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Research Article



Modeling of Cr³⁺ doped Cassiterite (SnO₂) Single Crystals

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Abstract

Using the superposition model, the crystal field and zero-field splitting parameters of Cr³⁺ doped cassiterite (tin oxide), SnO₂ single crystals are computed. For calculations, the appropriate locations for Cr³⁺ ions in SnO₂ with distortion are taken into account. The experimental values and the zero-field splitting parameters in theory with local distortion agree fairly well. Using the Crystal Field Analysis Program and crystal field parameters, the optical energy bands for Cr³⁺ in SnO₂ are calculated. The findings indicate that in SnO₂ single crystals, one of the Sn⁴⁺ ions is replaced by Cr³⁺ ions.

Introduction

When examining the local symmetry of transition ions in crystals, electron paramagnetic resonance, or EPR, is thought to be a crucial tool. The Cr³⁺ ion introduced into different crystals provides good information about the Crystal Field (CF) and zero field splitting (ZFS) parameters [1-4]. When divalent or trivalent impurities are used in place of monovalent ions, it is crucial to compensate for the charge imbalance. In such systems positive ion vacancies fulfill the charge compensation [5]. The optical characteristics of the crystal are impacted by substituted impurities that cause very little structural change. The Superposition Model (SPM) is mostly used for the theoretical estimation of ZFS and CF parameters [6-8]. It is worth mentioning various semiempirical approaches developed for modeling CF parameters (CFPs) based on crystal structure data. Apart from the historically first, Point Charge Model (PCM), other CFP modeling approaches are Superposition Model (SPM), Angular Overlap Model (AOM), and Simple Overlap Model (SOM). These approaches may yield varying results even using the same crystallographic data as input. Various modeling techniques for the analysis and interpretation of EMR data for transition ions at low symmetry sites in crystals have been reviewed [8]. The superposition model was originally developed and applied first to CFPs for lanthanide ions in various crystals and later to CFPs for transition metal ions. Subsequently, its applications

have been extended to the semi-empirical parameterization of Zero-Field Splitting Parameters (ZFSPs) and interpretation of EPR spectra for the S-state 3d⁵ and 4f⁷ transition ions. It should be emphasized that out of the semi-empirical approaches applicable for CFPs: PCM, SPM, AOM, and SOM, only SPM is also applicable to ZFSPs. In fact, SPM may be employed independently for modeling both CFPs and ZFSPs, whereas attempts to use PCM for ZFSPs occasionally appear in EMR literature. SPM calculations of CFPs and those of ZFSPs utilize the same mathematical framework [8]. Accurate interpretation of EMR experimental spectra and modeling of ZFSPs is important for proper understanding of spectroscopic and magnetic properties of crystals containing 4f^N and 3d^N ions. SPM yields calculable predictions for EMR experiments in which transition ions are used as probes to investigate the structure and nature of paramagnetic centers. Modeling using SPM may also help predict characteristics important for potential applications. Hence, SPM calculations of ZFS parameters are of prime importance.

SnO₂ is one of the important semiconducting oxides having desirable qualities such as optical transmittance, mechanical hardness, low resistivity, stability under heat treatment, uniformity, and piezoelectric behavior. This semiconductor, which is of the n-type and has a wide band gap of 3.6 eV at 300 K, is highly iconic and has a wide range of uses. Some of these uses include gas sensors, catalyst supports, dye-sensitized solar cells, supercapacitors, and transparent conducting



electrodes [9-13]. Recently, some researchers have added metal or halogen ions to SnO₂ as impurities, changing its surface states, electronic structure, and optical characteristics in the process, which has improved the material's qualities and potential applications [10,14,15]. Moreover, the Cr³⁺-doped SnO₂ materials are useful in solid-state lighting [16].

EPR study for Cr³⁺ ions in SnO₂ was performed and spin Hamiltonian parameters were evaluated [17]. Sn⁴⁺ ions have an ionic radius of 0.069 nm, which is marginally greater than Cr³⁺ ions' ionic radius of 0.0615 nm. Hence Cr³⁺ substitutes for one of the Sn⁴⁺ ions as discussed in [17].

The crystallographic axes (a, b, and c) and the laboratory axes (x, y, and z) are chosen in parallel. The symmetry-adopted axes (magnetic axes) have labels (X, Y, Z). The crystallographic c axis is found to correspond with the principal Z axis of the g and D tensors of Cr³⁺ ions.

