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An EPR theory for $C_{2v}(d^6)$ and the spectral analysis of $ZnS:Fe^{2+}$

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Abstract. The $C_{2v}(d^6)$ strong-field matrices for $S = 2$ are given in an O_h point-group representation and an EPR theory for d^6-C_{2v} systems is established in this paper. By means of the eigenvalues and eigenvectors of these matrices, the EPR spectrum of Fe^{2+} in $ZnS:Fe^{2+}$ is analysed, the fine structure of the absorption spectrum with $\Delta S = 0$ is explained, the paramagnetic g -factors, the zero-field splitting parameters and the Zeeman energy corrections are obtained. The experimental requirements for realising those EPR transitions are discussed and the influences of the excited states on the ground-state spin-Hamiltonian parameters are analysed. Information which can be obtained from the eigenvectors is discussed.

1. Introduction

There have been many works researching the structure and absorption spectrum of the $ZnS:Fe^{2+}$ complex (Low and Weger 1960, Dietz and Pappalardo 1960, 1961, Slack *et al* 1966, Ham and Slack 1971, Skowronski *et al* 1982, 1985, Zhao *et al* 1989). But there has so far been no systematical theory for the analysis of its EPR spectrum. In ligand field theory, the usual calculation scheme of g -factors is employed only for degenerate eigenstates of spin, onto which some high state perturbation terms have sometimes also been added (Bleaney and Stevens 1953, Bowers and Owen 1955, Griffith 1961, Chakravarty 1980). However, the $ZnS:Fe^{2+}$ complex is of the $C_{2v}(C_2, \sigma_d)$ symmetrical tetrahedral type (Vasiliev *et al* 1975, Marfunin *et al* 1967, 1975, Zhao *et al* 1989): the energy degeneracy of the valence electron states of Fe^{2+} is entirely removed by the central field of the atomic kernel, the electrostatic interaction among the valence electrons, the spin-orbit coupling and the low symmetrical crystal field. Moreover, a complete configuration mixing occurs in the wavefunctions.

In order that all factors mentioned above be taken into account, an analysis scheme with a complete configuration-mixing EPR theory will be established in this paper. In this theory the $C_{2v}(d^6, S = 2)$ strong-field matrices will be established in an O_h point group representation, by means of the eigenvalues and eigenvectors; the fine structure of the absorption spectrum for $\Delta S = 0$ will be studied; and the zero-field splitting parameters of the ground state, the paramagnetic g -values and the Zeeman energy corrections will

be obtained. That is, by means of the complete configuration-mixing eigenvectors of ZnS:Fe²⁺, a complete theoretical analysis for its EPR spectrum will be given.

2. The energy matrix

In analysing the EPR spectrum of Fe²⁺(d⁶), only its spin-quintet should be considered. This is because the behaviour of its spatial part in a crystal field is similar to that of a single d-electron and the transition energies within its spin-quintets are usually below 12000 cm⁻¹ and can be separated entirely from the transitions with $\Delta S = 1$ (>12000 cm⁻¹). Thus, the effects of spin-triplets on the zero-field splitting of the ground state and the paramagnetic *g*-factor values can entirely be neglected.

According to the resolution of the group chain $SO_3 \times SU_2 \supset Td \times SU_2 \supset C_{2v} \times SU_2$, the 25 degenerate states of ⁵D can be linearly combined to obtain a set of base functions of the 11 irreducible representations of T_d^{*}, and the latter can again be linearly combined to obtain a set of bases for the four irreducible representations $\Gamma[A_1'(7), A_2'(6), B_1'(6), B_2'(6)]$ of the spin-orbit direct-product group C_{2v}^{*} of C_{2v}(C₂, σ_d). Then, the energy matrices in the T_d^{*} representation of the spin-quintets of d⁶[C_{2v}(C₂, σ_d)] can be established (as in Appendix 1) according to the scheme of Zhao *et al* (1986b, 1989). The matrix elements are expressed by *B*, *C*, ζ , *D_q*, *d_i* and *d₄₅*, where

$$\begin{aligned} d_i &= \langle \psi_i | V(C_{2v}) | \psi_i \rangle, & i &= 1, 2, 3, 4, 5 \\ d_{45} &= \langle \psi_4 | V(C_{2v}) | \psi_5 \rangle \end{aligned} \quad (1)$$

are single electron crystal field matrix elements and

$$\begin{aligned} \psi_1 &= (1/\sqrt{2})(\eta + \xi) & (B_1) \\ \psi_2 &= (1/\sqrt{2})(\eta - \xi) & (B_2) \\ \psi_3 &= \varepsilon & (A_2) \\ \psi_4 &= \theta & (A_1) \\ \psi_5 &= \zeta & (A_1). \end{aligned} \quad (2)$$

3. EPR theory

Using the eigenvectors of the strong-field matrices of d⁴(C_{2v}^{*}) with *S* = 2, we can establish an EPR theory for d⁶-C_{2v} systems.

