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Rare Earth Ions in a Hexagonal Field III*

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Energy levels and magnetic moments of rare earth ions in a crystal field of hexagonal symmetry have been obtained using a Hamiltonian of the form,

$$\mathscr{H} = \mu_B g\, \mathbf{J}\cdot\mathbf{H} + B_4^0 O_4^0 + B_6^0(O_6^0 + 77/8\, O_6^6).$$

Selected results are presented for all J values appearing in the rate earth series and for values of the parameters covering the situations in which the crystal field is dominant, in whkch the interaction with the magnetic field is dominant and in which the two interactions are comparable in magnitude The present treatment is confined to the case in which the magnetic field is directed perpendicular to the hexagonal axis.

I. Introduction

Rare earth systems have attracted attention for a number of years. Interest in these systems, particularly those with the rare earth in a hexagonal environment, has intensified recently because of the usefulness of $SmCO_5$ and related materials in the fabrication of permanent magnets. The magnetic behavior, and other physical properties, of rare earth systems are significantly influenced by the crystal field interaction (*1*). For this reason it has seemed useful to present the results of calculations on these systems, showing how the ground state multiplet of the various rare earths is split under the combined influence of an electric and magnetic field, and the energies and magnetic moments of the various states.

In previous works in the series (*2*, *3*), designated SW I and SW II, eigenfunctions, energy levels and magnetic moments were obtained for rare earth ions in a hexagonal field using the Hamiltonian

$$\mathscr{H} = \mu_B g\, \mathbf{J}\cdot\mathbf{H} + B_4^0 O_4^0 + B_4^0(O_4^0 + 77/8\, O_6^6).$$

In SW I, H was set equal to zero. In SW II, H was non vanishing and was applied along the hexagonal axis. In the present calculation H is applied perpendicular to the hexagonal.(*4*). This information is needed in the calculation of the susceptibilities of polycrystalline materials (*5*) and in the treatment of magnetically ordered systems in which the direction of magnetization is perpendicular to the hexagonal axis.

II. The Calculations

Nomenclature and procedure are essentially identical with that employed in SW II. Since H is applied perpendicular to the hexagonal axis

$$\mathbf{J}\cdot\mathbf{H} = J_x H_x + J_y H_y. \quad (1)$$

With no loss of generality we may assume the magnetic field to be applied in the x direction. The operator J_x is given by

$$J_x = \tfrac{1}{2}(J_+ + J_-). \quad (2)$$

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Accordingly,

$$\langle JM'|J_x|JM\rangle = \tfrac{1}{2}\{\langle JM'|J_+|JM\rangle + \langle JM'|J_-|JM\rangle\} \quad (3)$$

where

$$\langle M+1|J_x|M\rangle = \tfrac{1}{2}\langle J, M+1|J_+|J, M\rangle = \tfrac{1}{2}((J-M)(J+M+1))^{\frac{1}{2}} \quad (4)$$

$$\langle M-1|J_x|M\rangle = \tfrac{1}{2}\langle J, M-1|J_-|J, M\rangle = \tfrac{1}{2}((J+M)(J-M+1))^{\frac{1}{2}} \quad (5)$$

and all the other elements are zero. The operator J_x is a symmetrical matrix. For example, for $2J$ odd the matrix has the form

$$\begin{pmatrix}
0 & \frac{1}{2}(1\cdot 2J)^{1/2} & & & & & & & \\
\frac{1}{2}(1\cdot 2J)^{1/2} & 0 & \frac{1}{2}(2(2J-1))^{1/2} & & & & & & \\
& \frac{1}{2}(2(2J-1))^{1/2} & 0 & \frac{1}{2}(3(2J-2))^{1/2} & & & & & \\
& & \frac{1}{2}(3(2J-2))^{1/2} & 0 & & & & & \\
& & & & \ddots & & & & \\
& & & & 0 & \frac{1}{2}(J+\frac{1}{2}) & & & \\
& & & & \frac{1}{2}(J+\frac{1}{2}) & 0 & & & \\
& & & & & & \ddots & & \\
& & & & & & 0 & \frac{1}{2}(2(2J-1))^{1/2} & \\
& & & & & & \frac{1}{2}(2(2J-1))^{1/2} & 0 & \frac{1}{2}(1\cdot 2J)^{1/2} \\
& & & & & & & \frac{1}{2}(1\cdot 2J)^{1/2} & 0
\end{pmatrix}$$

All the matrix elements except those shown vanish. Matrix elements associated with O_4^0, O_6^0 and O_6^6 have been tabulated by Hutchings (*6*).

For the calculations the Hamiltonian given in the Introduction was, as in SW II, expressed in terms of 3 parameters—W, x and C. Definitions of these are given in SW II.

III. Results

The parameter $C = 2\mu H_{\perp}/W_{cr}$, where $\mu =$ the moment in the direction of the field and W_{cr} is the splitting due to the crystal field

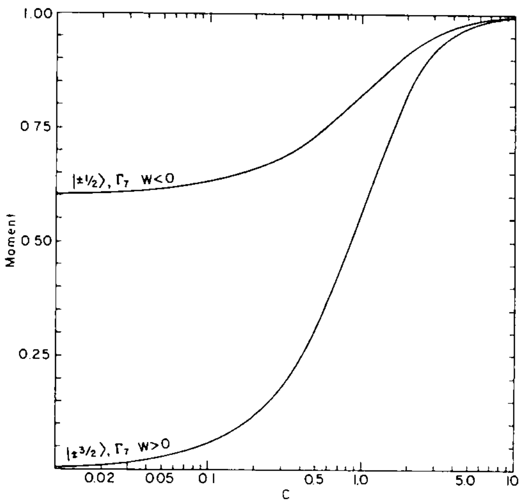

FIG. 1. Moment vs C for $J = 5/2$. (For definitions of C and W see text.) The moment is given in units of $gJ\mu_B$; the same practice is followed in the ensuing diagrams.

