Modeling of Cr\textsuperscript{3+} doped Single Crystals of Lithium Sulfate Monohydrate

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Abstract: Crystal field parameters and zero field splitting parameters of Cr\textsuperscript{3+} doped lithium sulphate monohydrate, Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O single crystals are computed with the help of superposition model. The appropriate sites for Cr\textsuperscript{3+} ions in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O with distortion are considered for calculation. Theoretical zero field splitting parameters obtained including local distortion in the calculation correspond well with the values obtained from the experiment. The optical energy bands for Cr\textsuperscript{3+} in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O are evaluated with the Crystal Field Analysis Program and crystal field parameters. The results suggest that Cr\textsuperscript{3+} ions substitute for one of the Li\textsuperscript{+} ions, and the charge compensation occurs by the proton vacancies in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O single crystals.

Keywords: superposition model; crystal field; zero-field splitting; optical spectroscopy; Cr\textsuperscript{3+} ions in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O

1. Introduction

The electron paramagnetic resonance (EPR) provides the nature of the electric field symmetry produced by the ligands about the paramagnetic ions, permits the determination of the flaw causing the charge compensation in impurity doped crystals [1] and the zero field splitting (ZFS) of impurity ions added to crystals [2-4]. Superposition model (SPM) [5-7] is used most commonly for theoretically determining zero field splitting (ZFS) and crystal field (CF) parameters.

Lithium sulphate monohydrate single crystals have a wide spectrum of applications in non-linear optical (NLO) assistant devices used in telecommunications, laser technology, THz imaging, optical communication, and optical storage technologies [8]. The optical, electrical, and thermal properties of this crystal mark it as a potential candidate for modern optoelectronic applications [9]. It is found that the intoxication of a dopant in lithium sulphate monohydrate increases the efficacy of the grown single crystals [8].

Cr\textsuperscript{3+} ions have extensively been used as probe to study the symmetries of the crystalline electric fields. An important interest is the compensation of the charge imbalance when divalent or trivalent impurities are incorporated in place of monovalent ions. In these cases positive ion vacancies are supposed to fulfil the charge compensation [10]. Incorporated impurities yielding microscopic structural change affect the optical properties of the crystal. The Cr\textsuperscript{3+} ion is a very good probe for obtaining information on lithium sulphate monohydrate, Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O crystal [11].

EPR measurements for Cr\textsuperscript{3+} ions in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O were done and spin Hamiltonian parameters reported [11]. The consistency of the EPR spectra with the monoclinic symmetry of the crystal indicates the substitution of Cr\textsuperscript{3+} at Li\textsuperscript{+} site. The ionic radius of Li\textsuperscript{+} ion (0.078 nm) is larger than that of the Cr\textsuperscript{3+} ion (0.0615 nm). Therefore
Cr$^{3+}$ substitutes for one of the Li$^+$ ions, and the charge compensation takes place in this case by the proton vacancies, since no superhyperfine of the protons with the electron spin of Cr$^{3+}$ was observed [11].

The laboratory axes ($x, y, z$) are selected so that they align with the crystallographic axes ($a^*, b, c$). The symmetry adopted axes (magnetic axes) are labeled ($X, Y, Z$). The principal $Y$ axis of $g$ and $D$ tensors of Cr$^{3+}$ ions is found corresponding to the crystallographic $c$ axis.

This study examines the superposition model (SPM) of the CF parameters and the ZFS parameters for Cr$^{3+}$ ions in Li$_2$SO$_4$.H$_2$O crystal. Due to continued interest in the compound by other workers [12, 13], this study is undertaken. The objective is to find the ZFS parameters, the lattice distortion and the CF parameters for the Cr$^{3+}$ ions in Li$_2$SO$_4$.H$_2$O at octahedral sites. The optical energy bands for Cr$^{3+}$ ions in Li$_2$SO$_4$.H$_2$O are determined using CF parameters and Crystal Field Analysis (CFA) computer program. Both the ZFS and CF parameters obtained may be useful in future investigations for scientific and industrial applications of such crystals.

