HDL-TR-1788

RARE EARTH ION-HOST LATTICE INTERACTIONS
13. Lanthanides in $YAlO_3$

Host Lattice Interactions. 13. Lanthanides in YAlO3.
Ion, Nick Karayianis, and Donald E. Wortman

February 1977

U.S. Army Material Development and Readiness Command
HARRY DIAMOND LABORATORIES
Adelphi, Maryland 20783

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Phenomenological even-fold crystal field parameters, B_{km}, are obtained for triply ionized Nd, Tb, Dy, Ho, Er, and Tm in $YAlO_3$ by diagonalizing a $C_s(C_{1h})$ crystal field Hamiltonian in a free-ion wave-function basis. These parameters are reduced to give the part of the crystal field components, A_{km}, due solely to the crystal lattice, and new B_{km} are then calculated for all the lanthanides by using previously derived ρ_k, where $B_{km} = \rho_k A_{km}$.

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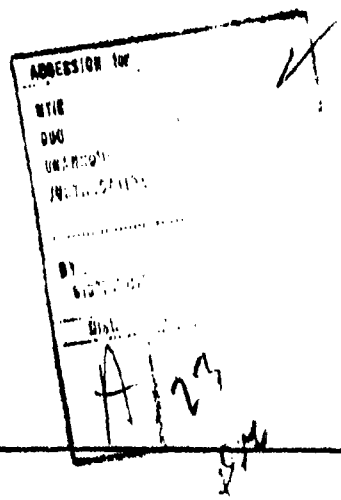
The latter B_{km} are used to calculate the energy levels of the lower J-multiplets for the lanthanide series in $YAlO_3$.



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TABLES (CONT'D)

1. INTRODUCTION

The optical spectra of a number of triply ionized lanthanides in yttrium orthoaluminate ($YAlO_3$) have been reported.[1-6] Because of the excellent laser properties of this material,[1] we have examined these reported spectra in order to obtain a unified theory of the crystal field interactions at the laser ion site in $YAlO_3$. In this report, phenomenological crystal field parameters, B_{km}, for triply ionized Nd, Tb, Dy, Ho, Er, and Tm were obtained by diagonalizing a $C_s(C_{1h})$ crystal field Hamiltonian in a free-ion wave-function basis. The parameters were reduced to give the part of the crystal field components, A_{km}, due solely to the crystal lattice, and new B_{km} were then calculated for all the lanthanides by using previously derived[7] ρ_k, where $B_{km} = \rho_k A_{km}$. These B_{km} were then used to calculate the energy levels of the lower J-multiplets for the lanthanide series in $YAlO_3$.

2. CALCULATIONS

The point group symmetry[8] at the yttrium site in $YAlO_3$ is $C_s(C_{1h})$, which includes a reflection plane in addition to the identity operation.

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[1] *M. Bass and M. J. Weber, Laser Focus, 7 (1971), 34-36.*

[2] *M. J. Weber and T. E. Varitimos, J. Appl. Phys., 42 (1971), 4996-5005.*

[3] *Kh. S. Bagdasarov, A. A. Kaminskii, and G. I. Rogov, Sov. Phys. Doklady, 14 (1969), 346-348.*

[4] *J. L. Berg, High Resolution Low Temperature Spectra of Tb^{3+} in $YAlO_3$, Master's Thesis, Air Force Institute of Technology, Wright-Patterson Air Force Base, OH (June 1973).*

[5] *V. A. Antanov, P. A. Arsenev, K. E. Bienert, and A. V. Potemkin, Phys. Status Solidi A, 19 (1973), 289-299.*

[6] *V. L. Donlan and A. A. Santiago, Jr., J. Chem. Phys., 57 (1972), 4717-4723.*

[7] *D. E. Wortman, C. A. Morrison, and N. Karayianis, Rare Earth Ion-Host Lattice Interactions 11. Lanthanides in $Y_3Al_5O_{12}$, Harry Diamond Laboratories TR-1773 (August 1976).*

[8] *R. Diehl and G. Brandt, Materia Research Bulletin, 10 (1975), 85-90.*

If the z-axis is taken perpendicular to the reflection plane, the crystal field Hamiltonian is of the form

$$H_x = \Sigma_{km} B_{km} C_{km}, \; k = 2, 4, 6; \; m = 0, \pm 2, \ldots \pm k , \qquad (1)$$

where the B_{km} for $m \neq 0$ may be complex. With no loss in generality, we chose real B_{22} and imaginary $B_{42} \neq 0$.

The crystal field Hamiltonian was diagonalized in the low-lying J-multiplets of free-ion wave functions,[9] and the B_{km} were varied to obtain best fits between theoretical and experimental energy levels reported for Nd,[2,3] Tb,[4] Dy,[5] Ho,[5] Er[5,6] and Tm.[5] The resultant best-fit parameters are given in table I, where the next to last four columns give the number of J-multiplets diagonalized, the number of levels in these multiplets, the number of experimental energies used, and finally the rms deviation between these energies and their corresponding theoretical energies. The multiplets included for each ion were (1) the ^4I term, $^4F_{3/2}$, and $^4F_{9/2}$ for Nd; (2) the ^7F term and $^5D_4$ for Tb; (3) $^6H_{15/2, 13/2, 11/2, 5/2}$ and $^6F_{7/2, 5/2}$ for Dy; (4) $^5I_{8,7,6,5}$ and $^5F_{5,4}$ for Ho; (5) the ^4I term, $^4F_{9/2}$, and $^4S_{3/2}$ for Er; and (6) the ^3H term, $^3F_{3/2}$, and $^1G_4$ for Tm. The lack of sufficient data in some cases plus ambiguities owing to overlapping multiplets governed the choice of

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[2] *M. J. Weber and T. E. Varitimos, J. Appl. Phys., 42 (1971), 4996-5005.*

[3] *Kh. S. Bagdasarov, A. A. Kaminskii, and G. I. Rogov, Sov. Phys. Doklady, 14 (1969), 346-348.*

[4] *J. L. Berg, High Resolution Low Temperature Spectra of Tb^{3+} in $YAlO_3$, Master's Thesis, Air Force Institute of Technology, Wright-Patterson Air Force Base, OH (June 1973).*

[5] *V. A. Antanov, P. A. Arsenev, K. E. Bienert, and A. V. Potemkin, Phys. Status Solidi A, 19 (1973), 289-299.*

[6] *V. L. Donlan and A. A. Santiago, Jr., J. Chem. Phys., 57 (1972), 4717-4723.*

[9] *W. T. Carnall, P. R. Fields, and K. Rajnak, J. Chem. Phys., 49 (1968), 4412-4455.*

TABLE I. PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS, B_{km}, FOR TRIPLY IONIZED LANTHANIDES IN $YAlO_3$

Ion	B_{20}	B_{22}	B_{40}	B_{42} Real	B_{42} Imaginary	B_{44} Real	B_{44} Imaginary	B_{60}	B_{62} Real	B_{62} Imaginary	B_{64} Real	B_{64} Imaginary	B_{66} Real	B_{66} Imaginary	Multiplets Used	Levels (%)	Energy Levels Used	χ^2	Table
Pr	814	-18	-1345	-521	525	-214	-575	-1810	-348	-155	1,114	231	-62	370	6	33	244	A,196	A
Tb	567	-233	-1060	-217	497	-398	-82	-751	-317	-425	740	-508	-230	91	4	58	32	0,641	A
Dy	653	-163	-882	-616	300	151	-405	-888	156	-203	649	-97	-440	-8	6	31	31	0,130	A111
Ho	716	-248	-838	-544	384	-63	-360	-963	211	-214	-41	563	-750	19	4	56	44	0,333	A
Er	547	-8	-793	-487	391	-482	-416	-877	-304	-175	325	210	33	259	10	48	48	0,385	A111
Er	431	-170	-838	-346	365	-218	-709	-742	-241	-180	534	17	23	224	4	33	33	0,461	A111
Tm	675	-76	-784	-480	367	-64	-445	-750	-72	-184	601	59	-218	-18	6	43	34	0,160	A

[illegible]

[illegible]

[illegible]

multiplets and experimental energies that were used in the fitting procedure. Table I, line 6, gives the set of initial B_{km} for Er that were chosen to begin the fitting procedure. For starting parameters, previously reported parameters for Er:yttrium aluminum garnet (YAG)[10] were used. Since the YAG crystal field is real, imaginary B_{kq} was arbitrarily set at 200 cm^{-1}.

Subsequent choices for starting parameters for the other ions were chosen by scaling the Ho parameters, which were obtained by averaging the best-fit Dy and Er phenomenological B_{km}, according to the ρ_k in table II. These ρ_k, given by

TABLE II. VALUES FOR $\rho_k = \tau^{-k}\langle r^k\rangle (1 - \sigma_k)$ IN Å^k TO CONVERT LATTICE SUMS CRYSTAL FIELD COMPONENTS, A_{km}, TO CRYSTAL FIELD PARAMETERS, B_{km}, AS $B_{km} = \rho_k A_{km}$

Ion	ρ_2	ρ_4	ρ_6
Ce	0.1841	0.7546	2.3417
Pr	0.1756	0.6464	1.8754
Nd	0.1706	0.5776	1.5897
Pm	0.1679	0.5339	1.4218
Sm	0.1668	0.5069	1.3210
Eu	0.1666	0.4936	1.2504
Gd	0.1668	0.4866	1.1873
Tb	0.1673	0.4790	1.1232
Dy	0.1681	0.4761	1.0614
Ho	0.1692	0.4717	1.0119
Er	0.1706	0.4726	0.9826
Tm	0.1722	0.4753	0.9669
Yb	0.1737	0.4838	0.9720

[10] C. A. Morrison, D. E. Wortman, and N. Karayianis, J. Phys. C: Solid State Phys., 9 (1976), L191.

$$\rho_k = \tau^{-k} \langle r^k \rangle (1 - \sigma_k) , \qquad (2)$$

are rare-earth-ion dependent and relate the B_{km} to the lattice sum field A_{km} by

$$B_{km} = \rho_k A_{km} , \qquad (3)$$

where it is assumed that the A_{km} are host dependent only. The $\langle r^k \rangle$ are smoothed values of Freeman and Watson,[11] the σ_k are linearly interpolated calculations of Erdos and Kang,[12] and the τ are quadratically fit wave-function expansion parameters found in studies of lanthanides in $CaWO_4$.[13] The B_{km} for the lanthanide series obtained by using these σ_k values of table II in equation (3) and the B_{km} for Dy and Er of table I are given in table III.

Energy levels calculated by using the B_{km} of tables I and III for the lowest-lying six to eight multiplets of the lanthanides in $YAlO_3$ are given in tables IV to XXI.

To make intensity calculations, some estimates of the odd-fold (odd-k) A_{km} are necessary. These can be obtained by appropriate lattice sums.[14] In this work, we have performed the lattice sums for $YAlO_3$ using the x-ray data of Diehl and Brandt[8] for oxygen charges $q_0 = -1$ and -2; the results are given in table XXII. The one-fold field, A_{1m}, was not

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[8] R. Diehl and G. Brandt, *Materia Research Bulletin*, 10 (1975), 85-90.