The eigenvector corresponding to the *J*th eigenvalue *E*(*J*) of a given Γ'_α -matrix can be denoted by $|\Gamma'_\alpha(J)\rangle$, which is a combination of the basic vectors $\phi(\Gamma'_\alpha, p)$ of Γ'_α as follows:

$$|\Gamma'_\alpha(J)\rangle = \sum_p \gamma_{\alpha p}(J) \phi(\Gamma'_\alpha, p) \quad (3)$$

where the combination coefficient $\gamma_{\alpha p}(J)$ (i.e. *A*_{1*p*}(*J*), *A*_{2*p*}(*J*), *B*_{1*p*}(*J*) and *B*_{2*p*}(*J*)) is the *p*th component of $|\Gamma'_\alpha(J)\rangle$. Obviously, each level includes the contributions from all configurations of the Γ'_α -space to which it belongs. This is just the meaning of 'complete configuration mixing'. In addition, the degeneracy is entirely removed. EPR absorptions can only occur between some pairs of neighbouring eigenstates with an interval of about 1 cm⁻¹ in an external magnetic field.

3.1. On EPR g -factors

For $ZnS:Fe^{2+}$, there have been no works calculating its g -factors because the influence from excited states is very strong and can hardly be figured out. Now, we will discuss this problem in some detail.

Since the transformation character of L and S is the same as the rotation operator $R(R_x, R_y, R_z)$, thus we have, in the C_{2v} coordinate system (x, y, z) :

$$L_x, S_x \in B_2 \quad L_y, S_y \in B_1 \quad L_z, S_z \in A_2 \quad (4)$$

and the following equations hold:

$$\langle \Gamma'_i | L_\alpha^2 | \Gamma'_j \rangle = M \delta_{i,j} \quad \langle \Gamma'_i | L + 2S | \Gamma'_j \rangle = M(\Gamma'_i, \Gamma'_j)(1 - \delta_{i,j}). \quad (5)$$

From these and the Wigner–Eckart theorem in point group, we can obtain the symmetry selection rule for the magnetic dipole transitions and the g -factors among the four irreducible representations of C_{2v}^* , as shown in table 1, in which the coordinate system of $C_{2v}(C_2, \sigma_d)$ is used and can be easily transformed into that of T_d .

Table 1. The symmetry selection rule for the magnetic dipole transitions and the g -factors among the four irreducible representations of C_{2v}^* , here the $C_{2v}(C_2, \sigma_d)$ coordinate system is used.

g_α	A'_1	A'_2	B'_1	B'_2
A'_1	0	g_z	g_y	g_x
A'_2	g_z	0	g_x	g_y
B'_1	g_y	g_x	0	g_z
B'_2	g_x	g_y	g_z	0

Since the effective spin S' is equal to the real spin S for the ground state of d^6 system, we have, for two eigenvectors $|\Gamma'_1(J)\rangle$ and $|\Gamma'_2(K)\rangle$ belonging to the orbital ground state of d^6-C_{2v} ,

$$g_\alpha[\bar{\Gamma}'_1(J), \bar{\Gamma}'_2(K)] = 2 + \sum_{ij} \gamma_{1i}^*(J) \gamma_{2j}(K) \langle \varphi(\bar{\Gamma}'_1, i) | L_\alpha | \varphi(\bar{\Gamma}'_2, j) \rangle + \sum_{ij} \gamma_{1i}^*(J) \gamma_{2j}(K) \langle \varphi(\bar{\Gamma}'_1, i) | S_\alpha | \varphi(\bar{\Gamma}'_2, j) \rangle. \quad (6)$$

Generally, the spin Hamiltonian parameters (g', D', E' etc) of an orbital excited state do not equal those (g^0, D^0, E^0 etc) of the orbital ground state. In order to reflect this situation we may divide the basic vectors $\varphi(\Gamma', i)$ into two groups, by symbols $\varphi^0(\Gamma', i)$ and $\varphi'(\Gamma', i)$ belonging to orbital excited states and the ground state (both are spatial singlets) respectively, and rewriting expression (3) as

$$|\Gamma'(J)\rangle = \sum_i^0 \gamma_i(J) \varphi^0(\Gamma', i) + \sum_j' \gamma_j(J) \varphi'(\Gamma', j) \quad (7)$$

where Σ^0 and Σ' sum only over the Γ' -basic vectors belonging respectively to the orbital ground state and excited states. If in both Σ^0 and Σ' only one term is retained, expression (7) will become

$$|\Gamma'(J)\rangle \cong \gamma_i(J) \varphi^0(\Gamma', i) + \gamma_j(J) \varphi'(\Gamma', j). \quad (7')$$