TABLE I

x-VALUES USED IN THE CALCULATIONS

	x
$J = 5/2$	1.0
$J = 7/2$	1.0, 0.6, −0.4
$J = 4$	1.0, 0.6, 0, −0.8
$J = 9/2$	1.0, 0.6, 0.2, −0.8
$J = 6$	1.0, 0.8, 0, −0.8
$J = 15/2$	1.0, 0.8, 0.1, −0.5
$J = 8$	1.0, 0.6, 0, −0.2, −0.6

interaction acting alone. Thus C describes the relative importance of the magnetic and crystal field interactions. Calculations were made for a large number of C values (20–40) covering the range from 0 to 10. In SW II values of the parameter x, which describes the relative importance of the fourth and sixth order interactions, were chosen to cover all possible ground states. The same x values, enumerated in Table I, were made use of in the present calculations.

The program used in making the calculations is given in the appendix.

It is feasible to report only a portion of the results obtained. Representative results are given in Table II for $J = 5/2$, 4, and 15/2. To conserve space only energies and magnetic moments are given.

The ground state moments are given in Figs. 1–13 for the 2 cases W >O and W< O. It is to be noted that in all cases the moment at high values of C approaches the free ion value. Thus in the limit of high field the full

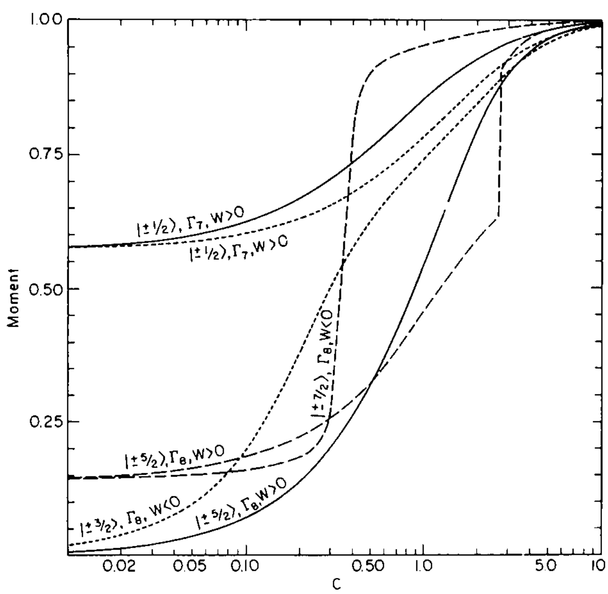

FIG. 2. Moment vs C for $J = 7/2$. short dashes $x = -0.40$; long dashes $x = 0.60$; solid line $x = 1.00$.

TABLE II

ENERGIES AND MAGNETIC MOMENTS FOR RARE EARTH IONS IN A HEXAGONAL FIELD[a]

$J = 5/2$

$C = .100$ Energy	Moment	$C = 10.000$ Energy	Moment	$C = 1.000$ Energy	Moment
2.153889E + 00	.6307	2.553315E + 01	.9940	3.813983E + 00	.8218
1.854133E + 00	−.5663	1.401132E + 01	.5945	1.500000E + 00	.3000
1.003109E + 00	.0248	5.723980E + 00	.2008	1.243662E + 00	.1617
1.003104E + 00	.0247	−4.213564E + 00	−.2017	7.360680E − 01	−.3382
−3.006998E + 00	−.0554	−1.625713E + 01	−.5949	−3.557645E + 00	−.3835
−3.007237E + 00	−.0583	−2.479776E ∓ 01	−.9928	−3.736068E + 00	−.5618

$J = 4$

$x = 1.000$ Energy	$C = .100$ Moment	$x = 1.000$ Energy	$C = 1.000$ Moment	$x = 1.000$ Energy	$C = 10.000$ Moment
1.825773E + 01	.2582	3.057758E + 01	.8652	2.014112E + 02	.9946
1.401359E + 01	.0139	1.565132E + 01	.2377	1.391948E + 02	.7457
1.401359E + 01	.0139	1.543370E + 01	.1538	9.365819E + 01	.4974
9.053404E + 00	.0547	1.348724E + 01	.3399	5.324475E + 01	.2445
8.795893E + 00	−.2030	2.942196E + 00	−.1290	6.584543E + 00	.0017
−1.097077E + 01	.0295	−1.012030E + 01	−.0063	−4.653912E + 01	−.2440
−1.097099E + 01	.0290	−1.180236E + 01	−.2907	−1.014904E + 02	−.5017
−2.109622E + 01	−.0981	−2.801825E + 01	−.5713	−1.549005E ∓ 02	−.7462
−2.109622E + 01	−.0981	−2.815112E + 01	−.5983	−1.911635E + 02	−.9921
$x = .600$	$C = .100$	$x = .600$	$C = 1.000$	$x = .600$	$C = 10.000$
1.318822E + 01	.9826	2.464955E + 01	.9511	2.047515E + 02	.9995
1.314184E + 01	.0353	1.721453E + 01	.4330	1.452518E + 02	.7444
6.553163E + 00	.6239	1.526453E + 01	.3386	1.011758E + 02	.4970
5.896026E + 00	.0942	1.046103E + 01	.2493	5.300892E + 01	.2469
2.154393E + 00	−.5066	7.965381E − 01	.0389	1.716080E + 00	.0002
−9.853394E − 01	−.0773	−4.900196E + 00	−.2478	−4.867692E + 01	−.2474
−1.026985E + 00	−.1314	−1.260672E + 01	−.5680	−1.010069E + 02	−.4973
−1.176879E + 01	−.0684	−1.900390E + 01	−.7605	−1.586838E + 02	−.7439
−2.715253E + 01	−.0522	−3.187536E + 01	−.4346	−1.975366E + 02	−.9994
$x = .0000$	$C = .100$	$x = 0.000$	$C = 1.000$	$x = 0.000$	$C = 10.000$
3.032313E + 01	.1278	4.570241E + 01	.7505	3.341682E + 02	.9962
3.020023E + 01	.0543	3.811962E + 01	.4345	2.463042E + 02	.7428
2.153929E + 00	−.0350	1.754634E + 01	.5952	1.716974E + 02	.5018
1.347813E + 00	.1777	6.001953E + 00	.2461	8.278756E + 01	.2514
1.062291E + 00	.0375	−5.368408E + 00	−.0394	−5.777973E + 00	−.0000
−4.154881E + 00	−.0271	−7.960013E + 00	−.1995	−8.229378E + 01	−.2509
−4.250795E + 00	−.0773	−8.920686E + 00	−.4505	−1.590632E + 02	−.5013
−2.032407E + 01	−.1932	−3.970965E + 01	−.8557	−2.560480E + 02	−.7433
−3.635764E + 01	−.0647	−4.541156E + 01	−.4811	−3.317745E + 02	−.9967
$x = -.800$	$C = .100$	$x = -.800$	$C = 1.000$	$x = -.800$	$C = 10.000$
1.747015E + 01	.2363	2.631143E + 01	.6817	1.758705E + 02	.9905
1.373191E + 01	.1942	2.195153E + 01	.6401	1.394904E + 02	.7474
1.338628E + 01	−.1768	1.103572E + 01	.1605	9.302002E + 01	.5046
9.440457E + 00	−.1171	7.461436E + 00	.0041	4.248857E + 01	.2457