The superposition model (SPM) analysis of the ZFS and CF parameters for Cr³⁺ ions in SnO₂ single crystal is presented in the current work. Investigating the ZFS parameters, the CF parameters, and the lattice distortion for the Cr³⁺ ions in SnO₂ at octahedral sites is the goal. The Crystal Field Analysis (CFA) computer program and CF parameters are used to determine the optical energy bands for Cr³⁺ ions in SnO₂. The estimated CF and ZFS parameters could both be helpful in later research for obtaining crystals of various scientific and industrial applications.

Crystal structure

SnO₂ belongs to the TiO₂ (Rutile) crystal class, which crystallizes in a space group P4₂ 2₁/n 2/m-D_{4h}¹⁴ tetragonal crystal system [18]. The unit cell has the following parameters: a = 0.4737 nm, b = 0.4737 nm, and c = 0.3185 nm. Two nonequivalent Sn⁴⁺ sites make up the unit cell, and they can be converted into one another by rotating 90° around the c-axis. Due to a slight deformation of the SnO₆ octahedra, an orthorhombic local symmetry D_{2h} is formed around the Sn⁴⁺ site. Figure 1 shows the SnO₂ crystal structure with the Symmetry-Adopted Axis System (SAAS).

The directions of metal-ligand bonds that are mutually perpendicular are the symmetry adopted axes (SAA) or local site symmetry axes. For centers I, the two other axes (X, Y) are perpendicular to the Z axis of SAAS, which is along the metal-ligand bond Sn-O (crystal c-axis) (Figure 1). This suggests that in the SnO₂ crystal, Cr³⁺ takes the place of Sn⁴⁺ with approximately orthorhombic symmetry. The ionic radius of Cr³⁺ ions (0.0615 nm) is slightly less than that of Sn⁴⁺ ions (0.069 nm), suggesting that Cr³⁺ ions can, with some distortion, occupy the position of Sn⁴⁺ ions. The ligands' spherical polar coordinates and the position of the Cr³⁺ ion for center I in SnO₂ are shown in Table 1 [18]. These specifics are employed for Cr³⁺ ion CF and ZFS computations in SnO₂.

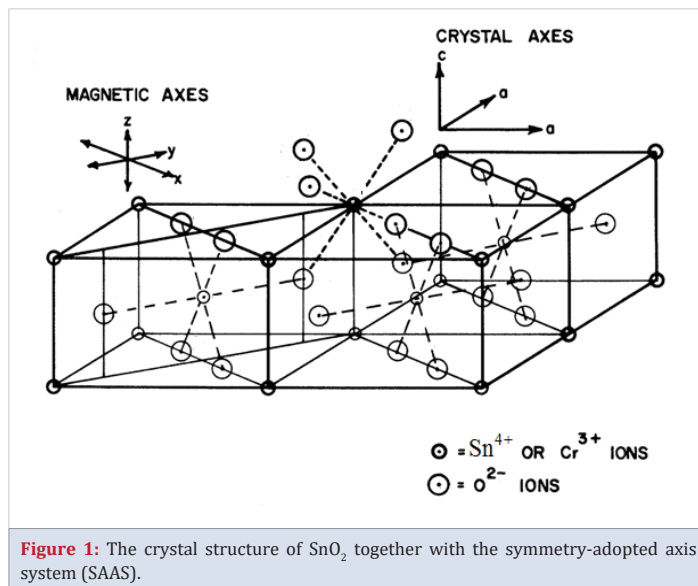


Figure 1: The crystal structure of SnO₂ together with the symmetry-adopted axis system (SAAS).

Table 1: The Cr³⁺ ion's fractional coordinates and the spherical polar co-ordinates (R, θ, φ) of ligands (center I) in a single crystal of SnO₂.

