Theoretical Zero Field Splitting Parameters of Fe^{3+} doped $(NH_4)_2[AlF_5.H_2O]$ Single Crystal

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Abstract— Zero field splitting parameters (ZFSPs) D and E of Fe^{3+} doped $(NH_4)_2[AlF_5.H_2O]$ (AAF) crystals are determined theoretically at room temperature (RT) using Crystal field parameters (CFPs) from superposition model. The obtained theoretical D and E are in reasonable agreement with the experimental values. The experimental conclusion that Fe^{3+} substitutes for Al^{3+} in AAF is supported by the present study. The parameters D and E are computed without and with local distortion. These D and E provide reasonable agreement with the experimental ones when we consider the local distortion.

Keywords— Inorganic compounds; Single crystal; Crystal fields; Optical properties; Electron paramagnetic resonance.

I. INTRODUCTION

Electron paramagnetic resonance (EPR) provides local site symmetry and zero field splitting parameters (ZFSPs) of transition ions in crystals [1, 2]. Fe^{3+} ion in the iron group with the ground state ^6S has spin S = 5/2. The electron spins being affected by the crystal field through high order interaction become free to orient themselves in the external magnetic field.

The superposition model (SPM) yields physical and geometrical information included in crystal field parameters [3, 4]. The positions of different ligands in the crystal are required to apply this model. Therefore, the theories of local distortion in crystals are quite important. In order to discuss the location of Fe^{3+} ion with respect to the surrounding oxygen ligands a one-parameter model was used [5].

Theoretical studies of spin Hamiltonian parameters of d^5 ions have been done by various workers [6-8]. A number of mechanisms have been advised to contribute to the ground state splitting of the paramagnetic ions in crystals [9]. The effect of spin Hamiltonian is generally studied by perturbation methods. In most of the cases, cubic field and the diagonal part of free-ion Hamiltonian are assumed as unperturbed terms whereas the spin-orbit coupling, the low-symmetry field, and the off-diagonal part of free-ion Hamiltonian are considered as the perturbation terms [10].

EPR absorption of Fe^{3+} doped $(NH_4)_2[AlF_5.H_2O]$ (AAF) single crystals has been reported earlier [11]. Two possibilities are there for Fe^{3+} site in the AAF crystal, substitutional and interstitial. It is worth to find the site of the impurity in AAF crystal. It was concluded that Fe^{3+} ion substitutes at Al^{3+} site in AAF lattice [11]. In the present study, the zero-field splitting parameters (ZFSPs) D and E are evaluated for the Fe^{3+} ion at substitutional Al^{3+} site in AAF; using crystal field parameters (CFPs) determined from superposition model and perturbation theory [12]. The aim of study is to gather information of Fe^{3+} ion being entering the crystal lattice substitutionally or interstitially and also about the distortion occurring in the lattice. The results provided from this model give reasonable agreement with the experimental ones when we consider the local distortion for the Fe^{3+} ion at substitutional Al^{3+} site in AAF crystal.

This section was provided to the brief introduction of SPM methodology and Hamiltonians. The remaining part of the paper is organized as follows. Section II gives the related work associated with the CF and ZFS analysis. Section III provides the methods employed for calculation of CFPs and ZFSPs. Section IV describes the results and its discussion based on the analysis performed. In section V, conclusion of the study and future scope for improvement are provided.

II. RELATED WORK

The CF and ZFS analysis have been carried out for various ion-host systems [6-8, 10, 12]. The crystal structure of $(NH4)_2[AlF_5.H_2O]$ [AAF] crystal is orthorhombic having unit cell parameters a = 1.01924 nm, b = 0.80372 nm, c = 0.78441 nm and Z = 4 [13, 14]. Because of the positions of the eight $[NH_4]^+$ and four $[AlF_5.H_2O]^{2-}$ ions in the unit cell, the crystal has an anti-fluorite structure [14]. The space group is Pbcn. Each ammonium ion is surrounded by four

