	50 1I + 19 1D2 + 19 1G1
60	1	27878	47 3D + 47 3F2 + 2 1I	104	2,3	45741	46 1I + 24 1D2 + 19 1G1
61	2,3	28094	53 3D + 43 3F2 + 2 1I	105	2,3	49708	41 1I + 31 1G2 + 18 1D2
62	1	28104	55 3D + 44 3F2 + 1 3F1	106	1	49839	60 1F + 38 1I + 1 1G1
63	2,3	30678	46 1G2 + 24 1G1 + 23 1I	107	1	50546	40 1S2 + 40 1G2 + 11 1S1
64	2,3	30883	48 1I + 17 1G2 + 16 1D2	108	2,3	52683	72 1F + 10 1I + 10 1G1
65	1	31302	48 1I + 15 1D2 + 12 1G2	109	1	53530	76 1F + 9 1I + 7 1G1
66	1	31751	50 1I + 18 1S2 + 13 1G2	110	1	54027	51 3F1 + 47 3F2 + 1 3P1
67	2,3	32911	50 3F2 + 46 3F1 + 2 1I	111	2,3	54032	51 3F1 + 47 3F2 + 1 3P1
68	1	32942	48 3F2 + 44 3F1 + 4 1I	112	1	55108	46 1G2 + 33 1F + 11 1G1
69	1	35653	27 1G2 + 24 1I + 17 3H	113	2,3	55641	48 1G2 + 34 1F + 8 1G1
70	2,3	35706	31 1G2 + 20 1I + 16 3H	114	1	57473	58 3P1 + 12 3F1 + 9 3H

Table 24. Energy levels (cm⁻¹) of Co³⁺ in Y₃Al₅O₁₂ using parameters of table 17 with $\alpha = 30$ and $\zeta = 484.80$ (cm⁻¹) (cont'd)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
115	1	57542	56 3P1 + 14 3F1 + 9 3H	129	1	64043	61 3F1 + 11 3P2 + 7 3F2
116	2,3	57570	55 3P1 + 15 3F1 + 9 3H	130	2,3	65366	58 3F1 + 15 3P2 + 8 3P1
117	2,3	57791	48 3P1 + 23 3F1 + 9 3H	131	1	65388	60 3F1 + 13 3P2 + 8 3G
118	2,3	58032	57 3P1 + 15 3F1 + 10 3H	132	2,3	65395	57 3F1 + 15 3P2 + 9 3P1
119	1	58061	57 3P1 + 14 3F1 + 10 3H	133	1	65399	60 3F1 + 14 3P2 + 8 3G
120	2,3	59977	63 3F1 + 15 3F2 + 7 3D	134	1	69443	62 1G1 + 33 1G2 + 3 1I
121	2,3	60007	64 3F1 + 15 3F2 + 8 3D	135	2,3	69469	59 1G1 + 32 1G2 + 4 1F
122	1	60048	66 3F1 + 16 3F2 + 9 3D	136	1	70869	53 1G1 + 22 1G2 + 14 1S2
123	1	60099	64 3F1 + 15 3F2 + 9 3D	137	2,3	73112	41 1D2 + 34 1G1 + 17 1G2
124	2,3	60776	68 3F1 + 19 3F2 + 9 3D	138	2,3	76771	78 1D1 + 10 1G1 + 6 1I
125	1	60806	68 3F1 + 19 3F2 + 9 3D	139	2,3	87513	73 1D1 + 15 1D2 + 9 1F
126	2,3	61798	66 1G1 + 20 1I + 9 1D2	140	1	88855	71 1D1 + 16 1D2 + 9 1F
127	1	62077	62 1G1 + 19 1I + 10 1D2	141	1	108376	71 1S1 + 13 1S2 + 11 1G1
128	2,3	63996	63 3F1 + 11 3P2 + 7 3F2				

^aLabels 1 and 2,3 are abbreviations for the Γ_1 and $\Gamma_{2,3}$ irreducible representations of the C_{3i} group.