Now, for an arbitrary pair of eigenvectors, say $|\Gamma'_1(J)\rangle$ and $|\Gamma'_2(K)\rangle$, belonging to the orbital ground state, we have, according to (7'),

$$\begin{aligned} |\Gamma'_1(J)\rangle &\equiv \gamma_{1p}(J)\varphi^0(\Gamma'_1, p) + \gamma_{1q}(J)\varphi'(\Gamma'_1, q) \\ |\Gamma'_2(K)\rangle &\equiv \gamma_{2i}(K)\varphi^0(\Gamma'_2, i) + \gamma_{2j}(K)\varphi'(\Gamma'_2, j). \end{aligned} \quad (7'')$$

Thus we get

$$\begin{aligned} \langle \Gamma'_1(J) | g_\alpha S_\alpha | \Gamma'_2(K) \rangle &\equiv g_\alpha^0 \gamma_{1p}^*(J) \gamma_{2i}(K) \langle \varphi^0(\Gamma'_1, p) | S_\alpha | \varphi^0(\Gamma'_2, i) \rangle \\ &+ g'_\alpha \gamma_{1q}^*(J) \gamma_{2j}(K) \langle \varphi'(\Gamma'_1, q) | S_\alpha | \varphi'(\Gamma'_2, j) \rangle \\ &\times \langle \Gamma'_1(J) | S_\alpha | \Gamma'_2(K) \rangle = \gamma_{1p}^*(J) \gamma_{2i}(K) \langle \varphi^0(\Gamma'_1, p) | S_\alpha | \varphi^0(\Gamma'_2, i) \rangle \\ &+ \gamma_{1q}^*(J) \gamma_{2j}(K) \langle \varphi'(\Gamma'_1, q) | S_\alpha | \varphi'(\Gamma'_2, j) \rangle. \end{aligned} \quad (8)$$

Then we have

$$g_\alpha[\Gamma'_1(J), \Gamma'_2(K)] = g_\alpha^0/[1 + \chi] + g'_\alpha/[1 + \chi^{-1}], \quad (9)$$

where

$$\chi = \gamma_{1q}^*(J) \gamma_{2j}(K) \langle \varphi'(\Gamma'_1, q) | S_\alpha | \varphi'(\Gamma'_2, j) \rangle / \gamma_{1p}^*(J) \gamma_{2i}(K) \langle \varphi^0(\Gamma'_1, p) | S_\alpha | \varphi^0(\Gamma'_2, i) \rangle. \quad (10)$$

It can be seen from (9) and (10) that the g_α -values must be corresponding to the observed values and contain contributions from not only the ground state g_α^0 -factors but also the excited state g'_α -factors. For different eigenstates of the ground state, owing to the influences on which from various excited states are different, the g_α -values calculated with this formula can thus also be different. If they do equal to each other, that is to say the influences are equivalent. The above conclusions can easily be also applied to the cases which involve all of the excited states. In what follows the degree of such influences will be discussed.

3.2. On the zero-field splitting parameters

When the external magnetic field is absent, the spin Hamiltonian, omitting its higher order terms, can be written as

$$H(S) = D[S_z^2 - \frac{1}{3}S(S+1)] + E(S_x^2 - S_y^2). \quad (11)$$

Owing to the joint effect of C_{2v} crystal field and spin-orbit coupling, the degeneracy of $d^{6-5}D$ states is entirely removed and each eigenstate contains complete configuration mixing. Thus the ground state zero-field splitting parameters D and E should be determined by the secular equation of the spin Hamiltonian matrix within the group of eigenstates $|\Gamma'_\alpha(J_\alpha)\rangle$ belonging to the orbital ground state ${}^5A_1(C_{2v})$. Since S_x^2 , S_y^2 and S_z^2 belong to $A_1(C_{2v})$, such secular equation can be written as

$$|H_{\alpha\beta}(s) - \lambda \delta_{\alpha\beta}| = 0 \quad (12)$$

where

$$H_{\alpha\beta}(s) = \langle \Gamma'_\alpha(J_\alpha) | H(s) | \Gamma'_\beta(J_\beta) \rangle. \quad (13)$$

This shows that the zero-field splitting parameters are determined by the complete configuration mixed eigenvectors. If the approximation of (7'') is used to (13), that is, if

$$\begin{aligned} |\Gamma'_\alpha(J_\alpha)\rangle &= \gamma_{\alpha p}(J_\alpha)\varphi^0(\Gamma'_\alpha, p) + \gamma_{\alpha q}(J_\alpha)\varphi'(\Gamma'_\alpha, q) \\ |\Gamma'_\beta(J_\beta)\rangle &= \gamma_{\beta p'}(J_\beta)\varphi^0(\Gamma'_\beta, p') + \gamma_{\beta q'}(J_\beta)\varphi'(\Gamma'_\beta, q') \end{aligned}$$

