# Investigation of the Spin-Hamiltonian Parameters and the Local Structure of $Ni^{2+}$ Ions in $CsMgX_3$ (X = Cl, Br, I) Crystals

Qun Wei

Department of Physics, Baoji University of Arts and Science, Baoji 721007, P. R. China

Reprint requests to Q. W.; E-mail: weiaqun@163.com

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Taking into account spin-spin (SS), spin-other-orbit (SOO), and orbit-orbit (OO) interactions in addition to general spin-orbit (SO) interactions, the local structures of $Ni^{2+}$ in $CsMgX_3$ (X = Cl, Br, I) are theoretically investigated by using the complete diagonalization method (CDM). On this basis, it is found that the local angles, at the $Ni^{2+}$ centres are larger than those, at the hosts. The contributions to the spin-Hamiltonian parameters from spin triplets and slight magnetic interactions are discussed.

*Key words:* Spin-Hamiltonian Parameters; Local Structure; $Ni^{2+}$; $CsMgX_3$ (X = Cl, Br, I).

## 1. Introduction

Electron paramagnetic resonance (EPR) spectra and optical spectra of $CsMgX_3$ (X = Cl, Br, I) crystals doped with transition metal (TM) ions have been extensively investigated experimentally and theoretically [1 – 13]. As known, the microscopic spin-Hamiltonian (MSH) theory has been extensively used in the area of the EPR of transition ions [14 – 17]. The MSH theory enables to correlate optical spectroscopy and structural data with the spin-Hamiltonian (SH) parameters extracted from the EPR spectra. Hence, the MSH studies of transition metal ions in crystals can provide a great deal of microscopic insight concerning the crystal structure, structural disorder, phase transitions and pressure behaviour as well as the observed magnetic and spectroscopic properties [17]. To study these properties, using the perturbation method (PTM), Pereosyan and Mirzakhanyan [18], Shang et al. [19], and Huang [20] obtained a high-order perturbation formula for the SH parameters of $d^8$ ions at trigonal symmetry, including spin-orbit (SO) interaction only. The accuracy of the approximate PTM developed by Pereosyan and Mirzakhanyan has been checked in [17] by using the complete diagonalization method (CDM). This investigation indicated that the PTM formulas for the *g*-factors indeed work well, whereas the PTM formula for zero-field splitting (ZFS) of the ground $^3A_2$ state exhibits serious shortcomings. Recently, a more complete diagonalization method has been developed by Hao and Yang [21]. In this CDM, some slight magnetic interactions, omitted in previous work, including spin-spin (SS), spin-other-orbit (SOO), and orbit-orbit (OO) interactions were considered. In the present paper, by taking into account SS, SOO, and OO interactions, the local structure and SH parameters of $Ni^{2+}$ ions in $CsMgX_3$ (X = Cl, Br, I) are investigated, and the contributions to the spin-Hamiltonian from spin triplets and slight magnetic interactions are discussed, respectively.

## 2. Theory

In the crystal-field (CF) framework, the total Hamiltonian can be written as [21, 22]

$$H = H_{\mathrm{ee}}(B,C) + H_{\mathrm{CF}}(B_{kq}) + H_{\mathrm{M}}(\xi, M_0, M_2), \quad (1)$$

where $H_{\mathrm{ee}}$ represents the Coulomb interactions, $H_{\mathrm{CF}}$ represents CF interactions, and $H_{\mathrm{M}}$ represents magnetic interactions. In addition to the magnetic spin-orbit interaction parameterized by $\xi$, slight magnetic interactions including SS, SOO, and OO interactions parameterized by the Marvin integrals [23, 24], $M_0$ and $M_2$, are included [25 – 28]:

$$\begin{aligned} H_{\mathrm{M}} = {} & H_{\mathrm{SO}}(\xi) + H_{\mathrm{SS}}(M_0, M_2) \\ & + H_{\mathrm{SOO}}(M_0, M_2) + H_{\mathrm{OO}}(M_0, M_2). \end{aligned} \quad (2)$$