[AlF$_5$(H$_2$O)] octahedra, each N-hydrogen being bonded to a fluorine in a different octahedron. The orientations of the *(x, y, z)* axes (SAAS-symmetry adopted axis system) relative to the *(a, b, c)* crystallographic axes in the [AIF$_5$.H$_2$O]$^{2-}$ complex ion are *(x → a, y → c, z → b)* as shown in Fig. 1.
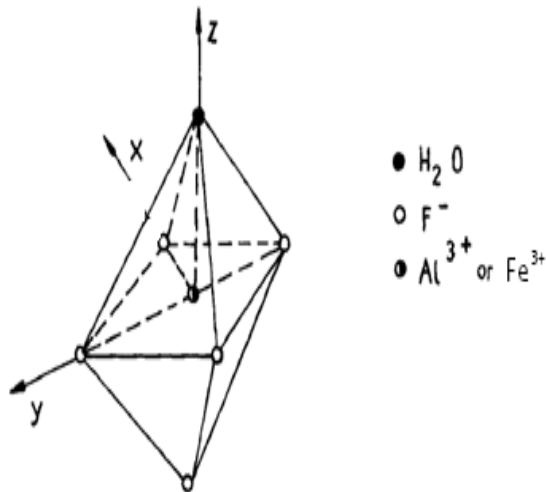

Figure 1. Crystal structure of AAF with symmetry adopted axis system (SAAS).

III. MATERIALS AND METHODS

The experimental resonance magnetic fields are analyzed using the spin Hamiltonian [15, 16],

$$\mathcal{H} =$$

$$\mu_B B.g.S + D\left\{S_z^2 - \frac{1}{3}S(S+1)\right\} + E(S_x^2 - S_y^2) + \frac{a}{6}[S_x^4 + S_y^4 + S_z^4 - \frac{1}{5}S(S+1)(3S^2 + 3S+1)]$$

$$(1)$$

where g is the spectroscopic splitting factor, μ_B is the Bohr magneton and B is the external magnetic field. D and E are the second rank axial and rhombic ZFSPs, while *a* is the fourth rank cubic ZFSP [17, 18]. The maximum overall splitting of the EPR spectrum is taken along the z axis and the minimum along the x axis [19]. The laboratory axes (x, y, z) are parallel to the crystallographic axes. The local site symmetry axes, i. e. the symmetry adopted axes (SAA) are the nearly orthogonal directions of metal-ligand bonds. The Z-axis of SAAS in four equivalent sites is coincident with the crystal **b**-axis and the other two axes (X, Y) lie in the ac plane (Fig. 1). This indicates that Fe^{3+} substitutes Al^{3+} in the crystal lattice. The ionic radius of Fe^{3+} ion 0.064 nm is slightly larger than the ionic radius of Al^{3+} (0.054 nm), thus Fe^{3+} ion can substitute at the location of Al^{3+} with some distortion [20].

The ZFSPs of Fe^{3+} ion at four equivalent sites are determined using the perturbation theory [21, 22]. These values are then compared with the experimental result.

Spin Hamiltonian of a d^5 (^{6}S state) ion may be written as sum of free ion ($\mathcal{H}_o$), spin-orbit coupling ($\mathcal{H}_{so}$), spin-spin coupling ($\mathcal{H}_{ss}$) and crystal field ($\mathcal{H}_c$) Hamiltonians,

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_{so} + \mathcal{H}_{ss} + \mathcal{H}_c \qquad (2)$$

where $\mathcal{H}_c = \sum B_{kq} C_q^{(k)}$ \qquad (3)

where B$_{kq}$ are the crystal-field parameters and $C_q^{(k)}$ are the Wybourne spherical tensor operators. For the orthorhombic symmetry crystal field, B$_{kq}$ ≠ 0 only with k = 2, 4, q = 0, 2, 4. The crystal-field theory has been widely used for the study of spin Hamiltonian parameters of transition ions doped in different crystals [12, 23-25]. In the our study, we have calculated the CFPs, B$_{kq}$ employing SPM [21].

