RESEARCH REVIEW JOURNALS
Volume-04
Issue-02
February -2019

ISSN: 2455-3085 (Online)
RESEARCH REVIEW International Journal of Multidisciplinary
www.rrjournals.com [UGC Listed Journal]

Magnetic Susceptibilities and Energy Levels of Potassium Neodymium Fluoride (KNd_3F_{10})

Somnath Bhattacharya

Assistant Teacher in Physics, Sutahata Janakalyan Sikshaniketan (H.S), Haldia , West Bengal , Pin Code - 721635

ARTICLE DETAILS

Article History
Published Online: 20 February 2019

Keywords
Potassium, Magnetic, Energy.

ABSTRACT

KNd_3F_{10} has tetragonal structure with site symmetry C_{4v} .The energy levels and wavefunctions of the 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 for the first time

1. Introduction

Since Er^{3+} -compounds are highly magnetic the optical and magnetic properties of trivalent erbium compounds have been studied enormously [1-3] . 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 [4] has shown that the ground term splitting is 308 cm^{-1} with |±5/2> as ground state . Again magnetic and EPR studies on some other compounds furnish that $g_{II} \rangle g_{\perp}$ for different Nd^{3+} compounds. Recently magnetic susceptibility measurements have been done on potassium erbium fluoride by Chemberlein and Corruccini [5] at low temperatures . Again a detailed magnetic study have been done on potassium europium fluoride over a wide range of temperatures by Bhattacharyya [6] . The magnetic , optical and thermal properties of potassium praseodymium fluoride have been calculated theoretically very recently [7] . But no study on potassium neodymium fluoride have been done as yet. Hence in the present paper we report the magnetic susceptibilities and energy levels in IR , visible and UV range for KNd_3F_{10}.

2. Theoretical Consideration

KNd_3F_{10} is a tetragonal sample having site symmetry C_{4v} for Nd^{3+} [Fig .1]

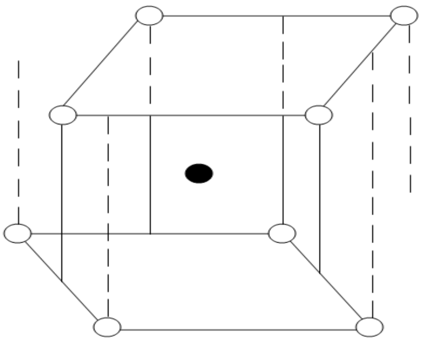


Fig . 1 Structure of KNd_3F_{10} (not in scale)

The free ion ground term for Nd^{3+} is $^4I_{9/2}$ followed by $^4I_{11/2}$ at about 1867 cm^{-1} which is well separated . So here we adopt the crystal field (CF) theory to find optical levels and magnetic susceptibilities for different temperatures for this sample .

The Hamiltonian of Nd^{3+} inside the crystal is

$$H = H_0 + H_V \qquad \text{................(1)}$$

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

For C_{4v} site symmetry , H_V is given by

$$H_V = B_2^0V_2^0 + B_4^0V_4^0 + B_6^0V_6^0 + B_4^4(V_4^4 + V_4^{-4}) + B_6^4(V_6^4 + V_6^{-4}) \qquad \text{................(2)}$$

Here V_k^q and B_k^q are CF potential and CF parameters (CFP) respectively.

Operating by H on | J,m_J > basis states of Nd^{3+} the CF energy levels and corresponding wave functions have been determined in terms of four CFP . Magnetic susceptibilities along symmetry axis (K_{II}) and perpendicular to symmetry axis ($K_{\perp}$) were calculated using Van – Vleck's formula [8] 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 five CFP were varied in such a way so that the ground term splitting becomes close to 300 cm^{-1} , |±5/2> 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 five CFP were determined.

3. Results and Discussions

The most appropriate CFP (all in cm^{-1}) are $B_2^0 = 96$, $B_4^0 = -270$, $B_6^0 = -1$, $B_4^4 = 5$ $B_6^4 = -240$. The energy levels and CF wave functions are given in Table 1.

