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Research Paper

Magnetic Susceptibilities and Energy Levels of Neodymium Chloride ($NdCl_3$)

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Abstract: ***NdCl3 has hexagonal structure with site symmetry C3h. The energy levels of ground term, magnetic susceptibilities and energy levels of excited states in visible and UV range of this compound has been calculated with the help of crystal field theory.***

Keywords: Neodymium, Energy, $NdCl_3$

1. Introduction

Studies on optical and magnetic properties of trivalent erbium compounds have been done extensively [1,2] since Er^{3+} - compounds are highly magnetic. But similar studies on Nd^{3+} compounds are very few. The magnetic moment of Nd^{3+} ion is 3.62 BM , and magnetic study on Nd-ethylsulphate [3] has shown that the ground term splitting is 308 cm^{-1} with $\left|\pm\frac{5}{2}\right\rangle$ as ground state. Again magnetic and EPR studies [4,5] on some other compounds furnish that $g_{II} \rangle g_{\perp}$ for different Nd^{3+} compounds. Hence in the present paper we report the magnetic susceptibilities and energy levels in visible and UV range for $NdCl_3$ for the first time.

2. Theoretical Consideration

$Ndcl_3$ is a hexagonal sample having site symmetry C_{3h} for Nd^{3+} [Fig .1]

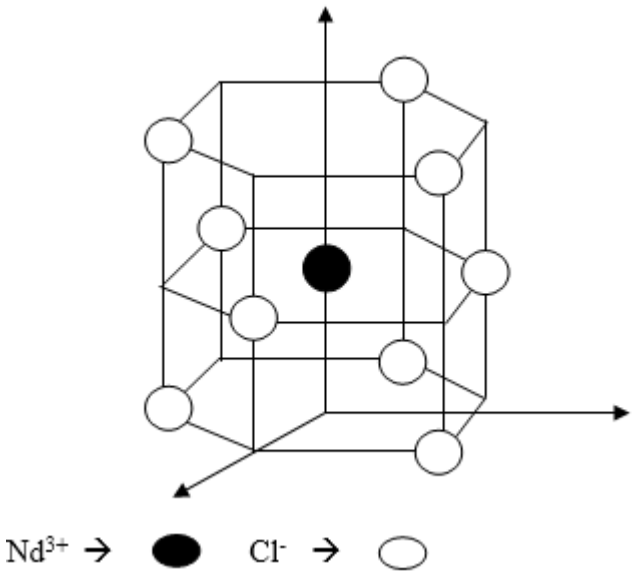

Fig . 1 Structure of $NdCl_3$ (not in scale)

The free ion ground term for Nd^{3+} is $^4I_{9/2}$ followed by $^4I_{11/2}$ at about 1867cm^{-1}. Since no ordering has been found for Nd-compounds down to 4.2K (Liquid He temperature) , We determined its optical levels and magnetic susceptibilities by considering only the crystal field (CF) owing to the Chloride anions about the Nd-cation.

The Hamiltonian of the crystal is $H = H_0 + H_V$ .....(1)

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For C_{3h} site symmetry , H_V is given by

$$H_V = B_2^0 V_2^0 + B_4^0 V_4^0 + B_6^0 V_6^0 + B_6^6 (V_6^6 + V_6^{-6}) \qquad \text{……..(2)}$$

Here V_k^q 's represent CF potential and B_k^q are treated as CF parameters (CFP).

Operating by H on $|J, m_J\rangle$ basis states of Nd^{3+} the CF energy levels and corresponding wave functions have been determined in terms of four CFP.The CF states are operated with magnetic perturbation $H_M = \beta \vec{\mu}.\vec{H}$ where β = Bohr Magneton , μ=vector operator corresponding to magnetic moment and H = applied magnetic field. Magnetic susceptibilities along symmetry axis (K_{II}) and

Where H_0 is the free ion Hamiltonian and H_V is that due to CF.

perpendicular to symmetry axis ($K_{\perp}$) were calculated using Van – Vleck's formula [6] as

$$K_J = \frac{N\beta^2 g^2 \sum_{nm} \{\frac{(E_{nm}^{(1)})^2}{kT} - 2E_{nm}^{(2)}\} \exp(-\frac{E_{nm}^{(0)}}{kT})}{\sum_{nm} \exp(-\frac{E_{nm}^{(0)}}{kT})}$$

Where J = parallel and perpendicular in case of axial CF,

$E_{nm}^{(0)}$ = Zero field energy , $E_{nm}^{(1)}$ = First order perturbed energy , $E_{nm}^{(2)}$ = Second order perturbed energy . Here n and m are quantum numbers (in M_J)

The four CFP were varied in such a way so that the ground term splitting becomes close to $300cm^{-1}$, $\left|\pm\frac{5}{2}\right\rangle$ be the ground state , g_{II} is greater than $g_{\perp}$ and mean magnetic moment becomes close to 3.62 BM. Thus the most accurate set of CFP were determined.