2. Crystal structure

Li$_2$SO$_4$.H$_2$O crystallizes in a monoclinic crystal system with space group P2$_1$ [14]. The unit cell dimensions are $a = 0.5454$ nm, $b = 0.4857$ nm, $c = 0.8173$ nm, and $\beta = 107.22^\circ$. The compound contains the two Li atoms Li$_1$ and Li$_2$, Li$_1$ being coordinated only to the oxygen atoms of the SO$_4$ groups, while one of the O atoms around Li$_2$ is the oxygen of the water molecule. Li$_2$SO$_4$.H$_2$O crystal structure with symmetry adopted axis system (SAAS) is shown in Fig.1.
The symmetry adopted axes (SAA) (local site symmetry axes) are the mutually perpendicular directions of metal-ligand bonds. The Z axis of SAA is along the metal-ligand bond Li-O (crystal a*-axis) and the two other axes (X, Y) are perpendicular to the Z axis for center I (Fig. 1). This indicates that Cr\(^{3+}\) substitutes for Li\(^+\) in the crystal of Li\(_2\)SO\(_4\)\(_2\)H\(_2\)O with approximately orthorhombic symmetry and charge compensation. Cr\(^{3+}\) ion’s ionic radius (0.0615 nm) is marginally smaller than Li\(^+\) ionic radius (0.076 nm), indicating that Cr\(^{3+}\) ion can sit at the position of Li\(^+\) with charge compensation and certain distortion.

Table 1 displays the ligands’ spherical polar coordinates and Cr\(^{3+}\) ion position for center I in Li\(_2\)SO\(_4\)\(_2\)H\(_2\)O [14]. Cr\(^{3+}\) ion ZFS and CF calculations in Li\(_2\)SO\(_4\)\(_2\)H\(_2\)O use these data.

### 3. Calculations of zero field splitting parameters

The energy states of Cr\(^{3+}\) ions in crystals were obtained utilizing the spin Hamiltonian [15, 16, 17]:

\[
\mathcal{H} = \mathcal{H}_{zh} + \mathcal{H}_{ZFS} = \mu_B g_B S + \sum B_k^q O_k^q = \mu_B g_B S + \sum f_k b_k^q O_k^q,
\]

where \(g, \mu_B\) and \(B\) are the spectroscopic splitting factor, Bohr magneton and steady magnetic field, respectively. \(S\) represents the effective spin operator and \(O_k^q\) are the extended Stevens operators (ESO) [18, 19]; \(B_k^q\) and \(b_k^q\) give the ZFS parameters, \(f_k = 1/3\) and 1/60 the scaling factors for \(k = 2\) and 4, respectively. For the Cr\(^{3+}\) ion \((S = 3/2)\) at orthorhombic symmetry sites, the ZFS terms in (1) are given as [20, 21]:

### Table 1. The spherical polar co-ordinates (R, θ, φ) of ligands and fractional coordinates of Cr\(^{3+}\) ion (center I) in Li\(_2\)SO\(_4\)\(_2\)H\(_2\)O single crystal

<table>
<thead>
<tr>
<th>Position of Cr(^{3+})</th>
<th>Ligands</th>
<th>Spherical polar co-ordinates of ligands</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(R^b)</td>
</tr>
<tr>
<td>ND: Substitutional</td>
<td>O1</td>
<td>6.7696</td>
</tr>
<tr>
<td></td>
<td>O2</td>
<td>11.5987</td>
</tr>
<tr>
<td></td>
<td>O3</td>
<td>7.8598</td>
</tr>
<tr>
<td></td>
<td>O4</td>
<td>6.5226</td>
</tr>
<tr>
<td></td>
<td>O1'</td>
<td>3.8625</td>
</tr>
<tr>
<td></td>
<td>O2'</td>
<td>4.8637</td>
</tr>
<tr>
<td>WD: substitutional Centre I</td>
<td>O1</td>
<td>7.6250</td>
</tr>
<tr>
<td></td>
<td>O2</td>
<td>11.2440</td>
</tr>
<tr>
<td></td>
<td>O3</td>
<td>6.2035</td>
</tr>
<tr>
<td></td>
<td>O4</td>
<td>7.5444</td>
</tr>
<tr>
<td></td>
<td>O1'</td>
<td>6.0650</td>
</tr>
<tr>
<td></td>
<td>O2'</td>
<td>7.8415</td>
</tr>
</tbody>
</table>

WD = No distortion, ND = With distortion

\[
\mathcal{H}_{ZFS} = B_2^0 O_2^0 + B_2^2 O_2^2 = \frac{1}{3} b_2^0 O_2^0 + \frac{1}{3} b_2^2 O_2^2 = D(S^2 - \frac{1}{3} S(S + 1)) + E(S^2 - S_z^2).
\]