we will have

$$\begin{aligned} H_{\alpha\beta}(S) &= D^0\gamma_{\alpha p}^*(J_\alpha)\gamma_{\beta p'}(J_\beta)\langle\varphi^0(\Gamma'_\alpha, p)|S_z^2|\varphi^0(\Gamma'_\beta, p')\rangle \\ &+ E^0\gamma_{\alpha p}^*(J_\alpha)\gamma_{\beta p'}(J_\beta)\langle\varphi^0(\Gamma'_\alpha, p)|S_x^2 - S_y^2|\varphi^0(\Gamma'_\beta, p')\rangle \\ &+ D'\gamma_{\alpha q}^*(J_\alpha)\gamma_{\beta q'}(J_\beta)\langle\varphi'(\Gamma'_\alpha, q)|S_z^2|\varphi'(\Gamma'_\beta, q')\rangle \\ &+ E'\gamma_{\alpha q}^*(J_\alpha)\gamma_{\beta q'}(J_\beta)\langle\varphi'(\Gamma'_\alpha, q)|S_x^2 - S_y^2|\varphi'(\Gamma'_\beta, q')\rangle. \end{aligned} \quad (14)$$

If the eigenvectors in expression (13) belong to an orbital excited state ${}^5\Gamma(C_{2v})$, the values of D and E so obtained will also belong to ${}^5\Gamma(C_{2v})$.

3.3. On the Zeeman correction

For the $d^6-{}^5D(C_{2v})$ states, although the degeneracy is entirely removed, the level intervals are very small. Thus in order to give Zeeman correction, the contribution of the applied magnetic field \mathbf{B} (we have $H_B = \beta(\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B}$) should be introduced into the complete matrix of $d^6-{}^5D(C_{2v}^*)$ before its diagonalisation. Since

$$\begin{aligned} \langle\Gamma'_i(J)|S_\alpha|\Gamma'_j(K)\rangle &= C_s[\Gamma'_i(J), \Gamma'_j(K)](1 - \delta_{ij}) \\ \langle\Gamma'_i(J)|L_\alpha|\Gamma'_j(K)\rangle &= C_l[\Gamma'_i(J), \Gamma'_j(K)](1 - \delta_{ij}) \end{aligned} \quad (15)$$

the new matrix so obtained will be of 25×25 order and consist of the four Γ' -matrices of C_{2v}^* by the coupling of H_B as shown in Appendix 2. From the Zeeman energy diagram so obtained one can calculate the required condition for the EPR experiments. If the external magnetic field is along some special direction, the Zeeman energy matrix will reduce to a product sum of lower order matrices.

It should be indicated that the complete configuration mixing is closer to the real situation of low symmetrical complexes, thus the above calculation scheme with the eigenvectors of the $d^6-C_{2v}^*$ strong-field matrices is even more reasonable.

4. The numerical results

4.1. Analysis on the absorption spectrum

We neglect the effects of the triplets. Since the spatial part of 5D states behave like single d-electron states, thus every d_i and d_{45} can easily be determined by the observed spin-allowed spectrum of $ZnS:Fe^{2+}$, according to the method of Zhou *et al* (1984) and Zhao *et al* (1986b, 1989), as follows:

$$\begin{aligned} d_5 - d_4 &= 3550 \text{ cm}^{-1} & d_1 - d_4 &= 3250 \text{ cm}^{-1} \\ d_2 - d_4 &= 2950 \text{ cm}^{-1} & d_3 - d_4 &= 29.6 \text{ cm}^{-1}. \end{aligned} \quad (16)$$

These are similar values to those of Zhao *et al* (1989), except for $d_3 - d_4$, which has a large effect on the zero-field splitting of the ground state. As $ZnS:Fe^{2+}$ is of $C_{2v}(C_2, \sigma_d)$

symmetrical tetrahedral form, its T_d ground state is ${}^5E(T_d)$. Because of energy region of the splitting of 5E caused by the spin-orbit coupling and the low symmetrical crystal field is only about 100 cm^{-1} , the relative occupation probability of these split states is in the range 1–0.7 at room temperature ($kT \sim 200$). Thus each of the ten undegenerate split states of 5E can be occupied by a complex with almost equal probability and can therefore be taken as an initial state of the absorption transitions. Then, the fine structure of the observed absorption spectrum with $\Delta S = 0$ can be well explained by the eigenvalues (cf table 2) of the matrices in Appendix 1, in which $\zeta = 380\text{ cm}^{-1}$, $d_{45} = 250\text{ cm}^{-1}$.

Table 2. The fine structure of the spin-allowed absorption spectrum.