TABLE II—*Continued*

$x = -.800$ Energy	$C = .100$ Moment	$x = -.800$ Energy	$C = 1.000$ Moment	$x = -.800$ Energy	$C = 10.000$ Moment
−6.867715E + 00	.1457	−2.237842E + 00	.1085	−6.435757E + 00	−.0014
−7.039272E + 00	−.0439	−9.834100E + 00	−.2197	−4.773033E + 01	−.2472
−1.076667E + 01	−.0144	−1.182654E + 01	−.1263	−8.423931E + 01	−.5006
−1.078310E + 01	−.0332	−1.422877E + 01	−.4245	−1.288986E + 02	−.7469
−1.857204E + 01	−.1907	−2.863277E + 01	−.8244	−1.835655E + 02	−.9931

$J = 15/2$

$x = 1.00$ Energy	$C = .10$ Moment	$x = 1.00$ Energy	$C = 1.00$ Moment	$x = 1.00$ Energy	$C = 10.00$ Moment
2.7311E + 02	.0090	3.9786E + 02	.9318	2.5852E + 03	.9958
2.7311E + 02	.0090	2.8432E + 02	.0936	2.1248E + 03	.8597
2.0446E + 02	.6995	2.8431E + 02	.0928	1.7308E + 03	.7313
1.7930E + 02	−.2302	2.8084E + 02	.6770	1.4031E + 03	.6006
1.2824E + 02	−.0418	1.7933E + 02	.4576	1.1235E + 03	.4615
1.2707E + 02	−.1783	9.3917E + 01	.2606	8.5207E + 02	.3240
2.2668E + 01	−.0269	2.2478E + 01	.1984	5.5799E + 02	.1954
2.2665E + 01	−.0273	−1.8244E + 01	.1019	2.3646E + 02	.0691
−9.0525E + 01	.0387	−4.4883E + 01	.1941	−1.0613E + 02	−.0603
−9.0525E + 01	.0387	−5.7337E + 01	−.1555	−4.6320E + 02	−.1934
−1.0090E + 02	.0082	−1.1938E + 02	−.2261	−8.2825E + 02	−.3290
−1.0090E + 02	.0082	−1.2664E + 02	−.3802	−1.1940E + 03	−.4659
−1.9791E + 02	.1986	−2.2917E + 02	−.4231	−1.5516E + 03	−.6024
−1.9791E + 02	.1986	−2.2975E + 02	−.4381	−1.8883E + 03	−.7380
−2.2598E + 02	−.3521	−3.5882E + 02	−.6923	−2.1941E + 03	−.8589
−2.2598E + 02	−.3521	−3.5884E + 02	−.6928	−2.3883E + 03	−.9894
$x = .80$	$C = .10$	$x = .80$	$C = 1.00$	$x = .80$	$C = 10.00$
2.3158E + 02	.0086	3.1636E + 02	.9495	2.1538E + 03	.9977
2.3158E + 02	.0086	2.4075E + 02	.1066	1.7666E + 03	.8604
1.5015E + 02	.7313	2.4077E + 02	.0868	1.4520E + 03	.7287
1.2979E + 02	−.1168	2.2402E + 02	.6641	1.1792E + 03	.6002
9.8219E + 01	−.0321	1.5942E + 02	.5271	9.4128E + 02	.4631
9.6490E + 01	−.2646	7.5042E + 01	.3655	7.1414E + 02	.3233
3.2564E + 01	.0843	2.1806E + 01	.1251	4.6634E + 02	.1937
2.6134E + 01	−.2098	−1.2303E + 01	.0295	1.9163E + 02	.0692
−6.2668E + 01	.1588	−4.4033E + 01	.1859	−9.8020E + 01	−.0590
−6.9142E + 01	−.1413	−6.0753E + 01	−.0332	−3.9219E + 02	−.1927
−9.5863E + 01	.0527	−9.7799E + 01	−.1756	−6.8822E + 02	−.3297
−9.5953E + 01	.0484	−1.0667E + 02	−.5578	−9.8866E + 02	−.4665
−1.4887E + 02	.0790	−1.8011E + 02	−.4469	−1.2923E + 03	−.6009
−1.4892E + 02	.0713	−1.9284E + 02	−.4702	−1.5847E + 03	−.7331
−1.8750E + 02	−.2372	−2.8996E + 02	−.6613	−1.8349E + 03	−.8603
−1.8760E + 02	−.2411	−2.9299E + 02	−.6953	−1.9859E + 03	−.9942
$x = .10$	$C = .10$	$x = .10$	$C = 1.00$	$x = .10$	$C = 10.00$
1.3382E + 02	.5931	2.2310E + 02	.8420	1.3477E + 03	.9892
1.2137E + 02	−.3258	1.4712E + 02	.4347	1.0974E + 03	.8660
9.2648E + 01	−.0082	1.1213E + 02	.4187	9.3350E + 02	.7349
9.2509E + 01	−.0390	9.6751E + 01	.3011	8.0333E + 02	.5909
7.2049E + 01	−.0120	8.4407E + 01	.1307	6.2236E + 02	.4711
7.1902E + 01	−.0460	7.8721E + 01	.6272	4.4350E + 02	.3348