Position of Cr ³⁺	Ligands	Spherical polar co-ordinates of ligands		
		R ^Å	θ ^o	φ ^o
ND: Substitutional (0.0000, 0.0000, 0.0000)	01	2.2772	64.57	45.00
	02	2.0566	89.91	45.00
	03	4.2409	67.94	13.44
	04	4.2409	67.94	76.55
	05	2.0566	89.91	-45.00
	06	2.0566	89.91	-45.00
WD: substitutional Centre I (-0.1662, -0.1185, -0.0022)	01	3.1712	71.91	41.95
	02	1.1145	89.47	53.24
	03	5.0978	71.71	17.74
	04	4.9672	71.21	68.78
	05	2.4128	89.92	-21.71
	06	2.1230	89.91	-71.69

Computations of splitting parameters for zero field

The energy levels of Cr³⁺ ions in crystals are found using the spin Hamiltonian [19-21]:

$$H = H_{Ze} + H_{ZFS} = \mu_B B \cdot g \cdot S + \sum B_k^q O_k^q = \mu_B B \cdot g \cdot S + \sum f_k b_k^q O_k^q \quad (1)$$

Where spectroscopic splitting factor, Bohr magneton, and steady magnetic field are represented by g, μ_B, and B, respectively. S represents the effective spin operator and O_k^q(S_x, S_y, S_z) are the extended Stevens operators (ESO) [22,23]; B_k^q and b_k^q are the parameters of ZFS, f_k = 1/3 and 1/60 give the scaling factors for k = 2 and 4, respectively. At orthorhombic symmetry sites, the ZFS terms in (1) for the Cr³⁺ ion (S = 3/2) are evaluated as [24,25]:

$$H_{ZFS} = B_2^0 O_2^0 + B_2^2 O_2^2 = \frac{1}{3} b_2^0 O_2^0 + \frac{1}{3} b_2^2 O_2^2 = D(S_z^2 - \frac{1}{3} S(S+1)) + E(S_x^2 - S_y^2) \quad (2)$$

The traditional orthorhombic ZFS parameters D, E and B_k^q, b_k^q have relations :

$$b_2^0 = D = 3B_2^0, b_2^2 = 3E = B_2^2 \quad (3)$$

In ESO notation, the parameters of ZFS for any symmetry utilizing SPM [24,25] are obtained as:

$$b_k^q = \sum_i \bar{b}_k^q (R_0) \left(\frac{R_0}{R_i} \right)^{t_k} K_k^q(\theta_i, \varphi_i) \quad (4)$$

Where $(R_i, \theta_i, \varphi_i)$ present the spherical polar coordinates of the i -th ligand. The intrinsic parameters \bar{b}_k^q represent the magnitude of a ligand's k -th rank ZFS contribution at a distance R_i and the coordination factors K_k^q provide the geometrical data. K_k^q for $k = 1$ to 6 in ESO notation [26] are given in Appendix A1 of [27].

Eq. (4), in terms of the intrinsic parameters \bar{b}_k^q , the power-law exponents t_k and the reference distance R_0 , provide traditional ZFS parameters, D and E as given below [27,28-30]:

$$b_2^0 = D = \frac{\bar{b}_2^0 (R_0)}{2} \left[\left(\frac{R_0}{R_1} \right)^{t_2} \sum_i (3 \cos^2 \theta_i - 1) \right] \quad (5)$$

$$b_2^2 = 3E = \frac{\bar{b}_2^2 (R_0)}{3} \left[\left(\frac{R_0}{R_1} \right)^{t_2} \sum_i \sin^2 \theta_i \cos 2\varphi_i \right]$$

The Sn^{4+} ion site and the interstitial site with a comparable ligand environment are expected to be substituted by the Cr^{3+} ion in SnO_2 . The Cr^{3+} ion's local symmetry is orthorhombic. In LiNbO_3 having octahedral coordination of Cr^{3+} ion with $\text{Cr}^{3+}-\text{O}^{2-}$ bond, $t_2 = -0.12$ and $t_2 = 2.34 \text{ cm}^{-1}$ [31] were taken to compute b_2^0 and b_2^2 . Since oxygen serves as a ligand and the Cr^{3+} ion in SnO_2 has distorted octahedral coordination (Figure 1), the b_k^q in the current study is established using $\bar{b}_2(R_0) = 2.34 \text{ cm}^{-1}$ and $t_2 = -4.173$ for the center I.

