ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

ДУБНА

19/IV-76

H-54

E17 - 9535

1388/2-76

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Submitted to"Journal Phys. Chem. Solids"

ядерных исследований
БИБЛИОТЕКА

1. Introduction

A crystal field, which removes the degeneracies of rare earth ion multiplets (configuration ($4f$ $)^n$) in a crystal compound, can be rather well described by the Hamiltonian[1]

$$H_{cr} = \sum_{i=1}^{n} \sum_{\ell=2,4,6} \sum_{m=-\ell}^{\ell} A_{\ell,m} Y_{\ell,m}(\Omega_i). \tag{1}$$

The crystal field parameters $A_{\ell,m}$ are equal or not equal to zero depending on the symmetry of the field at the rare earth ion site. The energies of electronic levels are defined by these parameters and can be found by diagonalization of (1). For n = 2 (Pr^{3+}) the matrix elements are [2]

$$\begin{aligned} &\langle (4f)^2 L\,S\,J\,M \,|\, \sum_{i=1}^{2} Y_{\ell,m}(\Omega_i) \,|\, (4f)^2 L'\,S'\,J'\,M' \rangle = \\ &= -14 \left\{ \frac{2\ell+1}{4\pi} \right\}^{1/2} (-1)^{M+S+J+J'} \delta_{SS'} \times \\ &\times \left\{ (2L+1)(2L'+1)(2J+1)(2J'+1) \right\}^{1/2} \times \\ &\times \begin{Bmatrix} \ell & L' & L \\ 3 & 3 & 3 \end{Bmatrix} \begin{Bmatrix} \ell & J & J' \\ S & L' & L \end{Bmatrix} \begin{pmatrix} \ell & 3 & 3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J & \ell & J' \\ -M & m & M' \end{pmatrix}. \end{aligned} \tag{2}$$

Within the approximation, which considers by diagonalization of (1) only one-multiplet states ($L = L'$, $S = S'$, $J = J'$), the Hamiltonian (1) can be rewritten using the so-called operator equivalents O_ℓ^m for which the calculation of the matrix elements is simplified to a considerable extent [3, 4]

$$H_{cr} = \sum_{\ell=2,4,6} \sum_{m=-\ell}^{\ell} B_\ell^m O_\ell^m . \tag{3}$$

The parameters $A_{\ell,m}$ and $\mathcal{B}_{\ell}^{m}$ are linearly dependent. Comparing experimentally obtained crystal field energies of a given multiplet with theoretical values for these levels depending on the parameters $A_{\ell,m}$ (or $\mathcal{B}_{\ell}^{m}$) one may find the parameters of the crystal field.

Most simple is the case of a crystal field of cubic symmetry for which only parameters $\mathcal{B}_4^4/5 = \mathcal{B}_4^0 \equiv \mathcal{B}_4$ and $-\mathcal{B}_6^4/21 = \mathcal{B}_6^0 \equiv \mathcal{B}_6$ are non-zero. From this it follows

$$H_{cr} = \mathcal{B}_4\left(O_4^0 + 5\,O_4^4\right) + \mathcal{B}_6\left(O_6^0 - 21\,O_6^4\right) \equiv \mathcal{B}_4 O_4 + \mathcal{B}_6 O_6 \quad (4)$$

Picking out a scaling factor W in (4) one finds the problem of level energy determination to be a single parameter one. In paper/5/, the results of which owing to their clearness are widely used by the experimentators Lea, Leask and Wolf carried out an investigation of the ground multiplet splitting of all threevalent rare earth elements from Ce^{3+} to Yb^{3+} depending on the parameter x $(-1 \leq x \leq 1)$, defined as follows:

$$\mathcal{B}_4 = \frac{Wx}{F(4)} \qquad \text{and} \qquad \mathcal{B}_6 = \frac{W(1-|x|)}{F(6)} . \qquad (5)$$

The normalization factors $F(4)$ and $F(6)$ for Pr^{3+} - $^3H_4$ are 60 and 1260, respectively.

2. A combination of magnetic and crystal fields.

If a homogeneous magnetic field is present at the rare earth ion site an interaction Hamiltonian should be added

$$H_M = \frac{|e|\hbar}{2mc}\left((\vec{L}+2\vec{S})\cdot\vec{H}\right) + \frac{e^2}{8mc^2}\sum_{i=1}^{n}\left[\vec{H}\times\vec{r}_i\right]^2 . \quad (6)$$

This magnetic field may originate from both external and inner fields (ordered magnetic structures of crystal compounds, consideration of the dynamical exchange interaction/7/ and so on). For magnetic fields up to the order of several thousand kOe the second term in (6) may be neglected in comparison with the first one. Earlier, simultaneous consideration of Hamiltonians (4) and (6) within some range of the parameter x and with increasing magnetic fields $\vec{H}$ was carried out, for instance, for Nd^{3+} /7/. In the following the $^3H_4$ multiplet of Pr^{3+} is discussed. The parameter x was varied from -1 to 1. The homogeneous magnetic field directed along the Z-axis (parallel to the axis of rotation C_4) was changed in the limit from y = 0 to y = 4.0. For given y and scaling factor W (in meV) the magnetic field intensity is