Table 25. Energy levels (cm⁻¹) of Ni³⁺ in Y₃Al₅O₁₂ using parameters of table 17 with $\alpha = 30$ and $\zeta = 599.20$ (cm⁻¹)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	4,5	0	94 4F + 6 4P	22	4,5	22407	61 2P + 21 2H + 13 2F
2	6	354	92 4F + 7 4P	23	4,5	22948	62 2P + 22 2H + 13 2F
3	4,5	385	94 4F + 5 4P	24	4,5	25548	87 4P + 12 4F + 1 2P
4	4,5	908	90 4F + 6 4P + 2 2G	25	6	25648	85 4P + 12 4F + 1 2P
5	6	910	91 4F + 6 4P + 2 2G	26	4,5	26478	94 4P + 6 4F
6	4,5	1109	94 4F + 6 4P	27	6	26799	91 4P + 6 4F + 1 2H
7	4,5	4682	42 2G + 28 2H + 13 2D2	28	4,5	26989	92 4P + 5 4F + 1 2H
8	6	4729	43 2G + 29 2H + 13 2D2	29	4,5	27143	91 4P + 5 4F + 1 2P
9	6	14038	97 4F + 2 2G + 1 2D2	30	4,5	29650	88 4F + 5 4P + 3 2H
10	4,5	14066	98 4F + 1 2G	31	6	29656	87 4F + 5 4P + 4 2H
11	4,5	14305	98 4F + 1 2G	32	4,5	30250	97 2G + 1 2H + 1 2P
12	6	14350	97 4F + 2 2G	33	4,5	31055	55 2H + 28 2G + 9 2D1
13	4,5	14383	95 4F + 3 2G + 1 2D2	34	6	31307	54 2H + 24 2G + 9 2D1
14	4,5	14624	98 4F + 1 2G	35	4,5	31594	59 2H + 22 2G + 8 2D1
15	4,5	17383	50 2G + 46 2H + 2 4F	36	6	33728	66 2H + 19 2G + 12 2P
16	6	17542	53 2G + 42 2H + 2 4F	37	4,5	33838	66 2H + 21 2G + 11 2P
17	4,5	17995	51 2G + 46 2H + 2 4F	38	4,5	33937	61 2H + 27 2G + 10 2P
18	4,5	18248	59 2G + 16 2H + 15 2D2	39	4,5	35857	53 2H + 37 2D2 + 8 2D1
19	6	18272	58 2G + 16 2H + 16 2D2	40	6	35909	52 2H + 37 2D2 + 9 2D1
20	4,5	18424	57 2G + 19 2D2 + 15 2H	41	4,5	38962	72 2D2 + 12 2G + 11 2H
21	6	22265	60 2P + 21 2H + 12 2F	42	4,5	39156	68 2D2 + 17 2H + 11 2G

Table 25. Energy levels (cm^{-1}) of Ni^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 599.20$ (cm^{-1}) (cont'd)

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
43	6	39210	69 2D2 + 18 2H + 10 2G	52	4,5	48499	100 2F
44	4,5	40856	48 2H + 38 2F + 13 2G	53	6	51917	43 2F + 24 2P + 18 2H
45	4,5	41769	45 2F + 40 2H + 9 2G	54	4,5	52066	44 2F + 24 2P + 18 2H
46	6	41894	45 2F + 40 2H + 11 2G	55	4,5	52796	48 2F + 25 2P + 16 2H
47	4,5	42731	73 2F + 15 2H + 8 2D1	56	4,5	68497	65 2D1 + 31 2D2 + 3 2H
48	6	43482	77 2F + 11 2H + 8 2D1	57	6	68511	64 2D1 + 32 2D2 + 3 2H
49	4,5	43799	78 2F + 10 2D1 + 9 2H	58	4,5	71390	76 2D1 + 12 2F + 6 2H
50	6	46346	53 2G + 17 2H + 15 2D1	59	6	72396	75 2D1 + 12 2F + 7 2D2
51	4,5	46352	53 2G + 16 2H + 15 2D1	60	4,5	72890	73 2D1 + 13 2F + 8 2D2

^aLabels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and Γ_6 irreducible representations of the C_{3i} double group. Levels labeled 6 are also doublets.

Table 26. Energy levels (cm^{-1}) of Cu^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 728.80$ (cm^{-1})

Level No.	IR ^a	Energy	Free ion state (%)	Level No.	IR ^a	Energy	Free ion state (%)
1	1	0	100 3F	16	1	26964	85 1G + 10 1S + 3 3F
2	2,3	3	100 3F	17	2,3	29617	74 1D + 21 1G + 3 3P
3	2,3	1400	281 3F + 13 1D + 6 1G	18	1	303' -	71 1D + 25 1G + 3 3P
4	2,3	14434	99 3F	19	2,3	34653	80 1G + 15 3P + 5 3F
5	1	14583	100 3F	20	1	34780	44 1G + 42 3P + 14 3F
6	1	14814	100 3F	21	2,3	35026	57 3P + 29 3F + 13 1G
7	2,3	15000	98 3F + 1 1D + 1 1G	22	1	35114	70 3P + 27 3F + 1 1D
8	1	15162	100 3F	23	2,3	35133	61 3P + 30 3F + 7 1G
9	2,3	15969	53 1D + 24 1G + 22 3F	24	1	35388	56 1G + 30 3P + 14 3F
10	1	21784	74 3F + 24 3P + 2 1G	25	2,3	36821	71 3P + 27 3F + 1 1G
11	2,3	22141	74 3F + 26 3P	26	1	36855	71 3P + 27 3F + 1 1G
12	1	22698	72 3F + 27 3P	27	1	46631	75 1G + 25 1D
13	1	22893	68 3F + 31 3P	28	2,3	46686	68 1G + 32 1D
14	2,3	23128	67 3F + 32 3P	29	2,3	47877	77 1G + 23 1D
15	2,3	23313	65 3F + 33 3P + 1 1G	30	1	72868	89 1S + 11 1G