The spherical polar coordinates of ligands and the Cr^{3+} ion's location as shown in Table 1 are considered for computation. The traditional ZFS parameters, D and E of Cr^{3+} ion in a single crystal of SnO_2 are calculated using Eq. (5). The reference distance $R_0 = 0.200 \text{ nm}$ is used [32] to find the ZFS parameters, and the values are: $|D| = 2395.2 \times 10^{-4} \text{ cm}^{-1}$ and $|E| = 4.2 \times 10^{-13} \times 10^{-4} \text{ cm}^{-1}$ for center I. For symmetry that is orthorhombic, the ratio b_2^2 / b_2^0 should fall between 0 and 1 [33]. In the current calculation, the ratio $|b_2^2| / |b_2^0| = 5.2 \times 10^{-16}$ and $|E| / |D| = 1.74 \times 10^{-16}$ for the center I. It is seen that the calculated values of $|D|$ and $|E|$ do not match with the experimental ones though $|b_2^2| / |b_2^0|$ falls in the specified range [33]. Therefore, with the above t_2 and reference distance R_0 , the ZFS parameters $|D|$ and $|E|$ are calculated for Cr^{3+} at the Sn^{4+} site with distortion having position $\text{Sn}^{4+} (-0.1662, -0.1185, -0.0022)$ for center I. The local environment about Cr^{3+} is shown in Figure 2. The traditional ZFS parameters obtained now are $|D| = 5778.1 \times 10^{-4} \text{ cm}^{-1}$, $|E| = 953.6 \times 10^{-4} \text{ cm}^{-1}$ for center I, which are matching fairly well with the values found from the experiment. The

ratio $|b_2^2| / |b_2^0| = 0.495$ and $|E| / |D| = 0.165$ for the center I are in the specified range [34]. Further, with the above t_2 and reference distance R_0 , the ZFS parameters $|D|$ and $|E|$ are calculated for Cr^{3+} at the interstitial site but the values discovered differ significantly from the experimental ones. For this reason, they are not included here.

Table 2 gives the experimental and calculated ZFS parameters of the Cr^{3+} ion in SnO_2 . It shows that the ZFS parameters $|D|$ and $|E|$ are in fair agreement with the values of the experiment [17] when the distortion is introduced into the calculation.

Computations of the crystal field's parameters

The transition ion CF energy states in crystals [34-37] can be obtained using Wybourne operators as follows [19,38,39]:

$$H_{\text{CF}} = \sum_{kq} B_{kq} C_q^{(k)} \quad (6)$$

Where H_{CF} is CF Hamiltonian. The metal-ligand complex's CF parameters in equation (6) are found using SPM [24,25] as follows:

$$B_{kq} = \sum_i A_k \left(\frac{R_0}{R_i} \right)^{t_k} K_{kq}(\theta_i, \varphi_i) \quad (7)$$

R_0 denotes the reference distance, R_i, θ_i, φ_i provide the i^{th}

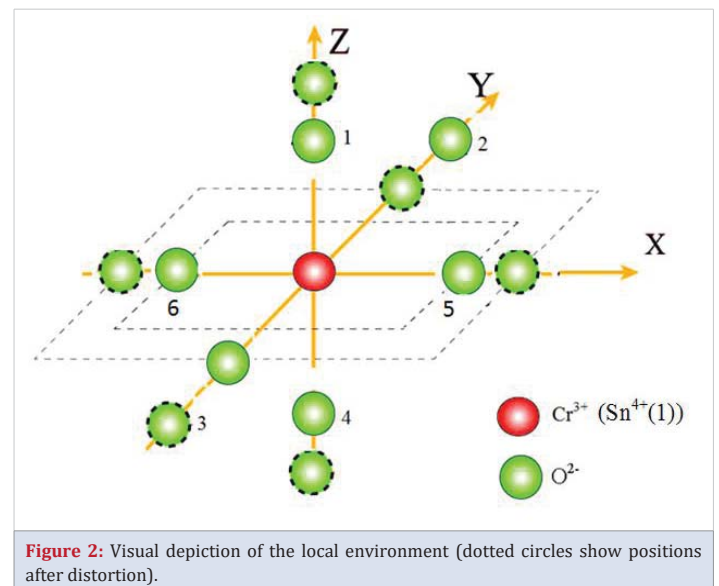


Figure 2: Visual depiction of the local environment (dotted circles show positions after distortion).

Table 2: The reference distance and calculated and Cr^{3+} 's experimental ZFS parameters in a single crystal of SnO_2 for the center I.