The traditional orthorhombic ZFS parameters \(D, E\) and \(B_k^q\), \(b_k^q\) are related as:

\[
b_2^0 = D = 3 B_2^0, \quad b_2^2 = E = 3 B_2^2.
\]

The parameters of ZFS (in ESO notation) for any symmetry using SPM [20-21] are found as:

\[
b_k^q = \sum_i \bar{b}_k (R_i) \left( \frac{R_i}{R_k} \right)^{i/3} K_k^q (\theta_i, \phi_i),
\]

where \((R, \theta, \phi)\) are the spherical polar coordinates of \(i\)-th ligand. The intrinsic parameters \(\bar{b}_k\) provide the strength of the \(k\)-th rank ZFS contribution from a ligand at the distance \(R\), and the coordination factors \(K_k^q\) give the geometrical information. \(K_k^q\) for \(k = 1\) to \(6\) in ESO notation [22] are given in Appendix A1 of [23].

Eq. (4) yields traditional ZFS parameters, \(D\) and \(E\), in terms of the intrinsic parameters \(\bar{b}_k\), the power-law exponents \(i_k\) and the reference distance \(R_0\), as [23, 24-26]:

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**Figure 1.** Li\(_2\)SO\(_4\)\(_2\)H\(_2\)O crystal structure with symmetry adopted axis system (SAAS)
\[ b_2^0 = D = \frac{b_z(R_o)}{2} \sum_i \left[ \frac{R_o}{R_i} \right]^2 \sum_i (3 \cos^2 \theta_i - 1) \]
\[ b_2^2 = 3E = \frac{b_z(R_o)}{3} \sum_i \left[ \frac{R_o}{R_i} \right]^2 \sum_i \sin^2 \theta_i \cos 2\varphi_i \]

(5)

Cr\(^{3+}\) ion in Li\(_2\)SO\(_4\).H\(_2\)O may be assumed to substitute at the Li\(^+\) ion site, and the interstitial site with similar ligand arrangement. The Cr\(^{3+}\) ion's local symmetry is supposed to be approximately orthorhombic. In LiNbO\(_3\) with octahedral coordination of Cr\(^{3+}\) ion having Cr\(^{3+}\)-O\(^2-\) bond, \( b_z(R_o) = 2.34 \text{ cm}^{-1} \) and \( t_2 = -0.12 \) [27] were used to obtain \( b_2^0 \) and \( b_2^2 \). Since Cr\(^{3+}\) ion in Li\(_2\)SO\(_4\).H\(_2\)O has distorted octahedral coordination (Fig.1) with oxygen as ligands, the \( b_k^0 \) in the current research are established using \( b_z(R_o) = 2.34 \text{ cm}^{-1} \) and \( t_2 = -0.77 \) for center I.

The ligands' spherical polar coordinates and the position of the Cr\(^{3+}\) ion displayed in Table 1 are considered for calculation. The traditional ZFS parameters, D and E of Cr\(^{3+}\) ion in Li\(_2\)SO\(_4\).H\(_2\)O single crystal are decided using Eq. (5). To determine the ZFS parameters, the reference distance \( R_0 = 0.200 \text{ nm} \) was used [28], and the values are: \(|D| = 1605.3 \times 10^{-4} \text{ cm}^{-1}\) and \(|E| = 33.4 \times 10^{-4} \text{ cm}^{-1}\) for center I. For symmetry that is orthorhombic, the ratio \( |b_2^2| / |b_2^0| \) should fall between 0 and 1 [29]. In the current calculation, the ratio \(|b_2^2| / |b_2^0| = 0.062\) and \(|E| / |D| = 0.020\) for center I. It is seen that the calculated values of \(|D|\) and \(|E|\) do not agree with the experimental ones though \(|b_2^2| / |b_2^0|\) is in the specified range [29]. Therefore, with above \( t_2 \) and reference distance \( R_0 \), the ZFS parameters \(|D|\) and \(|E|\) are calculated for Cr\(^{3+}\) at the Li\(^+\) site with distortion having position Li\(^+\)(0.8240, 0.7450, 0.9988) for center I. The local environment about Cr\(^{3+}\) is shown in Fig. 2. The traditional ZFS parameters obtained now are \(|D| = 1420.3 \times 10^{-4} \text{ cm}^{-1}\), \(|E| = 177.6 \times 10^{-4} \text{ cm}^{-1}\) for center I, which correspond well with the values obtained from the experiment. The ratio \(|b_2^2| / |b_2^0| = 0.375\) and \(|E| / |D| = 0.125\) for center I are in the given range [30]. Further, with above \( t_2 \) and reference distance \( R_0 \), the ZFS parameters \(|D|\) and \(|E|\) are determined for Cr\(^{3+}\) at the interstitial site but the values acquired are quite distinct from the values found in the experiment. Therefore, these are not shown here.