^aLabels 1 and 2,3 are abbreviations for the Γ_1 and $\Gamma_{2,3}$ irreducible representations of the C_{3i} group.

Table 27. Energy levels (cm^{-1}) of Zn^{3+} in $\text{Y}_3\text{Al}_5\text{O}_{12}$ using parameters of table 17 with $\alpha = 30$ and $\zeta = 923.88^a$ (cm^{-1})

Level No.	IR ^b	Energy	Free ion state (%)
1	6	0	100 2D
2	4,5	105	100 2D
3	4,5	13303	100 2D
4	4,5	14616	100 2D
5	6	15116	100 2D

^aHartree-Fock value (ref 18).

^bLabels 4,5 and 6 are abbreviations for the $\Gamma_{4,5}$ and Γ_6 irreducible representations of the C_{3i} double group. Levels labeled 6 are also doublets.

4.2 Discussion of Results

Because of the sparse experimental data on the fine structure, a detailed comparison of the calculation given in tables 19 through 27 is not possible. The only ion with reliable fine structure reported is Cr^{3+} [7, 9, 10, 22], and these data were used to determine the crystal field parameter B_{20} for Cr^{3+} .

The results given for Ti^{3+} in table 19 show considerable splitting of the lower levels, but since only room temperature absorption was reported by Karpov et al [4], no comparison can be made. The absorption spectra at room temperature were reported by Bantien et al [23] as having bands at 25,600, 19,800, and 17,100 cm^{-1} , with the band at 25,600 cm^{-1} being very strong compared to the other two bands. The two lower energy bands were assumed to be $3d^1 \rightarrow 3d^1$ transitions, but the high-energy band is unknown and under investigation.

The energy levels of V^{3+} given in table 20 show considerable splitting of the ground state (3T_1 in cubic approximation) so that if the absorption spectra were taken at low temperature rather than at room temperature as reported by Weber and Riseberg [5], the lines should be much narrower. Surprisingly, the spin-orbit and the two-fold field B_{20} do not mix the states much, and the usual assumption of spin-forbidden transitions in the analysis of the absorption spectra should be reasonably valid. It should be interesting to analyze the spectra taken at low temperature.

There are a considerable number of papers reporting the experimental data and analysis of experimental data on Cr^{3+} in YAG. The calculated splitting of the ground state, 0.62 cm^{-1} , is slightly larger than the experimental value [10] 0.53 cm^{-1} , but the splitting of the R lines calculated to be 19.5 cm^{-1} compares well with the experimental value [10] 19.6 cm^{-1} (levels 3 and 4 in table 21). The calculated centroid of the R lines is shifted approximately 600 cm^{-1} from the experimental value reported by Henry et al [10]. Comparison of the results in table 21 with the experimental results given in tables 4 through 7 shows, in general, that the calculated values are slightly higher than the experimental results. Slight adjustment of the parameters can bring the calculated values into better agreement with any one set of the experimental results. Also, mixing of the states by the spin-orbit does not occur below level number 32 ($37,935 \text{ cm}^{-1}$) in table 21, which should make identification of the fine structure somewhat easier.

Using the parameters of table 17, we calculated the energy levels for Mn^{3+} , and the results are given in table 22. For this set of parameters, the high spin state 5D is the lowest, which contradicts the assumptions made by Arsenov and Sviridov [11] in analyzing the experimental data. However, only three energy levels were reported so that a re-analysis of the experimental data would be inconclusive. We found that if we reduced $F^{(4)}$ from $41,688 \text{ cm}^{-1}$ to $33,332 \text{ cm}^{-1}$, the ground state became mixed with the 3H levels (the low spin ground states assumed in ref 11).