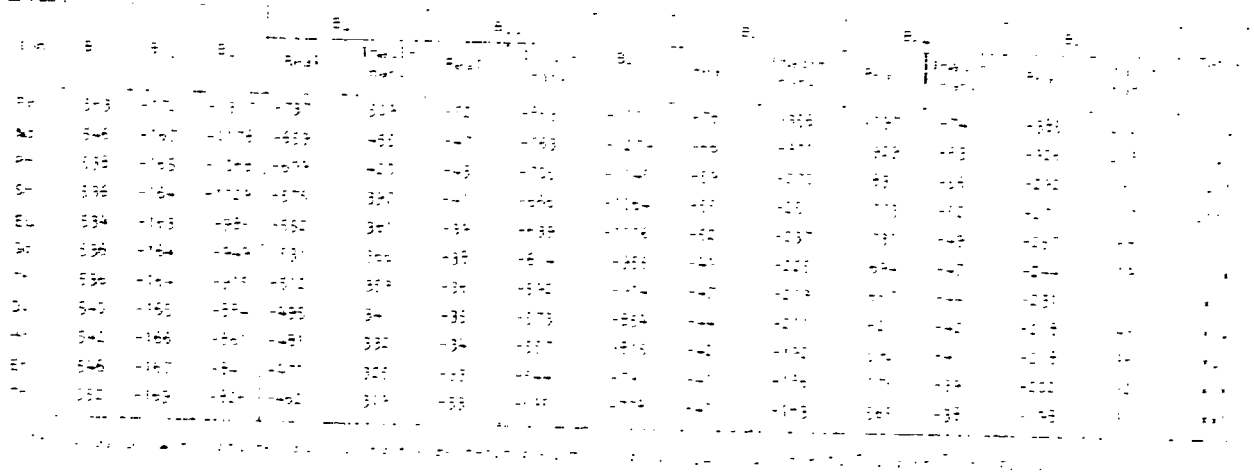
[11] A. J. Freeman and R. E. Watson, *Phys. Rev.*, 127 (1962), 2058-2075.

[12] P. Erdos and J. H. Kang, *Phys. Rev. B*, 6 (1972), 3393-3408.

[13] R. P. Leavitt, C. A. Morrison, and D. E. Wortman, *Rare Earth Ion-Host Crystal Interactions 3. Three-Parameter Theory of Crystal Fields, Harry Diamond Laboratories TR-1673 (June 1975).*

[14] N. Karayianis and C. A. Morrison, *Rare Earth Ion-Host Lattice Interactions 1. Point Charge Lattice Sum in Scheelites, Harry Diamond Laboratories TR-1648 (October 1973).*

TABLE III. CRYSTAL FIELD PARAMETERS, B_{km}, FOR TRIPLY IONIZED LANTHANIDES IN $YAlO_3$[a]



included because of its slow convergence. By appropriate rotations of the coordinate system chosen for the calculation of the A_{km} of table XXII, different sets of A_{km} can be generated. Thus by appropriate rotation, the sets of A_{km} for $q_0 = -1$ and -1.5 given in table XXIII were calculated. Since the A_{km} are linear functions of q_0, a value of q_0 can be chosen by using equation (3) and the ρ_k of table II to obtain a best fit of calculated B_{km} to phenomenological B_{km}. The results of this calculation give $q_0 = -1.52$, and the corresponding A_{km} are reported elsewhere.[15]

3. SUMMARY

Reported energy levels for Nd, Tb, Dy, Ho, Er, and Tm were used to obtain phenomenological B_{km} that yielded least-rms deviations between these levels and levels calculated by using the Hamiltonian given in equation (1) and unpublished theoretical methods and computer programs. These parameters were then scaled to get even-k B_{km} for the entire lanthanide series in $YAlO_3$. It is expected that these B_{km} will at least serve as starting parameters for the analysis of yet unreported ions in $YAlO_3$. No intensities were calculated because the symmetry of the Y^{3+} site was low and because no reasonable higher symmetry approximation could be made as was done[7] for the lanthanides in YAG.

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[7] *D. E. Wortman, C. A. Morrison, and N. Karayianis, Rare Earth Ion-Host Lattice Interactions 11. Lanthanides in $Y_3Al_5O_{12}$, Harry Diamond Laboratories TR-1773 (August 1976).*

[15] *N. Karayianis, D. E. Wortman, and C. A. Morrison, Solid State Comm., 18 (1976).*

TABLE IV. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Pr^{3+} IN $YAlO_3$[a]

PR IN YALO3. SCALED EXP FROM MO DETERMINED BY AVERAGING BY AND ER HOMED RESULTS
INIT. EKM AND OPSTM.IOS. Q = -0.301

563.000 = B20	-272.000 = B22	-1317.000 = B40	-737.000 = B42	509.000 = B62	-52.000 = B44	-853.000 = B64
-1210.300 = B60	-78.000 = B62	-356.000 = B62	1097.000 = B64	-74.000 = B64	-385.000 = B66	252.000 = B66

3H 4	2514.3
3H 5	2354.3
3H 6	4527.3
3F 2	5101.3
3F 3	6478.3
3F 4	6953.3
1G 4	9923.3
1D 2	16802.9

			FREE ION	PCT PURE	CM1	THEO.ENERGY	EXP.ENERGY		
1	3H 4	93.2	0	-189.5	0.0	30 3H 5	95.5	0	4713.4	0.0
2	3H 4	89.4	0	-46.7	0.0	31 3H 6	92.3	2	4913.5	0.0
3	3H 4	93.1	2	10.2	0.0	32 3H 6	91.8	1	4966.7	0.0
4	3H 4	98.1	2	76.4	0.0	33 3H 6	93.3	2	4983.2	0.0
5	3H 4	94.8	0	165.8	0.0					
6	3H 4	87.5	0	247.4	0.0	34 3F 2	96.9	2	5103.6	0.0
7	3H 4	97.1	2	312.4	0.0	35 3F 2	94.1	0	5164.6	0.0
8	3H 4	96.3	2	457.4	0.0	36 3F 2	93.2	2	5180.6	0.0
9	3H 4	98.8	0	573.3	0.0	37 3F 2	91.1	0	5246.4	0.0
						38 3F 2	75.8	0	5389.0	0.0
10	3H 5	96.5	2	2043.2	0.0					
11	3H 5	95.3	0	2095.4	0.0	39 3F 3	96.7	2	6364.5	0.0
12	3H 5	96.1	2	2146.1	0.0	40 3F 3	94.3	0	6443.8	0.0
13	3H 5	97.4	0	2161.3	0.0	41 3F 3	94.1	2	6491.1	0.0
14	3H 5	97.7	2	2245.3	0.0	42 3F 3	94.9	2	6527.3	0.0
15	3H 5	95.5	0	2249.2	0.0	43 3F 3	93.1	2	6594.8	0.0
16	3H 5	97.4	2	2301.2	0.0					
17	3H 5	94.7	0	2444.9	0.0	44 3F 3	90.4	0	6614.3	0.0
18	3H 5	95.6	2	2534.1	0.0	45 3F 3	68.6	2	6683.2	0.0
19	3H 5	96.4	2	2535.1	0.0					
20	3H 5	97.3	0	2562.4	0.0	46 3F 4	80.2	2	6823.4	0.0
						47 3F 4	66.7	2	6870.8	0.0
21	3H 6	99.7	0	4042.6	0.0	48 3F 4	92.1	0	6894.0	0.0
22	3H 6	94.7	2	4105.7	0.0	49 3F 4	95.7	0	6967.7	0.0
23	3H 6	95.6	0	4163.9	0.0	50 3F 4	83.3	2	6998.4	0.0
24	3H 6	95.8	2	4190.7	0.0	51 3F 4	95.9	0	7033.9	0.0
25	3H 6	96.2	0	4253.4	0.0	52 3F 4	94.4	2	7162.0	0.0
26	3H 6	93.3	2	4344.4	0.0	53 3F 4	97.3	0	7162.2	0.0
27	3H 6	96.3	2	4434.5	0.0	54 3F 4	92.7	0	7244.0	0.0
28	3H 6	92.4	2	4512.6	0.0					
29	3H 6	93.4	0	4571.9	0.0					

[a] See footnote at end of table.

TABLE IV. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR PR^{3+} IN $YAlO_3$[a] (CONT'D)

	FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
55	16 4	99.4	2	9520.5	0.0
56	16 4	99.3	2	9603.6	0.0
57	16 4	99.4	0	9721.9	0.0
58	16 4	99.5	0	9795.6	0.0
59	16 4	99.6	2	9894.0	0.0
60	16 4	99.5	0	10078.6	0.0
61	16 4	99.6	0	10164.4	0.0
62	16 4	99.5	2	10255.4	0.0
63	16 4	99.6	0	10507.9	0.0
64	16 2	100.0	0	16435.2	0.0
65	16 2	99.9	0	16715.0	0.0
66	16 2	99.7	2	16777.1	0.0
67	16 2	99.9	2	17016.0	0.0
68	16 2	99.9	0	17114.9	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ϵ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE V. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Nd^{3+} IN $YAlO_3$[a]

NO [illegible] YALO MEHER DATA 6 MULTIPLETS EXP FROM DY & ER HOME 9/16/75

FINAL P&M AND CENTROIDS. Q = 6.786

-214.035 = 829	-1[illegible].035 = 822	-1344.537 = 840	-521.130 = 842	525.202 = 842	-214.375 = 844	-574.625 = 844
-1113.469 = 863	-347.745 = 862	-155.494 = 862	1214.405 = 864	221.375 = 864	-82.365 = 866	370.375 = 866

4I 9/2	336.1
4I11/2	2214.2
4I13/2	4131.2
4I15/2	6142.4
4F 3/2	11464.2
4F 9/2	14760.3

			FREE ION	PCT PURE	ZMU	THEO.ENERGY	EXP.ENERGY
1 4I 9/2	98.3	1	0.3	0.0			
2 4I 9/2	98.2	1	113.2	117.0			
3 4I 9/2	96.4	1	219.2	-0.0			
4 4I 9/2	97.6	1	482.6	-0.0			
5 4I 9/2	96.7	1	595.1	-0.0			
6 4I11/2	97.3	1	2333.4	2023.0*			
7 4I11/2	96.4	1	2203.0	2094.0			
8 4I11/2	97.3	1	2159.0	2157.0			
9 4I11/2	93.4	1	2259.1	2269.0*			
10 4I11/2	93.7	1	2313.4	2320.0			
11 4I11/2	96.4	1	2368.3	2368.0			
12 4I13/2	97.7	1	3953.2	3951.0			
13 4I13/2	96.4	1	4024.7	4017.0*			
14 4I13/2	96.5	1	4097.3	4087.0*			
15 4I13/2	96.9	1	4183.2	4190.0*			
16 4I13/2	96.2	1	4249.1	-0.0			
17 4I13/2	96.6	1	4317.8	4324.0			
18 4I13/2	94.0	1	4429.5	4433.0*			
19 4I15/2	97.4	1	5746.8	5760.0*			
20 4I15/2	96.7	1	5931.0	5896.0			
21 4I15/2	99.0	1	6018.2	6011.0			
22 4I15/2	99.1	1	6208.9	6197.0			
23 4I15/2	96.3	1	6246.9	6242.0			
24 4I15/2	97.7	1	6317.8	6311.0*			
25 4I15/2	98.0	1	6597.1	-0.0			
26 4I15/2	98.1	1	6682.0	-0.0			
27 4F 3/2	99.6	1	11413.3	11413.0			
28 4F 3/2	99.7	1	11546.7	11542.0			
29 4F 9/2	99.5	1	14674.0	14680.0			
30 4F 9/2	99.4	1	14722.3	14730.0*			
31 4F 9/2	99.3	1	14763.0	14746.0			
32 4F 9/2	99.9	1	14803.5	14795.0*			
33 4F 9/2	100.0	1	14930.5	14925.0			