$$H_z\,(kOe) = -W\cdot y\cdot 1000.$$

The matrix which had to be diagonalized had the form

$$W\left[\left\langle J=4,M\right|\frac{x}{F(4)}O_4 + \frac{(1-|x|)}{F(6)}O_6\left|J=4,M'\right\rangle + \right.$$
$$\left. + \; C\cdot M\cdot y\cdot\delta_{M,M'}\right], \qquad (7)$$

where $C = -4{,}63061.$

In table 1 the eigenvalues E and the parameters $a_M^{i/j}$ of the eigenfunctions of matrix (7) (W=1) as a combination of $|J=4,M\rangle$ functions are given for x = -1.0; (0.2); 1.0 and y = 0;0.3; 0.7; 1.0; 2.0; 3.0; and 4.0. For y = 0 the results of our calculations are consistent with those of ref./5/. If y is non-zero the symmetry of the problem lowers down from cubic to tetragonal C_{4h}, which leads to a complete splitting of the multiplet under consideration. The eigenfunctions $|\Gamma_i^j>$, which are transformed in the case of y = 0 as the j-th component of the irreducible representation Γ_i of cubic groups, are transformed for y ≠ 0 as the irreducible representations $\tilde{\Gamma}_i$ of the group C_{4h}:

$$\Gamma_1 \to \tilde{\Gamma}_1,\ \Gamma_3^1 \to \tilde{\Gamma}_1,\ \Gamma_3^2 \to \tilde{\Gamma}_2,\ \Gamma_4^1 \to \tilde{\Gamma}_4,\ \Gamma_4^2 \to \tilde{\Gamma}_3,\ \Gamma_4^3 \to \tilde{\Gamma}_1,$$
$$\Gamma_5^1 \to \tilde{\Gamma}_4,\ \Gamma_5^2 \to \tilde{\Gamma}_3,\ \Gamma_5^3 \to \tilde{\Gamma}_2.$$

Non-zero parameters $a_M^{5/j}$ of the Γ_5^j level eigenfunctions

$$|\Gamma_5^j> = \sum_M a_M^{5/j}\ |J=4, M>$$

may be found from table 1 with the help of the following relations:

$$a_3^{5/1} = a_{-1}^{4/1},\ a_{-1}^{5/1} = -a_3^{4/1},\ a_{-3}^{5/2} = a_1^{4/2},\ a_1^{5/2} = -a_{-3}^{4/2},$$
$$a_{-2}^{5/3} = -a_2^{3/2},\ a_2^{5/3} = a_{-2}^{3/2}.$$

The dependence of level energies on parameters x and y (W = 1) is given in figs. 1 - 11.

If y is varied from y > 0 (+) to y < 0 (-) the picture of level positions changes for a fixed x symmetrically with respect to y = 0. In this case the relations

$$E(\Gamma_i^j)^+ = E(\Gamma_i^j)^-,\ a_M^{i/j+} = a_{-M}^{i/j-}$$

hold, except for the $\Gamma_4^1, \Gamma_4^2, \Gamma_5^1$ and Γ_5^2 levels, for which we have

$$E(\Gamma_4^1)^\pm = E(\Gamma_4^2)^\mp,\ a_M^{4/1\pm} = a_{-M}^{4/2\mp},$$
$$E(\Gamma_5^1)^\pm = E(\Gamma_5^2)^\mp,\ a_M^{5/1\pm} = a_{-M}^{5/2\mp}.$$

Table 1

Γ_i^j	$\tilde{\Gamma}_i$	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	I	E	-28.0	-28.9	-32.6	-36.7	-53.I	-70.9	-89.I
		-4	.456	.29I	.I47	.090	.026	.0I2	.007
		0	.764	.7I3	.553	.44I	.238	.I58	.II8
		4	.456	.638	.820	.893	.97I	.987	.993
3/I	I	E	-4.00	-2.38	2.77	7.47	24.7	42.7	6I.0
		-4	.540	.779	.904	.94I	.980	.990	.994
		0	-.645	-.564	-.4II	-.332	-.I96	-.I38	-.I06
		4	.540	.275	.II6	.069	.022	.0I0	.006
3/2	2	E	-4.00	-4.26	-5.34	-6.63	-I2.8	-20.6	-29.0
		-2	.707	.639	.549	.487	.334	.245	.I9I
		2	.707	.769	.836	.873	.943	.970	.982
4/I	4	E	-I4.0	-I3.4	-I3.0	-I3.I	-I7.0	-26.3	-38.2
		-I	.935	.9I6	.878	.836	.609	.39I	.267
		3	.354	.40I	.479	.549	.793	.92I	.964
4/2	3	E	-I4.0	-I4.8	-I6.0	-I7.0	-20.8	-24.9	-29.2
		-3	.354	.3I4	.272	.247	.I87	.I49	.I24
		I	.935	.949	.962	.969	.982	.989	.992
4/3	I	E	-I4.0	-I4.7	-I6.2	-I6.8	-I7.6	-I7.8	-I7.9
		-4	-.707	-.556	-.40I	-.327	-.I96	-.I38	-.I06
		0	.000	-.4I7	-.725	-.834	-.95I	-.978	-.987
5/I	4	E	26.0	22.6	I8.5	I5.8	I0.4	I0.5	I3.2
5/2	3	E	26.0	29.5	34.5	38.3	5I.3	64.7	78.2
5/3	2	E	26.0	26.3	27.3	28.6	34.8	42.6	5I.0

x=-I.0

Table 1 (continued)