The energy levels of Fe^{3+} given in table 23 were obtained using the parameters given in table 17 with $\alpha = 30 \text{ cm}^{-1}$ and $\gamma = 0$. The ground state (6A_1 in the cubic approximation) is split by the spin orbit and the two-fold field, B_{20} . We have been unable to find any reported measurement of this ground state splitting. The spin-orbit coupling mixes the spin of a large number of levels, and the calculated energy levels appear to be considerably higher than experiment. We have not tried to fit the experimental data starting with the parameters of table 23. A comparison of the parameters obtained here for Fe^{3+} in YAG with the parameters for Fe^{3+} in $\text{Ho}_3\text{Al}_5\text{O}_{12}$ or $\text{Er}_3\text{Al}_5\text{O}_{12}$ shows that the $F^{(k)}$ for YAG are larger but B_{20} is smaller than these compounds [2]. The B_{40} and B_{43} crystal field parameters are approximately the same. The experimental data for Fe^{3+} in the rare earth garnets were considerably different than reported for Fe^{3+} in YAG [12,13].

The energy levels for Co^{3+} were calculated using the parameters given in table 17 with $\alpha = 30 \text{ cm}^{-1}$ and $\gamma = 0$; the results are given in table 24. As for Mn^{3+} , the calculated ground state disagrees with that given by Arsenev and Sviridov [11]. However, we have observed that a reduction of the parameter α causes the ground state, which in table 24 is predominately 5D , to become significantly mixed with 3F_2 , 3H , and 1I . If more data were available, a fitting starting with the parameters of table 17 could be undertaken.

The energy levels for Ni^{3+} , Cu^{3+} , and Zn^{3+} were calculated using the parameters in table 17. We are unaware of any data reported on these ions in YAG, and we are uncertain as to the possibility of doping YAG with these ions. It would seem that doping with Ni^{3+} would be possible since the spectrum of this ion in the rare earth garnets has been reported [24].

Author's note: Since this report has been written an article has appeared (in Russian) by Yu. A. Voitukevich, M. V. Konzhik, V. V. Kuz'min, M. G. Livshitz and M. L. Meil'man: *Energy Structure of Fe^{3+} Impurity Ions in Yttrium Aluminum Garnet ($\text{Y}_3\text{Al}_5\text{O}_{12}$) Crystals*, Opt. Spectrosc. 63 (1987), 810. Consequently, a supplement to this report will be issued which will include an analysis of this latest data.

References

1. D. L. Wood and J. P. Remeika, *Optical Absorption of Tetrahedral Co^{3+} and Co^{2+} in Garnets*, J. Chem. Phys. 46 (1967), 3595.
2. C. A. Morrison, J. D. Bruno, and G. A. Turner, *Analysis of the Spectra of Triply Ionized Iron in Rare-Earth Aluminum Garnets*, Harry Diamond Laboratories, HDL-TR-2113 (September 1987).
3. E. Konig and S. Kremer, *Ligand Field Energy Diagrams*, Plenum Press, New York (1977).
4. I. I. Karpov, B. N. Grechusnikov, and Kh. S. Bagdarsarov, *Use of Polarized Luminescence to Investigate Luminescence in Yttrium-Aluminum Garnet Crystals with Added Titanium*, Sov. Phys. Crystallogr. 23 (1978), 688.
5. M. J. Weber and L. A. Riseberg, *Optical Spectra of Vanadium Ions in Yttrium Aluminum Garnet*, J. Chem. Phys. 55 (1971), 2032.
6. B. K. Sevast'yanov, D. T. Sviridov, V. P. Grekhovo, L. B. Pasternak, R. K. Sviridova, and T. F. Vermeichik, *Optical Absorption Spectra of Excited Cr^{3+} Ions in Yttrium Aluminum Garnet*, Sov. J. Electron. 2 (1973), 339.
7. D. T. Sviridov, R. K. Sviridova, N. I. Kulik, and V. B. Glasko, *Optical Spectra of the Iso-Electronic Ions V^{2+} , Cr^{3+} , and Mn^{4+} in an Octahedral Coordination*, J. Appl. Spectrosc. 30 (1979), 334.
8. B. N. Grechusnikov, T. F. Veremeichik, and I. N. Kalinkina, *Analysis of Spectra of Cr^{3+} Impurity Ions in Series of Crystals Allowing for the Tree's Correction*, Sov. Phys. Crystallogr. 22 (1978), 525.
9. Z. T. Azamatov, P. A. Arsenev, T. Yu. Geraskina, and M. V. Chukichev, *Properties of Chromium Ions in the Lattice of Yttrium Aluminum Garnet (YAG)*, Phys. Status Solidi A: 1 (1970), 801.