TABLE II—*Continued*

$x = .10$ Energy	$C = .10$ Moment	$x = .10$ Energy	$C = 1.00$ Moment	$x = .10$ Energy	$C = 10.00$ Moment
6.6541E + 00	.3506	3.6798E + 01	.4359	2.7190E + 02	.1904
−3.5374E + 00	−.4174	2.8804E + 01	−.3973	8.2673E + 01	.0621
−8.5257E + 00	.6019	−1.2141E + 01	−.1490	−1.1020E + 02	−.0582
−2.0891E + 01	−.2944	−4.1523E + 01	.0635	−2.7327E + 02	−.1932
−5.5807E + 01	−.0052	−5.8745E + 01	−.4154	−4.1605E + 02	−.3382
−5.6140E + 01	−.0809	−7.4749E + 01	−.0083	−5.8589E + 02	−.4692
−8.6230E + 01	.0782	−1.1288E + 02	−.4231	−7.8850E + 02	−.5897
−9.0582E + 01	−.2472	−1.4257E + 02	−.3812	−9.6661E + 02	−.7402
−1.3060E + 02	.2324	−1.5741E + 02	−.7556	−1.1651E + 03	−.8660
−1.3863E + 02	−.3790	−2.0763E + 02	−.7240	−1.2968E + 03	−.9845
$x = -.50$	$C = .10$	$x = -.50$	$C = 1.00$	$x = -.50$	$C = 10.00$
1.3808E + 02	.3408	2.2568E + 02	.8011	1.3582E + 03	.9757
1.3767E + 02	.2628	2.0394E + 02	.6396	1.1987E + 03	.8565
1.1272E + 02	.1540	1.4183E + 02	.3544	1.0128E + 03	.7533
1.0390E + 02	−.4319	1.0979E + 02	.3398	8.6249E + 02	.6046
9.4070E + 01	−.0681	6.9994E + 01	.3414	6.7568E + 02	.4634
9.3443E + 01	−.1211	6.8505E + 01	−.0103	4.6212E + 02	.3304
5.6902E − 01	.3862	1.5984E + 01	−.4019	2.4726E + 02	.1985
−8.6063E + 00	−.2712	1.4388E + 01	.4641	4.5851E + 01	.0654
−1.0306E + 01	.0052	−1.9634E + 01	−.1940	−1.3679E + 02	−.0678
−1.0743E + 01	−.0285	−2.2295E + 01	−.1377	−3.0134E + 02	−.2007
−7.9416E + 01	.0298	−6.6353E + 01	−.0758	−4.5695E + 02	−.3315
−7.9536E + 01	.0035	−9.0091E + 01	−.1953	−6.1472E + 02	−.4603
−1.0694E + 02	.0317	−1.1678E + 02	−.1772	−7.7449E + 02	−.5983
−1.0706E + 02	.0061	−1.1682E + 02	−.2159	−9.5046E + 02	−.7418
−1.3187E + 02	.3447	−1.7207E + 02	−.6465	−1.1960E + 03	−.8599
−1.4598E + 02	−.6441	−2.4618E + 02	−.8857	−1.4323E + 03	−.9873

[a] These are taken directly from the computer sheets. Energy is expressed as multiples of the scaling parameter W. Moment is given as multiples of $gJ\mu_B$.

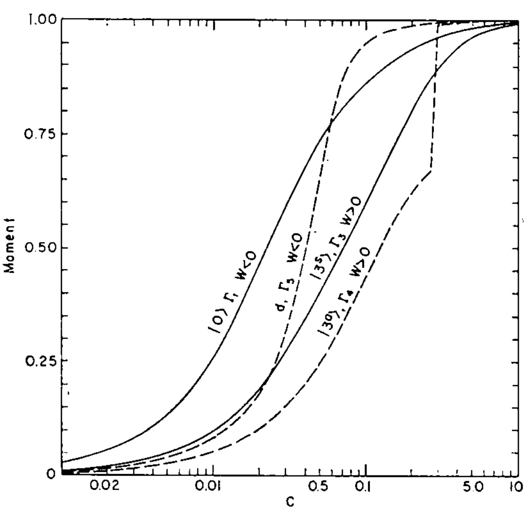

FIG. 3. Moment vs C for $J = 4$. Solid line $x = 1.00$; dashed line $x = 0.60$.

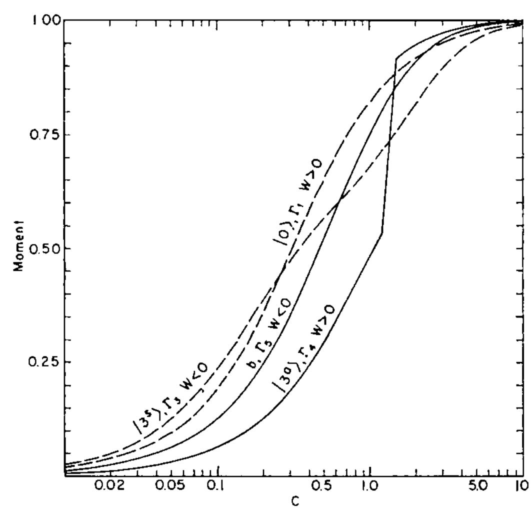

FIG. 4. Moment vs C for $J = 4$. Solid line $x = 0.00$; dashed line $x = 0.80$.