Table 1: Ground term energy levels and wave functions of KNd_3F_{10}

CF energy levels (cm^{-1})	CF wave functions
-103.135	$0.996\left\|\pm\frac{5}{2}\right\rangle - 0.085\left\|\mp\frac{3}{2}\right\rangle$
-85.889	$0.267\left\|\pm\frac{9}{2}\right\rangle - 0.818\left\|\mp\frac{1}{2}\right\rangle + 0.509\left\|\pm\frac{7}{2}\right\rangle$
-56.962	$-0.866\left\|\pm\frac{9}{2}\right\rangle + 0.368\left\|\pm\frac{1}{2}\right\rangle + 0.338\left\|\mp\frac{7}{2}\right\rangle$
31.663	$0.085\left\|\pm\frac{5}{2}\right\rangle + 0.996\left\|\mp\frac{3}{2}\right\rangle$
214.323	$0.434\left\|\pm\frac{9}{2}\right\rangle + 0.896\left\|\pm\frac{1}{2}\right\rangle - 0.096\left\|\mp\frac{7}{2}\right\rangle$

The ground term splits into 5 Kramers' doublets with splitting 317 cm^{-1}.

3.1 g- values

The g –values were calculated with the following 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 KNd_3F_{10} the g – values are obtained as g_{II} =3.594 and $g_{\perp}$ = 1.132 which are consistent with the g – values of other compounds [4] .

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 468 × 10^{-6} emu/mole which increases to 6% at 80K.

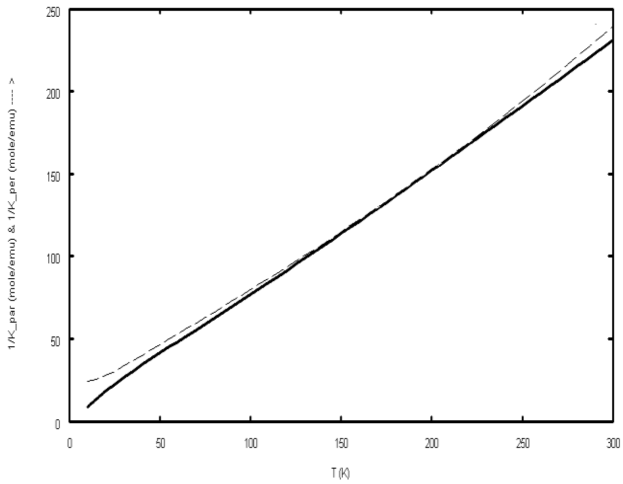


Fig 2a. Thermal variation of ($1/K_{par}$) and ($1/K_{per}$)

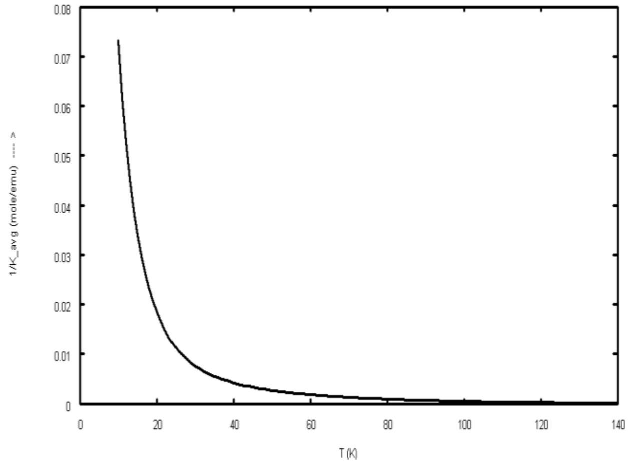


Fig 2b. Thermal variation of ΔK

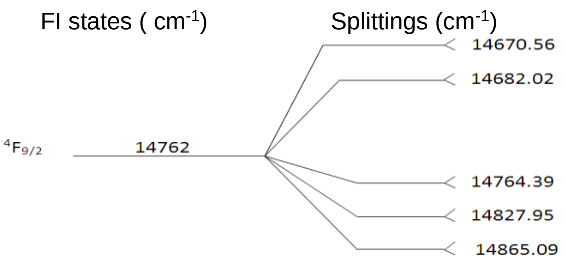
It was found that thermal variation of both K_{II} and $K_{\perp}$ follow Curie – Weiss law within a certain range of temperature as follows.