In AAF crystal the local symmetry around Fe^{3+} ions is considered to be orthorhombic of type I (OR-I) [11, 20]. In OR-I symmetry, the ZFSPs D and E are given by [12]

$$D^{(4)}(SO) = \left(\frac{3\xi^2}{70P^2D}\right)[-B_{20}^2 - 21\xi B_{20} + 2B_{22}^2] + \left(\frac{\xi^2}{63P^2G}\right)[-5B_{40}^2 - 4B_{42}^2 + 14B_{44}^2]$$

$$E^{(4)}(SO) = \left(\frac{\sqrt{6}\xi^2}{70P^2D}\right)[2B_{20} - 21\xi]B_{22} + \left(\frac{\xi^2}{63P^2G}\right)[3\sqrt{10}B_{40} + 2\sqrt{7}B_{44}]B_{42}$$

$$(4)$$

$$(5)$$

where P = 7B+7C, G = 10B+5C, D = 17B+5C. B and C are Racah parameters, giving electron-electron repulsion and ξ is the spin-orbit coupling parameter. It is found that the values of B and C for transition metal ion in a crystal are less than those of the free ion. By taking the average covalency parameter N, we can write the Racah parameters and spin-orbit coupling parameter as B = N^{4}B$_0$, C = N^{4}C$_0$, ξ = N$^2\xi_0$, where B$_0$ and C$_0$ are Racah parameters for free ion and ξ_0 is free ion spin-orbit coupling parameter [21, 26]. For free Fe^{3+}ion, B$_0$ = 1130 cm^{-1}, C$_0$ = 4111 cm^{-1} and ξ_0 = 589 cm^{-1} are used [21].

Considering the values of Racah parameters (B = 899 cm^{-1}, C = 3198 cm^{-1}) evaluated from optical study of the Fe^{3+} ion with F ligand, the average parameter N is obtained from N = ($\sqrt{B/B_0} + \sqrt{C/C_0}$)/2 [27].

The CFPs from SPM are given as

$$B_{kq} = \sum_j \overline{A_k}(R_j) K_{kq}(\theta_j, \phi_j) \qquad (6)$$

where the co-ordination factor K$_{kq}(\theta_j, \varphi_j)$ is an explicit function of the angular position of the ligand [12, 28]. The intrinsic parameter $\overline{A_\kappa}(R_j)$ is written as

$$\overline{A_k}(R_j) = \overline{A_k}(R_0)\left(\frac{R_0}{R_j}\right)^{t_k}$$

where R_j is the distance between the d^n ion and the ligand, $\overline{A_k}(R_0)$ represents the intrinsic parameter of the reference crystal, t_k is the power law exponent and R_0 is the reference distance between metal and ligand. For Fe^{3+} doped in different crystals having various ligands, $t_2 = 3$ and $t_4 = 5$ [25]. The above values are used here in this calculation. As the co-ordination around Fe^{3+} ion is octahedral, $\overline{A_4}$ and Dq are related as

$$\overline{A_4}(R_0) = \frac{3}{4}Dq$$

[29]. From optical study [27], the value of Dq = 1390 cm^{-1}. Thus, the relation gives the value of $\overline{A_4}(R_0)$ = 1042.5 cm^{-1}. It is noted that for $3d^5$ ions the ratio of $\overline{A_2}(R_0)$ and $\overline{A_4}(R_0)$ lies between 8 to 12 [21, 30, 31]. In this study,

$$\frac{\overline{A_2}}{\overline{A_4}} = 10$$ is taken, which gives $\overline{A_2}$ = 10425 cm^{-1}.

IV. RESULTS AND DISCUSSION

The CFPs B_{kq} of Fe^{3+} ion at four equivalent sites are calculated using SPM with the help of parameters $\overline{A_2}$ and $\overline{A_4}$ and arrangement of ligand ions around Fe^{3+} ion (Fig. 1). Atomic coordinates in AAF crystal and bond length R (without and with distortion) together with angle θ, φ (one site) are shown in Table 1. The calculated CFPs and ZFSPs along with reference distance R_0 are shown in Table 2. It is noted from Table 2 that the value of R_0 = 0.108 nm slightly less than the lowest of four ligand distances from the central metal ion (0.1782 nm) together with local distortion yield ZFSPs for all the four equivalent sites in reasonable agreement with the experimental values [11]. The ZFSPs calculated using R_0 = 0.108 nm and without local distortion are quite larger than the experimental values. For comparison the interstitial sites for Fe^{3+} ions were also calculated. The calculated values of ZFSPs are found to be different from the experimental ones and hence are not provided here.

Table 1. Atomic coordinates in AAF crystal and bond length R (without and with distortion) together with angle θ, φ (one site).