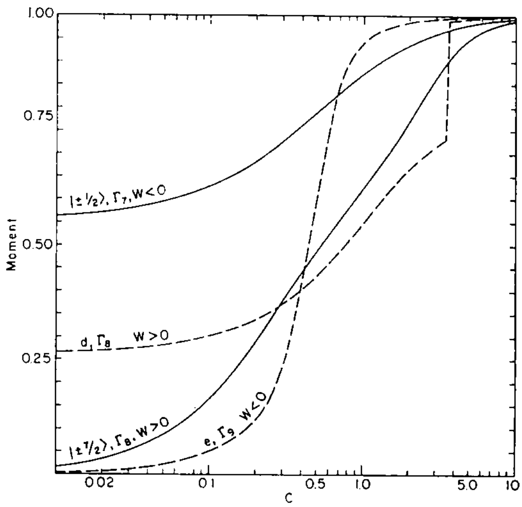

FIG. 5. Moment vs C for $J = 9/2$. Solid line $x = 1.00$; dashed line $x = 0.60$.

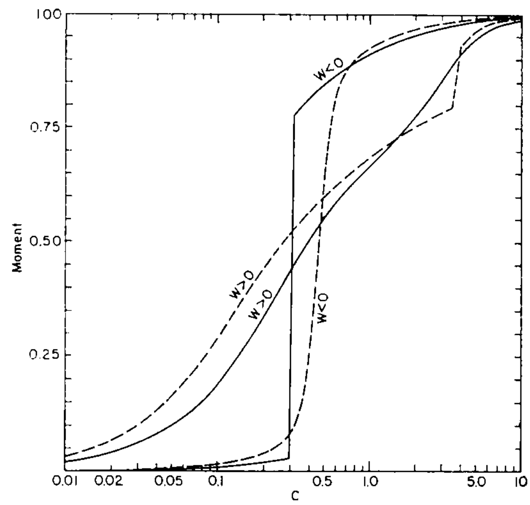

FIG. 7. Moment vs C for $J = 6$. Solid line $x = 1.00$; dashed line $x = 0.80$.

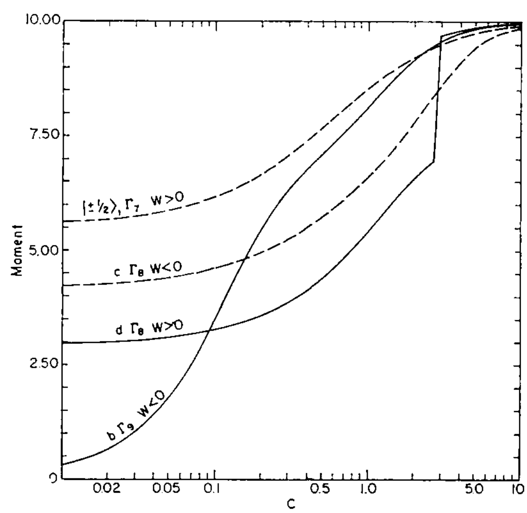

FIG. 6. Moment vs C for $J = 9/2$. Solid line $x = 0.20$; dashed line $x = -0.80$.

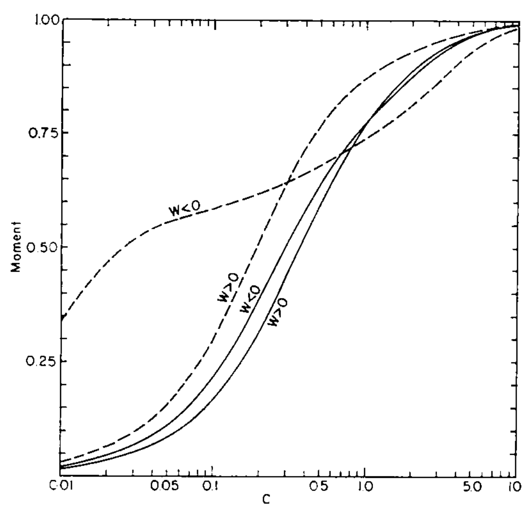

FIG. 8. Moment vs C for $J = 6$. Solid line $x = 0.00$; dashed line $x = -0.60$.

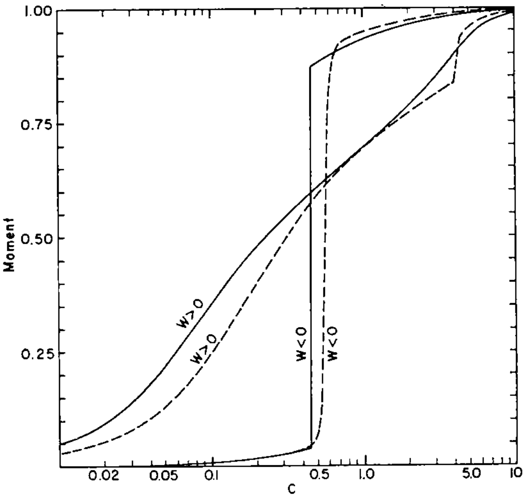

FIG. 9. Moment vs C for $J = 15/2$. Solid line $x = 1.00$ dashed line $x = 0.80$.