Γ_i^j	M	ν=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E -4 0 4	-38.4 .456 .764 .456	-38.9 .369 .750 .548	-40.9 .268 .696 .666	-43.3 .207 .638 .742	-55.7 .090 .44I .893	-7I.5 .045 .3I3 .949	-88.0 .026 .238 .97I
3/I	E -4 0 4	9.60 .540 -.645 .540	I0.5 .678 -.62I .393	I3.9 .803 -.543 .244	I7.5 .859 -.48I .I74	32.5 .94I -.332 .069	49.4 .968 -.248 .036	67.0 .980 -.I96 .022
3/2	E -2 2	9.60 .707 .707	8.65 .44I .897	5.78 .25I .968	3.26 .I84 .983	-5.67 .096 .995	-I4.8 .064 .998	-24.0 .048 .999
4/I	E -I 3	-I0.4 .935 .354	-9.85 .905 .426	-9.77 .83I .556	-I0.5 .743 .669	-I8.3 .40I .9I6	-30.4 .234 .972	-43.6 .I6I .987
4/2	E -3 I	-I0.4 .354 .935	-II.2 .298 .954	-I2.5 .245 .970	-I3.6 .2I5 .977	-I7.6 .I5I .989	-2I.9 .II6 .993	-26.4 .094 .996
4/3	E -4 0 4	-I0.4 -.707 -.000 .707	-I0.8 -.635 -.227 .738	-I2.2 -.53I -.470 .705	-I3.4 -.468 -.60I .648	-I6.0 -.327 -.834 .444	-I7.2 -.246 -.9I7 .3I4	-I7.7 -.I96 -.95I .238
5/I	E	I6.8	I3.5	9.69	7.6I	6.I9	9.06	I3.0
5/2	E	I6.8	20.4	25.4	29.3	42.6	56.I	69.8
5/3	E	I6.8	I7.7	20.6	23.I	32.I	4I.2	50.4

x=-0.8

Table 1 (continued)

Γ_i^j	M	ν=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E -4 0 4	-48.8 .456 .764 .456	-49.I .397 .758 .5I8	-50.5 .325 .732 .599	-52.I .276 .702 .657	-6I.5 .I55 .567 .809	-74.8 .090 .44I .893	-90.2 .056 .348 .936
3/I	E -4 0 4	23.2 .540 -.645 .540	23.8 .636 -.634 .440	26.3 .739 -.59I .323	29.I .796 -.550 .254	42.0 .898 -.422 .I23	57.6 .94I -.332 .069	74.4 .962 -.27I .044
3/2	E -2 2	23.2 .707 .707	23.7 .8I7 .576	25.5 .905 .425	27.5 .939 .343	35.5 .980 .I98	44.3 .99I .I36	53.3 .995 .I04
4/I	E -I 3	-6.80 .935 .354	-6.43 .86I .509	-7.73 .624 .782	-I0.4 .430 .903	-22.8 .I73 .985	-36.4 .I05 .995	-50.I .075 .997
4/2	E -3 I	-6.80 .354 .935	-7.67 .26I .965	-9.I6 .I89 .982	-I0.4 .I56 .988	-I4.7 .098 .995	-I9.2 .07I .997	-23.8 .056 .998
4/3	E -4 0 4	-6.80 -.707 .000 .707	-7.09 -.662 -.I54 .734	-8.20 -.590 -.338 .733	-9.33 -.539 -.452 .7I0	-I3.0 -.4II -.707 .575	-I5.3 -.327 -.834 .444	-I6.5 -.269 -.897 .350
5/I 5/2 5/3	E E E	7.60 7.60 7.60	4.45 II.3 7.I2	2.04 I6.4 5.26	I.90 20.4 3.29	5.I0 34.I -4.70	9.39 47.8 -I3.5	I3.9 6I.6 -22.5

x=-0.6

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-59.2	-59.4	-60.4	-6I.7	-69.0	-80.I	-93.8
	-4	.456	.4I2	.355	.3I6	.207	.I35	.090
	0	.764	.760	.746	.728	.638	.533	.44I
	4	.456	.502	.564	.609	.742	.835	.893
3/I	E	36.8	37.2	39.2	4I.4	52.6	66.9	82.7
	-4	.540	.6I3	.698	.750	.859	.9I2	.94I
	0	-.645	-.639	-.6I3	-.585	-.48I	-.396	-.332
	4	.540	.465	.37I	.3I0	.I74	.I05	.069
3/2	E	36.8	37.0	37.9	38.9	44.3	5I.4	59.3
	-2	.707	.756	.8I2	.847	.920	.955	.972
	2	.707	.655	.583	.532	.39I	.298	.237
4/I	E	- 3.2	-6.03	-II.5	-I5.7	-29.6	-43.5	-57.4
	-I	.935	.II9	.045	.03I	.0I5	.0I0	.007
	3	.354	.993	.999	.999	.999	.999	.999
4/2	E	- 3.2	-4.43	-6.26	-7.64	-I2.3	-I6.9	-2I.5
	-3	.354	.078	.037	.027	.0I4	.009	.007
	I	.935	.997	.999	.999	.999	.999	.999
4/3	E	- 3.2	-3.42	-4.3I	-5.30	-9.I8	-I2.4	-I4.5
	-4	-.707	-.674	-.622	-.582	-.468	-.387	-.327
	0	.000	-.II6	-.262	-.358	-.60I	-.748	-.834
	4	.707	.729	.738	.730	.648	.539	.444
5/I	E	-I.60	-I.55	0.265	I.65	6.27	I0.9	I5.5
5/2	E	-I.60	2.4I	7.94	I2.I	26.0	39.9	53.8
5/3	E	-I.60	-I.80	-2.66	-3.72	-9.08	-I6.2	-24.I