Position of Fe''	Ligands				Spherical co-ordinates of ligands		
		x	y	z	R(nm)	θ⁰	φ°
					(A)		
Site 1							
Site I: Substitutional Al(	F(1) 0	0.4226	0.2500	0.1792	R₁ 90	θ₁ 90	φ₁
Al (0, 0.1996, 0.2500)	F(1') 0	-0.4226	0.7500	0.6355	R₂ 85.48	θ₂ 90	φ₂
	F(2) 0.0400	0.1966	0.0288	0.1782	R₃ 97.12	θ₃ 88.70	φ₃
	F(3) 0.1713	0.1975	0.3012	0.1791	R₄ 88.36	θ₄ 84.51	φ₄
	F(3') 0.5000	0.3025	0.7500	0.6483	R₅ 85.57	θ₅ 85.56	φ₅
	O 0	-0.0412	0.2500	0.1935	R₆ 90	θ₆ 90	φ₆
With distortion							
	F(1)				0.2790 R₁+ΔR₁		
	F(1')				0.7235 R₂+ΔR₂		
	F(2)				0.3022 R₃+ΔR₃		
	F(3)				0.3011 R₄+ΔR₄		
	F(3')				0.7363 R₅+ΔR₅		
	O				0.3285 R₆+ΔR₆		

Table 2 Crystal field parameters and zero field splitting parameters of Fe^{3+} doped AAF single crystal.

		Crystal- field parameters (cm⁻¹)				Zero-field splitting parameters (×10⁻⁴cm⁻¹)		
Site	R₀(nm)	B₂₀	B₂₂	B₄₀	B₄₂	B₄₄	|D|	|E|	E|/|D|
Without distortion								
Site I								
$\frac{\overline{A_2}}{\overline{A_4}}$=10	0.108	-8679.25	-10669.2	882.0244	933.1926	4965.281 2521		
	1182	0.468						
With distortion								
Site I								
$\frac{\overline{A_2}}{\overline{A_4}}$=10	0.108	-1974.33	-2426.23	73.44317	77.65143	4119.371 668.1		
	137.3	0.205						
Exp.						668.1	176.6	0.263

Using CFPs and CFA program with OR-I symmetry of the crystal field the optical spectra of Fe^{3+} doped AAF crystals are computed [32, 33]. The energy levels of the impurity ion are obtained by diagonalization of the complete Hamiltonian within the $3d^N$ basis of states in the intermediate crystal field coupling scheme. The calculated energy values are presented in Table 3 along with the experimental values for comparison. There we obtain a reasonable agreement between the two. Thus, the results obtained on the basis of superposition model support the experimental finding that Fe^{3+} ions substitute at Al^{3+} site in the crystal [11].

Table 3. Experimental and calculated (CFA package) energy band positions of Fe^{3+} doped AAF single crystal.

Transition from $^6A_{1g}(S)$	Observed wave number (cm^{-1})	Calculated wave number (cm^{-1})
$^4T_{1g}(G)$	16300	
$^4T_{2g}(G)$	22000	
$^4A_{1g}(G)$	25100	24508
$^4E_g(G)$	26750	26720, 26764
$^4T_{2g}(D)$	29600	8716, 28764, 29021, 29063, 30139, 30281
$^4E_g(D)$	31850	31833, 31915
$^4T_{1g}(P)$	37050	37468, 37580, 37707, 37835, 37956, 38772
$^4T_{1g}(F)$	42550	42097, 42285, 42347, 42509, 42839, 42992
$^4T_{2g}(F)$	46750	45945, 46131, 46338, 46797, 46857, 46993

V. CONCLUSION AND FUTURE SCOPE

CFPs and ZFSPs for Fe^{3+} ion doped AAF have been obtained using superposition model and perturbation theory, respectively. The determined ZFSPs give a reasonable agreement with the experimental values. The calculated optical spectra are also in reasonable agreement with the experimental result. The conclusion found on the basis of superposition model supports the experimental result that Fe^{3+} ions substitute at Al^{3+} site in the AAF crystal. Modeling methods used here may be useful in future to correlate EPR and optical data for various ion-host systems. The combined modeling approaches: CF, ZFS and Microscopic Spin Hamilton may yield better correlation of EPR and optical data.

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