The $^4I_{9/2}$ term is not 100% (nearly 98%) pure but is admixtures of $^4I_{11/2}$, $^4I_{13/2}$ and $^4I_{15/2}$ terms . The intermediate coupling constants for V_2^0 , V_4^0 and V_6^0 were found to be 0.955 , 0.958 and 0.958 respectively. The most appropriate CFP (all in cm^{-1}) are $B_2^0 = 52$, $B_4^0 = -61$, $B_6^0 = -44$, $B_6^6 = 625$. The energy levels and CF wave functions are given in Table 1.

Table 1: Ground term energy levels and wave functions of $NdCl_3$

CF energy levels (cm^{-1})	CF wave functions
-179.337	$0.901\left\|\pm\frac{7}{2}\right\rangle + 0.434\left\|\mp\frac{5}{2}\right\rangle$
-31.180	$\left\|\pm\frac{1}{2}\right\rangle$
-27.263	$0.752\left\|\pm\frac{9}{2}\right\rangle + 0.658\left\|\mp\frac{3}{2}\right\rangle$

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113.621	$0.434\left\|\pm\frac{7}{2}\right\rangle - 0.901\left\|\mp\frac{5}{2}\right\rangle$
124.159	$0.658\left\|\pm\frac{9}{2}\right\rangle - 0.752\left\|\mp\frac{3}{2}\right\rangle$

3. Results and Discussions

The ground term splits into 5 Kramer's doublets with splitting 303 cm^{-1}.

3.1 g- values

The g –values were calculated with the following well – known relation $g_{II} = 2\, g_J \left|\langle \psi_0 | J_Z | \psi_0 \rangle\right|$ and $g_{\perp} = 2\, g_J \left|\langle \psi_0 | J_X | \psi_0 \rangle\right|$ where g_J is the Lande' splitting factor and $|\psi_0\rangle$ represents the ground CF eigen state . For $NdCl_3$ g – values are obtained as g_{II} =3.444 and $g_{\perp}$ = 2.277 which are consistent with the g – values of other compounds [4,5] .

3.2 Magnetic Susceptibilities

The thermal variation of both K_{II} and $K_{\perp}$ and their anisotropy $\Delta K = (K_{II} - K_{\perp})$ is shown in Fig 2a and 2b . It has been found that both K_{II} and $K_{\perp}$ follows the Curie – Weiss law down to 40K and 50K respectively. At room temperature the value of ΔK was 300 × 10^{-6} emu/mole which increases nearly 17 times at 80K .

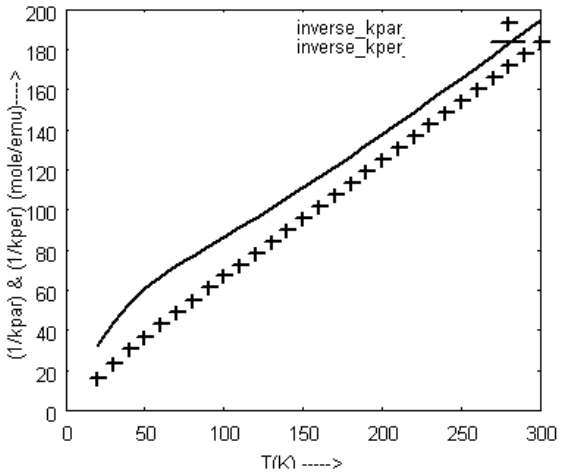


Fig 2a. Thermal variation of ($1/K_{par}$) and ($1/K_{per}$)