The CF Hamiltonian for trigonal symmetry in the Wybourne notation [14, 28, 29] is given as [21, 22, 30]

$$H_{\mathrm{CF}} = B_{20}C_0^{(2)} + B_{40}C_0^{(4)} + B_{43}C_3^{(4)} + B_{4-3}C_{-3}^{(4)}, \quad (3)$$

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where $B_{kq}$ are the CF parameters and $B_{43} = -B_{4-3}$ for trigonal symmetry ($C_{3v}$, $D_3$, $D_{3d}$), and they are real. The methods of calculation of the matrix elements for $H_{\mathrm{ee}}$, $H_{\mathrm{SO}}$, and $H_{\mathrm{CF}}$ have been described in [31,32], whereas those of $H_{\mathrm{SS}}$, $H_{\mathrm{SOO}}$, and $H_{\mathrm{OO}}$ in [21,25,33].

For Ni$^{2+}$ ions with trigonal symmetry, the effective spin-Hamiltonian [14,29], taking into account the ZFS and Zeeman terms [14,15,29], can be written as [17]

$$\begin{aligned} H_{\mathrm{S}} = D\left[S_z^2 - \frac{1}{3}S(S+1)\right] \\ + \mu_{\mathrm{B}} g_{\parallel} B_z S_z + \mu_{\mathrm{B}} g_{\perp}(B_x S_x + B_y S_y) \end{aligned} \tag{4}$$

with the $z$-axis along the [111] direction. The ZFS parameter $D$ is the splitting of a spin doublet and spin singlet for trigonal symmetry, and is given by

$$\begin{aligned} D = \varepsilon(|\mathrm{E}(^3\mathrm{F}\downarrow {}^3\mathrm{A}_{2g}\downarrow {}^3\mathrm{A}_2)\rangle) \\ - \varepsilon(|\mathrm{A}(^3\mathrm{F}\downarrow {}^3\mathrm{A}_{2g}\downarrow {}^3\mathrm{A}_2)\rangle). \end{aligned} \tag{5}$$

The expressions for the Zeeman $g$-factors are given as [34]

$$g_{\parallel} = \langle \psi_{+1} | kL_z + g_{\mathrm{s}} S_z | \psi_{+1} \rangle, \tag{6}$$

$$g_{\perp} = \sqrt{2}\langle \psi_{+1} | kL_x + g_{\mathrm{s}} S_x | \psi_0 \rangle, \tag{7}$$

where $k$ is the orbital reduction factor and $g_{\mathrm{s}}$ is the free-spin $g$-value of 2.0023. $|\psi_0\rangle$ and $|\psi_{\pm1}\rangle$ are the eigenfunctions of the ground $^3\mathrm{A}_2$ state obtained by complete diagonalization of the three $15 \times 15$ matrices in the form of linear combinations of the basis $LS$ states as [25,35,36]

$$\psi_{\pm1} = \sum_{j=1}^{15} a_{\pm1,j} |\varphi_j\rangle, \tag{8}$$

$$\psi_0 = \sum_{j=1}^{15} a_{0,j} |\varphi_j\rangle. \tag{9}$$

Equations (5) – (7) have been built in our CDM/MSH program. For taking into account SS, SOO, and OO interactions, the present program can provide a more accurate determination of the SH parameters.

## 3. Local Structure and SH Parameters of Ni$^{2+}$ Ions in CsMgX$_3$

In CsMgX$_3$ crystals, the Mg$^{2+}$ ion is in the local symmetry $D_{3d}$ with the threefold symmetry axis coincident with the crystallographic $c$-axis [1,2]. When Ni$^{2+}$ ions are doped into CsMgX$_3$ crystals, Ni$^{2+}$ will replace Mg$^{2+}$ ions, and occupy the $D_{3d}$ site. The Mg-X bonding lengths are $R_0 = 0.2496$ nm, 0.2662 nm, and 0.2899 nm, and the bonding angles are $\theta_0 = 51.73°$, 52.44°, and 52.89° for X = Cl, Br, and I, respectively. Because of the difference between the ionic radii of impurities Ni$^{2+}$ and hosts Mg$^{2+}$, the local structure will change.