Observed (cm^{-1}) Skowronski <i>et al</i> (1982, 1985) Vasiliev <i>et al</i> (1975)	Calculated (cm^{-1})	Assignment ^a $C_{2v}(C_2, \sigma_a)$
	ground state	
	0	$A'_1(1)$
	5.2467	$B'_2(1)$
	22.133	$B'_1(1)$
	23.401	$A'_2(2)$
	33.776	$A'_1(5)$
15 ± 2	16.88	$B'_2(1) \rightarrow B'_1(1)$
27 ± 2	28.53	$B'_2(1) \rightarrow A'_1(5)$
46 ± 2	49.44	$A'_1(5) \rightarrow A'_2(4)$
63 ± 2	63.30	$B'_1(1) \rightarrow A'_1(3)$
2899	2901.8	$A'_2(1) \rightarrow A'_2(6)$
2919	2918.1	$A'_1(5) \rightarrow B'_1(6)$
2930	2928.5	$A'_2(2) \rightarrow B'_1(6)$
2945	2947.4	$B'_2(1) \rightarrow B'_2(6)$
2964	2969.0	$A'_1(5) \rightarrow A'_2(6)$
2984	2980.7	$B'_1(1) \rightarrow A'_2(6)$
3040	3031.5	$B'_2(1) \rightarrow B'_2(3)$
3050	3036.8	$A'_1(1) \rightarrow B'_2(3)$
3129	3157.9	$A'_2(1) \rightarrow A'_1(7)$
3182	3182.5	$A'_2(4) \rightarrow B'_2(3)$
3241	3238.3	$B'_1(1) \rightarrow B'_1(3)$
3263	3260.4	$A'_1(1) \rightarrow B'_1(3)$
3276	3276.5	$A'_2(1) \rightarrow B'_2(2)$
3293	3292.0	$A'_1(3) \rightarrow B'_2(2)$
3342	3343.6	$A'_1(5) \rightarrow B'_2(2)$
3374	3374.5	$A'_1(1) \rightarrow B'_1(2)$
3550		$A'_1(1) \rightarrow B'_1(2) + \bar{\nu}_1$
3840		$A'_1(1) \rightarrow B'_1(5) + \bar{\nu}_2$

Parameters (cm^{-1}): $d_3 - d_4 = 29.6$, $d_1 - d_4 = 2950$; $d_{45} = 250$; $d_3 - d_4 = 3250$; $\zeta = 380$; $d_5 - d_4 = 3550$; $\bar{\nu}_1, \bar{\nu}_2$ —vibronic basic frequencies.

^a The initial states are the eigenstates belonging to ${}^5E_g(A)$.

The absorption spectrum with $\Delta S = 1$ can be well explained by the above view point and parameters. It is found that the effects of the states with $S = 2$ and $S = 1$ caused by spin-orbit coupling each with the other are very weak.

4.2. EPR spectrum analysis

By means of the eigenvectors of the matrices in appendix 1, the non-zero magnetic dipole matrix elements and the corresponding g -factors between neighbouring eigenstates belonging to the orbital ground state can be obtained according to formula (9). The results calculated (in the T_d coordination system) for $ZnS:Fe^{2+}$ are as follows:

$$\begin{aligned}
 g_z[A'_1(5), A'_2(2)] &= 2.1247 & g_z[B'_1(1), B'_2(1)] &= 2.0444 \\
 g_x[A'_2(2), B'_1(1)] &= g_y[A'_2(2), B'_1(1)] & &= 2.3067 \\
 g_x[B'_1(1), A'_1(1)] &= g_y[B'_1(1), A'_1(1)] & &= 2.2192.
 \end{aligned}
 \tag{17}$$

Firstly, it must be indicated that the g -factors calculated from the complete configuration mixed wavefunctions have already contained the effects of all spin Hamiltonian parameters of each orbital excited state. Because excited states have different effects on different energy levels of the ground state, thus the g -values (g_z or $g_{x,y}$) calculated are different for different pairs of eigenstates of the ground state. In fact, the energy gap between the T_d ground state ${}^5E_g(A_1)$ and the first excited state ${}^5E_g(A_2)$ is only about 50 cm^{-1} . Thus, the effects of the excited states on the ground state are very large. This has already been shown from the numerical results of g -factors. However, whether the transition corresponding to a g -factor can be realised still depends on the Zeeman energy levels and the conditions required by EPR experiments.