x=-0.4

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-69.6	-69.8	-70.6	-7I.6	-77.6	-86.9	-99.0
	-4	.456	.42I	.375	.342	.247	.I74	.I24
	0	.764	.762	.752	.740	.678	.596	.5I3
	4	.456	.493	.542	.579	.693	.784	.849
3/I	E	50.4	50.8	52.3	54.2	63.9	77.0	9I.8
	-4	.540	.599	.670	.7I6	.825	.885	.9I9
	0	-.645	-.64I	-.624	-.604	-.522	-.444	-.38I
	4	.540	.480	.402	.349	.2I7	.I4I	.096
3/2	E	50.4	50.5	5I.I	5I.8	55.6	6I.I	67.8
	-2	.707	.738	.777	.803	.87I	.9I4	.94I
	2	.707	.674	.630	.596	.49I	.405	.338
4/I	E	0.4	I.3I	2.87	4.I3	8.56	I3.I	I7.7
	-I	.935	.970	.986	.99I	.997	.998	.999
	3	.354	.242	.I66	.I34	.08I	.058	.045
4/2	E	0.4	0.I57	2.39	5.70	I8.9	32.6	46.4
	-3	.354	.566	.873	.95I	.992	.997	.998
	I	.935	.824	.488	.3II	.I26	.078	.056
4/3	E	0.4	0.225	-0.5I2	-I.37	-5.I4	-8.83	-II.7
	-4	-.707	-.682	-.64I	-.608	-.509	-.432	-.373
	0	.000	-.093	-.2I3	-.295	-.5I8	-.669	-.769
	4	.707	.726	.738	.737	.688	.604	.5I9
5/I	E	-I0.8	-I4.5	-I9.7	-23.8	-37.5	-5I.3	-65.I
5/2	E	-I0.8	-7.78	-6.3I	-6.84	-I0.7	-I5.2	-I9.7
5/3	E	-I0.8	-I0.9	-II.5	-I2.2	-I6.0	-2I .5	-28.2

x=-0.2

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-80.0	-80.2	-80.8	-8I.7	-86.7	-94.7	-I05.0
	-4	.456	.427	.388	.360	.276	.207	.I55
	0	.764	.762	.756	.747	.702	.638	.567
	4	.456	.487	.528	.558	.657	.742	.809
3/I	E	64.0	64.3	65.6	67.2	75.8	87.7	I02.0
	-4	.540	.589	.650	.69I	.796	.859	.898
	0	-.645	-.643	-.630	-.6I6	-.550	-.48I	-.422
	4	.540	.490	.424	.378	.254	.I74	.I23
3/2	E	64.0	64.I	64.5	65.0	67.9	72.4	78.0
	-2	.707	.730	.759	.780	.838	.88I	.9II
	2	.707	.683	.65I	.626	.546	.473	.4II
4/I	E	4.0	4.8I	6.I6	7.28	II.4	I5.7	20.2
	-I	.935	.956	.972	.979	.990	.994	.996
	3	.354	.292	.235	.204	.I40	.I06	.085
4/2	E	4.0	3.47	3.57	4.57	I3.7	26.3	39.7
	-3	.354	.438	.59I	.7I9	.940	.980	.99I
	I	.935	.899	.807	.695	.340	.I99	.I37
4/3	E	4.0	3.85	3.23	2.48	-I.06	-4.97	-8.34
	-4	-.707	-.686	-.653	-.626	-.539	-.468	-.4II
	0	.000	-.078	-.I79	-.250	-.452	-.60I	-.707
	4	.707	.723	.736	.738	.7I0	.648	.575
5/I	E	-20.0	-23.6	-28.6	-32.5	-45.9	-59.5	-73.2
5/2	E	-20.0	-I6.7	-I3.I	-II.3	-II.I	-I4.5	-I8.6
5/3	E	-20.0	-20.I	-20.5	-2I.0	-23.9	-28.4	-34.0