10. M. O. Henry, J. P. Larkin, and G. F. Imbusch, *Luminescence from Chromium Doped Yttrium Aluminum Garnet*, Proceedings of the Royal Irish Academy, 75 (1975) 97.
11. P. A. Arsenov and D. T. Sviridov, *Absorption Spectra of Yttrium Aluminum Garnet (YAG) with Contaminant Ions of the Iron Group*, Sov. Phys. Crystallogr. 14 (1970), 578.
12. T. F. Veremeichik, B. N. Grechusnikov, T. M. Varina, D. T. Sviridov, and I. N. Kalinkina, *Absorption Spectra and Calculation of Energy-Level Diagram of Fe^{3+} and Mn^{2+} Ions in Single Crystals of Yttrium Aluminum Garnet, Orthoclase, and Manganese Silicate*, Sov. Phys. Crystallogr. 19 (1975), 742.
13. Y. Sugitani, K. Tagawa, and K. Kato, *Optical Absorption Spectra of Iron (III) and Chromium (III) Doped in Synthetic Yttrium-Aluminum-Garnets (YAG)*, Mineral J. 7 (1974), 445.
14. F. Euler and J. A. Bruce, *Oxygen Coordinates of Compounds with Garnet Structure*, Acta Cryst. 19 (1965), 971.
15. P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. B19 (1979), 5525.
16. N. Karayianis, C. A. Morrison, and D. E. Wortman, *Crystal Field Parameters for the Pentaphosphates of Neodymium and Europium*, J. Chem. Phys. 64 (1976), 3890.
17. R. P. Leavitt, *On the Rule of Certain Rotation Invariants in Crystal-Field Theory*, J. Chem. Phys. 77 (1982), 1661.
18. S. Fraga, K. M. S. Saxena, and J. Karwowski, *Physical Science Data: 5. Handbook of Atomic Data*, Elsevier, New York (1976). Also see C. A. Morrison and R. G. Schmalbach, *Approximate Values of $\langle r^k \rangle$ for the Divalent, Trivalent, and Quadrivalent Ions with the $3d^N$ Electronic Configuration*, Harry Diamond Laboratories, HDL-TL-85-3 (July 1985). Also see C. A. Morrison, N. Karayianis, and D. Wortman, *Rare-Earth Ion-Host Lattice Interactions 4. Predicting Spectra and Intensities of Lanthanides in Crystals*, Harry Diamond Laboratories, HDL-TR-1816 (June 1977).

19. R. M. Macfarlane, *Analysis of the Spectrum of d^3 Ions in Trigonal Crystal Fields*, J. Chem. Phys. 39 (1963), 3118.
20. C. J. Ballhausen, *Ligand Field Theory*, McGraw-Hill, New York (1962), 104.
21. P. H. M. Uylings, A. J. J. Raassen, and J. F. Wyart, *Energies of N Equivalent Electrons Expressed in Terms of Two-Electron Energies and Independent Three-Electron Parameters: A New Complete Set of Orthogonal Operators: II. Applications of $3d^N$ Configurations*, J. Phys. B17 (1984), 4103.
22. G. Burns, E. A. Geiss, B. A. Jenkins, and M. I. Nathan, *Cr^{3+} Fluorescence in Garnets and Other Crystals*, Phys. Rev. 139A (1965), 1687. (This reference gives the ground state splitting as 0.53 cm^{-1} reported by J. W. Carson and R. L. White, J. Appl. Phys. 32 (1961), 1787. Also see L. J. Schruke and J. R. Cunningham, Jr., J. Appl. Phys. 37 (1966), 449.)
23. F. Bantien, P. Albers, and G. Huber, *Optical Transitions in Titanium-Doped YAG*, J. Lumin. 36 (1987), 363.
24. P. A. Arsenev, N. L. Perlova, and D. T. Sviridov, *Absorption Spectra of Nickel Ions in the Crystals of Some Rare Earth Aluminum Garnets*, Sov. Phys. Crystallogr. 16 (1971), 196.

DISTRIBUTION

ADMINISTRATOR
DEFENSE TECHNICAL INFORMATION CENTER
ATTN DTIC-DDA (12 COPIES)
CAMERON STATION, BUILDING 5
ALEXANDRIA, VA 22314

DIRECTOR
NIGHT VISION & ELECTRO-OPTICS LABORATORY
ATTN TECHNICAL LIBRARY
ATTN R. BUSER
ATTN A. PINTO
ATTN J. HABERSAT
FT BELVOIR, VA 22060