Figure 2. Graphical presentation of local environment (dotted circles show positions after distortion)
Table 2 lists the experimental and calculated ZFS parameters for the Cr$^{3+}$ ion in Li$_2$SO$_4$.H$_2$O. This table shows that the ZFS parameters [D] and [E] are in good match with the values of the experiment [11] when the distortion is included into calculation.

| Site     | $R_0$ | $|b_{20}^{0}|$ | $|b_{22}^{0}|$ | $|b_{20}^{2}|$ | $|b_{22}^{2}|$ | $|D|$   | $|E|$   | $|E/D|$ |
|----------|-------|----------------|----------------|----------------|----------------|--------|--------|--------|
|          |       |                |                |                |                |        |        |        |
| Center I |       |                |                |                |                |        |        |        |
| ND       | 2.00  | 0.16053        | 0.01005        | 0.062          | 1605.3         | 33.4   | 0.020  |        |
| WD       | 2.00  | 0.14203        | 0.05330        | 0.375          | 1420.3         | 177.6  | 0.125  |        |
|          |       |                |                |                |                | 1420.3 |        | 0.124  |

ND = No distortion, WD = With distortion, $^*$ = experimental

### 4. Calculations of crystal field parameters

In crystals [30–33], the CF energy states of transition ions by using Wybourne operators are given by [15, 34, 35]:

$$\mathcal{H}_{\text{CF}} = \sum_{kq} B_{kq} C_q^{(k)}$$  \hspace{1cm} (6)

where $\mathcal{H}_{\text{CF}}$ is CF Hamiltonian. The CF parameters in (6) for a metal-ligand complex are evaluated using SPM [20-21] as follows:

$$B_{kq} = \sum_i \tilde{A}_i \left( \frac{R_0}{R_i} \right)^{\frac{t_i}{4}} K_{kq} (\theta_i, \phi_i).$$  \hspace{1cm} (7)

$R_0$ is the reference distance, $R_i$, $\theta_i$, $\phi_i$ are the $i^{th}$ ligand spherical polar coordinates and $K_{kq}$ are the coordination factors [30]. $\tilde{A}_2 = 40$, 400 cm$^{-1}$, $\tilde{t}_2 = 1.3$, $\tilde{A}_4 = 11$, 700 cm$^{-1}$ and $t_4 = 3.4$ are used to find $B_{kq}$ ($k = 2, 4; q = 0, 2, 4$) [30]. Table 3 displays the $B_{kq}$ parameters that were computed. The ratio $|B_{22}|/|B_{20}| = 0.184$ for center I indicating that $B_{4q}$ parameters are standardized [29]. Using $B_{kq}$ parameters in Table 3 and CFA computer program [31, 32], the CF energy levels of Cr$^{3+}$ in Li$_2$SO$_4$.H$_2$O single crystals are calculated by diagonalizing the entire Hamiltonian. Table 4 gives the energy values that were computed. The comparison of calculated energy values is done with the experimental energy values for Cr$^{3+}$: NiMTH [36] having similar ligands as in Li$_2$SO$_4$.H$_2$O single crystal is reported in literature. From Table 4, the experimental and theoretical band positions are seen to be reasonably consistent. Therefore the theoretical study of Cr$^{3+}$ ions at Li$^+$ sites in Li$_2$SO$_4$.H$_2$O supports the experimental one [11, 36].