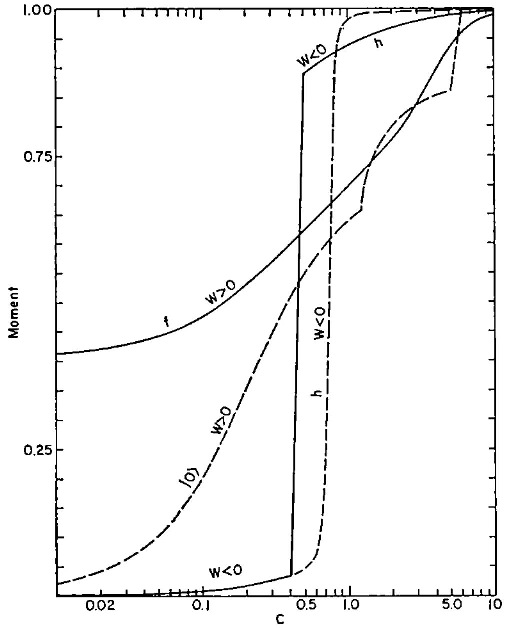

FIG. 11. Moment vs C for $J = 8$. Solid line $x = 1.00$; dashed line $x = 0.60$.

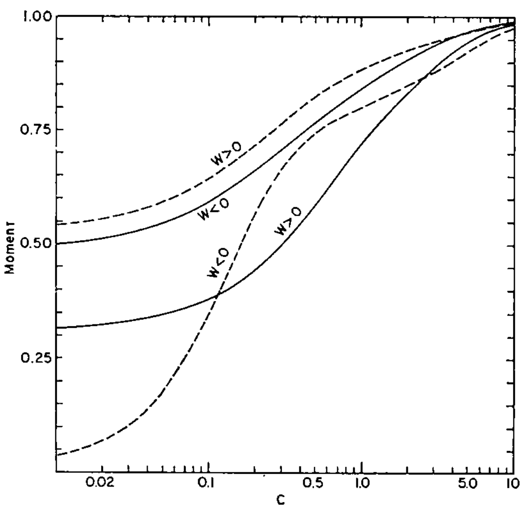

FIG. 10. Moment vs C for $J = 15/2$. Solid line $x = 0.10$; dashed line $x = -0.50$.

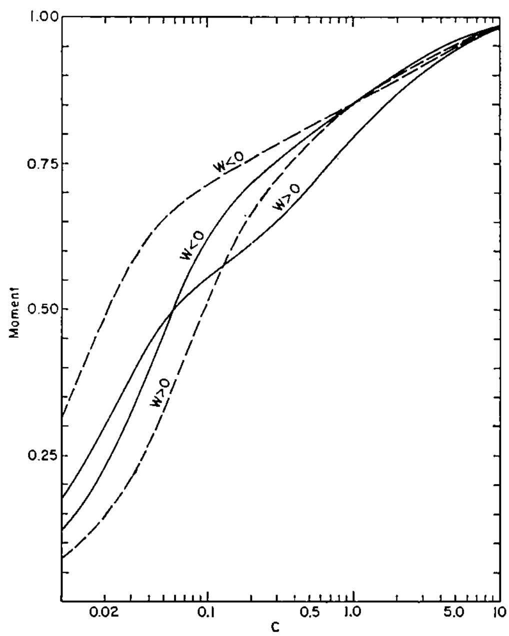

FIG. 12. Moment vs C for $J = 8$. Solid line $x = 0.00$; dashed line $x = -0.20$.

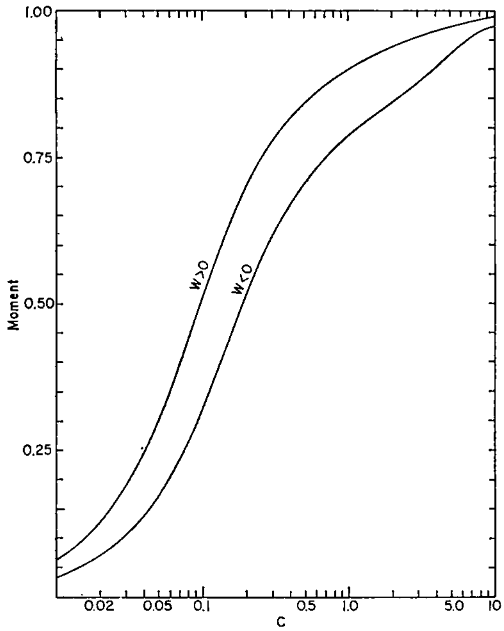

FIG. 13. Moment vs C for $J = 8$, for $x = -0.60$.

moment is developed when the magnetic field is applied perpendicular to the hexagonal axis. Similar behavior was observed in SW II when the magnetic field is applied along the hexagonal axis.

References

1. For details see W. E. WALLACE, "Rare Earth Intermetallics," Academic Press, New York (1973).
2. E. SEGAL AND W. E. WALLACE, *J. Solid State Chem.* **2**, 347 (1970).
3. E. SEGAL AND W. E. WALLACE, *J. Solid State Chem.* **6**, 99 (1973).
4. In SW II it was stated that the next contribution in the series would be for the situation in which the axial ratio is non ideal and hence the second order term must be included. These calculations have now been published as an appendix to Ref. 1.
5. See for example R. S. CRAIG, S. G. SANKAR, V. U. S. RAO, W. E. WALLACE, AND E. SEGAL, *J. Phys. Chem. Solids* **33**, 2267 (1972).
6. M. T. HUTCHINGS, *Solid State Phys.* **16**, 277 (1966).