x=0.0

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-58.4	-58.6	-59.5	-60.6	-67.0	-77.0	-89.7
	-4	.456	.4I8	.368	.333	.232	.I59	.II0
	0	.764	.76I	.750	.736	.664	.573	.486
	4	.456	.496	.550	.589	.7II	.804	.867
3/I	E	52.0	52.4	54.I	56.I	66.4	79.9	95.I
	-4	.540	.604	.680	.728	.838	.896	.928
	0	-.645	-.64I	-.620	-.598	-.508	-.426	-.363
	4	.540	.475	.39I	.335	.20I	.I27	.086
3/2	E	52.0	52.I	52.6	53.2	56.4	6I.4	67.5
	-2	.707	.733	.766	.789	.852	.896	.925
	2	.707	.680	.642	.6I4	.524	.445	.380
4/I	E	6.0	6.8	8.II	9.2I	I3.2	I7.5	22.0
	-I	.935	.954	.970	.977	.989	.993	.996
	3	.354	.298	.245	.2I5	.I5I	.II6	.094
4/2	E	6.0	5.45	5.37	6.08	I3.9	26.0	39.2
	-3	.354	.426	.556	.669	.9I6	.972	.987
	I	.935	.905	.83I	.743	.40I	.234	.I6I
4/3	E	6.0	5.8I	5.02	4.II	0.27I	-3.26	-5.84
	-4	-.707	-.679	-.634	-.599	-.494	-.4I5	-.356
	0	.000	-.I0I	-.230	-.3I8	-.594	-.700	-.795
	4	.707	.727	.738	.735	.674	.58I	.49I
5/I	E	-2I.2	-24.8	-29.8	-33.7	-47.0	-60.5	-74.2
5/2	E	-2I.2	-I7.9	-I4.I	-I2.0	-I0.6	-I3.5	-I7.4
5/3	E	-2I.2	-2I.3	-2I.8	-22.4	-25.6	-30.6	-36.7

x=0.2

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-36.8	-37.I	-38.4	-39.9	-48.8	-6I.6	-76.7
	-4	.456	.40I	.332	.286	.I67	.099	.062
	0	.764	.758	.736	.709	.585	.462	.368
	4	.456	.5I4	.59I	.645	.794	.88I	.928
3/I	E	40.0	40.6	42.9	45.6	58.I	73.5	90.0
	-4	.540	.630	.729	.785	.890	.935	.958
	0	-.645	-.635	-.597	-.559	-.436	-.346	-.284
	4	.540	.446	.334	.267	.I34	.077	.049
3/2	E	40.0	40.I	40.7	4I.3	45.I	50.6	57.2
	-2	.707	.738	.776	.80I	.869	.9I2	.939
	2	.707	.675	.63I	.598	.495	.409	.343
4/I	E	8.0	8.79	I0.I	II.I	I5.I	I9.4	23.8
	-I	.935	.953	.967	.974	.987	.992	.995
	3	.354	.304	.253	.225	.I6I	.I25	.I02
4/2	E	8.0	7.43	7.23	7.7I	I4.4	25.9	38.9
	-3	.354	.4I8	.529	.629	.888	.962	.983
	I	.935	.909	.848	.777	.459	.272	.I86
4/3	E	8.0	7.73	6.67	5.56	I.83	-0.673	-2.II
	-4	-.707	-.665	-.598	-.550	-.424	-.340	-.28I
	0	.000	-.I45	-.3I9	-.430	-.684	-.8I7	-.885
	4	.707	.733	.735	.7I6	.593	.466	.370
5/I	E	-22.4	-26.0	-3I.0	-34.8	-48.0	-6I.5	-75.2
5/2	E	-22.4	-I9.I	-I5.2	-I2.8	-I0.3	-I2.5	-I6.2
5/3	E	-22.4	-22.5	-23.I	-23.7	-27.5	-33.0	-39.6

x=0.4

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E	-I5.2	-I5.7	-I7.9	-20.6	-33.8	-50.0	-67.4
	-4	.456	.360	.25I	.I88	.076	.037	.02I
	0	.764	.744	.682	.6I4	.406	.284	.2I4
	4	.456	.558	.687	.766	.9II	.958	.977
3/I	E	28.0	29.0	32.6	36.5	5I.9	69.I	86.8
	-4	.540	.69I	.820	.874	.949	.973	.984
	0	-.645	-.6I6	-.527	-.460	-.309	-.228	-.I79
	4	.540	.378	.223	.I54	.059	.030	.0I8
3/2	E	28.0	28.I	28.8	29.6	34.0	40.I	47.3
	-2	.707	.744	.789	.8I8	.890	.93I	.954
	2	.707	.668	.6I5	.575	.457	.366	.300
4/I	E	I0.0	I0.8	I2.0	I3.I	I7.0	2I.2	25.6
	-I	.935	.95I	.965	.972	.985	.99I	.994
	3	.354	.308	.26I	.233	.I7I	.I34	.II0
4/2	E	I0.0	9.42	9.I3	9.43	I5.I	25.9	38.6
	-3	.354	.4II	.509	.597	.857	.95I	.977
	I	.935	.9I2	.86I	.802	.5I5	.3II	.2I2
4/3	E	I0.0	9.54	8.08	6.95	4.62	3.73	3.35
	-4	-.707	-.626	-.5I4	-.447	-.305	-.227	-.I79
	0	.000	-.350	-.508	-.64I	-.860	-.93I	-.960
	4	.707	.738	.692	.624	.409	.285	.2I4
5/I	E	-23.6	-20.2	-I6.2	-I3.8	-I0.I	-II.7	-I5.I
5/2	E	-23.6	-27.2	-32.I	-36.0	-49.I	-62.6	-76.2
5/3	E	-23.6	-23.7	-24.4	-25.2	-29.6	-35.7	-42.9