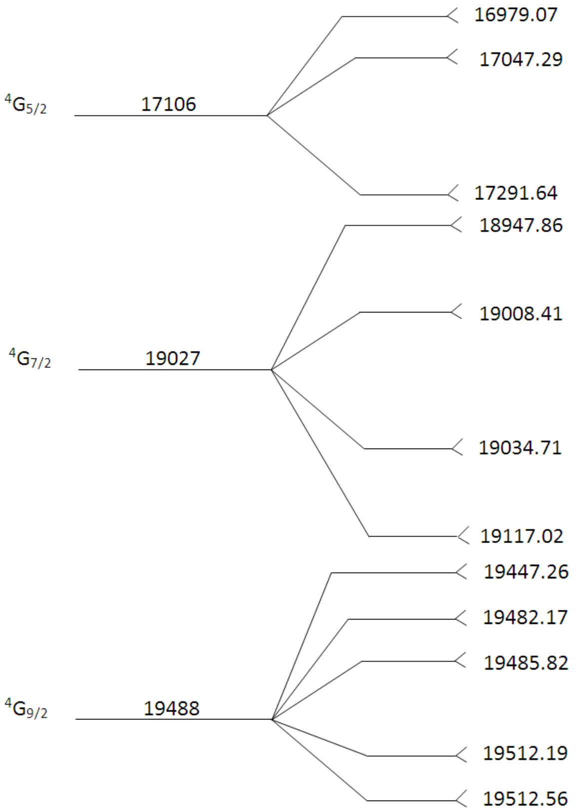
$$K_{II} = \frac{1.357}{T + 5.429}$$ (down to 30K) and

$$K_{\perp} = \frac{1.486}{T + 19.318}$$ (down to 20K)

3.3 Optical studies

The optical energy levels for $^4F_{9/2}$, $^4G_{5/2}$, $^4G_{7/2}$ $^4G_{9/2}$, $^2G_{9/2}$, $^2D_{3/2}$ of KNd_3F_{10} were calculated. The levels belongs to visible and ultraviolet region . The splitting of the above levels are 194.53 cm^{-1} , 312.57 cm^{-1} , 169.16 cm^{-1} , 65.30 cm^{-1} ,154.88 cm^{-1} and 13.87cm^{-1} respectively.





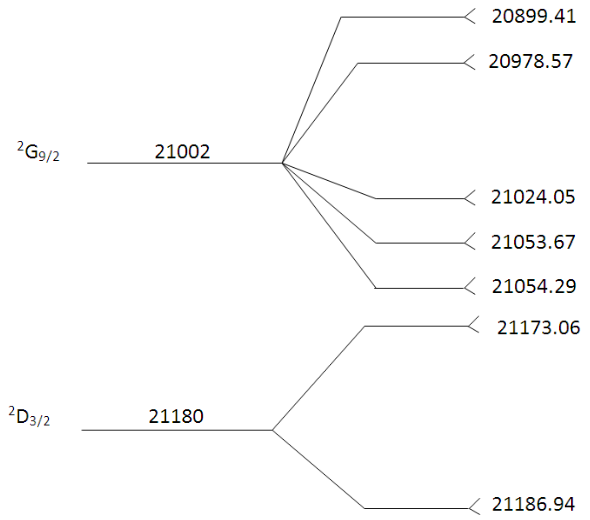


Fig 3 Energy levels in visible and UV range

4. Conclusions

The mean magnetic moment of KNd_3F_{10} 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 KNd_3F_{10} is not as anisotropic as Er^{3+} in compounds [2]. Measurements of g-values and magnetic susceptibilities at low temperatures are welcome.

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