In order to determine the Zeeman corrections, we must diagonalise the matrices in Appendix 2. The Zeeman corrections calculated for $ZnS:Fe^{2+}$ are shown in figure 1. It

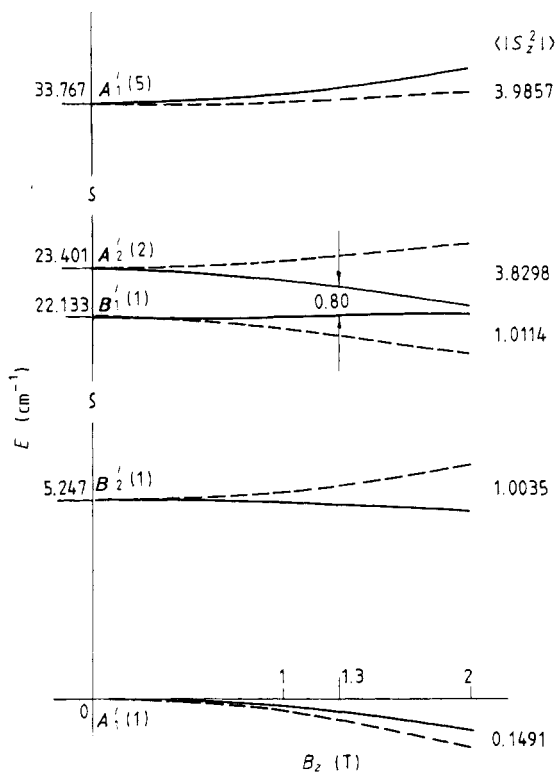


Figure 1. Zeeman energy corrections of the eigenstates belonging to the orbital ground state. — $\mathbf{B} = (0, 0, B_z)$, - - - $\mathbf{B} = (B_x, 0, 0)$.

can be seen from the diagram for $\mathbf{B} = (0, 0, B_z)$ that when $B_z = 1.3 \text{ T}$ an EPR transition of $\tilde{\nu} = 0.80 \text{ cm}^{-1}$ can indeed occur between $A_2'(1)$ and $B_1'(2)$. This is just the expected result of experiments.

It can be seen from the above that the transition corresponding to

$$g_{x0}(A_2'(2) - B_1'(1)) = g_{y0}(A_2'(2) - B_1'(1)) = 2.3063$$

(in the case of a T_d coordinate system) is just the one that can actually be observed, that is to say we have $g_{\parallel} = 2.3063$ along the X -direction of $C_{2v}(C_2, \sigma_d)$. On the other hand, any other EPR absorption cannot be observed. This is fully consistent with experiment (Skowronski *et al* 1985, Low and Weger 1960).

The ground-state zero-field splittings can be obtained by diagonalising the Γ' matrices. The results are shown in figure 2. The five undegenerate split states result from complete configuration mixing, that is, in some cases, mixing within the orbital ground state (by spin-orbit coupling), and in other cases, mixing with excited states (by crystal field together with the spin-orbit coupling).

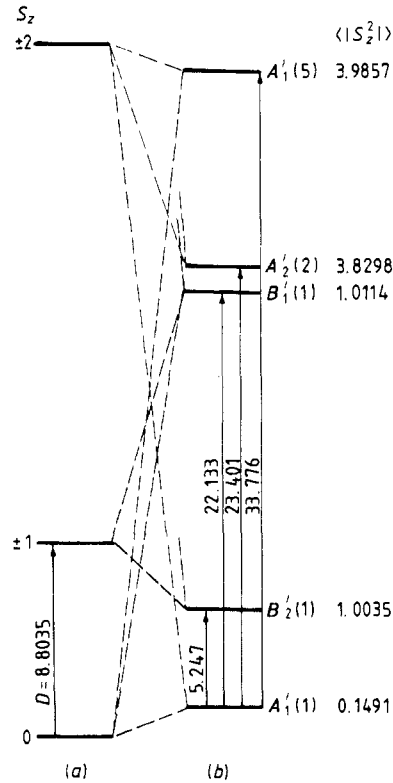


Figure 2. The zero-field splitting of the ground state ${}^5E_g(\text{cm}^{-1})$. (a) non-mixed, (b) mixed.

It can be proved that, for the eigenvectors of all Γ' of $d^6(C_{2v}^*, S = 2)$, we have

$$\begin{aligned} \langle \Gamma'_i(I) | S_\alpha^2 | \Gamma'_j(J) \rangle &= M_{ij}(I, J) \delta_{ij}, & \alpha = x, y, z \\ \langle \Gamma'_i(I) | S_x^2 | \Gamma'_j(J) \rangle &= \langle \Gamma'_i(I) | S_y^2 | \Gamma'_j(j) \rangle. \end{aligned} \tag{18}$$

That is, the spin-Hamiltonian parameter E equals zero and only D exists. From figure 2 we can see that, among the split states of the ground state, $A_2'(2)$, $B_1'(1)$ and $B_2'(1)$ are influenced mainly by orbital excited states and therefore their energies deviate obviously from those of the non-mixed spin-eigenstates. While $A_1'(1)$ and $A_1'(5)$ are mainly influenced by each other within the orbital ground state (of course still due to the results of the complete configuration mixing). Therefore the zero-field splitting parameter D can be determined by the secular equation of H_s between only $A_1'(1)$ and $A_1'(5)$:

$$\begin{vmatrix} \langle A_1'(1) | S_z^2 | A_1'(1) \rangle D - \lambda & \langle A_1'(1) | S_z^2 | A_1'(5) \rangle D \\ \langle A_1'(5) | S_z^2 | A_1'(1) \rangle D & \langle A_1'(5) | S_z^2 | A_1'(5) \rangle D - \lambda \end{vmatrix} = 0 \quad (19)$$

where $\langle \Gamma'(i) | S_z^2 | \Gamma'(j) \rangle$ can be calculated according to the relations shown in Appendix 3 by the eigenvectors. Using the calculated values of $\langle A_1'(i) | S_z^2 | A_1'(j) \rangle$, the $\Gamma_1' | S_z^2 | \Gamma_2' \rangle D$ of two observed energies $A_1'(1)[0]$ and $A_1'(5)[33.767]$ must correspond to $0.1491D$ ($A_1'(1)$) and $3.9857D$ ($A_1'(5)$) respectively. From these values we have determined $D = 8.8035 \text{ cm}^{-1}$.

A comparison of the low-lying Γ' levels with the corresponding levels of spin eigenstates is shown in figure 2.

5. Conclusion

To sum up, we have proposed an EPR theory for cases of undegenerated complete configuration-mixed wavefunctions. An important modification in concept is that the EPR is calculated between different eigenstates of the irreducible representations of C_{2v}^* , which are spin-projection-mixed states in this paper, instead of spin eigenstates with $\Delta S = \pm 1$ as for the previous concept. Only when the applied magnetic field is very strong can these states be superimposed to get spin eigenstates and the EPR absorption occur between spin eigenstates.

By our theory, good calculated results have been obtained for $ZnS:Fe^{2+}$. They are the fine structure of the absorption spectrum with $\Delta S = 0$, the selection rule for magnetic dipole transitions, the g -values of the spin-Hamiltonian, the zero-field splitting parameters and the Zeeman corrections. All these are calculated by means of the strong-field matrix of $C_{2v}^*(d^6)$ for $S = 2$. All formulae obtained in this paper can easily be generalised to complex ions with various types of C_{2v} distortion. At the same time they can be also applied to a d^4 system (such as Cr^{2+}).

It should be indicated that the EPR absorption of customary Fe^{2+} complexes can hardly be observed, owing to the large zero-field splitting. However, in the cases of very low symmetry, such as C_{2v} symmetrical $ZnS:Fe^{2+}$, the spin degeneracy of the spatial ground state is completely removed and between some of its higher lying split states the Zeeman energy interval may be near 1 cm^{-1} . Thus if the condition $M_s = \pm 1$ is satisfied an EPR will possibly be observed. This possibility has already been proved in the calculated result of this paper, as shown in figure 2. Of course the measurement is difficult. This is why there is very little experimental EPR data on complexes of this kind.

Acknowledgment

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Appendix 1
The strong-field matrices of $d^4(C_{2v}^*)$ with $S = 2^+$.