x=0.6

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E -4 0 4	6.40 .456 .764 .456	4.3I .I35 .533 .835	-I.9I .034 .27I .962	-7.I7 .0I7 .I90 .983	-25.4 .004 .094 .996	-43.8 .002 .062 .998	-62.2 .00I .046 .999
3/I	E -4 0 4	I6.0 .540 -.645 .540	I9.0 .9I2 -.396 .I05	25.7 .975 -.2I9 .028	3I.I .987 -.I62 .0I4	49.3 .996 -.086 .004	67.8 .998 -.058 .002	86.2 .999 -.044 .00I
3/2	E -2 2	I6.0 .707 .707	I6.2 .753 .658	I7.0 .807 .590	I8.0 .84I .542	23.2 .9I4 .405	30.I .950 .3II	37.9 .968 .249
4/I	E -I 3	I2.0 .935 .354	I2.8 .950 .3II	I4.0 .964 .267	I5.0 .97I .240	I8.9 .984 .I79	23.0 .990 .I42	27.4 .993 .II7
4/2	E -3 I	I2.0 .354 .935	II.4 .405 .9I4	II.0 .492 .870	II.2 .570 .82I	I5.9 .825 .565	26.0 .937 .350	38.4 .97I .239
4/3	E -4 0 4	I2.0 -.707 .000 .707	II.I -.387 -.748 .539	I0.6 -.2I8 -.937 .27I	I0.5 -.I62 -.968 .I90	I0.4 -.086 -.992 .094	I0.4 -.058 -.996 .062	I0.4 -.044 -.998 .046
5/I	E	-24.8	-28.4	-33.3	-37.I	-50.2	-63.6	-77.2
5/2	E	-24.8	-2I.4	-I7.4	-I4.8	-I0.2	-II.0	-I4.I
5/3	E	-24.8	-25.0	-25.8	-26.8	-32.0	-38.9	-46.7

x=0.8

Table 1 (continued)

Γ_i^j	M	y=0	0.3	0.7	I.0	2.0	3.0	4.0
I	E -4 0 4	28.0 .456 .764 .456	28.9 .638 .7I3 .29I	32.6 .820 .553 .I47	36.7 .893 .44I .090	53.I .97I .238 .026	70.9 .987 .I58 .0I2	89.I .993 .II8 .007
3/I	E -4 0 4	4.00 .540 -.645 .540	2.38 .275 -.564 .779	-2.77 .II6 -.4II .904	-7.47 .069 -.332 .94I	-24.7 .022 -.I96 .980	-42.7 .0I0 -.I38 .990	-6I.0 .006 -.I06 .994
3/2	E -2 2	4.00 .707 .707	4.26 .769 .639	5.34 .836 .549	6.63 .873 .487	I2.8 .943 .334	20.6 .970 .245	29.0 .982 .I9I
4/I	E -I 3	I4.0 .935 .354	I4.8 .949 .3I4	I6.0 .962 .272	I7.0 .969 .247	20.8 .982 .I87	24.9 .989 .I49	29.2 .992 .I24
4/2	E -3 I	I4.0 .354 .935	I3.4 .40I .9I6	I3.0 .479 .878	I3.I .549 .836	I7.0 .793 .609	26.3 .92I .39I	38.2 .964 .267
4/3	E -4 0 4	I4.0 -.707 .000 .707	I4.7 -.7I9 .4I7 .556	I6.2 -.56I .725 .40I	I6.8 -.444 .834 .327	I7.6 -.238 .95I .I96	I7.8 -.I58 .978 .I38	I7.9 -.II0 .987 .I06
5/I	E	-26.0	-29.5	-34.5	-38.3	-5I.3	-64.7	-78.2
5/2	E	-26.0	-22.6	-I8.5	-I5.8	-I0.4	-I0.5	-I3.2
5/3	E	-26.0	-26.3	-27.3	-28.6	-34.8	-42.6	-5I.0