DIRECTOR
DEFENSE ADVANCED RESEARCH
PROJECTS AGENCY
ATTN J. FRIEBELE
1400 WILSON BLVD
ARLINGTON, VA 22209

DIRECTOR
DEFENSE NUCLEAR AGENCY
ATTN TECH LIBRARY
WASHINGTON, DC 20305

UNDER SECRETARY OF DEFENSE RES
& ENGINEERING
ATTN TECHNICAL LIBRARY, 3C128
WASHINGTON, DC 20301

OFFICE OF THE DEPUTY CHIEF OF STAFF,
FOR RESEARCH, DEVELOPMENT,
& ACQUISITION
DEPARTMENT OF THE ARMY
ATTN DAMA-ARZ-A, CHIEF SCIENTIST,
L. CAMERON
ATTN DAMA-ARZ-B, I. R. HERSHNER
WASHINGTON, DC 20310

COMMANDER
US ARMY ARMAMENT MUNITIONS &
CHEMICAL COMMAND (AMCCOM)
US ARMY ARMAMENT RESEARCH &
DEVELOPMENT CENTER
ATTN DRDAR-TSS, STINFO DIV
DOVER, NJ 07801

COMMANDER
ATMOSPHERIC SCIENCES LABORATORY
ATTN TECHNICAL LIBRARY
WHITE SANDS MISSILE RANGE, NM 88002

DIRECTOR
US ARMY BALLISTIC RESEARCH LABORATORY
ATTN DRDAR-TSB-S (STINFO)
ABERDEEN PROVING GROUND, MD 21005

DIRECTOR
US ARMY ELECTRONICS WARFARE LABORATORY
ATTN J. CHARLTON
ATTN DELET-DD
FT MONMOUTH, NJ 07703

COMMANDING OFFICER
USA FOREIGN SCIENCE & TECHNOLOGY CENTER
FEDERAL OFFICE BUILDING
ATTN DRXST-BS, BASIC SCIENCE DIV
CHARLOTTESVILLE, VA 22901

COMMANDER
US ARMY MATERIALS & MECHANICS
RESEARCH CENTER
ATTN DRXMR-TL, TECH LIBRARY
WATERTOWN, MA 02172

US ARMY MATERIEL COMMAND
5001 EISENHOWER AVE
ALEXANDRIA, VA 22333-0001

US ARMY MATERIEL SYSTEMS ANALYSIS
ACTIVITY
ATTN DRXSY-MP (LIBRARY)
ABERDEEN PROVING GROUND, MD 21005

COMMANDER
US ARMY MISSILE & MUNITIONS
CENTER & SCHOOL
ATTN ATSK-CTD-F
ATTN DRDMI-TB, REDSTONE SCI INFO CENTER
REDSTONE ARSENAL, AL 35809

COMMANDER
US ARMY RESEARCH OFFICE (DURHAM)
PO BOX 12211
ATTN ROBERT J. LONTZ
ATTN M. STROSIO
ATTN M. CIFTAN
ATTN B. D. GUENTHER
ATTN CHARLES BOGOSIAN
RESEARCH TRIANGLE PARK, NC 27709

COMMANDER
US ARMY RSCH & STD GRP (EUROPE)
FPO NEW YORK 09510

COMMANDER
US ARMY TEST & EVALUATION COMMAND
ATTN D. H. SLINEY
ATTN TECH LIBRARY
ABERDEEN PROVING GROUND, MD 21005

DISTRIBUTION (cont'd)

COMMANDER
US ARMY TROOP SUPPORT COMMAND
ATTN DRXRES-RTL, TECH LIBRARY
NATICK, MA 01762

OFFICE OF NAVAL RESEARCH
ATTN J. MURDAY
ARLINGTON, VA 22217

DIRECTOR
NAVAL RESEARCH LABORATORY
ATTN CODE 2620, TECH LIBRARY BR
ATTN G. QUARLES
ATTN G. KINTZ
ATTN A. ROSENBAUM
ATTN G. RISENBLATT
ATTN CODE 5554, F. BARTOLI
ATTN CODE 5554, L. ESTEROWITZ
ATTN CODE 5554, R. E. ALLEN
WASHINGTON, DC 20375

COMMANDER
NAVAL WEAPONS CENTER
ATTN CODE 3854, R. SCHWARTZ
ATTN CODE 3854, M. HILLS
ATTN CODE 3844, M. NADLER
ATTN CODE 385, R. L. ATKINS
ATTN CODE 343, TECHNICAL INFORMATION
DEPARTMENT
CHINA LAKE, CA 93555

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
ATTN MAJOR H. V. WINSOR, USAF
BOLLING AFB
WASHINGTON, DC 20332

HQ, USAF/SAMI
WASHINGTON, DC 20330

DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS
ATTN LIBRARY
WASHINGTON, DC 20234

NASA LANGLEY RESEARCH CENTER
ATTN N. P. BARNES (2 COPIES)
ATTN P. CROSS
ATTN D. GETTENY
ATTN J. BARNES
ATTN C. BAIR
HAMPTON, VA 23665

