IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

ANALYSIS AND COMPARISON OF OPTICAL ENERGY LEVELS OF SOME ERBIUM AND NEODYMIUM COMPOUNDS

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Abstract : $NdCl_3$ and $ErCl_3$ both has hexagonal structure with site symmetry C_{3h} for trivalent rare earth ion and KNd_3F_{10} has tetragonal structure with site symmetry C_{4v} for the same.The energy levels (all in cm^{-1} units) of ground term , magnetic splitting factors i.e g-values and magnetic susceptibilities were calculated with the help of crystal field theory . Then using the corresponding crystal field parameters (CFP) energy levels of some excited states in visible and UV range of this compound has been calculated and compared with some other compounds from different references..As they belong to visible range so they are called optical energy levels. Possible Zeeman splitting was also shown for two states of $ErCl_3$.

Keywords *:* Crystal field effect, g-values, excited energy levels with spectroscopic notation, Zeeman effect.

1. Introduction :-

Studies on magnetic , EPR optical properties of Nd^{3+} [1 ,8] and Er^{3+} [7 , 9] compounds had been done extensively. Both of the ion are strongly magnetic and high anisotropic. When Nd^{3+} ion (ground term symbol $^4I_{9/2}$) and Er^{3+} ion (ground term symbol $^4I_{15/2}$) sit in the neighbourhood of 9 chloride ions its site symmetry becomes C_{3h}. Again when Nd^{3+} ion sits in the surroundings of fluoride ions in KNd_3F_{10} compound its site symmetry becomes C_{4v}. Then FI terms of Nd^{3+} ion and Er^{3+} ions splits into 5 and 8 Kramer's doublets respectively. Then values of the crystal field parameters (CFP) were determined keeping in mind about the referred values of magnetic splitting factors , total splitting of the ground term with a particular lowest level etc . After that using the values of CFP the energy splitting of the levels belonging to the visible and UV region were calculated.

2. Theoretical considerations :-

The RE ion normally exists as tripositive ion in solid crystal with spherical symmetry and (2J+1) fold degenerate energy level . The ion embedded in a crystalline lattice is acted upon by a number of interaction forces which were not present in the free ion . The electrostatic crystal field (CF) , produced by surrounding anions modifies the energy levels and eigen functions of the free ion which is the object of CF theory . Under the action of CF the symmetry becomes lower than that of the free ion and the degree to which (2J+1) degeneracy is removed will depend on the point symmetry of the RE ion called its site symmetry . The static crystal field acting on the free ion in terms of the spherical harmonics (since the unperturbed energy functions would have complete spherical symmetry) can be expressed as

$$H_V = \sum_{k,q} B_k^q\, V_k^q \quad (\text{ with condition } |q| \le k \text{ and } 0 \le k \le \infty) \qquad \ldots\ldots\ldots\ldots (1)$$

Here B_k and V_k denote corresponding crystal field parameter (CFP) and CF potential respectively. The value of k , q will be limited by the point symmetry of RE ion . For example for C_{3h} symmetry ,

$$H_v = B_2^0 V_2^0 + B_4^0 V_4^0 + B_6^0 V_6^0 + B_6^6 \left(V_6^6 + V_6^{-6} \right) \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

In C_{3h} symmetry ($NdCl_3$ and $ErCl_3$) there are three fold axis of rotational symmetry with a mirror plane perpendicular to the rotational axis . The electric field produced in this case is similar due to same symmetry . If a rotation of 120° is made followed by a reflection on the potential V , the new potential may be equated with the original potential if and only q = 0 or q = ±6 . The term with q = 0 do not mix the eigenstates with different quantum no m_J and the others arise due to the rotational elements of finite symmetry . For C_{4v} symmetry

$$H_v = B_2^0 V_2^0 + B_4^0 V_4^0 + B_6^0 V_6^0 + B_4^4 \left(V_4^4 + V_4^{-4} \right) + B_6^4 \left(V_6^4 + V_6^{-4} \right) \qquad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

which has lower symmetry than the previous potential expressed in equation (2) . For the sample Potassium Neodymium Fluoride (PNF) the CF potential has the above form . H_v will act upon the state vectors and give non-zero values when V_2^0,V_4^0,V_6^0 acts without any change in wave function and V_6^6 and V_6^{-6} act upon the ket states less or greater than the bra states by 6 . Similarly the potential V_4^4 and V_4^{-4} act upon the ket states less or greater than the bra states by 4 .