x=I.0

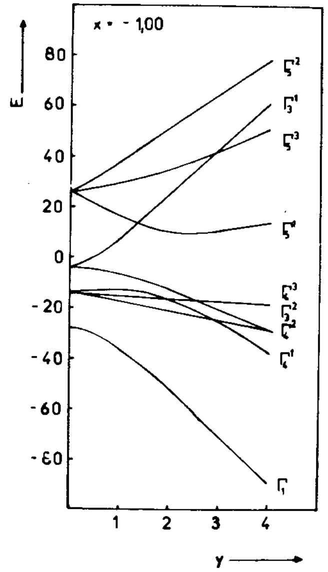


Fig. 1

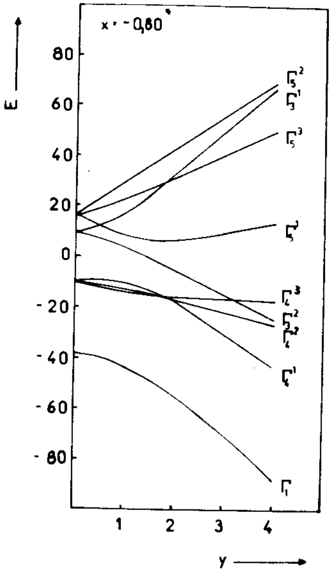


Fig. 2

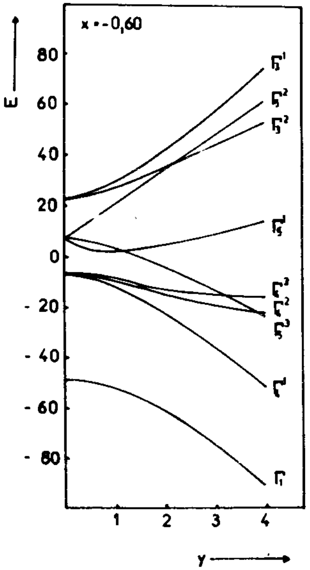
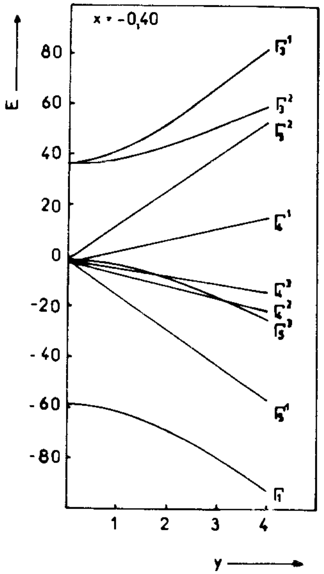


Fig. 3



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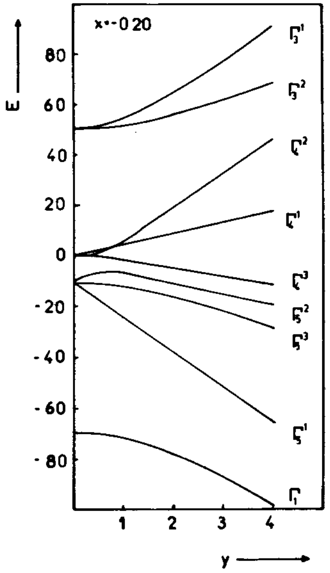

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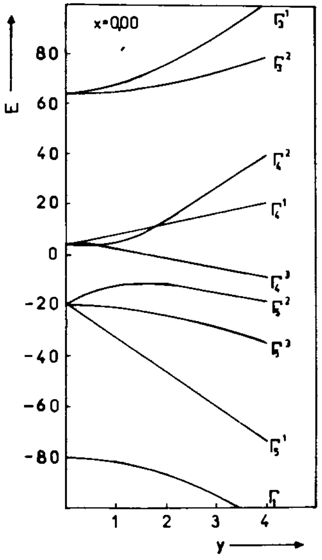

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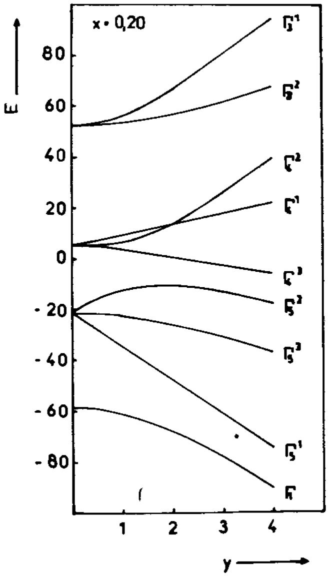

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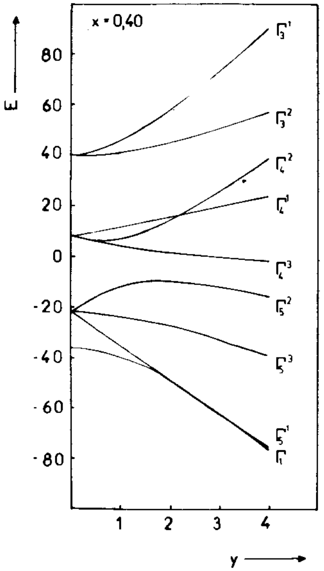

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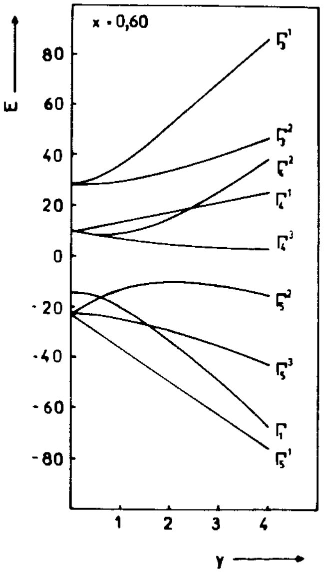