### Table 3. $B_{kq}$ parameters of Cr$^{3+}$ in Li$_2$SO$_4$.H$_2$O single crystal for center I with distortion

| Site     | $R_0$ | $B_{20}$ | $B_{22}$ | $B_{40}$ | $B_{42}$ | $B_{44}$ | $|D|/|E|$ |
|----------|-------|----------|----------|----------|----------|----------|--------|
|          |       |          |          |          |          |          |        |
| Center I |       |          |          |          |          |          |        |
| WD       | 2.00  | 22741.12 | 4192.224 | 2626.792 | –428.516 | –428.989 | 0.184  |

WD = With distortion

The spectra of optical absorption of Cr$^{3+}$-activated phosphors have been explained using Franck-Condon analysis with the configurational-coordinate (CC) model [37]. The different excited-state transitions in Cr$^{3+}$ are due to strong coupling with the lattice vibrations (CC model) [37]. The CC model is not being used and hence there is difference between excited-state peak energies obtained here and zero-phonon line (ZPL) energies discussed in [37,38].The oxide- phosphors doped with Cr$^{3+}$ are classified into two groups: (i) type O–Cr–A, (ii) type O–Cr–B. The crystal-field strength of type O–Cr–A phosphors fall in the region of Dq/B > 2.1 and, hence, their luminescence properties is determined by the $^2E_g$-related luminescence transitions while the crystal-field strength of type O–Cr–B phosphors fall in the region of Dq/B < 2.1 and, so, their luminescence properties is determined by the $^4T_{2g}$-related optical transitions.

Li$_2$SO$_4$.H$_2$O: Cr$^{3+}$ comes under O–Cr–A type phosphors (Dq/B =2.649 which is >2.1) [38].
5. Summary and conclusions

The zero-field splitting (ZFS) and crystal field (CF) parameters for Cr\textsuperscript{3+} ions in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O single crystals are computed employing the superposition model (SPM). Cr\textsuperscript{3+} ions in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O crystal at Li\textsuperscript{+} ion sites, interstitial site and distortion models are taken up for calculation. The calculated traditional ZFS parameters for Cr\textsuperscript{3+} ion at Li\textsuperscript{+} sites in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O single crystal give excellent conform to the experimental values when distortion is introduced in the calculation. It is discovered that the Cr\textsuperscript{3+} ions substitute at Li\textsuperscript{+} ion sites in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O lattice with charge compensation.

The CF energy values for Cr\textsuperscript{3+} ions at Li\textsuperscript{+} sites calculated using CFA package and CF parameters are reasonably in agreement with the experimental ones. Thus, the theoretical findings corroborate the experimental investigation.

Table 4. Energy bands determined through experimentation and computation (center I) of Cr\textsuperscript{3+} in Li\textsubscript{2}SO\textsubscript{4}.H\textsubscript{2}O single crystal

<table>
<thead>
<tr>
<th>Transition from ( ^4A_{2g}(F) )</th>
<th>Experimentally observed band (cm\textsuperscript{-1})</th>
<th>Calculated energy band from CFA (cm\textsuperscript{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^2E_g(G) )</td>
<td>13967, 14135</td>
<td></td>
</tr>
<tr>
<td>( ^2T_{1g}(G) )</td>
<td>15143, 15192, 15630</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{2g}(F) )</td>
<td>17725</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{2g}(F) )</td>
<td>24505</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{1g}(G) )</td>
<td>16053, 16334, 16943</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{1g}(G) )</td>
<td>17176, 17218, 17944</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{2g}(F) )</td>
<td>22654, 22965, 23427</td>
<td></td>
</tr>
<tr>
<td>( ^4T_{2g}(F) )</td>
<td>24339, 24919, 26075</td>
<td></td>
</tr>
<tr>
<td>( ^2T_{1g}(P) )</td>
<td>31161, 31466, 34333</td>
<td></td>
</tr>
<tr>
<td>( ^2T_{1g}(aD) )</td>
<td>34843, 35405, 37345</td>
<td></td>
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<tr>
<td>( ^2T_{1g}(bD) )</td>
<td>39481, 44015, 45117</td>
<td></td>
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<tr>
<td>( ^2E_g(bD) )</td>
<td>52393, 54981</td>
<td></td>
</tr>
</tbody>
</table>

(Racah parameters A, B and C, spin-orbit coupling constant and Trees correction are 0, 668, 2672 (= 4B), 276 and 70 cm\textsuperscript{-1}, respectively)

The modeling approach taken up in this work could prove helpful in the future in correlating EPR and optical data for different ion-host systems to investigate crystals for a variety of industrial and scientific applications.

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