The g-values for ground level along and perpendicular to the symmetry axis of the sample are obtained from the relations $g_{II} = 2g_J \langle\psi_0|J_z|\psi_0\rangle$ and $g_\perp = 2g_J \langle\psi_0|J_x|\psi_0\rangle$ ....
(4) Where g_J = Lande' splitting factor and $|\psi_0>$= ground state CF wave function .

For Zeeman splitting **a**n electronic energy level with given n and l splits in a magnetic field into (2l+1) equidistant terms corresponding to 2l+1 settings , each with a slightly different energy determined by m_l . It can be shown that when the spin of the electron is also considered , the energy change of the electron due to the field is given by $\Delta E = g_J \mu_B m_j H$ where g_J=Lande' splitting factor .

Here optical energy levels for $^4F_{9/2}$, $^4G_{5/2}$, $^4G_{7/2}$, $^4G_{9/2}$, $^2G_{9/2}$ and $^2D_{3/2}$ for the two Nd-compounds and $^4F_{9/2}$, $^4S_{3/2}$, $^2H_{11/2}$, $^4F_{7/2}$, $^4F_{5/2}$, $^4F_{3/2}$ for $ErCl_3$ were calculated after determining the values of CFP effective for g values for ground term.

3. Results and Discussion :-

3.1 The obtained set of CF parameters (in cm^{-1}) are

$B_2^0 = 52$, $B_4^0 = -61$, $B_6^0 =-44$, and $B_6^6 = 625$ for $NdCl_3$

$B_2^0 = 96$, $B_4^0 =-270$, $B_6^0 = -1$, $B_4^4 = 5$ and $B_6^4 = -240$ for KNd_3F_{10}

$B_2^0 = 75$, $B_4^0 = -43$, $B_6^0 = -41$, and $B_6^6 = 540$ for $ErCl_3$

Table -1 g-values of different Nd and Er-Compounds :-

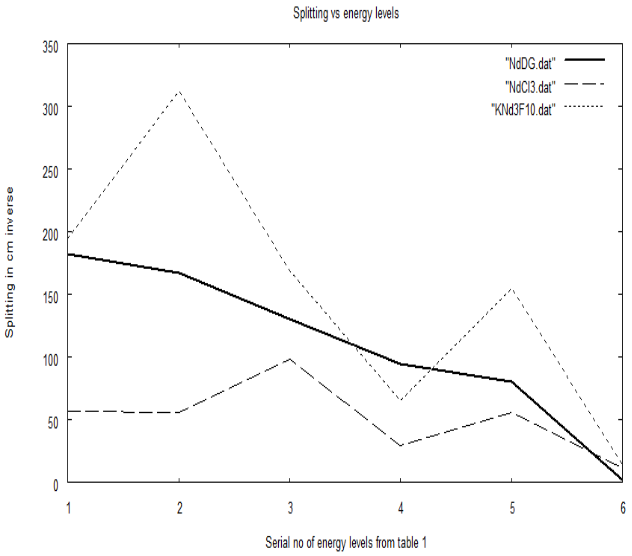
Sample	Symmetry	g_{II}	$g_\perp$	Ref
$Nd^{3+}:LaCl_3$	C_{3h}	3.996	1.763	[11]
$Nd^{3+}:Y(OH)_3$	C_{3h}	3.630	1.960	[12]
NdES	C_{3h}	3.594	2.039	[10]
$NdCl_3$	C_{3h}	3.444	2.277	[3]
KNd_3F_{10}	C_{4v}	3.594	1.132	[5]
ErES	C_{3h}	1.47	8.85	[2]
$Er^{3+}:Y(OH)_3$	C_{3h}	1.70	8.75	[6]
$Er(OH)_3$	C_{3h}	1.693	8.848	[9]
$ErCl_3$	C_{3h}	2.079	8.832	[4]