To study the local structure of Ni$^{2+}$ in CsMgX$_3$ (X = Cl, Br, I), the relation between the lattice structure and CF parameters, using the superposition model [37,38], can be established as

$$B_{20} = 6\bar{A}_2[3\cos^2(\theta_0 + \Delta\theta) - 1], \tag{10}$$

$$\begin{aligned} B_{40} = 6\bar{A}_4\big[35\cos^4(\theta_0 + \Delta\theta) \\ - 30\cos^2(\theta_0 + \Delta\theta) + 3\big], \end{aligned} \tag{11}$$

$$B_{43} = -12\sqrt{35}\bar{A}_4 \sin^3(\theta_0 + \Delta\theta)\cos(\theta_0 + \Delta\theta), \tag{12}$$

where $\bar{A}_2$ and $\bar{A}_4$ are intrinsic parameters [22,38,39], following the relationships $\bar{A}_4 = \frac{3}{4}Dq$ [37,40] and $\bar{A}_2 = 10.8\bar{A}_4$ [40], and $\Delta\theta$ describes the local distortion.

In our calculations we take the following spectral parameters of Ni$^{2+}$ ions in CsMgX$_3$ (X = Cl, Br, I): $B = 828$ cm$^{-1}$, 765 cm$^{-1}$, 750 cm$^{-1}$, and $C = 3206$ cm$^{-1}$, 2958 cm$^{-1}$, 2800 cm$^{-1}$ for the Racah parameters, $Dq = 695$ cm$^{-1}$, 655 cm$^{-1}$, 650 cm$^{-1}$ for the cubic CF parameters [3,4,13], and $k = 0.8317$, 0.7656, 0.6368 for the orbital reduction factors, and the spin-orbit coupling parameter $\xi = k\xi_0$ with $\xi_0 = 668$ cm$^{-1}$ [5]. Marvin's radial integrals [23,24] $M_0$ and $M_2$ can be obtained by the relations [22] $M_0 = k^2 M_{0\mathrm{F}}$, $M_2 = k^2 M_{2\mathrm{F}}$, here $M_{0\mathrm{F}} = 0.3382$ cm$^{-1}$, $M_{2\mathrm{F}} = 0.0264$ cm$^{-1}$ for free Ni$^{2+}$ ions. Substituting the parameters into the above equations, one can obtain the complete energy matrices. Diagonalizing the obtained complete energy matrices, the SH parameters including the ZFS parameters of the ground state and the anisotropic $g$-factors (characterized by $\Delta g_{\parallel} = g_{\parallel} - g_{\mathrm{s}}$, $\Delta g_{\perp} = g_{\perp} - g_{\mathrm{s}}$, and $\Delta g = g_{\parallel} - g_{\perp}$) can be calculated. By fitting the calculated $D$ to the observed values, one can obtain the local distortion $\Delta\theta = 3.43°$, 2.70°, 1.88° for X = Cl, Br, I, respectively. Then the local bonding angles are $\theta = 55.16°$, 55.14°, 54.77°. In Tables 1 – 3, the calculated results [column (F), row II] and experimental values are listed. It can be seen that the inclusion of small lattice distortions leads to agreement between the experimental and theoretical spin-

Table 1. SH parameters of $Ni^{2+}$ in $CsMgCl_3$ crystal.

| | | Calculated in this work | | | | | | Exp. [2, 3] |
|---|---|---|---|---|---|---|---|---|
| | | (A) | (B) | (C) | (D) | (E) | (F) | |
| $D$ / cm$^{-1}$ | I | −2.16676 | −0.05278 | −0.00062 | −0.06087 | −2.28103 | −2.28047 | |
| | II | −1.87055 | −0.05278 | −0.00061 | −0.06466 | −1.98860 | −1.98912 | −2.0000 ± 0.0008 |
| $g_{\parallel} - g_s$ | I | 0.25530 | 0.00000 | 0.00446 | −0.0006 | 0.25916 | 0.25916 | |
| ($g_s = 2.0023$) | II | 0.25222 | 0.00000 | 0.00446 | −0.00056 | 0.25612 | 0.25613 | 0.2547 ± 0.005 |
| $g_{\perp} - g_s$ | I | 0.24153 | 0.00000 | 0.00423 | −0.00058 | 0.24518 | 0.24518 | |
| ($g_s = 2.0023$) | II | 0.23845 | 0.00000 | 0.00423 | −0.00054 | 0.24214 | 0.24215 | 0.2387 ± 0.008 |
| $\Delta g = g_{\parallel} - g_{\perp}$ | I | 0.01377 | 0.00000 | 0.00023 | −0.00001 | 0.01399 | 0.01398 | |
| | II | 0.01377 | 0.00000 | 0.00023 | −0.00002 | 0.01398 | 0.01398 | 0.016 ± 0.013 |