CENTROIDS. CRYSTAL = 5779.8 FREE ION = 5770.9

[a] *The calculated and experimental energy levels rms deviation is 6.786 cm^{-1}.*

TABLE VI. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Nd^{3+} IN $YAlO_3$[a]

ND IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
INIT. BKM AND CENTROIDS. Q = -0.000

546.000 = B20 -167.000 = B22 -1178.000 = B40 -659.000 = B42 459.000 = B42 -67.000 = B44 -763.000 = B44
-1279.000 = B60 -66.000 = B62 -301.000 = B62 929.000 = B64 -63.000 = B64 -326.000 = B66 213.000 = B66

4I 9/2	352.0
4I11/2	2219.0
4I13/2	4192.0
4I15/2	6180.0
4F 3/2	11500.0
4F 5/2	12403.0
2H 9/2 2	12670.0
4F 7/2	13476.0
4S 3/2	13583.0
4F 9/2	14746.3

			FREE ION	PCT PURE	2MJ
1	4I 9/2	97.9	1	2.9	0.0
2	4I 9/2	98.2	1	167.1	0.0
3	4I 9/2	94.6	1	273.6	0.0
4	4I 9/2	98.2	1	460.4	0.0
5	4I 9/2	97.6	1	604.6	0.0
6	4I11/2	97.4	1	2048.4	0.0
7	4I11/2	96.3	1	2111.4	0.0
8	4I11/2	97.9	1	2158.3	0.0
9	4I11/2	97.3	1	2267.7	0.0
10	4I11/2	96.4	1	2304.2	0.0
11	4I11/2	97.2	1	2347.4	0.0
12	4I13/2	97.5	1	3994.7	0.0
13	4I13/2	96.5	1	4040.2	0.0
14	4I13/2	97.6	1	4103.0	0.0
15	4I13/2	97.2	1	4213.8	0.0
16	4I13/2	97.2	1	4253.2	0.0
17	4I13/2	97.1	1	4297.8	0.0
18	4I13/2	98.0	1	4388.2	0.0
19	4I15/2	97.5	1	5778.2	0.0
20	4I15/2	98.3	1	5893.2	0.0
21	4I15/2	99.3	1	6012.3	0.0
22	4I15/2	94.3	1	6131.6	0.0
23	4I15/2	96.3	1	6276.7	0.0
24	4I15/2	99.2	1	6318.5	0.0
25	4I15/2	98.5	1	6500.6	0.0
26	4I15/2	93.6	1	6599.2	0.0

39	4F 7/2	94.6	1	13557.5	0.0				
40	4S 3/2	83.1	1	13591.3	0.0				
41	4S 3/2	70.0	1	13599.7	0.0				
42	4F 7/2	56.5	1	13605.9	0.0				
43	4F 9/2	99.3	1	14664.5	0.0				
44	4F 9/2	99.0	1	14712.3	0.0				
45	4F 9/2	98.5	1	14754.3	0.0				
46	4F 9/2	93.3	1	14828.0	0.0				
47	4F 9/2	93.5	1	14833.9	0.0				
27	4F 3/2	98.0	1	11447.0	0.0				
28	4F 3/2	97.8	1	11532.2	0.0				
29	4F 5/2	94.6	1	12314.2	0.0				
30	4F 5/2	78.3	1	12408.3	0.0				
31	4F 5/2	92.4	1	12447.0	0.0				
32	2H 9/2 2	81.4	1	12523.7	0.0				
33	2H 9/2 2	93.6	1	12604.5	0.0				
34	2H 9/2 2	98.5	1	12654.1	0.0				
35	2H 9/2 2	97.4	1	12799.1	0.0				
36	2H 9/2 2	98.1	1	12828.7	0.0				
37	4F 7/2	97.1	1	13357.6	0.0				
38	4F 7/2	96.7	1	13469.2	0.0				

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE VII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Pm^{3+} IN $YAlO_3$[a]

PM I+ YA. D3. SCALED BKM FROM HO DETERMINED BY AVERAGING BY AND FR HOMED RESULTS
INIT. B M AND CENTROIDS. Q = 0.00
-536.000 = 622 -1165.000 = 632 -1348.000 = 640 -699.000 = 642 420.000 = 642 -63.000 = 644 -705.000 = 644
-1145.000 = 660 -59.000 = 662 -270.000 = 662 831.000 = 664 -56.000 = 664 -292.000 = 666 191.000 = 666
SI 4 233.0
SI 5 1731.0
SI 6 3366.0
SI 7 4953.0
SI 8 6716.0
SF 1 12298.0

				FREE ION	PCT PURE	/MU	THEO.ENERGY		EXP.ENERGY	
1	SI 4	98.9	0	-53.1	0.0	29 SI 6	97.6	0	3146.2	0.0
2	SI 4	96.6	2	17.9	0.0	30 SI 6	95.9	2	3161.1	0.0
3	SI 4	98.7	0	83.4	0.0	31 SI 6	96.3	2	3173.9	0.0
4	SI 4	95.3	3	147.0	0.0	32 SI 6	97.3	0	3179.5	0.0
5	SI 4	96.9	2	157.3	0.0	33 SI 6	97.3	0	3194.0	0.0
6	SI 4	99.0	0	235.6	0.0					
7	SI 4	96.2	2	326.6	0.0	34 SI 7	96.4	0	4465.4	0.0
8	SI 4	94.3	3	360.9	0.0	35 SI 7	94.6	2	4465.7	0.0
9	SI 4	97.9	2	424.2	0.0	36 SI 7	95.9	2	4471.0	0.0
						37 SI 7	97.0	0	4474.4	0.0
10	SI 5	96.4	0	1619.8	0.0	38 SI 7	97.3	2	4415.4	0.0
11	SI 5	94.1	2	1618.2	0.0	39 SI 7	95.6	2	4421.5	0.0
12	SI 5	94.0	2	1648.4	0.0	40 SI 7	97.1	0	4426.3	0.0
13	SI 5	96.2	0	1673.7	0.0	41 SI 7	97.3	2	4435.5	0.0
14	SI 5	96.9	0	1724.1	0.0	42 SI 7	97.4	2	4451.4	0.0
15	SI 5	97.6	2	1742.3	0.0	43 SI 7	95.8	0	4459.5	0.0
16	SI 5	97.1	0	1750.6	0.0	44 SI 7	95.7	0	4499.0	0.0
17	SI 5	95.8	2	1752.7	0.0	45 SI 7	96.0	2	5033.5	0.0
18	SI 5	97.3	0	1784.3	0.0	46 SI 7	96.3	2	5047.6	0.0
19	SI 5	93.4	2	1819.1	0.0					
20	SI 5	94.2	2	1836.9	0.0	47 SI 7	97.4	2	5067.2	0.0
						48 SI 7	97.6	0	5074.0	0.0
21	SI 6	93.1	2	3134.2	0.0					
22	SI 6	97.5	0	3199.3	0.0	49 SI 8	97.3	2	6441.1	0.0
23	SI 6	97.7	2	3211.9	0.0	50 SI 8	95.1	2	6446.6	0.0
24	SI 6	95.2	3	3221.6	0.0	51 SI 8	97.3	0	6470.4	0.0
25	SI 6	96.7	0	3246.3	0.0	52 SI 8	94.6	3	6524.3	0.0
26	SI 6	96.3	2	3306.5	0.0	53 SI 8	97.9	2	6533.5	0.0
27	SI 6	96.4	0	3323.5	0.0	54 SI 8	93.5	4	6634.7	0.0
28	SI 6	97.1	2	3326.7	0.0	55 SI 8	93.4	2	6670.0	0.0
						56 SI 8	94.1	4	6674.4	0.0

[a] *See footnote at end of table.*

TABLE VII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Nd^{3+} IN $YAlO_3$[a] (CONT'D)

FREE ION	PCT PURE	ZMU	THEO. ENERGY	EXP. ENERGY
57 5I 4	[illegible]	[illegible]	6721.6	[illegible]
58 5I 4	[illegible]	[illegible]	6724.7	[illegible]
59 5I 4	[illegible]	[illegible]	6783.6	[illegible]
60 5I 4	[illegible]	[illegible]	6[illegible]5.4	[illegible]
61 5I 4	[illegible]	[illegible]	6[illegible]1.4	[illegible]
62 5I 4	[illegible]	[illegible]	7[illegible]1.3	[illegible]
63 5I 4	[illegible]	[illegible]	7[illegible]5.3	[illegible]
64 5I 4	[illegible]	[illegible]	7[illegible]7.9	[illegible]
65 5I 4	[illegible]	[illegible]	7[illegible]6.3	[illegible]
66 5F 1	[illegible]	[illegible]	12[illegible]4.4	[illegible]
67 5F 1	[illegible]	[illegible]	12[illegible]4.1	[illegible]
68 5F 1	[illegible]	[illegible]	12454.8	[illegible]

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE VIII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Sm^{3+} IN $YAlO_3$[a]

SM IN YALO3. SCALED PRM FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
INIT. PRM AND CENTROIDS. Q = 0.000

536.000 = B20 -164.000 = B22 -1025.000 = B40 -575.000 = B42 397.000 = B62 -41.000 = B44 -666.000 = B44
-1064.000 = B60 -59.000 = B62 -251.000 = B62 773.000 = B64 -52.000 = B64 -271.000 = B66 177.000 = B66

6H 5/2	1346.
6H 7/2	1143.
6H 9/2	2338.
6H11/2	3737.
6H13/2	5038.
6F 1/2	6356.
6H15/2	6550.
6F 3/2	6700.
6F 5/2	7116.
6F 7/2	7935.
6F 9/2	9147.

		FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	6H 5/2	97.1	-67.4	0.0		
2	6H 5/2	96.5	94.3	0.0		
3	6H 5/2	97.2	214.4	0.0		
4	6H 7/2	95.1	381.5	0.0		
5	6H 7/2	95.6	1139.1	0.0		
6	6H 7/2	96.7	1197.2	0.0		
7	6H 7/2	93.0	1339.1	0.0		
8	6H 9/2	97.1	2211.4	0.0		
9	6H 9/2	96.3	2311.1	0.0		
10	6H 9/2	93.0	2356.4	0.0		
11	6H 9/2	97.1	2479.2	0.0		
12	6H 9/2	98.7	2654.4	0.0		
13	6H11/2	97.3	3644.6	0.0		
14	6H11/2	95.9	3761.8	0.0		
15	6H11/2	97.0	3777.6	0.0		
16	6H11/2	97.5	3[illegible].1	0.0		
17	6H11/2	94.2	3[illegible].7	0.0		
18	6H11/2	94.7	[illegible]	0.0		
19	6H13/2	94.7	4596.3	0.0		
20	6H13/2	96.5	4774.1	0.0		
21	6H13/2	95.7	5220.7	0.0		
22	6H13/2	95.9	5.62.4	0.0		
23	6H13/2	97.4	5113.3	0.0		
24	6H13/2	97.5	5239.5	0.0		
25	6H13/2	97.3	5.35.3	0.0		
26	6H15/2	93.6	621[illegible]	0.0		
27	6H15/2	93.[illegible]	6[illegible]6.2	0.0		
28	6F 1/2	92.9	6336.4	0.0		
29	6H15/2	92.9	6472.9	0.0		
30	6H15/2	92.5	6524.3	0.0		
31	6H15/2	92.9	6593.4	0.0		
32	6H15/2	93.5	6662.7	0.0		
33	6H15/2	92.2	6[illegible]4.4	0.0		
34	6F 3/2	91.[illegible]	6724.9	0.0		
35	6F 3/2	91.4	6762.4	0.0		

[a] *See footnote at end of table.*

TABLE VIII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Sm^{3+} IN $YAlO_3$[a] (CONT'D)

	FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
36	6H15/2	[illegible]	1	6422.3	0.0
37	6F 5/2	[illegible]	1	7145.8	0.0
38	6F 5/2	[illegible]	1	7170.6	0.0
39	6F 5/2	[illegible]	1	7236.4	0.0
40	6F 7/2	[illegible]	1	7980.2	0.0
41	6F 7/2	[illegible]	1	8018.4	0.0
42	6F 7/2	[illegible]	1	8049.8	0.0
43	6F 7/2	[illegible]	1	8116.8	0.0
44	6F 9/2	[illegible]	1	9115.8	0.0
45	6F 9/2	[illegible]	1	9157.4	0.0
46	6F 9/2	[illegible]	1	9182.1	0.0
47	6F 9/2	[illegible]	1	9216.5	0.0
48	6F 9/2	[illegible]	1	9246.4	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the θ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE IX. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Eu^{3+} IN $YAlO_3$[a]

EU IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER -OMED RESULTS
INIT. BKM AND CENTROIDS: C = -0.000

534.000 = B20	-163.000 = B22	-385.000 = B40	-552.000 = B42
-1006.000 = B60	-52.000 = B62	-237.000 = B64	731.000 = B66

381.000 = B42	-39.000 = B44	-639.000 = B46	
-49.000 = B64	-257.000 = B66	168.000 = B66	

7F 0		96.0	
7F 1		473.0	
7F 2		1175.0	
7F 3		1998.0	
7F 4		3000.0	
7F 5		4073.0	
7F 6		5096.0	
5D 0	3	17220.0	
5D 1	3	18960.0	
5D 2	3	21422.0	
5D 3	3	24653.0	

				FREE ION	PCT PURE	2MJ	THEO.ENERGY	EXP.ENERGY
1	7F 0	97.8	0	52.7	0.0			
2	7F 1	96.3	2	333.5	0.0			
3	7F 1	98.0	2	423.6	0.0			
4	7F 1	96.8	0	525.5	0.0			
5	7F 2	98.0	0	1003.8	0.0			
6	7F 2	96.7	2	1038.7	0.0			
7	7F 2	92.2	2	1119.4	0.0			
8	7F 2	95.0	0	1159.8	0.0			
9	7F 2	96.8	0	1323.9	0.0			
10	7F 3	96.7	2	1902.7	0.0			
11	7F 3	91.6	0	1910.4	0.0			
12	7F 3	96.2	2	1922.3	0.0			
13	7F 3	91.3	0	1952.3	0.0			
14	7F 3	94.6	0	2019.8	0.0			
15	7F 3	93.1	2	2043.4	0.0			
16	7F 3	94.5	2	2069.8	0.0			
17	7F 4	94.4	0	2734.3	0.0			
18	7F 4	94.9	2	2817.2	0.0			
19	7F 4	93.6	0	2891.0	0.0			
20	7F 4	94.6	0	2914.1	0.0			
21	7F 4	94.2	2	2983.2	0.0			
22	7F 4	94.4	0	3083.4	0.0			
23	7F 4	96.6	0	3117.1	0.0			
24	7F 4	96.6	2	3153.0	0.0			
25	7F 4	96.8	2	3211.0	0.0			
26	7F 5	95.1	0	3454.7	0.0			
27	7F 5	94.6	2	3486.7	0.0			
28	7F 5	93.0	2	3942.7	0.0			
29	7F 5	93.5	0	3983.8	0.0			
30	7F 5	92.6	0	4096.1	0.0			
31	7F 5	95.3	2	4102.9	0.0			
32	7F 5	95.0	2	4114.5	0.0			
33	7F 5	92.1	0	4134.6	0.0			
34	7F 5	97.7	0	4216.3	0.0			
35	7F 5	97.2	2	4234.8	0.0			
36	7F 5	97.8	2	4285.3	0.0			
37	7F 6	97.1	2	4911.2	0.0			
38	7F 6	95.8	0	4927.0	0.0			
39	7F 6	96.5	2	5024.0	0.0			
40	7F 6	96.8	0	5074.6	0.0			
41	7F 6	96.1	0	5173.9	0.0			
42	7F 6	97.3	2	5187.1	0.0			
43	7F 6	95.3	0	5191.0	0.0			
44	7F 6	97.7	2	5173.2	0.0			
45	7F 6	97.6	0	5215.3	0.0			
46	7F 6	95.4	2	5244.3	0.0			
47	7F 6	95.3	2	5244.8	0.0			
48	7F 6	99.1	0	5381.3	0.0			
49	7F 6	99.1	0	5390.5	0.0			
50	5D 0	100.0	0	17219.7	0.0			

[a] *See footnote at end of table.*

TABLE IX. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Eu^{3+} In $YAlO_3$[a] (CONT'D)

	FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
51	SD 1 3	100.0	2	18932.9	0.0
52	SD 1 3	100.0	2	18955.3	0.0
53	SD 1 3	100.0	0	18990.5	0.0
54	SD 2 3	100.0	0	21391.1	0.0
55	SD 2 3	100.0	0	21401.0	0.0
56	SD 2 3	100.0	2	21422.0	0.0
57	SD 2 3	100.0	0	21436.2	0.0
58	SD 2 3	100.0	2	21458.3	0.0
59	SD 3 3	100.0	0	24624.0	0.0
60	SD 3 3	100.0	0	24626.2	0.0
61	SD 3 3	100.0	2	24637.4	0.0
62	SD 3 3	100.0	2	24656.6	0.0
63	SD 3 3	100.0	0	24658.4	0.0
64	SD 3 3	100.0	2	24691.2	0.0
65	SD 3 3	100.0	2	24695.4	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the θ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE X. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Gd^{3+} IN $YAlO_3$[a]

GD IN YALO3. SCALED B4M FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
INIT. B4M AND CENTROIDS. Q = 0.000

536.000 = B21 -104.000 = B22 -349.000 = B40 -531.000 = B42 366.000 = B42 -38.000 = B44 -614.000 = B44
-355.000 = B61 -41.000 = B62 -225.000 = B62 696.000 = B64 -47.000 = B64 -244.000 = B66 159.000 = B66

6S 7/2 0.0
6P 7/2 32210.0
6P 5/2 32753.0
6P 3/2 33289.0
6I 7/2 35465.0
6I 3/2 36217.0
6I17/2 36448.0
6I11/2 36516.0
6I13/2 36700.0
6I15/2 36711.0

	FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	8S 7/2	100.0	1	-0.4	0.0
2	8S 7/2	100.0	1	-0.2	0.0
3	8S 7/2	100.0	1	0.0	0.0
4	8S 7/2	100.0	1	0.2	0.0
5	6P 7/2	99.4	1	32117.3	0.0
6	6P 7/2	99.1	1	32171.9	0.0
7	6P 7/2	99.2	1	32701.3	0.0
8	6P 7/2	99.4	1	32736.9	0.0
9	6P 5/2	99.4	1	32694.3	0.0
10	6P 5/2	99.1	1	32715.7	0.0
11	6P 5/2	99.4	1	32750.2	0.0
12	6P 3/2	99.7	1	33136.5	0.0
13	6P 3/2	99.4	1	33274.0	0.0
14	6I 7/2	99.4	1	35533.4	0.0
15	6I 7/2	99.7	1	35560.2	0.0
16	6I 7/2	99.3	1	35636.2	0.0
17	6I 7/2	99.5	1	35703.3	0.0
18	6I 5/2	99.2	1	36188.9	0.0
19	6I 5/2	99.6	1	36204.2	0.0
20	6I 5/2	99.4	1	36227.6	0.0
21	6I 5/2	99.1	1	36241.8	0.0
22	6I 5/2	99.1	1	36256.7	0.0
23	6I17/2	97.4	1	36448.0	0.0
24	6I17/2	97.7	1	36448.3	0.0
25	6I17/2	99.3	1	36448.7	0.0
26	6I17/2	99.7	1	36449.0	0.0
27	6I17/2	97.1	1	36451.4	0.0
28	6I17/2	97.0	1	36451.8	0.0
29	6I17/2	98.3	1	36455.4	0.0
30	6I17/2	96.7	1	36457.3	0.0
31	6I17/2	92.1	1	36472.1	0.0
32	6I11/2	92.4	1	36491.3	0.0
33	6I11/2	93.1	1	36501.4	0.0
34	6I11/2	95.9	1	36515.0	0.0
35	6I11/2	96.4	1	36534.9	0.0
36	6I11/2	97.3	1	36547.4	0.0
37	6I11/2	97.4	1	36556.7	0.0
38	6I13/2	98.7	1	36660.9	0.0
39	6I13/2	91.6	1	36674.4	0.0
40	6I13/2	74.7	1	36681.6	0.0
41	6I15/2	62.4	1	36690.5	0.0
42	6I15/2	63.5	1	36691.5	0.0
43	6I15/2	65.0	1	36701.3	0.0
44	6I15/2	68.6	1	36707.4	0.0
45	6I13/2	50.0	1	36712.9	0.0
46	6I15/2	67.4	1	36723.7	0.0
47	6I13/2	66.9	1	36725.6	0.0
48	6I13/2	56.8	1	36737.9	0.0
49	6I15/2	63.0	1	36742.2	0.0
50	6I15/2	65.8	1	36745.5	0.0
51	6I15/2	56.9	1	36752.0	0.0
52	6I15/2	74.4	1	36757.4	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XI. ENERGY LEVELS AND PHENOMENOLOGICAL B_{km} FOR Tb^{3+} IN $YAlO_3$[a]

TB IN YALO RUSSIAN DATA 7 MULTIPLETS 4713/75 RUN NO. 5
FINAL RKM AND CENTROIDS. Q = 7.521

567.335 = B20	-233.157 = B22	-1060.235 = B40	-717.484 = B42
476.378 = B44	-338.484 = B44	-81.516 = B44	-751.000 = B60
-317.404 = B62	-424.488 = B62	740.373 = B64	-508.102 = B64
-223.503 = B66	31.309 = B66		