DIRECTOR
ADVISORY GROUP ON ELECTRON DEVICES
ATTN SECTRY, WORKING GROUP D
201 VARICK STREET
NEW YORK, NY 10013

AEROSPACE CORPORATION
PO BOX 92957
ATTN M. BIRNBAUM
ATTN N. C. CHANG
LOS ANGELES, CA 90009

COLORADO STATE UNIVERSITY
PHYSICS DEPARTMENT
ATTN S. KERN
FORT COLLINS, CO 80523

ALLIED
ADVANCED APPLICATION DEPT
ATTN A. BUDGOR
31717 LA TIEMDA DRIVE
WESTLAKE VILLAGE, CA 91362

AMES LABORATORY DOE
IOWA STATE UNIVERSITY
ATTN K. A. GSCHNEIDNER, JR. (2 COPIES)
AMES, IA 50011

ARGONNE NATIONAL LABORATORY
ATTN W. T. CARNALL
9700 SOUTH CASS AVENUE
ARGONNE, IL 60439

ARIZONA STATE UNIVERSITY
DEPT OF CHEMISTRY
ATTN L. EYRING
TEMPE, AZ 85281

BRIMROSE CORP OF AMERICA
ATTN R. G. ROSEMEIER
7527 BELAIR ROAD
BALTIMORE, MD 21236

CARNEGIE MELLON UNIVERSITY
SCHENLEY PARK
ATTN PHYSICS & EE, J. O. ARTMAN
PITTSBURGH, PA 15213

ENGINEERING SOCIETIES LIBRARY
ATTN ACQUISITIONS DEPT
345 EAST 47TH STREET
NEW YORK, NY 10017

IBM RESEARCH DIVISION
ALMADEN RESEARCH CENTER
ATTN R. M. MACFARLANE
MAIL STOP K32 802(D)
650 HARRY ROAD
SAN JOSE, CA 95120

DISTRIBUTION

JOHNS HOPKINS UNIVERSITY
DEPT OF PHYSICS
ATTN B. R. JUDD
BALTIMORE, MD 21218

KALAMAZOO COLLEGE
DEPT OF PHYSICS
ATTN K. RAJNAK
KALAMAZOO, MI 49007

DIRECTOR
LAWRENCE RADIATION LABORATORY
ATTN MARVIN J. WEBER
ATTN HELMUT A. KOEHLER
ATTN W. KRUPKE
LIVERMORE, CA 94550

MARTIN MARIETTA
ATTN F. CROWNE
ATTN R. LEAVITT
ATTN J. LITTLE
ATTN T. WORCHESKY
ATTN D. WORTMAN
1450 SOUTH ROLLING ROAD
BALTIMORE, MD 21227

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
CRYSTAL PHYSICS LABORATORY
ATTN H. P. JENSSEN
ATTN A. LINZ
CAMBRIDGE, MA 02139

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
77 MASS AVE
ROOM 26-251
ATTN V. BAGNATO
CAMBRIDGE, MA 02139

MIT LINCOLN LAB
PO BOX 73
ATTN PETER MOULTON,
ATTN B. AULL
LEXINGTON, MA 02173

DEPARTMENT OF MECHANICAL, INDUSTRIAL,
& AEROSPACE ENGINEERING
PO BOX 909
ATTN S. TEMKIN
PISCATAWAY, NJ 08854

NATIONAL OCEANIC & ATMOSPHERIC ADM
ENVIRONMENTAL RESEARCH LABS
ATTN LIBRARY, R-51, TECH RPTS
BOULDER, CO 80302

OAK RIDGE NATIONAL LABORATORY
ATTN R. G. HAIRE
OAK RIDGE, TN 37830

SCIENCE APPLICATIONS, INC
ATTN T. ALLIK
1710 GOODRIDGE DRIVE
McLEAN, VA 22102

UNION CARBIDE CORP
ATTN M. R. KOKTA
ATTN J. H. W. LIAW
750 SOUTH 32ND STREET
WASHOUGAL, WA 98671

UNIVERSITY OF MINNESOTA, DULUTH
DEPARTMENT OF CHEMISTRY
ATTN L. C. THOMPSON
DULUTH, MN 55812

OKLAHOMA STATE UNIVERSITY
DEPT OF PHYSICS
ATTN R. C. POWELL
STILLWATER, OK 74078

PENNSYLVANIA STATE UNIVERSITY
MATERIALS RESEARCH LABORATORY
ATTN W. B. WHITE
ATTN B. K. CHANDRASEKHAR
UNIVERSITY PARK, PA 16802