Appendix—Program Used in Making the Calculations

```
   PROGRAM JEQ1502 (INPUT,OUTPUT)
   DIMENSION  ENERGY(16),EVEC(16,16),HAMILT(16,16),OJ(8),VS(8,16)
  1,C(40),X(10),Y(10)
   REAL  JX(16,16),MU(16),MUPAL(16),MUPER(16)
   REAL  J
   COMMON /LICH/ ILOC(16),IMAX,IMIN
                        DATA INPUT
NC=NOMBER OF C VALUES. NOTE THAT C(1)=0 AND THE READ IS FROM 2 UP TO NC.
NX=NO. OF X VALUES.  NY=NO. OF Y VALUES.
F2,F4,F6,=L.L.W. CONSTANTS.  W246=ENERGY SCALE
WCR=CRYSTAL FIELD OVERALL SPLITTINGS IN UNITS OF W246
     THE $ SIGN INDICATES A NEW STATEMENT
   NCM1=3 $ NC=NCM1+1 $ NX=2 $ NY=1
   PI=3.14159265358979323846264 3 $ RADIAN=PI/180.
   C(1)=0.$ W246=1.$ Z=1.E-12 $THETA=90.$ RAD=RADIAN*THETA $PRINT130
   J=15./2. $ N=2.*J+1.5
   AN=N $ NM1=N-1 $ NP1=N+1 $ NO2=N/2 $ NO2M3=NO2-3
   F2=3. $ F4=60. $ F6=13600. $ F=(77./4.)*(360.*SQRT(11.)/F5)
   READ 202, (C(IC),IC=2,NC) $ PRINT 102, (C(IC),IC=2,NC)
   READ 202, (X(IX),IX=1,NX) $ PRINT 102, (X(IX),IX=1,NX)
   READ 202, (Y(IY),IY=1,NY) $ PRINT 102, (Y(IY),IY=1,NY)
   PRINT 100 $ DO 21 I=1,N $ DO 21 K=I,N $ JX(I,K)=0.
21 CONTINUE
   DO 22 M=1,NM1 $ AM=M $ JX(M,M+1)=0.5*SQRT(AM*(AN-AM))
22 CONTINUE
   DO 23 I=2,N $ IM1=I-1 $ DO 23 K=1,IM1 $ JX(I,K)=JX(K,I)
23 CONTINUE
   DO 50 IY=1,NY $ B2F2=W246*(1.-ABS(Y(IY)))
   DO 40 IX=1,NX
   B4F4=W246*Y(IY)*X(IX) $ B6F6=W246*Y(IY)*(1.-ABS(X(IX))) $ WCR=1.
   DO 30 IC=1,NC $ CFOAS=W246*WCR
   WH=C(IC)*CFOAS/(2.*J) $ WHPAL=WH*COS(RAD) $ WHPER=WH*SIN(RAD)
                THE MATRIX ELEMENTS
   DO 24 I=1,NM1 $ IP1=I+1 $ DO 24 K=IP1,N $ HAMILT(I,K)=0.
24 CONTINUE
   OJ(1)=35.*B2F2+273.*B4F4+55.*B6F6
   OJ(2)=21.*B2F2-31.*B4F4-117.*B6F6
   OJ(3)=9.*B2F2-221.*B4F4-33.*B6F6 $ OJ(4)=-B2F2-201.*B4F4+59.*B6F6
   OJ(5)=-9.*B2F2-111.*B4F4+67.*B6F6
   OJ(6)=-15.*B2F2+23.*B4F4+45.*B6F6
   OJ(7)=-19.*B2F2+129.*B4F4-25.*B6F6
   OJ(8)=-21.*B2F2+169.*B4F4-75.*B6F6
   DO 25 IA=1,NO2 $ AI=IA $ NP1MIA=NP1-IA $ WHPALM=(J+1.-AI)*WHPAL
   HAMILT(IA,IA)=-WHPALM+OJ(IA) $ HAMILT(NP1MIA,NP1MIA)=WHPALM+OJ(IA)
25 CONTINUE
   DO 26 IA=1,NM1 $ HAMILT(IA,IA+1)=WHPER*JX(IA,IA+1)
26 CONTINUE
   HAMILT(1,7)=F*SQRT(35.*13.)*B6F6 $HAMILT(2,8)=F*7.*SQRT(39.)*B6F6
   HAMILT(3,9)=F*4.*SQRT(2/3.)*B6F6 $ HAMILT(4,10)=F*34.*B6F5
   HAMILT(5,11)=F*42.*SQRT(6.)*B6F5
   DO 27 I=1,NO2M3
   NP1MI=NP1-I $ HAMILT(NP1MI-6,NP1MI)=HAMILT(I,I+6)
27 CONTINUE
   DO 28 I=2,N $ IM1=I-1 $ DO 28 K=1,IM1 $ HAMILT(I,K)=HAMILT(K,I)
28 CONTINUE
   CALL LICHSUN (HAMILT,N,EVEC,ENERGY)
   OAS=ENERGY(IMAX)-ENERGY(IMIN) $ IF(C(IC).EQ.0.)  WCR=OAS
                 CALCULATING THE MAGNETIC MOMENTS
   DO 33 M=1,N $ SPAL=0.
   DO 29 I=1,N $ AI=I $ SPAL=SPAL+EVEC(I,M)**2*(AI-(J+1.))
29 CONTINUE
   MUPAL(M)=SPAL/J $ SPER=0.
   DO 32 L=1,N $ R=ABS(ENERGY(M)-ENERGY(L)) $ IF(R.LT.Z) 1,32
 1 DO 32 K=1,N $ SUM=0. $ DO 31 I=1,N $ SUM=SUM+EVEC(I,M)*JX(I,K)
31 CONTINUE
   SPER=SPER+SUM*EVEC(K,L)
32 CONTINUE
   MUPER(M)=SPER/J $ MU(M)=SQRT(MUPAL(M)**2+MUPER(M)**2)
33 CONTINUE