7F 6	303.2		
7F 5	2322.9		
7F 4	3560.1		
7F 3	4601.8		
7F 2	5224.7		
7F 1	5633.6		
7F 0	5839.4		
5D 4 3	20629.3		

FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1 7F 6	99.3	0	-2.4	-0.0
2 7F 6	99.6	0	-1.7	-0.0
3 7F 6	98.7	2	151.0	-0.0
4 7F 5	93.1	0	188.2	-0.0
5 7F 6	99.1	2	188.6	-0.0
6 7F 6	99.1	2	256.1	-0.0
7 7F 6	99.5	0	327.3	-0.0
8 7F 6	99.4	2	476.0	-0.0
9 7F 6	99.1	0	496.4	-0.0
10 7F 6	99.3	0	536.4	-0.0
11 7F 6	99.2	2	607.4	-0.0
12 7F 6	99.1	0	654.1	-0.0
13 7F 6	99.2	2	660.2	-0.0
14 7F 5	94.9	2	2114.5	2126.0*
15 7F 5	98.3	2	2169.9	2165.0
16 7F 5	97.4	0	2189.1	2183.0
17 7F 5	96.3	0	2222.9	2214.0*
18 7F 5	99.2	0	2247.1	2246.0
19 7F 5	97.1	2	2254.9	2244.0
20 7F 5	99.7	2	2279.2	2273.0
21 7F 5	97.2	0	2377.8	-0.0
22 7F 5	97.2	2	2477.7	-0.0
23 7F 5	96.4	2	2494.4	2494.0
24 7F 5	97.6	0	2511.2	2511.0*
25 7F 4	96.7	2	3155.2	-0.0
26 7F 4	99.0	2	3417.4	3421.0*
27 7F 4	99.0	0	3431.6	-0.0
28 7F 4	99.1	0	3466.7	3464.0*
29 7F 4	99.0	2	3540.3	3539.0
30 7F 4	99.2	0	3651.3	3650.0
31 7F 4	99.3	0	3668.9	3668.0
32 7F 4	99.7	2	3752.5	3751.0
33 7F 4	99.4	0	3802.4	-0.0
34 7F 3	99.3	2	4534.3	-0.0
35 7F 3	99.4	2	4546.2	4545.0
36 7F 3	99.1	0	4564.9	4573.0*
37 7F 3	99.1	0	4621.8	-0.0
38 7F 3	99.5	2	4664.7	-0.0
39 7F 3	99.3	0	4679.3	4684.0*
40 7F 3	99.3	2	4711.2	4697.0*
41 7F 2	99.1	0	5168.4	-0.0
42 7F 2	99.7	0	5256.0	-0.0
43 7F 2	99.4	2	5280.4	-0.0
44 7F 2	99.4	2	5284.4	-0.0
45 7F 2	99.1	0	5376.1	-0.0
46 7F 1	99.7	0	5431.0	5434.0
47 7F 1	99.7	2	5460.0	5464.0
48 7F 1	99.4	2	5488.2	5487.0
49 7F 0	99.4	0	5587.4	5589.0
50 5D 4 3	100.0	2	21 [illegible]	21564.0*
51 5D 4 3	100.0	2	21 [illegible]	21577.0
52 5D 4 3	100.0	0	21 [illegible]	21595.0
53 5D 4 3	100.0	0	21 [illegible]	21616.0
54 5D 4 3	100.0	0	21 [illegible]	-0.0
55 5D 4 3	100.0	2	21 [illegible]	21641.0
56 5D 4 3	100.0	2	21 [illegible]	21681.0*
57 5D 4 3	100.0	0	21 [illegible]	21687.0
58 5D 4 3	100.0	2	21 [illegible]	21702.0

[a] *The least rms deviation between the calculated and experimental energy levels is 7.521 cm^{-1}.*

TABLE XII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Tb^{3+} IN $YAlO_3$[a]

TB IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
INIT. BKM AND CENTROIDS. Q = -0.000

536.000 = B20	-164.000 = B22	-915.000 = B40	-512.000 = B42	353.000 = B62	-36.000 = B44	-592.000 = B64
-904.000 = B60	-47.000 = B62	-213.000 = B62	657.000 = B64	-44.000 = B64	-231.000 = B66	151.000 = B66

7F 6		310.3
7F 5		2347.0
7F 4		3580.0
7F 3		4573.0
		5155.0
7F 1		5432.3
7F 0		5766.0
5D 4	3	20569.0
	3	26357.0

	FREE ION	PCT PURE	2MJ	THEO.ENERGY	EXP.ENERGY
1 7F 6	99.7	3	38.2	0.0	
2 7F 6	99.7	0	38.3	0.0	
3 7F 6	99.0	2	186.9	0.0	
4 7F 6	98.7	2	134.0	0.0	
5 7F 6	99.4	0	214.7	0.0	
6 7F 6	99.3	2	253.5	0.0	
7 7F 6	98.7	0	310.1	0.0	
8 7F 6	99.3	2	344.0	0.0	
9 7F 5	98.3	0	349.7	0.0	
10 7F 5	99.1	0	386.9	0.0	
11 7F 6	99.6	2	393.3	0.0	
12 7F 6	99.1	0	439.7	0.0	
13 7F 6	99.2	2	507.4	0.0	
14 7F 5	99.0	2	2149.7	0.0	
15 7F 5	98.7	2	2205.6	0.0	
16 7F 5	98.8	0	2217.1	0.0	
17 7F 5	97.1	0	2266.0	0.0	
18 7F 5	99.4	2	2285.6	0.0	
19 7F 5	97.9	2	2309.9	0.0	
20 7F 5	96.3	0	2312.5	0.0	
21 7F 5	97.1	0	2408.5	0.0	
22 7F 5	95.9	2	2457.4	0.0	
23 7F 5	97.0	2	2504.2	0.0	
24 7F 5	96.7	0	2544.0	0.0	
25 7F 4	98.3	2	3376.6	0.0	
26 7F 4	98.0	2	3429.5	0.0	
27 7F 4	97.4	0	3469.7	0.0	
28 7F 4	95.6	0	3494.6	0.0	
29 7F 4	95.7	2	3541.3	0.0	
30 7F 4	95.5	0	3647.3	0.0	
31 7F 4	94.2	0	3668.4	0.0	
32 7F 4	96.3	2	3734.2	0.0	
33 7F 4	95.3	0	3810.4	0.0	
34 7F 3	91.6	2	4490.4	0.0	
35 7F 3	92.3	2	4511.8	0.0	
36 7F 3	93.4	0	4535.0	0.0	
37 7F 3	88.8	0	4569.0	0.0	
38 7F 3	95.8	2	4623.6	0.0	
39 7F 3	90.9	0	4643.9	0.0	
40 7F 3	96.5	2	4651.3	0.0	
41 7F 2	94.3		5704.0	0.0	
42 7F 2	93.3		5730.2	0.0	
43 7F 2	94.3	2	5811.6	0.0	
44 7F 2	93.3	2	5841.1	0.0	
45 7F 2	91.5	2	5895.4	0.0	

[a] See footnote at end of table.

TABLE XII. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Tb^{3+} IN $YAlO_3$[a] (CONT'D)

	FREE ION		PCT PURE	2MJ	THEO. ENERGY	EXP. ENERGY
46	7F	1	94.3	0	5490.3	0.0
47	7F	1	92.9	2	5491.9	0.0
48	7F	1	96.8	2	5573.3	0.0
49	7F	0	95.0	0	5820.4	0.0
50	5D	4	100.0	2	20513.7	0.0
51	5D	4	100.0	0	20522.6	0.0
52	5D	4	100.0	2	20524.3	0.0
53	5D	4	100.0	0	20534.4	0.0
54	5D	4	100.0	0	20569.8	0.0
55	5D	4	100.0	2	20592.1	0.0
56	5D	4	100.0	0	20610.7	0.0
57	5D	4	100.0	0	20620.9	0.0
58	5D	4	100.0	2	20626.6	0.0
59	5D	3	100.0	2	26334.7	0.0
60	5D	3	100.0	2	26347.2	0.0
61	5D	3	100.0	2	26354.6	0.0
62	5D	3	100.0	0	26357.7	0.0
63	5D	3	100.0	0	26363.6	0.0
64	5D	3	100.0	2	26365.1	0.0
65	5D	3	100.0	0	26373.7	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XIII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Dy^{3+} IN $YAlO_3$[a]

DY IN YALO3 RUSSELL DATA & MULTIPLETS 9/15/75
FINAL BKW AND CENTROIDS. Q = 0.010

532.856 = 420	-162.598 = 422	282.424 = 840	-616.006 = 842	239.789 = 842	151.364 = 844	-404.707 = 844
-328.389 = 863	156.011 = 862	-204.367 = 862	647.536 = 864	-96.759 = 864	-440.255 = 866	48.157 = 866

6H15/2 2684.3
6H13/2 3721.9
6H11/2 6876.4
6F 9/2 10397.0
6F 7/2 11106.1
6F 5/2 12646.9

			FREE ION	PCT PURE	ZNU	THEO.ENERGY	EXP.ENERGY
1	6H15/2	99.7	1	2.9	0.0		
2	6H15/2	99.3	1	56.1	65.0*		
3	6H15/2	99.1	1	134.8	142.0		
4	6H15/2	99.3	1	227.1	226.0		
5	6H15/2	99.7	1	284.3	286.0		
6	6H15/2	99.6	1	402.9	404.0		
7	6H15/2	99.6	1	484.4	484.0		
8	6H15/2	99.8	1	561.2	558.0		
9	6H13/2	99.7	1	3541.7	3536.0*		
10	6H13/2	99.7	1	3657.4	3587.0*		
11	6H13/2	99.7	1	3666.3	3664.0		
12	6H13/2	99.8	1	3741.1	3741.0		
13	6H13/2	99.2	1	3794.2	3804.0*		
14	6H13/2	99.5	1	3827.0	3833.0		
15	6H13/2	99.5	1	3876.4	3881.0		
16	6H11/2	99.7	1	5866.2	5865.0		
17	6H11/2	99.3	1	5944.8	5952.0		
18	6H11/2	99.5	1	6043.5	6043.0		
19	6H11/2	99.5	1	6072.1	6071.0		
20	6H11/2	99.2	1	6088.3	6085.0*		
21	6H11/2	99.6	1	6166.6	6173.0		
22	6F 9/2	98.9	1	10231.9	10235.0		
23	6F 9/2	99.4	1	10337.6	10337.0		
24	6F 9/2	99.6	1	10407.8	10404.0		
25	6F 7/2	99.1	1	11 [illegible].5	11074.0*		
26	6F 7/2	99.1	1	11113.6	11129.0*		
27	6F 7/2	99.7	1	11154.2	11165.0*		
28	6F 7/2	99.2	1	11211.9	11203.0		
29	6F 5/2	99.2	1	12462.-	12469.0*		
30	6F 5/2	99.7	1	12506.1	12500.0		
31	6F 5/2	99.7	1	12541.8	12555.0*		

CENTROIDS, CRYSTAL = 5724.7 FREE ION = 5724.9

[a] *The least-rms deviation between the calculated and experimental energy levels is 8.010 cm^{-1}.*

TABLE XIV. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Dy^{3+} IN $YAlO_3$[a]

DY IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
INIT. BKM AND CENTROIDS. Q = -0.000

540.000 = B20	-165.000 = B22	-884.000 = B40	-495.000 = B42	341.000 = B62	-35.000 = B44	-573.000 = B64
-854.000 = B60	-44.000 = B62	-201.000 = B62	621.000 = B64	-42.000 = B64	-218.000 = B66	143.000 = B66

6H15/2 270.0
6H13/2 3737.0
6H11/2 6052.0
6H 9/2 7806.0
6F11/2 7818.0
6F 9/2 9219.0
6H 7/2 9274.0
6H 5/2 10371.0
6F 7/2 11084.0
6F 5/2 12477.0

			FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY			
1	6H15/2	99.9	1	43.2	0.0					
2	6H15/2	99.9	1	75.1	0.0					
3	6H15/2	99.8	1	152.8	0.0					
4	6H15/2	99.9	1	211.2	0.0					
5	6H15/2	99.7	1	268.2	0.0					
6	6H15/2	99.6	1	323.1	0.0					
7	6H15/2	99.2	1	463.5	0.0					
8	6H15/2	99.8	1	549.0	0.0					
9	6H13/2	99.4	1	3566.7	0.0					
10	6H13/2	99.7	1	3603.9	0.0					
11	6H13/2	99.5	1	3690.9	0.0					
12	6H13/2	99.8	1	3740.1	0.0					
13	6H13/2	99.2	1	3779.5	0.0					
14	6H13/2	99.3	1	3810.7	0.0					
15	6H13/2	99.2	1	3874.4	0.0					
16	6H11/2	99.1	1	5301.8	0.0					
17	6H11/2	98.1	1	5345.1	0.0					
18	6H11/2	98.3	1	6033.3	0.0					
19	6H11/2	98.8	1	6075.1	0.0					
20	6H11/2	98.6	1	6093.2	0.0					
21	6H11/2	99.6	1	6153.2	0.0					
22	6H 9/2	72.1	1	7577.5	0.0					
23	6H 9/2	64.2	1	7593.1	0.0					
24	6F11/2	62.3	1	7719.5	0.0					
25	6F11/2	65.2	1	7747.6	0.0					
26	6F11/2	62.1	1	7783.3	0.0					
27	6F11/2	56.3	1	7796.6	0.0					
28	6F11/2	43.7	1	7862.2	0.0					
29	6F11/2	65.1	1	7872.3	0.0					
30	6H 9/2	91.0	1	7927.8	0.0					
31	6F11/2	66.7	1	8030.8	0.0					
32	6F11/2	96.5	1	8056.3	0.0					
33	6H 7/2	92.7	1	8086.4	0.0					
34	6F 9/2	57.7	1	9095.0	0.0					
35	6H 7/2	98.2	1	9140.3	0.0					
36	6F 9/2	93.7	1	9204.9	0.0					
37	6F 9/2	83.9	1	9256.3	0.0					
38	6F 9/2	69.0	1	9296.0	0.0					
39	6H 7/2	65.6	1	9327.7	0.0					
40	6H 7/2	57.0	1	9421.1	0.0					
41	6H 7/2	69.2	1	9484.4	0.0					
42	6H 5/2	93.8	1	10248.2	0.0					
43	6H 5/2	92.3	1	10357.2	0.0					
44	6H 5/2	91.6	1	10508.5	0.0					
45	6F 7/2	96.3	1	11079.2	0.0					
46	6F 7/2	96.1	1	11101.9	0.0					
47	6F 7/2	98.0	1	11131.5	0.0					
48	6F 7/2	93.9	1	11201.7	0.0					
49	6F 5/2	99.1	1	12469.7	0.0					
50	6F 5/2	99.5	1	12499.8	0.0					
51	6F 5/2	99.0	1	12547.1	0.0					

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XV. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Ho^{3+} IN $YAlO_3$[a]

HO IN YALO RUSSIAN DATA 9/18/75 RUNE NO. 6
FINAL B** AND CENTROIDS. S = 7.033
716.337 = 820 -246.198 = 822 -837.569 = 840 -543.630 = 842 384.231 = 842 -63.195 = 844 -359.912 = 844
-963.432 = 860 211.439 = 862 -213.585 = 862 -40.725 = 864 592.750 = 864 -749.981 = 866 19.183 = 866
5I 8 295.1
5I 7 5267.3
5I 6 8736.7
5I 5 11243.7

					FREE ION	PCT PURE	2RU	THEO.ENERGY	EXP.ENERGY				
1	5I	6	99.9	2	-2.1	0.0		33 5I 6	99.7	0	8634.5	8626.0*	
2	5I	6	99.8	2	6.2	-0.0		34 5I 6	99.6	0	8648.0	8647.0	
3	5I	6	99.9	0	41.1	44.0		35 5I 6	99.6	2	8661.7	-0.0	
4	5I	6	99.9	0	64.1	65.0		36 5I 6	99.9	2	8690.4	8690.0	
5	5I	6	99.9	4	110.6	-0.0		37 5I 6	99.9	0	8714.4	8708.0	
6	5I	6	99.8	0	161.4	155.0		38 5I 6	99.9	2	8727.1	8730.0*	
7	5I	6	99.8	2	191.7	196.0		39 5I 6	99.9	0	8735.1	8736.0	
8	5I	6	99.9	0	233.7	234.0		40 5I 6	99.9	2	8752.5	8760.0*	
9	5I	6	99.8	2	264.1	-0.0		41 5I 6	99.8	0	8775.8	8772.0	
10	5I	6	99.9	0	329.6	330.0		42 5I 6	99.8	0	8792.9	8800.0*	
11	5I	6	99.9	0	382.2	390.0		43 5I 6	99.9	2	8824.3	8807.0*	
12	5I	6	99.9	2	404.9	405.0		44 5I 6	99.8	2	8844.5	8837.0*	
13	5I	6	99.9	0	443.9	-0.0		45 5I 6	99.4	0	8854.4	8867.0*	
14	5I	6	99.8	2	480.4	-0.0							
15	5I	6	99.9	0	514.1	-0.0		46 5I 5	99.5	2	11232.4	-0.0	
16	5I	6	99.7	0	618.9	-0.0		47 5I 5	99.8	2	11219.2	11229.0*	
17	5I	6	99.8	2	616.3	-0.0		48 5I 5	99.5	0	11240.3	11247.0	
18	5I	7	99.7	0	5148.3	5137.0*		49 5I 5	99.8	0	11262.4	11252.0*	
19	5I	7	99.6	0	5151.2	-0.0		50 5I 5	99.4	2	11283.1	11274.0*	
20	5I	7	99.6	2	5171.5	-0.0		51 5I 5	99.7	2	11306.8	11303.0	
21	5I	7	99.6	2	5176.8	5183.0*		52 5I 5	99.4	0	11308.8	11312.0	
22	5I	7	99.5	0	5234.3	5225.0*		53 5I 5	99.4	0	11330.3	11327.0	
23	5I	7	99.7	2	5244.3	5246.0		54 5I 5	99.6	2	11354.2	11364.0*	
24	5I	7	99.6	2	5253.6	5256.0		55 5I 5	99.5	2	11384.0	11370.0*	
25	5I	7	99.5	0	5266.8	5269.0		56 5I 5	99.4	0	11398.2	11402.0	
26	5I	7	99.5	2	5284.3	5285.0							
27	5I	7	99.7	0	5307.7	5307.0							
28	5I	7	99.4	2	5319.0	5323.0							
29	5I	7	99.5	2	5331.3	5328.0							
30	5I	7	99.6	0	5342.2	5343.0							
31	5I	7	99.5	0	5363.9	5359.0							
32	5I	7	99.5	2	5366.0	5376.0*							

[a] *The least-rms deviation between the calculated and experimental energy levels is 7.033 cm^{-1}.*

TABLE XVI. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Ho^{3+} IN $YAlO_3$[a]

HO IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER HOPED RESULTS
INIT. BKM AND CENTROIDS. Q = 0.0CJ

542.000 = B23 -166.000 = B22 -860.000 = B40 -481.000 = B42 332.000 = B42 -34.000 = B44 -557.000 = B44
-815.000 = B60 -42.000 = B62 -192.000 = B62 592.000 = B64 -40.000 = B64 -208.000 = B66 136.000 = B66

5I 8 169.6
5I 7 5219.5
5I 6 8717.6
5I 5 11274.7
5I 4 13333.4

			FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	5I 8	99.9	2	-92.1	0.0		
2	5I 8	99.9	2	-84.4	0.0		
3	5I 8	100.0	0	-43.5	0.0		
4	5I 8	99.9	C	-27.1	0.0		
5	5I 8	99.9	2	51.3	0.0		
6	5I 8	100.0	0	72.3	0.0		
7	5I 8	99.8	2	147.3	0.0		
8	5I 8	100.0	0	177.8	0.0		
9	5I 8	99.9	2	180.6	0.0		
10	5I 8	100.0	0	212.1	0.0		
11	5I 8	100.0	2	216.5	0.0		
12	5I 8	100.0	0	234.2	0.0		
13	5I 8	99.9	0	307.2	0.0		
14	5I 8	99.9	2	322.0	0.0		
15	5I 8	99.9	0	351.5	0.0		
16	5I 8	99.9	2	378.6	0.0		
17	5I 8	99.9	0	386.4	0.0		
18	5I 7	99.8	0	5120.6	0.0		
19	5I 7	99.8	0	5124.1	0.0		
20	5I 7	99.7	2	5135.0	0.0		
21	5I 7	99.7	2	5140.5	0.0		
22	5I 7	99.7	0	5200.1	0.0		
23	5I 7	99.8	2	5211.9	0.0		
24	5I 7	99.7	0	5213.8	0.0		
25	5I 7	99.7	2	5225.5	0.0		
26	5I 7	99.8	2	5231.8	0.0		
27	5I 7	99.5	0	5235.2	0.0		
28	5I 7	99.8	2	5244.4	0.0		
29	5I 7	99.7	2	5285.0	0.0		
30	5I 7	99.8	0	5291.6	0.0		
31	5I 7	99.9	0	5301.2	0.0		
32	5I 7	99.9	2	5303.2	0.0		
33	5I 6	99.6	0	8643.2	0.0		
34	5I 6	99.6	0	8649.0	0.0		
35	5I 6	99.7	2	8653.5	0.0		
36	5I 6	99.7	2	8670.4	0.0		
37	5I 6	99.6	0	8688.6	0.0		
38	5I 6	99.6	C	8693.7	0.0		
39	5I 6	99.4	2	8696.3	0.0		
40	5I 6	99.4	2	8709.5	0.0		
41	5I 6	99.6	0	8726.9	0.0		
42	5I 6	99.7	0	8775.3	0.0		
43	5I 6	99.7	2	8783.2	0.0		
44	5I 6	99.9	2	8809.4	0.0		
45	5I 6	99.7	0	8809.9	0.0		
46	5I 5	98.9	2	11210.7	0.0		
47	5I 5	99.1	2	11215.9	0.0		
48	5I 5	99.4	0	11237.0	0.0		
49	5I 5	99.4	0	11244.4	0.0		
50	5I 5	98.8	2	11246.9	0.0		
51	5I 5	99.1	2	11256.4	0.0		
52	5I 5	99.3	0	11267.4	0.0		
53	5I 5	99.6	0	11304.1	0.0		
54	5I 5	99.5	2	11327.9	0.0		
55	5I 5	99.7	2	11347.4	0.0		
56	5I 5	99.2	0	11350.2	0.0		
57	5I 4	99.4	2	13174.6	0.0		
58	5I 4	99.6	0	13224.5	0.0		
59	5I 4	99.5	2	13239.1	0.0		
60	5I 4	99.6	0	13315.7	0.0		
61	5I 4	99.2	0	13362.4	0.0		
62	5I 4	99.3	2	13373.1	0.0		
63	5I 4	99.1	0	13437.1	0.0		
64	5I 4	99.1	2	13477.9	0.0		
65	5I 4	99.7	0	13523.9	0.0		

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XVII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Er^{3+} IN $YAlO_3$[a]