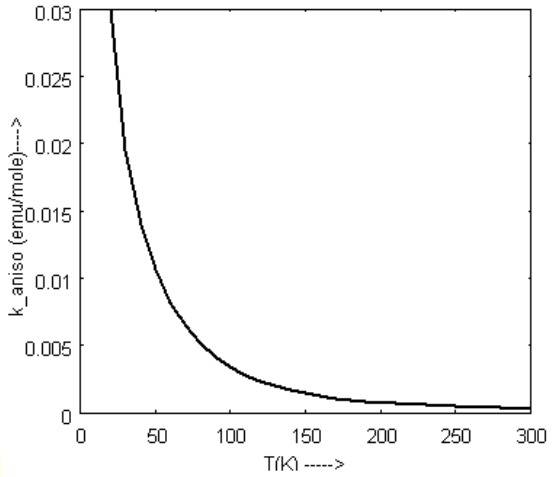


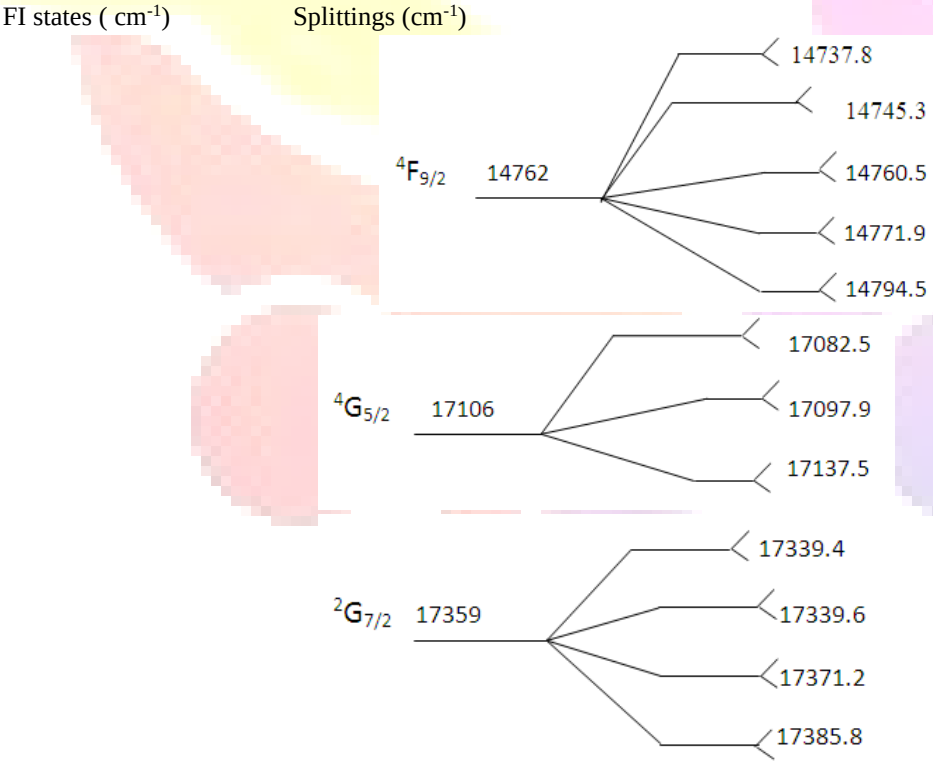
Fig 2b. Thermal variation of ΔK

It was found that thermal variation of both K_{II} and $K_{\perp}$ follow Curie – Weiss law within a certain range of temperature as follows.

$$K_{II} = \frac{1.737}{T + 15.631}$$ (down to 40K) and $$K_{\perp} = \frac{1.947}{T + 68.159}$$ (down to 50K)

3.3 Optical studies

The optical energy levels for $^4F_{9/2}$, $^4G_{5/2}$, $^2G_{7/2}$, $^4G_{7/2}$ $^4G_{9/2}$, $^2G_{9/2}$, $^2D_{3/2}$ of $Ndcl_3$ were calculated. The levels belongs to visible and ultraviolet region . The splitting of the above levels are 56.74 cm^{-1} , 55.0 cm^{-1} , 46.47 cm^{-1} , 98.18 cm^{-1} ,29.1 cm^{-1} , 54.94 cm^{-1} and 10.84 cm^{-1} respectively.



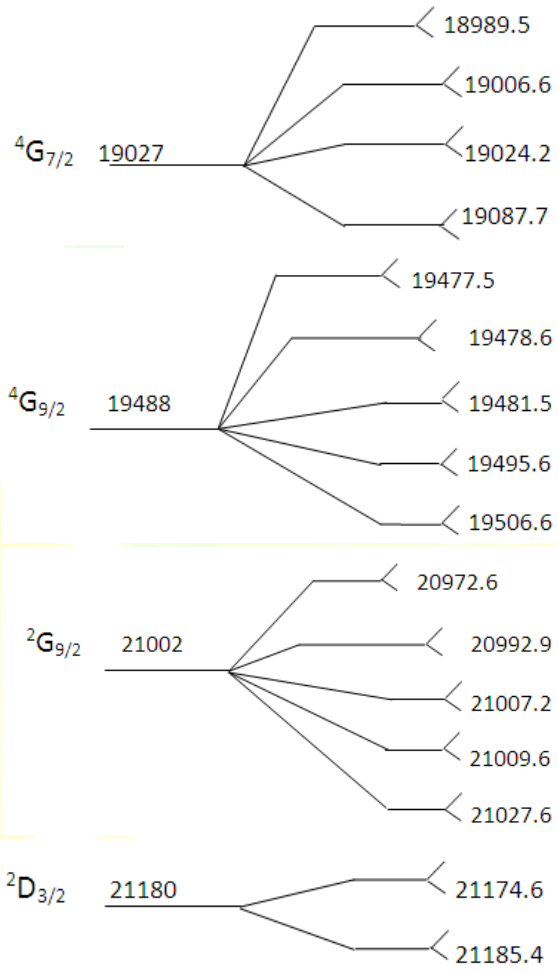


Fig 3 Energy levels in visible and UV range

4. Conclusions

The mean magnetic moment of $NdCl_3$ was found to be 3.546 BM which is very close to that of free ion . Nd^{3+} ion (in spite of being mirror image of Er^{3+} ion) in $NdCl_3$ is not as anisotropic as Er^{3+} in compounds [2]. Since $NdCl_3$ is nearly 5.4% anisotropic in nature the magnetic anisotropy measurement is welcome.

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