Table -2 **Optical level of different three Neodymium Compounds (in cm^{-1} unit):**

Sl No.	State (FI energy)	Ref [8] for NdDG	Splitting	$NdCl_3$	Splitting	KNd_3F_{10}	Splitting
1	$^4F_{9/2}$ (14762)	14670.3 14736.6 14753.7 14804.6 14853.0	182.7	14737.8 14745.3 14760.5 14771.9 14794.5	56.7	14670.6 14682.0 14764.4 14827.9 14865.1	194.5
2	$^4G_{5/2}$ (17106)	17022.4 17162.7 17189.6	167.2	17082.5 17097.9 17137.5	55.0	16979.1 17047.3 17291.6	312.6
3	$^4G_{7/2}$ (19027)	18962.1 19023.2 19067.4 19091.9	129.8	18989.5 19006.5 19024.2 19087.7	98.2	18947.8 19008.4 19034.7 19117.0	169.2
4	$^4G_{9/2}$ (19488)	19441.3 19483.1 19503.5 19528.9 19535.7	94.4	19477.5 19478.6 19481.6 19495.6 19506.6	29.1	19447.5 19482.2 19485.8 19512.2 19512.6	65.3
5	$^2G_{9/2}$ (21002)	20962.5 20986.8 21012.7 21019.0 21042.5	80.0	20972.6 20992.9 21007.2 21009.6 21027.6	55.0	20899.4 20978.6 21024.1 21053.7 21054.3	54.9
6	$^2D_{3/2}$ (21180)	21179.3 21180.7	1.4	21174.6 21185.4	10.8	21173.1 21186.9	13.8

Table - 3 **Optical level of two Erbium Compounds (in cm^{-1} unit) :**

Sl No.	State (FI energy)	$Er(OH)_3$ Ref [8]	Splitting	$ErCl_3$ (Present work)	Splitting
1	$^4F_{9/2}$ (15346)	15299.1 15335.9 15347.9 15387.4 15409.6	110.5	15317.1 15323.3 15328.9 15369.5 15391.1	74.0
2	$^4S_{3/2}$ (18470)	18448.4 18491.9	43.5	18461.3 18478.7	17.4
3	$^2H_{11/2}$ (19221)	19145.6 19201.5 19213.5 19221.3 19257.6 19259.3	113.7	19155.5 19202.6 19217.0 19226.2 19260.3 19264.4	108.9
4	$^4F_{7/2}$ (20594)	20516.0 20564.5 20617.5 20650.8	134.8	20542.5 20559.9 20634.8 20638.7	96.2
5	$^4F_{5/2}$ (22250)	22240.4 22247.7 22269.8	29.4	22245.7 22246.1 22258.2	12.5
6	$^4F_{3/2}$ (22590)	22559.9 22619.8	59.9	22577.9 22602.1	24.2