I, with spin triplets only; II, with all the 45 microscopic states. (A) SO mechanism; (B) SS mechanism; (C) SOO mechanism; (D) SO-SS-SOO combined mechanism; (E) with considering SO, SS and SOO mechanisms; (F) with considering SO, SS, SOO and OO mechanisms.

Table 2. SH parameters of $Ni^{2+}$ in $CsMgBr_3$ crystal.

| | | Calculated in this work | | | | | | Exp. [2, 3] |
|---|---|---|---|---|---|---|---|---|
| | | (A) | (B) | (C) | (D) | (E) | (F) | |
| $D$ / cm$^{-1}$ | I | −1.86568 | −0.04279 | −0.00045 | −0.04839 | −1.95731 | −1.95687 | |
| | II | −1.60324 | −0.04279 | −0.00044 | −0.05150 | −1.69797 | −1.69839 | −1.7000 ± 0.002 |
| $g_{\parallel} - g_s$ | I | 0.23062 | 0.00000 | 0.00372 | −0.00052 | 0.23382 | 0.23382 | |
| ($g_s = 2.0023$) | II | 0.22774 | 0.00000 | 0.00372 | −0.00048 | 0.23098 | 0.23098 | 0.2277 ± 0.01 |
| $g_{\perp} - g_s$ | I | 0.21865 | 0.00000 | 0.00353 | −0.00049 | 0.22169 | 0.22169 | |
| ($g_s = 2.0023$) | II | 0.21578 | 0.00000 | 0.00353 | −0.00046 | 0.21885 | 0.21885 | 0.2277 ± 0.01 |
| $\Delta g = g_{\parallel} - g_{\perp}$ | I | 0.01196 | 0.00000 | 0.00018 | 0.00000 | 0.01214 | 0.01213 | |
| | II | 0.01196 | 0.00000 | 0.00018 | −0.00001 | 0.01213 | 0.01213 | 0.0000 ± 0.02 |

The meaning of the symbols is the same as in Table 1.

Table 3. SH parameters of $Ni^{2+}$ in $CsMgI_3$ crystal.

| | | Calculated in this work | | | | | | Exp. [2, 3] |
|---|---|---|---|---|---|---|---|---|
| | | (A) | (B) | (C) | (D) | (E) | (F) | |
| $D$ / cm$^{-1}$ | I | −0.11394 | −0.00260 | −0.00002 | −0.00249 | −0.11905 | −0.11903 | |
| | II | −0.09803 | −0.00260 | −0.00002 | −0.00265 | −0.10330 | −0.10331 | −0.1030 ± 0.005 |
| $g_{\parallel} - g_s$ | I | 0.15650 | 0.00000 | 0.00209 | −0.00027 | 0.15832 | 0.15832 | |
| ($g_s = 2.0023$) | II | 0.15452 | 0.00000 | 0.00209 | −0.00025 | 0.15636 | 0.15636 | 0.1577 ± 0.02 |
| $g_{\perp} - g_s$ | I | 0.15577 | 0.00000 | 0.00208 | −0.00027 | 0.15758 | 0.15758 | |
| ($g_s = 2.0023$) | II | 0.15381 | 0.00000 | 0.00208 | −0.00025 | 0.15564 | 0.15564 | 0.1577 ± 0.02 |
| $\Delta g = g_{\parallel} - g_{\perp}$ | I | 0.00073 | 0.00000 | 0.00001 | 0.00000 | 0.00074 | 0.00074 | |
| | II | 0.00072 | 0.00000 | 0.00001 | 0.00000 | 0.00073 | 0.00073 | 0.0000 ± 0.04 |

The meaning of the symbols is the same as in Table 1.