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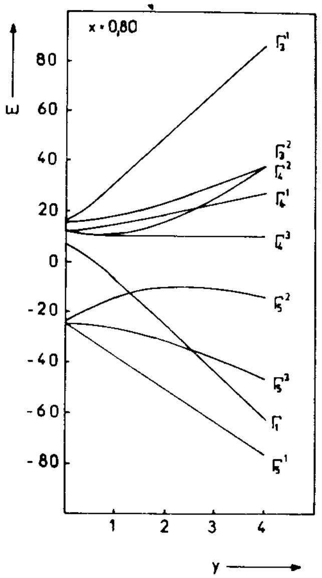
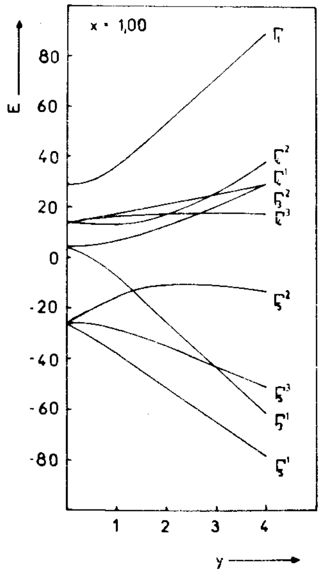


Fig. 10



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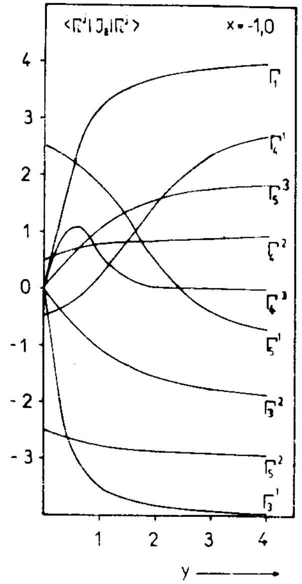

Fig. 12

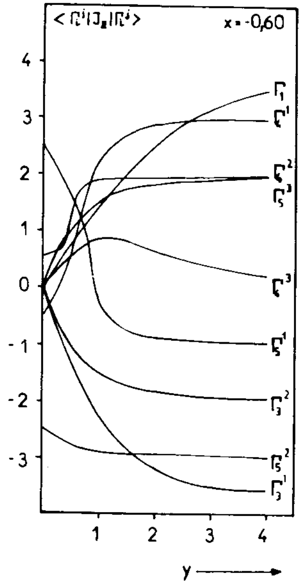

Fig. 13

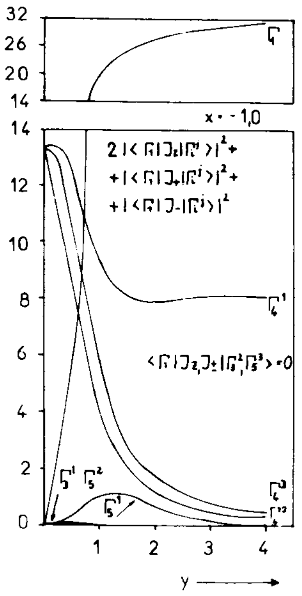

Fig. 14

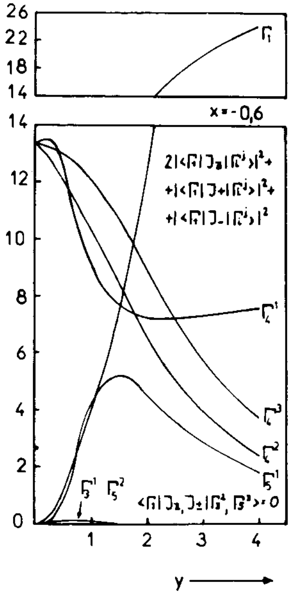

Fig. 15

The presence of a magnetic field effects noticeably not only the relative positions of electronic crystal field levels but other physical properties of this state as well. Figs. 12 and 13 give an example of (x = -1.0; -0.6) the dependence of magnetic moments $<\Gamma_i^j | \hat{J}_z | \Gamma_i^j>$ of Γ_i^j levels on y.

Figs. 14 and 15 show a similar dependence of the value

$$|<\Gamma_i^j|\hat{J}_\perp|\Gamma_{i'}^{j'}>|^2 =$$

$$= \frac{1}{3}\left(|<\Gamma_i^j|\hat{J}_+|\Gamma_{i'}^{j'}>|^2 + |<\Gamma_i^j|\hat{J}_-|\Gamma_{i'}^{j'}>|^2 + 2\,|<\Gamma_i^j|\hat{J}_z|\Gamma_{i'}^{j'}>|^2\right),$$

which within the dipole approximation determines the cross - section of elastic and inelastic scattering of neutrons on the electronic levels of polycrystalline samples /8/.

References.

/1/ G.H.Dieke. Spektra and Energy Levels of Rare Earth Ions in Crystals, Interience Publishers, New York (1968).

/2/ S.Matthies, D.Welsch. Phys.Sta.Sol. (b) 68, 125 (1975).

/3/ B.Bleaney, K.W.H.Stevens. Rep.Progr.Phys.16, 108 (1953).

/4/ M.T.Hutchings, Solid State Physics. 16, 227 (1964).

/5/ K.R.Lea, M.J.M.Leask, W.P.Wolf. J.Phys.Chem.Solids 23, 1381 (1962).

/6/ С.В.Вонсовский. Магнетизм, изд. Наука, М., 1971.

/7/ A.Furrer. Solid State Communications 16,839 (1975).

/8/ R.J.Birgeneau. J.Phys.Chem.Solids 33,59 (1972)

Received by Publishing Department
on February 12, 1976.