Site	R_0^A	Calculated ZFS parameters (cm^{-1}) parameters (10^{-4} cm^{-1})			Conventional ZFS		
		$ b_2^0 $	$ b_2^2 $	$ b_2^2 / b_2^0 $	$ D $	$ E $	$ E / D $
ND Center I	2.00	0.23953	1.2E-16	5.2E-16	2395.2	4.2E-13	1.74E-16
WD	2.00	0.57781	0.28607	0.495	5778.1	953.6	0.165
					5778.2 ^a	2785.5 ^a	0.482

WD = With Distortion; ND = No Distortion, E = Experimental.

ligand spherical polar coordinates and K_{kq} are the coordination factors [34]. $\bar{A}_2 = 40,400 \text{ cm}^{-1}$, $t_2 = 1.3$, $\bar{A}_4 = 11,700 \text{ cm}^{-1}$ and $t_4 = 3.4$ are used to find B_{kq} ($k = 2, 4$; $q = 0, 2, 4$) [34]. Table 3 contains a list of the calculated B_{kq} parameters. The ratio $|B_{22}|/|B_{20}| = 0.091$ for the center I, which suggests that B_{kq} parameters established are standardized [33]. In order to analyze the optical spectroscopy data using the crystal-field approach, an efficient computer program for diagonalization of a complete Hamiltonian (including electrostatic terms, Trees correction, spin-orbit interaction, and crystal-field) within the $3d^N$ configuration ($N = 2$ to 8) is essential. Yeung and Rudowicz [35,36] recently developed a computer program CFA for $3d^N$ configuration ($N = 2$ to 8) and for symmetry as low as orthorhombic. The CF analysis computer program is suitable for orthorhombic symmetry, tetragonal symmetry, cubic symmetry, trigonal symmetry, and hexagonal symmetry. Monoclinic and triclinic as well as trigonal and tetragonal symmetry cases involving "imaginary" CF terms are also included. Note that in the latter cases, the complex CF parameter can be made real by an appropriate rotation around the z-axis. Other low-spin states, e.g. $S = 1, 0$, for $3d^4$ and $3d^6$ ions and $S = 3/2, 1/2$ for $3d^5$ ions, arising at strong ligand fields, as well as the low spin to high spin transition can also be studied using the package. The Hamiltonian for a $3d^N$ ion in crystals can be written as the sum of the free-ion Hamiltonian, the spin-orbit interaction, and the Trees correction describing the two body orbit-orbit polarization. The crystal (ligand) field Hamiltonian in the equation in Wybourne's notation is taken in terms of the crystal field parameters B_{kq} and the renormalized spherical tensor operators. Since the ligand field is in the weak to intermediate range for most of the 3d transition metal ions in crystals, the basis of states in the LS coupling scheme can be taken. The Slater integrals F^k ($k = 0, 2$, and 4) are related to the Racah parameters A , B , and C as follows:

$$A = F_0 - 49F_4$$

$$B = F_2 - 5F_4$$

$$C = 35F_4$$

And $F_0 = F^0$, $F_2 = F^2/49$, $F_4 = F^4/441$. Usually, we set $A = 0$ since it will cause no energy

Level splittings apart from shifting the center of the whole spectrum. Racah parameters A , B , C , Tree's correction and spin-orbit coupling, and the CF parameters B_{kq} are taken as input parameters.

The total Hamiltonian is diagonalized to calculate the CF energy levels of the Cr^{3+} ion in SnO_2 single crystals using the B_{kq} parameters in Table 3 and the CFA computer program [35,36]. Table 4 shows the energy values that were calculated. The calculated and experimental energy values for Cr^{3+} : Cassiterite

Table 3: B_{kq} parameters of Cr^{3+} for center I with distortion in a single crystal of SnO_2 .

Calculated B_{kq} (cm^{-1}) Parameters used for the CFA program							
Site	$R0^A$	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}	$ B_{22} / B_{20} $
Center I WD	2	-86000.9	-7869.12	46442.65	10243.45	-94402.8	0.091

WD = With Distortion.

Table 4: Energy values of Cr^{3+} in SnO_2 single crystal determined by computation and experimentation (center I).