Hamiltonian parameters. The results indicate also that the distortion model, which we used, is reasonable.

## 4. Discussion and Conclusion

To study the contributions to the SH parameters from various magnetic interactions, we calculate the SH parameters in the following cases: (i) considering with SO interaction only, the results are listed in column (A) of Tables 1 – 3; (ii) with SS interaction only, the results are listed in column (B) of Tables 1 – 3; (iii) with SOO interaction only, the results are listed in column (C) of Tables 1 – 3; (iv) with SO, SS and SOO interactions, the results are listed in column (E) of Tables 1 – 3; (v) with all the interactions, i. e. SO, SS, SOO, and OO interactions, the results are listed in column (F) of Tables 1 – 3. In [41] it is referred that there exists an SO-SS-SOO combined mechanism, which is defined as [41]

$$D_{\text{SO-SS-SOO}} = D_{\text{Total}} - (D_{\text{SO}} + D_{\text{SS}} + D_{\text{SOO}}), \quad (13)$$

$$\begin{aligned}&\Delta g_{\parallel\text{SO-SS-SOO}}\\ &= \Delta g_{\parallel\text{Total}} - (\Delta g_{\parallel\text{SO}} + \Delta g_{\parallel\text{SS}} + \Delta g_{\parallel\text{SOO}}),\end{aligned} \quad (14)$$

Table 4. Percentage ratio of the contributions to the SH parameters of $Ni^{2+}$ in $CsMgX_3$ (in %).

| X | SH parameter | Percentage ratio $\eta_\gamma$ $\gamma = \text{SO}$ | $\gamma = \text{SS}$ | $\gamma = \text{SOO}$ | $\gamma = \text{SO-SS-SOO}$ | $\gamma = \text{OO}$ | $\gamma = \text{Total}$ |
|---|---|---|---|---|---|---|---|
| Cl | $D$ | 94.039 | 2.653 | 0.031 | 3.251 | 0.026 | 5.961 |
| | $\Delta g_\parallel$ | 98.473 | 0.000 | 1.741 | −0.219 | 0.004 | 1.527 |
| | $\Delta g_\perp$ | 98.472 | 0.000 | 1.747 | −0.223 | 0.004 | 1.528 |
| | $\Delta g$ | 98.498 | 0.000 | 1.605 | −0.143 | 0.000 | 1.502 |
| Br | $D$ | 94.398 | 2.519 | 0.026 | 3.032 | 0.025 | 5.602 |
| | $\Delta g_\parallel$ | 98.597 | 0.000 | 1.611 | −0.209 | 0.000 | 1.403 |
| | $\Delta g_\perp$ | 98.597 | 0.000 | 1.613 | −0.210 | 0.000 | 1.403 |
| | $\Delta g$ | 98.599 | 0.000 | 1.484 | −0.082 | 0.000 | 1.401 |
| I | $D$ | 94.889 | 2.517 | 0.019 | 2.565 | 0.009 | 5.111 |
| | $\Delta g_\parallel$ | 98.823 | 0.000 | 1.337 | −0.160 | 0.000 | 1.177 |
| | $\Delta g_\perp$ | 98.824 | 0.000 | 1.336 | −0.161 | 0.000 | 1.176 |
| | $\Delta g$ | 98.63 | 0.000 | 1.370 | 0.000 | 0.000 | 1.370 |

$$\Delta g_{\perp \text{SO-SS-SOO}} = \Delta g_{\perp \text{Total}} - (\Delta g_{\perp \text{SO}} + \Delta g_{\perp \text{SS}} + \Delta g_{\perp \text{SOO}}), \tag{15}$$

$$\Delta g_{\text{SO-SS-SOO}} = \Delta g_{\text{Total}} - (\Delta g_{\text{SO}} + \Delta g_{\text{SS}} + \Delta g_{\text{SOO}}). \tag{16}$$

The SH parameters due to an SO-SS-SOO combined mechanism are calculated, and the results are listed in column (D) of Tables 1 – 3. At the same time, we calculated these data in the two cases of considering spin triplets only and considering all the 45 microscopic terms. The results are shown in Tables 1 – 3 as row I and row II.