PRINCETON UNIVERSITY
DEPARTMENT OF CHEMISTRY
ATTN D. S. McCLURE
PRINCETON, NJ 08544

SAN JOSE STATE UNIVERSITY
DEPARTMENT OF PHYSICS
ATTN J. B. GRUBER
SAN JOSE, CA 95192

SETON HALL UNIVERSITY
CHEMISTRY DEPARTMENT
ATTN H. BRITTAIN
SOUTH ORANGE, NJ 07099

UNIVERSITY OF VIRGINIA
DEPT OF CHEMISTRY
ATTN DR. F. S. RICHARDSON (2 COPIES)
ATTN DR. M. REID
CHARLOTTESVILLE, VA 22901

UNIVERSITY OF WISCONSIN
CHEMISTRY DEPARTMENT
ATTN J. WRIGHT
ATTN B. TISSUE
MADISON, WI 53706

US ARMY LABORATORY COMMAND
ATTN TECHNICAL DIRECTOR, AMSLC-CT

DISTRIBUTION (cont'd)

INSTALLATION SUPPORT ACTIVITY
ATTN LEGAL OFFICE, SLCIS-CC
ATTN S. ELBAUM, SLCIS-CC

USAISC
ATTN RECORD COPY, ASNC-LAB-TS
ATTN TECHNICAL REPORTS BRANCH,
ASNC-LAB-TR (2 COPIES)

HARRY DIAMOND LABORATORIES
ATTN D/DIVISION DIRECTORS
ATTN HDL LIBRARY, SLCHD-TL (3 COPIES)
ATTN HDL LIBRARY, SLCHD-TL (WOODBRIDGE)
ATTN CHIEF, SLCHD-NW-E
ATTN CHIEF, SLCHD-NW-EP
ATTN CHIEF, SLCHD-NW-EH
ATTN CHIEF, SLCHD-NW-ES
ATTN CHIEF, SLCHD-NW-R
ATTN CHIEF, SLCHD-NW-TN
ATTN CHIEF, SLCHD-NW-RP
ATTN CHIEF, SLCHD-NW-CS
ATTN CHIEF, SLCHD-NW-TS
ATTN CHIEF, SLCHD-NW-RS
ATTN CHIEF, SLCHD-NW-P
ATTN CHIEF, SLCHD-PO
ATTN CHIEF, SLCHD-ST-C
ATTN CHIEF, SLCHD-ST-RS
ATTN CHIEF, SLCHD-ST-RP
ATTN CHIEF, SLCHD-TT
ATTN WILLIS, B., SLCHD-TA-ET
ATTN ZABLUDOWSKI, B., SLCHD-TA-ET
ATTN KENYON, C. S., SLCHD-NW-EP

HARRY DIAMOND LABORATORIES (cont'd)
ATTN MILETTA J. R., SLCHD-NW-EP
ATTN MCLEAN, F. B., SLCHD-NW-RP
ATTN LIBELO, L., SLCHD-ST-MW
ATTN BENCIVENGA, A. A., SLCHD-ST-SP
ATTN SATTLER, J., SLCHD-PO-P
ATTN NEMARICH, J., SLCHD-ST-CB
ATTN WEBER, B., SLCHD-ST-CB
ATTN BAHDER, T., SLCHD-ST-AP
ATTN BENCIVENGA, B. SLCHD-ST-AP
ATTN BRODY, P., SLCHD-ST-AP
ATTN BRUNO, J., SLCHD-ST-AP
ATTN DROPKIN, H., SLCHD-ST-AP
ATTN EDWARDS, A., SLCHD-ST-AP
ATTN HANSEN, A., SLCHD-ST-AP
ATTN HAY, G., SLCHD-ST-AP
ATTN KATZEN, E., SLCHD-ST-AP
ATTN NEIFELD, R., SLCHD-ST-AP
ATTN PENNISE, C., SLCHD-ST-AP
ATTN SCHMALBACH, R., SLCHD-ST-AP
ATTN SEMENDY, F., SLCHD-ST-AP
ATTN SIMONIS, G., SLCHD-ST-AP
ATTN SIMPSON, T., SLCHD-ST-AP
ATTN STEAD, M., SLCHD-ST-AP
ATTN STELLATO, J., SLCHD-ST-AP
ATTN TOBIN, M., SLCHD-ST-AP
ATTN TURNER, G., SLCHD-ST-AP (10 COPIES)
ATTN WONG, B., SLCHD-ST-AP
ATTN WORTMAN, D., SLCHD-ST-AP
ATTN GARVIN, C., SLCHD-ST-SS
ATTN GOFF, J., SLCHD-ST-SS
ATTN MORRISON, C., SLCHD-ST-AP (10 COPIES)