                     PRINTING THE RESULTS
   PRINT 104, X(IX),C(IC),THETA,OAS,WCR
   DO 34 I=1,N $ DO 34 L=1,NO2 $ NP1ML=NP1-L $ VS(L,I)=EVEC(NP1ML,I)
34 CONTINUE
   IF(C(IC).EQ.0.) GO TO 3 $ IF(THETA-30.)  3,2,3
 2 PRINT 111 $ GO TO  4
```

```
  3 PRINT 112
  4 DO 37 I=1,N $ II=ILOC(I)
                               ORTHOGONALITY CHECK
    DO 52 KK=1,N $ S=0. $ DO 51 K=1,N $ S=S+EVEC(K,II)*EVEC(K,KK)
 51 CONTINUE
 52 PRINT 131, II,S
    IF(C(10).EQ.0.) GO TO 6 $ IF(THETA-90.)  5,5,6
  5 PRINT 105
   1,II,ENERGY(II),MUPER(II),(EVEC(K,II),K=1,NO2),(VS(L,II),L=1,NO2)
    GO TO  37
  6 PRINT 106, II,ENERGY(II),MUPAL(II),MUPER(II),MU(II)
   1,(EVEC(K,II),K=1,NO2),(VS(L,II),L=1,NO2)
 37 CONTINUE
    IF(C(10).EQ.0.) GO TO 8 $ IF(THETA-90.)  8,7,8
  7 PRINT 111 $ GO TO  9
  8 PRINT 112
  9 PRINT 110
 39 CONTINUE
    PRINT 100
 40 CONTINUE
 50 CONTINUE
100 FORMAT(1H1)
102 FORMAT(1H0,8F10.3)
104 FORMAT(1H0,2X,2HX=,F6.3,5X,2HD=,F10.3,5X,*THETA=*,F5.1,* DEG*,10X
   1,6HD4S=,E20.13,5H*W26,5X,4HACP=,E20.13)
105 FORMAT(1H ,5X,I2,2H. ,E20.13,2X,F8.4,5X,2H-M,F8.5,7F9.5,3H -M
   1/45X,2H+M,F8.5,7F 9.5,3H +M)
106 FORMAT(1H ,I2,2H. ,E20.13,1X,3F8.4,3X,2H-M,F8.5,7F 9.5,3H -M
   1/53X,2H+M,F8.5,7F 9.5,3H +M)
110 FORMAT(1H0)
111 FORMAT(1H ,16X,6HENERGY,12X,5HMUPER,9X,5HM=15/2,3X,6HM=13/2,3X
   1,6HM=11/2,4X,5HM=9/2,4X,5HM=7/2,4X,5HM=5/2,4X,5HM=3/2,4X,5HM=1/2)
112 FORMAT(1H ,11X,6HENERGY,11X,5HMUPAL,3X,5HMUPER,5X,2HMU,8X
   1,6HM=15/2,3X,6HM=13/2,3X,6HM=11/2,4X,5HM=9/2,4X,5HM=7/2,4X
   2,5HM=5/2,4X,5HM=3/2,4X,5HM=1/2)
130 FORMAT(/////)
131 FORMAT(1H ,I2,2H. ,F25.13)
202 FORMAT(6F10.3)
    STOP $ END
```

```
    SUBROUTINE LICHSON (A,N,S,ROOT)
    DIMENSION  A(16,16),ROOT(16),S(16,16)
    COMMON /LICH/ ILOC(16),IMAX,IMIN
    NM1=N-1 $ SQ=0. $ S(1,1)=1. $ DO 3 I=2,N $ S(I,I)=1. $ IM = I - 1
    DO 3 K=1,IM $ IF(ABSF(A(I,K))-10.E-15) 2,2,1
  1 SQ=SQ+A(I,K)*A(I,K)
  2 S(I,K)=0.
  3 S(K,I)=0. $ V=SQRTF(2.*SQ) $ TOL=V*2.E-14 $ FN=N $ IF (V) 14,14,4
  4 V=V/FN
  5 JJ=0 $ DO 12 M=2,N $ MM=M-1 $ DO12L=1,MM$IF(ABSF(A(L,M))-V) 12,6,6
  6 ALM=-A(L,M) $ UM=.5*(A(L,L)-A(M,M)) $ OMGA=ALM/SQRT(ALM*ALM+UM*UM)
    IF(ABSF(OMGA)-10.E-15) 12,12,7
  7 JJ = 1 $ IF(UM) 8,9,9
  8 OMGA=-OMGA
  9 SNT=OMGA/SQRTF(2.*(1.+SQRTF(1.-OMGA*OMGA)))$ CST=SQRTF(1.-SNT*SNT)
    DO 10 I=1,N $ COM1=A(I,L) $ COM2=A(I,M) $ A(I,L)=COM1*CST-COM2*SNT
    A(I,M)=COM1*SNT+COM2*CST $ COM1=S(I,L) $ COM2=S(I,M)
    S(I,L)=COM1*CST-COM2*SNT
 10 S(I,M)=COM1*SNT+COM2*CST $ A(L,L)=A(L,L)*CST-A(M,L)*SNT
    A(M,M)=A(M,M)*CST+A(L,M)*SNT $ A(L,M)=0. $ A(M,L)=A(L,M)
    DO 11 I=1,N $ A(L,I)=A(I,L)
 11 A(M,I)=A(I,M)
 12 CONTINUE $ IF (JJ-1) 13,5,13
 13 IF(V-TOL) 14,14,4
 14 CONTINUE $ DO 15 I=1,N $ ROOT(I)=A(I,I)
 15 ILOC(I)=I $ DO 18 I=1,NM1 $ IP1=I+1 $ IL=ILOC(I) $ TEMP=ROOT(IL)
    DO 17 K=IP1,N $ KL=ILOC(K) $ IF(TEMP-ROOT(KL)) 16,17,17
 16 TEMP=ROOT(KL) $ ITEMP=ILOC(I) $ ILOC(I)=ILOC(K) $ ILOC(K)=ITEMP
 17 CONTINUE
 18 CONTINUE $ IMAX=ILOC(1) $ IMIN=ILOC(N) $ RETURN $ END
```