ER IN YALO ANTONOV'S DATA -HOPE 9/10/PK
FINAL BKM AND CENTROIDS. Q = 15.385

546.608 = B20	-7.553 = B22	-792.799 = B40	-487.332 = B42	391.316 = B42	-481.981 = B44	-466.919 = B44
-876.858 = B60	-304.470 = B62	-175.200 = B62	325.166 = B64	209.931 = B64	30.178 = B66	258.958 = B66

4I15/2	264.3
4I13/2	6737.3
4I11/2	10348.4
4I 9/2	12564.3
4F 9/2	15368.5
4S 3/2	18467.2
2H11/2 2	19192.1
4F 7/2	20581.5
4F 5/2	22229.8
4F 3/2	22564.5

			FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
1	4I15/2	99.9	1	-10.2		0.0	
2	4I15/2	100.0	1	57.8		50.0	
3	4I15/2	100.0	1	168.8		170.0	
4	4I15/2	100.0	1	212.4		217.0	
5	4I15/2	100.0	1	275.0		267.0	
6	4I15/2	100.0	1	378.0		389.0	
7	4I15/2	100.0	1	453.9		446.0	
8	4I15/2	100.0	1	528.5		525.0	
9	4I13/2	99.8	1	6589.0		6608.0*	
10	4I13/2	99.8	1	6643.8		6646.0	
11	4I13/2	99.7	1	6690.5		6674.0*	
12	4I13/2	99.9	1	6720.8		6720.0	
13	4I13/2	99.9	1	6773.4		6779.0	
14	4I13/2	99.8	1	6832.5		6820.0	
15	4I13/2	99.8	1	6871.3		6873.0	
16	4I11/2	99.7	1	10277.6		10290.0	
17	4I11/2	99.7	1	10300.8		10302.0	
18	4I11/2	99.7	1	10336.4		10330.0	
19	4I11/2	99.7	1	10354.5		10355.0	
20	4I11/2	99.7	1	10396.1		10390.0	
21	4I11/2	99.6	1	10413.4		10410.0	
22	4I 9/2	99.8	1	12374.3		12389.0	
23	4I 9/2	99.7	1	12458.1		12440.0*	
24	4I 9/2	99.9	1	12606.6		12617.0	
25	4I 9/2	99.9	1	12643.8		12642.0	
26	4I 9/2	99.8	1	12732.5		12726.0	
27	4F 9/2	99.9	1	15266.2		15263.0	
28	4F 9/2	99.8	1	15333.5		15346.0	
29	4F 9/2	99.8	1	15372.7		15375.0	
30	4F 9/2	99.8	1	15429.6		15397.0*	
31	4F 9/2	99.9	1	15461.4		15482.0*	
32	4S 3/2	96.8	1	18413.9		18409.0	
33	4S 3/2	97.2	1	18486.2		18490.0	
34	2H11/2 2	99.0	1	19116.5		19070.0*	
35	2H11/2 2	97.9	1	19139.0		19120.0*	
36	2H11/2 2	99.0	1	19175.6		19163.0	
37	2H11/2 2	99.5	1	19211.7		19243.0*	
38	2H11/2 2	97.5	1	19255.2		19278.0*	
39	2H11/2 2	98.5	1	19281.7		19305.0*	
40	4F 7/2	99.3	1	20518.3		20488.0*	
41	4F 7/2	99.1	1	20555.3		20560.0	
42	4F 7/2	98.6	1	20593.2		20623.0*	
43	4F 7/2	99.5	1	20694.3		20691.0	
44	4F 5/2	99.0	1	22211.2		22201.0	
45	4F 5/2	99.1	1	22217.7		22233.0	
46	4F 5/2	99.5	1	22272.9		22267.0	
47	4F 3/2	92.4	1	22552.8		22532.0*	
48	4F 3/2	94.7	1	22622.8		22643.0*	

[a] *The least-rms deviation between these calculated and experimental energy levels is 15.385 cm^{-1} (48 levels).*

TABLE XVIII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Er^{3+} IN $YAlO_3$

ER IN YALO RUSSELL DATA MULTIPLETS 7/15/75
FINAL EXP AND CALC DIFFS. Q = 7.461

430.390 = 842	1170.465 = 822	-835.695 = 842	-345.812 = 842	365.198 = 842	-218.279 = 844	-709.079 = 844
-742.421 = 863	-240.967 = 862	-1-0.513 = 862	534.345 = 864	17.009 = 864	23.210 = 866	223.613 = 866

4I15/2	262.4
4I13/2	6735.7
4I11/2	10345.6
4I 9/2	12560.3
4F 9/2	15364.9
4S 3/2	18443.8

			FREE ION	PCT PURE	THEO.ENERGY	EXP.ENERGY
1	4I15/2	99.9	1	2.9	0.0	
2	4I15/2	100.0	1	47.7	50.0	
3	4I15/2	100.0	1	172.3	170.0	
4	4I15/2	100.0	1	220.3	217.0	
5	4I15/2	100.0	1	264.8	267.0	
6	4I15/2	100.0	1	384.9	389.0	
7	4I15/2	100.0	1	453.1	446.0	
8	4I15/2	100.0	1	511.4	525.0	
9	4I13/2	99.9	1	6597.9	6606.0*	
10	4I13/2	99.9	1	6641.2	6646.0	
11	4I13/2	99.7	1	6686.0	6674.0*	
12	4I13/2	99.9	1	6723.7	6720.0	
13	4I13/2	99.9	1	6774.9	6779.0	
14	4I13/2	99.8	1	6830.2	6820.0*	
15	4I13/2	99.9	1	6868.8	6877.0	
16	4I11/2	99.9	1	10280.8	10290.0*	
17	4I11/2	99.9	1	10305.7	10302.0	
18	4I11/2	99.7	1	10331.6	10330.0	
19	4I11/2	99.9	1	10356.6	10359.0	
20	4I11/2	99.8	1	10390.9	10390.0	
21	4I11/2	99.7	1	10411.9	10410.0	
22	4I 9/2	99.9	1	12389.4	12394.0	
23	4I 9/2	99.9	1	12444.3	12440.0	
24	4I 9/2	100.0	1	12460.4	12617.0*	
25	4I 9/2	99.9	1	12647.9	12642.0	
26	4I 9/2	99.9	1	12727.4	12726.0	
27	4F 9/2	99.9	1	15287.6	15243.0*	
28	4F 9/2	99.9	1	15430.1	15346.0*	
29	4F 9/2	99.9	1	15476.1	15375.0	
30	4F 9/2	99.9	1	15614.6	15357.0*	
31	4F 9/2	99.9	1	15478.0	15492.0*	
32	4S 3/2	100.0	1	18415.2	18403.0*	
33	4S 3/2	99.9	1	18478.7	18460.0*	

CENTROIDS, CRYSTAL = 8722.4 FREE ION = 8722.3

TABLE XIX. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Er^{3+} IN $YAlO_3$[a]

ER IN YALO3. SCALED BKM FROM HO DETERMINED BY AVERAGING DY AND ER HOMED RESULTS
(NEIT. BKM AND CENTROIDS. Q = -0.00)

546.300 = B23 -167.000 = B22 -841.000 = B40 -470.000 = B42 325.000 = B42 -33.000 = B44 -544.000 = B44
-791.000 = B60 -41.000 = B62 -186.000 = B62 575.000 = B64 -39.000 = B64 -202.000 = B66 132.000 = B66

4I15/2	265.0
4I13/2	6738.3
4I11/2	10348.0
4I 9/2	12565.3
4F 9/2	15369.3
4S 3/2	18472.0
2H11/2 2	19150.3
4F 7/2	20582.3
4F 5/2	22230.3
4F 3/2	22561.3

	FREE ION		PCT PURE	2MU	THEO.ENERGY		EXP.ENERGY			
1 4I15/2	99.9	1	4.5	0.0		27 4F 9/2	99.3	1	15271.2	0.0
2 4I15/2	100.0	1	69.5	0.0		28 4F 9/2	99.8	1	15340.1	0.0
3 4I15/2	100.0	1	173.0	0.0		29 4F 9/2	99.9	1	15371.3	0.0
4 4I15/2	100.0	1	219.4	0.0		30 4F 9/2	99.4	1	15407.9	0.0
5 4I15/2	100.0	1	236.9	0.0		31 4F 9/2	99.9	1	15475.3	0.0
6 4I15/2	100.0	1	353.7	0.0						
7 4I15/2	100.0	1	462.9	0.0		32 4S 3/2	97.3	1	18421.1	0.0
8 4I15/2	100.0	1	542.9	0.0		33 4S 3/2	97.1	1	18493.3	0.0
9 4I13/2	99.9	1	6604.2	0.0		34 2H11/2 2	97.9	1	19115.7	0.0
10 4I13/2	99.8	1	6643.3	0.0		35 2H11/2 2	98.6	1	19139.0	0.0
11 4I13/2	99.8	1	6689.5	0.0		36 2H11/2 2	99.0	1	19183.1	0.0
12 4I13/2	99.8	1	6708.4	0.0		37 2H11/2 2	99.5	1	19205.6	0.0
13 4I13/2	99.8	1	6763.3	0.0		38 2H11/2 2	98.3	1	19248.7	0.0
14 4I13/2	99.8	1	6832.6	0.0		39 2H11/2 2	96.5	1	19269.5	0.0
15 4I13/2	99.9	1	6880.8	0.0						
						40 4F 7/2	99.4	1	20504.5	0.0
16 4I11/2	99.8	1	10281.9	0.0		41 4F 7/2	99.8	1	20554.3	0.0
17 4I11/2	99.7	1	10300.7	0.0		42 4F 7/2	99.9	1	20607.4	0.0
18 4I11/2	99.7	1	10331.0	0.0		43 4F 7/2	99.4	1	20694.5	0.0
19 4I11/2	99.8	1	10349.8	0.0						
20 4I11/2	99.6	1	10395.6	0.0		44 4F 5/2	99.2	1	22211.5	0.0
21 4I11/2	99.7	1	10418.5	0.0		45 4F 5/2	99.7	1	22217.7	0.0
						46 4F 5/2	99.4	1	22274.1	0.0
22 4I 9/2	99.8	1	12380.9	0.0						
23 4I 9/2	99.8	1	12462.7	0.0		47 4F 3/2	99.2	1	22537.4	0.0
24 4I 9/2	99.9	1	12577.9	0.0		48 4F 3/2	97.2	1	22626.2	0.0
25 4I 9/2	99.8	1	12664.1	0.0						
26 4I 9/2	99.8	1	12732.8	0.0						

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XX. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Tm^{3+} IN $YAlO_3$[a]

EP IN YALO RUSSIAN DATA 9/17/75
FINAL BK* AND CENTROIDS. Q = 6.16

675.198 = B20	-75.502 = B22	-783.36R = B40	-477.741 = B42	367.255 = B42	-54.338 = B44	-445.44 = B44
-752.332 = B60	-71.536 = B62	-153.912 = B62	609.*11 = B64	59.277 = B64	-218.224 = B66	115.257 = B66