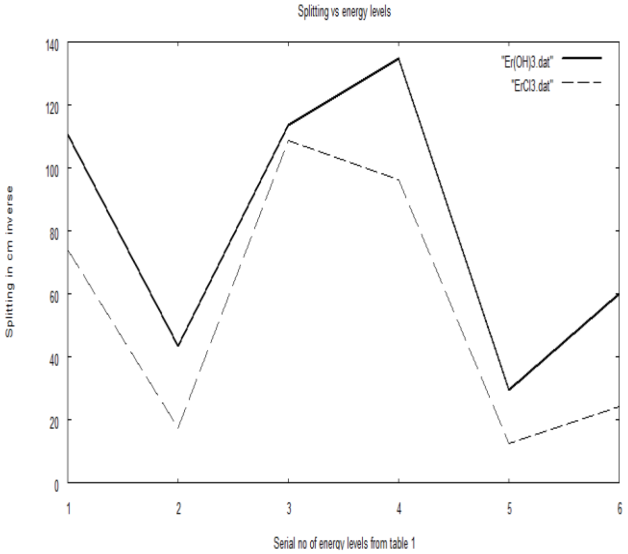


Fig – 1(a) (Nd – compounds) **Fig – 1(b) (Er - compounds)**

3.2 Zeeman Splitting of $^4S_{3/2}$ and $^4F_{3/2}$ for $ErCl_3$

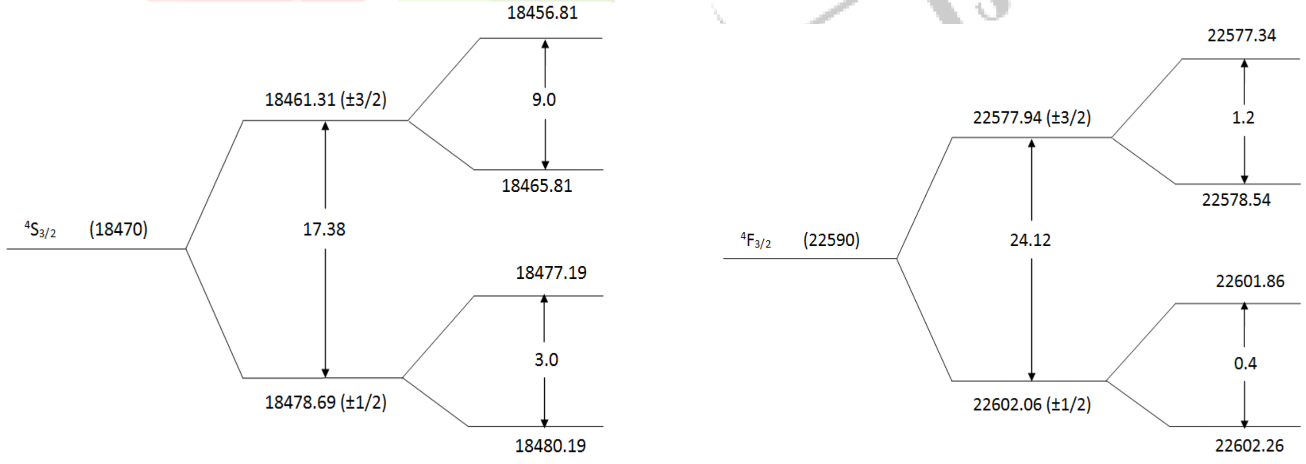


Fig.2 Zeeman splitting of $^4S_{3/2}$ and $^4F_{3/2}$ (all in cm^{-1} unit)

4. Conclusions

For the three samples the CF parameters do not change generally with temperature or by someway. So using the obtained CFP the energy levels of the aforesaid states were calculated. It was shown that the splitting was stronger for KNd_3F_{10} than $NdCl_3$ for the present work. But the splitting of NdDG is in between that of the two samples. For $ErCl_3$ the splitting is less than that of $Er(OH)_3$ but is of same pattern (Fig 1b).

For Zeeman splitting of $^4S_{3/2}$ and $^4F_{3/2}$ it can be said that after the first splitting due to crystal field effect , second one comes due to Zeeman effect in external magnetic field according to the formula $\Delta E = g_J \mu_B m_J H$ where symbols have their usual meaning. It is observed that the Zeeman splitting for both J = ±3/2 and J = ±1/2 are lesser for $^4F_{3/2}$ than $^4S_{3/2}$ state . For both cases the Zeeman splitting of J = ±3/2 is three times than that of J = ±1/2 . But the splitting of energy levels due to crystal field is in the reverse order .

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