From Tables 1 – 3 one can see that the contribution to the SH parameters (including the ZFS parameter $D$ and $g$-factors) from the SO mechanism is the most important one, where the contribution from triplets is dominant. There are no contributions to the ZFS due to the SS mechanism from spin singlet. That is, the ZFS from the SS mechanism depends on the spin triplets only. In the contributions to the ZFS due to the SOO mechanism and SO-SS-SOO combined mechanism, the contribution from spin triplets is dominant. For $g$-factors, it is found that there is almost no contribution from the SS and OO mechanism. The SOO mechanism has small influence on $g$-factors, in which the contribution from the spin singlet is almost zero. The SO-SS-SOO combined mechanism has slight influence on $g$-factors, in which the contribution from the spin singlet is slight. It is also found that in the $CsMgX_3$:$Ni^{2+}$ system, the following relationships hold:

$$|D_{\text{SO}}| > |D_{\text{SS}}| \approx |D_{\text{SO-SS-SOO}}| > |D_{\text{OO}}| \approx |D_{\text{SOO}}|, \tag{17}$$

$$|g_{\parallel \text{SO}}| > |g_{\parallel \text{SOO}}| > |g_{\parallel \text{SO-SS-SOO}}| > \\ > |g_{\parallel \text{OO}}| \approx |g_{\parallel \text{SS}}|, \tag{18}$$

$$|g_{\perp \text{SO}}| > |g_{\perp \text{SOO}}| > |g_{\perp \text{SO-SS-SOO}}| > \\ > |g_{\perp \text{OO}}| \approx |g_{\perp \text{SS}}|, \tag{19}$$

$$|\Delta g_{\text{SO}}| > |\Delta g_{\text{SOO}}| > |\Delta g_{\text{SO-SS-SOO}}| > \\ > |\Delta g_{\text{OO}}| \approx |\Delta g_{\text{SS}}|. \tag{20}$$

In order to illustrate the contributions to SH parameters from magnetic coupling mechanisms, including SO, SS, SOO, SO-SS-SOO, and OO mechanisms, it is convenient to define the percentage ratios

$$\eta_\gamma = 100 \left| \frac{\chi_\gamma}{\chi_{\text{Total}}} \right| \%, \tag{21}$$

in which $\gamma$ represents the SO mechanism, SS mechanism, SOO mechanism, or SO-SS-SOO combined mechanism, and $\chi = D$, $\Delta g_\parallel$, $\Delta g_\perp$, or $\Delta g$, and

$$\eta_{\text{OO}} = 100 \left| \frac{\chi_{\text{Total}} - \chi_{\text{SO+SS+SOO}}}{\chi_{\text{Total}}} \right| \% \tag{22}$$

for the OO mechanism. The calculated results are listed in Table 4.

The calculated results show that the contributions to the ZFS parameter $D$ from SS, SOO, and OO interactions are about 5 – 6% in the $CsMgX_3$:$Ni^{2+}$ system and those to the $g$-factors are less than 2%. It is found that the contributions to the SH parameters from slight magnetic interactions follow the order $CsMgCl_3$:$Ni^{2+}$ > $CsMgBr_3$:$Ni^{2+}$ > $CsMgI_3$:$Ni^{2+}$. It is interesting that the contributions to $\Delta g_\parallel$ and $\Delta g_\perp$ from slight magnetic interactions are almost the same.