3H 6	342.0	
3F 4	5862.8	
3H 5	8485.7	
3F 3	14546.4	
3F 2	15145.3	
1G 4	21343.6	

					FREE ION	PCT PURE	2PU	THEO.ENERGY	EXP.ENERGY				
1	3H	6	99.9	2	2.0	-0.0		29	3H	5	99.6	2	-0.0
2	3H	6	99.9	0	3.1	0.0		30	3H	5	99.5	0	8599.0*
3	3H	6	99.9	2	114.7	-0.0		31	3H	5	99.5	0	-0.0
4	3H	6	99.9	0	139.0	-0.0		32	3H	5	99.9	2	-0.0
5	3H	6	99.9	0	296.0	-0.0		33	3H	5	99.9	2	8396.0
6	3H	6	100.0	2	341.0	-0.0							
7	3H	6	100.0	2	385.4	-0.0		34	3F	3	99.6	2	14454.0*
8	3H	6	99.9	0	406.3	-0.0		35	3F	3	99.9	2	14493.0*
9	3H	6	99.9	0	460.3	-0.0		36	3F	3	99.9	0	14518.0
10	3H	6	100.0	2	473.2	472.0		37	3F	3	99.9	2	14564.4
11	3H	6	99.9	2	53[illegible]	-0.0		38	3F	3	99.7	2	14595.0*
12	3H	5	100.0	0	596.7	596.0		39	3F	3	99.1	0	14609.0
13	3H	5	100.0	0	621.5	628.0*		40	3F	3	99.9	2	14623.0
14	3F	4	99.7	2	5626.4	5631.0		41	3F	2	99.9	2	-0.0
15	3F	4	99.9	2	5714.3	5717.0		42	3F	2	99.9	0	-0.0
16	3F	4	99.1	0	5715.6	5729.0*		43	3F	2	99.7	2	-0.0
17	3F	4	99.7	0	5823.2	5825.0		44	3F	2	99.8	2	15197.9
18	3F	4	99.9	2	5830.4	5844.0		45	3F	2	99.1	0	15292.0
19	3F	4	99.6	0	5926.1	5919.0*							
20	3F	4	99.7	0	5980.6	-0.0		46	1G	4	[illegible]	2	21[illegible]
21	3F	4	99.9	2	5989.3	-0.0		47	1G	4	[illegible]	2	21[illegible]
22	3F	4	99.9	2	6033.8	-0.0		48	1G	4	[illegible]	2	21234.0*
								49	1G	4	[illegible]	0	21[illegible]
23	3H	5	99.6	0	8337.3	-0.0		50	1G	4	[illegible]	2	21329.4
24	3H	5	99.7	2	8257.3	8263.0		51	1G	4	[illegible]	2	21463.0
25	3H	5	99.8	2	8339.4	8344.0		52	1G	4	[illegible]	2	21491.0
26	3H	5	99.5	0	8377.4	8377.0		53	1G	4	[illegible]	2	-0.0
27	3H	5	99.7	0	8449.3	8485.0		54	1G	4	[illegible]	2	21[illegible]
28	3H	5	99.5	2	8535.5	8535.0							

[a] *The least-rms deviation between the calculated and experimental energy levels is 6.16 cm^{-1}.*

TABLE XXI. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Tm^{3+} IN $YAlO_3$[a]

TM IN YALO3. SCALED CRM FROM HO DETERMINED BY AVERAGING DY AND ER HOPED RESULTS
INIT. BKP AND CENTROIDS. Q = -0.020
552.000 = B20 -169.000 = B22 -826.000 = B40 -462.000 = B42 319.000 = B42 -33.000 = B44 -535.000 = B44
-778.000 = B60 -40.000 = B62 -183.000 = B62 565.000 = B64 -38.000 = B64 -196.000 = B66 130.000 = B66

3H 6	255.0	
3F 4	5820.0	
3H 5	8435.0	
3H 4	12731.0	
3F 3	14529.0	
3F 2	15133.0	
1G 4	21325.0	
1D 2	27892.0	

				FREE ION	PCT PURE	ZPU	THEO.ENERGY	EXP.ENERGY				
1	3H 6	99.9	0	-74.2	0.0		29	3H 5	99.6	2	8479.8	0.0
2	3H 6	99.9	2	-68.8	0.0		30	3H 5	99.5	0	8553.1	0.0
3	3H 6	99.9	2	31.4	0.0		31	3H 5	99.6	0	8573.2	0.0
4	3H 6	100.0	0	55.7	0.0		32	3H 5	99.7	2	8614.1	0.0
5	3H 6	99.8	0	202.6	0.0		33	3H 5	99.9	2	8631.9	0.0
6	3H 6	100.0	2	242.6	0.0							
7	3H 6	99.9	2	298.7	0.0		34	3H 4	99.5	0	12459.0	0.0
8	3H 6	99.9	0	323.2	0.0		35	3H 4	98.8	2	12570.1	0.0
9	3H 6	99.8	0	350.3	0.0		36	3H 4	99.6	2	12652.4	0.0
10	3H 6	99.9	2	392.4	0.0		37	3H 4	98.8	0	12681.9	0.0
11	3H 6	99.8	2	450.3	0.0		38	3H 4	98.8	2	12745.4	0.0
12	3H 6	99.9	0	484.7	0.0		39	3H 4	99.2	2	12765.0	0.0
13	3H 6	99.9	0	508.9	0.0		40	3H 4	99.4	0	12800.9	0.0
							41	3H 4	99.6	0	12886.4	0.0
14	3F 4	99.7	0	5583.2	0.0		42	3H 4	99.3	0	12938.5	0.0
15	3F 4	99.4	2	5664.9	0.0							
16	3F 4	99.2	0	5690.1	0.0		43	3F 3	98.9	2	14479.9	0.0
17	3F 4	99.6	0	5777.5	0.0							
18	3F 4	99.4	2	5840.9	0.0		44	3F 3	99.1	2	14494.7	0.0
19	3F 4	99.6	0	5883.4	0.0		45	3F 3	97.9	0	14526.6	0.0
20	3F 4	99.7	0	5925.2	0.0		46	3F 3	98.3	2	14532.4	0.0
21	3F 4	99.5	2	5956.9	0.0		47	3F 3	98.7	2	14560.3	0.0
22	3F 4	99.7	2	6002.3	0.0		48	3F 3	99.6	0	14591.9	0.0
							49	3F 3	97.9	0	14614.6	0.0
23	3H 5	99.6	0	8197.3	0.0							
24	3H 5	99.6	2	8214.7	0.0							
25	3H 5	99.6	2	8296.6	0.0							
26	3H 5	99.5	0	8331.1	0.0							
27	3H 5	99.5	0	8440.6	0.0							
28	3H 5	99.3	2	8460.6	0.0							

[a] *See footnote at end of table.*

TABLE XXI. CRYSTAL FIELD PARAMETERS, B_{km}, AND ENERGY LEVELS FOR Tm^{3+} IN $YAlO_3$ (CONT'D)

	FREE ION	PCT PURE	2MU	THEO.ENERGY	EXP.ENERGY
50	3F 2	[illegible]	[illegible]	[illegible]	0.0
51	3F 2	[illegible]	[illegible]	[illegible]	0.0
52	3F 2	[illegible]	[illegible]	[illegible]	0.0
53	3F 2	[illegible]	[illegible]	[illegible]	0.0
54	3F 2	[illegible]	[illegible]	[illegible]	0.0
55	1G 4	[illegible]	[illegible]	[illegible]	0.0
56	1G 4	[illegible]	[illegible]	[illegible]	0.0
57	1G 4	[illegible]	[illegible]	[illegible]	0.0
58	1G 4	[illegible]	[illegible]	[illegible]	0.0
59	1G 4	[illegible]	[illegible]	[illegible]	0.0
60	1G 4	[illegible]	[illegible]	[illegible]	0.0
61	1G 4	[illegible]	[illegible]	[illegible]	0.0
62	1G 4	[illegible]	[illegible]	[illegible]	0.0
63	1G 4	[illegible]	[illegible]	[illegible]	0.0
64	1D 2	[illegible]	[illegible]	[illegible]	0.0
65	1D 2	[illegible]	[illegible]	[illegible]	0.0
66	1D 2	[illegible]	[illegible]	[illegible]	0.0
67	1D 2	[illegible]	[illegible]	[illegible]	0.0
68	1D 2	[illegible]	[illegible]	[illegible]	0.0

[a] *These B_{km} values were obtained by scaling the Ho parameters by the ρ_k value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological B_{km} values.*

TABLE XXII. AMPLITUDES, CRYSTAL FIELD COMPONENTS, A_{km} IN cm^{-1} $Å^{-k}$, OF SPHERICAL DECOMPOSITION OF $YAlO_3$ LATTICE SUMS[a]

k	m	A_{km} [illegible]	A_{km} [illegible]
2	0	-811.2	1627
2	1	1703	[illegible]
2	2	68.17	816.8
3	0	-4442	9252
3	1	-1834	-1184
3	2	-1025	-1125
3	3	336.2	3230
4	0	-371.3	-627.0
4	1	-1976	-3918
4	2	1994	419.6
4	3	-659.1	-1231
4	4	1462	824.2
5	0	-812.3	-1553
5	1	-329.8	-779.6
5	2	53.93	128.1
5	3	-272.2	-932.3
5	4	-1321	-2673
5	5	794.9	1815
6	0	-738.4	-1751
6	1	32.35	60.47
6	2	-231.1	-554.4
6	3	110.3	224.5
6	4	435.9	1046
6	5	121.9	243.6
6	6	-282.9	-719.6
7	0	15.18	30.56
7	1	-160.1	-309.7
7	2	-72.75	-146.5
7	3	-26.31	-58.64
7	4	13.59	27.87
7	5	15.48	30.00
7	6	-27.56	-55.06
7	7	-21.40	-42.37

[a] [illegible] A_{km} [illegible]

[b] [illegible] q_Y [illegible] q_{Al} [illegible] respectively. The lattice constants [illegible] Å, [illegible] Å, [illegible] Å (R. Diehl and [illegible], Materials Research Bulletin, [illegible] (19[illegible]), 85-90). The atomic coordinates are as follows:

Atom	Y^{3+}	Al^{3+}	O_I^{2-}	O_{II}^{2-}
Position	4c	4b	4c	8d
x	0.0526(2)	0	0.475(2)	0.293(2)
y	0.025	0	0.025	0.044(2)
z	0.9896(2)	0.050	0.086(2)	0.703(2)

TABLE XXIII. AMPLITUDES, CRYSTAL FIELD COMPONENTS, A_{km} IN cm^{-1} $Å^{-k}$, OF SPHERICAL DECOMPOSITION OF $YAlO_3$ LATTICE SUMS FOR EVEN VALUES OF k^a

k	m	$A_{km}(\alpha_0 = 1)$		$A_{km}(\alpha_0 = 1.5)$	
		Real	Imaginary	Real	Imaginary
2	0	2365	0	3482	0
2	1	0	-384.5	0	-466.2
2	2	610.3	0	615.4	0
4	0	-3749	0	-3321	0
4	1	0	1401	0	2108
4	2	698.2	0	1007	0
4	3	0	860.0	0	1274
4	4	-779.5	0	167.3	0
6	0	-285.6	0	-502.2	0
6	1	0	36.68	0	62.46
6	2	-67.11	0	-101.0	0
6	3	0	96.78	0	146.2
6	4	739.6	0	125.9	0
6	5	0	-52.15	0	-77.24
6	6	137.8	0	204.2	0

[a] The coordinate system has been rotated so that the real part of A_{km} = 0 for m odd. The lattice constants and atomic positions are given in Table XXII.

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