Transition from	Observed	Calculated band using CFA (cm^{-1})
${}^4A_{2g}(F)$	band (cm^{-1})	Center I
${}^2E_g(G)$	14518	12396, 12533
${}^2T_{1g}(G)$		12669, 13605, 14076
${}^4T_{2g}(F)$	18389	14735, 14800, 15282, 15414, 15897, 20316
${}^4T_{1g}(F)$	23228	24334, 26120, 27018, 27597, 27897, 28835
${}^4T_{1g}(P)$		29673, 30762, 30961, 31575, 42777, 46856
${}^2T_{1g}(aD)$		49768, 52745, 79331
${}^2E_g(bD)$		79342, 83419

(The spin-orbit coupling constant, the Racah parameters A , B , and C , and the Trees correction have respective values of 276, 0, 442, 3676, and 70 cm^{-1}).

(SnO_2) [40] are contrasted. The experimental and theoretical energy values seem to be reasonably in agreement based on Table 4. Therefore, the experimental findings are supported by examining Cr^{3+} ions at Sn^{4+} sites in SnO_2 theoretically [17,40].

SPM studies of $3d^N$ ions in ferroelectrics, for example, Fe^{3+} ions in PbZrO_3 , $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ and PbTiO_3 and Cr^{3+} ions in PbTiO_3 and $\text{Ba}_x\text{Pb}_{1-x}\text{TiO}_3$ powders, Mn^{2+} ions in BaTiO_3 nanopowders, and other related ion-host systems as well as Fe^{3+} and Mn^{2+} in ZnO also back the experimental EPR findings [8]. The major usage of this investigation may be done in studies of Single Molecule Magnets (SMM), Single-Chain Magnets (SCM), and Single Ion Magnets (SIM) based on transition ions for computational modeling of their properties. The SMM, SCM, and SIM are formed by polynuclear clusters assembled from mononuclear coordination complexes. These systems have become a subject of large interest due to their unique magnetic properties like the phenomenon of macroscopic quantum tunneling of magnetization, as well as possible applications in high-density information storage and quantum computing [8]. Recently many novel SMM or SCM systems containing Cr^{3+} and/or Mn^{2+} ions as well as nanomagnets with elaborate coordination geometry containing Gd^{3+} ions have been synthesized [8].

The spectra of optical absorption of Cr^{3+} -activated phosphors are now explained using Franck-Condon analysis using the model known as configurational-coordinate (CC) [41]. The various excited state-ground state transitions in Cr^{3+} are a result of the lattice vibrations' strong coupling (CC model) [41]. The CC model is not being utilized so there is a difference between excited-state peak energies obtained here and energies of the zero-phonon line (ZPL) discussed in [41,42]. There are two types of oxide-phosphors that are doped with Cr^{3+} : the O-Cr-A type and the O-Cr-B type. The characteristics

of type O-Cr-A phosphors' luminescence are obtained from the 2E_g -related luminescence transitions as their crystal-field strength lies in the region of $Dq/B > 2.1$ while type O-Cr-B phosphors have a crystal-field strength falling within the range of $Dq/B < 2.1$, as a result, the transitions associated with ${}^4T_{2g}$ are used to find their luminescence properties. $\text{SnO}_2: \text{Cr}^{3+}$ is classified as an O-Cr-A type phosphor ($Dq/B = 4.15, > 2.1$) [42].

Summary and conclusion

The Crystal Field (CF) and Zero-Field Splitting (ZFS) parameters for Cr^{3+} ions in SnO_2 single crystals are determined using the Superposition Model (SPM). Calculations are performed using the interstitial site, distortion models, and Cr^{3+} ions in SnO_2 crystal at Sn^{4+} ion sites. When distortion is included in the calculation, the calculated conventional ZFS values for the Cr^{3+} ion at Sn^{4+} sites in SnO_2 single crystal give a reasonable accord with the experimental values. It is found that the Cr^{3+} ions in the SnO_2 lattice replace the Sn^{4+} ions at those locations. The CF energy values for Cr^{3+} ions at Sn^{4+} sites calculated with CF parameters and the CFA program show an adequate degree of conformity with the experimental ones. Therefore, the theoretical inferences support the experimental result.

The modeling approach adopted in this work could prove useful in the future to find crystals for different industrial and scientific applications by correlating EPR and optical data for several other ion-host systems. The major usage of this investigation may be done in studies of Single Molecule Magnets (SMM), Single-Chain Magnets (SCM), and Single Ion Magnets (SIM) based on transition ions for computational modeling of their properties.

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