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[1] G. L. McPherson and R. C. Koch, J. Chem. Phys. **60**, 1424 (1974).
[2] G. L. McPherson, T. J. Kistenmacher, and G. D. Stycky, J. Chem. Phys. **52**, 815 (1970).
[3] G. L. McPherson, J. E. Wall, and A. M. Hermann, Inorg. Chem. **13**, 2230 (1974).
[4] G. L. McPherson and G. D. Stycky, J. Chem. Phys. **57**, 3780 (1972).
[5] J. J. Chen and M. L. Du, Physica B **228**, 409 (1996).
[6] M. L. Du and C. Rudowicz, Phys. Rev. B **46**, 8974 (1992).
[7] H. Rinneberg and H. Hartmann, J. Chem. Phys. **52**, 5814 (1970).
[8] P. S. May and H. U. Gudel, Chem. Phys. Lett. **164**, 612 (1989).
[9] A. Hauser and H. U. Gudel, J. Lumin. **27**, 249 (1982).
[10] S. Y. Wu, W. Z. Yan, and X. Y. Gao, Spectrochim. Acta Part A **60**, 701 (2004).
[11] S. Y. Wu, X. Y. Gao, and H. N. Dong, J. Magn. Magn. Mater. **301**, 67 (2006).
[12] W. C. Zheng, Physica B **245**, 123 (1998).
[13] W. C. Zheng and X. X. Wu, Spectrochim. Acta Part A **64**, 628 (2006).
[14] C. Rudowicz, Magn. Reson. Rev. **13**, 1 (1987).
[15] C. Rudowicz and S. K. Misra, Appl. Spectrosc. Rev. **36**, 11 (2001).
[16] C. Rudowicz and H. W. F. Sung, Physica B **300**, 1 (2001).
[17] C. Rudowicz, Y. Y. Yeung, Z. Y. Yang, and J. Qin, J. Phys.: Condens. Matter **14**, 5619 (2002).
[18] A. K. Pereosyan and A. A. Mirzakhanyan, Phys. Status Solidi (b) **133**, 315 (1986).
[19] B. Shang, M. Huang, and M. G. Zhao, Phys. Status Solidi (b) **141**, K35 (1987).
[20] M. Huang, Phys. Status Solidi (b) **141**, K1 (1987).
[21] Y. Hao and Z. Y. Yang, J. Magn. Magn. Matter **299**, 445 (2006).
[22] Q. Wei, Solid State Commun. **138**, 427 (2006).
[23] H. H. Marvin, Phys. Rev. **71**, 102 (1947).
[24] G. Malli, J. Chem. Phys. **48**, 1088 (1967).
[25] C. Rudowicz, Z. Y. Yang, Y. Y. Yeung, and J. Qin, J. Phys. Chem. Solids **64**, 1419 (2003).
[26] M. Blume and R. E. Waston, Proc. R. Soc. (London) A **271**, 565 (1963).
[27] M. Blume and R. E. Waston, Proc. R. Soc. (London) A **270**, 127 (1963).
[28] B. G. Wybourne, Spectroscopic Properties of Rare Earths, Wiley, New York 1965.
[29] C. Rudowicz, Magn. Reson. Rev. **13**, 335 (1988).
[30] C. Rudowicz, Chem. Phys. **102**, 437 (1986).
[31] Y. Y. Yeung and C. Rudowicz, Comput. Chem. **16**, 207 (1992).
[32] Z. Y. Yang, Appl. Magn. Reson. **18**, 455 (2000).
[33] Z. Y. Yang, Y. Hao, C. Rudowicz, and Y. Y. Yeung, J. Phys.: Condens. Matter **16**, 3481 (2006).
[34] L. H. Xie, P. Hu, and P. Huang, J. Phys. Chem. Solids **66**, 918 (2005).
[35] Z. Y. Yang, C. Rudowicz, and Y. Y. Yeung, Physica B **348**, 151 (2004).
[36] Y. Y. Yeung and C. Rudowicz, Comput. Chem. **16**, 207 (1992).
[37] D. J. Newman and B. Ng, Rep. Prog. Phys. **52**, 699 (1989).
[38] C. Rudowicz, J. Phys. C: Solid State Phys. **20**, 6033 (1987).
[39] Z. Y. Yang and Q. Wei, Chin. J. Chem. Phys. **17**, 401 (2004).
[40] W. L. Yu, X. M. Zhang, L. X. Yang, and B. Q. Zen, Phys. Rev. B **50**, 6756 (1994).
[41] Z. Y. Yang, Acta Phys. Sin. **53**, 1981 (2004).