Γ'	Γ''	$S\Gamma'$	$S\Gamma''$	N	1	2	3	4	5	6	7
				O							
A_1	A_1	5E	$t_2^2(^4A_2)e$	1	$-\frac{1}{3}(d_3 - d_4)$	$-1\sqrt{6}\xi$	$\frac{1}{3}(d_4 - d_3)$			$-\frac{d_{45}}{\sqrt{5}}$	$\frac{\sqrt{3}}{\sqrt{10}}d_{45}$
A_1	A_1	5T_2	$t_2^2(^3T_1)e^2(^3A_2)$	2	$-1\sqrt{6}\xi$	$-\frac{1}{3}(d_1 + d_2 + d_3 + d_6) + d_4 - \frac{1}{3}\xi$		$\frac{d_1 + d_2}{3\sqrt{2}} - \frac{\sqrt{2}}{3}d_5$	$-\frac{d_{45}}{\sqrt{3}}$	$-\frac{d_1 - d_2}{\sqrt{10}}$	$-\frac{d_1 - d_2}{\sqrt{15}}$
A_1	E'	5E	$t_2^2(^4A_2)e$	3	$\frac{1}{3}(d_4 - d_3)$		$-\frac{1}{3}(d_3 - d_4)$	$-\frac{\sqrt{3}}{2}\xi$		$\frac{d_{45}}{\sqrt{5}}$	$-\frac{\sqrt{3}}{\sqrt{10}}d_{45}$
A_1	E'	5T_2	$t_2^2(^3T_1)e^2(^3A_2)$	4		$\frac{d_1 + d_2}{3\sqrt{2}} - \frac{\sqrt{2}}{3}d_5$	$-\frac{\sqrt{3}}{2}\xi$	$-\frac{1}{3}(d_1 + d_2) - \frac{1}{3}d_3 + d_4 + \frac{1}{4}\xi$	$-\frac{\sqrt{2}}{\sqrt{3}}d_{45}$	$\frac{1}{2\sqrt{5}}(d_1 - d_2)$	$\frac{1}{\sqrt{30}}(d_1 - d_2)$
A_1	T_2	5E	$t_2^2(^4A_2)e$	5		$-\frac{d_{45}}{\sqrt{3}}$		$-\frac{\sqrt{2}}{\sqrt{3}}d_{45}$		$\frac{3}{2\sqrt{10}}\xi$	$\frac{\sqrt{3}}{2\sqrt{5}}\xi$
A_1	T_2	$^5T_{21}$	$t_2^2(^3T_1)e^2(^3A_2)$	6	$-\frac{d_{45}}{\sqrt{5}}$	$-\frac{d_1 - d_2}{\sqrt{10}}$	$\frac{d_{45}}{\sqrt{5}}$	$\frac{d_1 - d_2}{2\sqrt{5}}$	$\frac{3}{2\sqrt{10}}\xi$	$-\frac{1}{10}(d_1 + d_2) - \frac{1}{3}d_3 + d_4 + \frac{1}{4}\xi$	$-\frac{\sqrt{6}}{10}(d_1 + d_2) + \frac{\sqrt{6}}{5}d_5$
A_1	T_2	$^5T_{23}$	$t_2^2(^3T_1)e^2(^3A_2)$	7	$\frac{\sqrt{3}}{\sqrt{10}}d_{45}$	$-\frac{d_1 - d_2}{\sqrt{15}}$	$-\frac{\sqrt{3}}{\sqrt{10}}d_{45}$	$\frac{d_1 - d_2}{\sqrt{30}}$	$\frac{\sqrt{3}}{2\sqrt{5}}\xi$	$-\frac{\sqrt{6}}{10}(d_1 + d_2) + \frac{\sqrt{6}}{5}d_5$	$-\frac{1}{10}(d_1 + d_2) - \frac{1}{3}d_3 + d_4 - \frac{1}{2}\xi$
B	T_1	5E	$t_2^2(^4A_2)e$	1	$\frac{1}{3}(d_4 - d_3)$	$\frac{d_{45}}{2\sqrt{2}}$	$-\frac{d_{45}}{2}$	$-\frac{\sqrt{3}}{4}(d_4 - d_3)$	$-\frac{3}{2\sqrt{10}}d_{45}$	$-\frac{\sqrt{3}}{2\sqrt{5}}d_{45}$	$-\frac{\sqrt{3}}{2\sqrt{5}}d_{45}$
B	T_1	$^5T_{22}$	$t_2^2(^3T_1)e^2(^3A_2)$	2	$\frac{d_{45}}{2\sqrt{2}} - \frac{\sqrt{6}}{4}\xi$	$-\frac{1}{6}\sqrt{6}\xi$	$-\frac{1}{3}\sqrt{3}\xi$	$-\frac{d_{45}}{2\sqrt{6}}$	$\frac{d_5 - d_1}{2\sqrt{5}}$	$\frac{\sqrt{3}}{2\sqrt{10}}d_1 - \frac{\sqrt{5}}{2\sqrt{6}}d_2 + \frac{d_5}{\sqrt{30}}$	$\frac{\sqrt{3}}{2\sqrt{10}}d_1 - \frac{\sqrt{5}}{2\sqrt{6}}d_2 + \frac{d_5}{\sqrt{30}}$
B	T_1	$^5T_{23}$	$t_2^2(^3T_1)e^2(^3A_2)$	3	$-\frac{d_{45}}{2} - \frac{\sqrt{3}}{2}\xi$	$-\frac{d_1 + d_2}{6\sqrt{2}} + \frac{d_5}{3\sqrt{2}} + d_4 - \frac{\xi}{6} + 4$	$\frac{d_1}{12} - \frac{d_2}{12} + \frac{d_5}{3\sqrt{2}} + d_4 - \frac{1}{3}\xi$	$-\frac{d_{45}}{2\sqrt{3}}$	$-\frac{d_1 + 2d_5}{2\sqrt{10}} - \frac{3d_2}{2\sqrt{10}}$	$-\frac{3d_1}{4\sqrt{15}} + \frac{d_2}{4\sqrt{15}} - \frac{d_5}{\sqrt{15}}$	

B_1^1	T_2^1	5E	$t_2^3({}^4A_2)e$	4	$-\frac{\sqrt{3}}{4}(d_4 - d_3)$	$\frac{d_{45}}{2\sqrt{6}}$	$-\frac{d_{45}}{2\sqrt{3}}$	$-\frac{3}{4}d_3 + \frac{3}{4}d_4$	$-\frac{\sqrt{3}}{2\sqrt{10}}d_{45}$	$-\frac{d_{45}}{2\sqrt{5}} + \frac{\sqrt{3}}{2\sqrt{10}}\zeta$
B_1^1	T_2^1	${}^5T_{21}$	$t_2^3({}^3T_1)e^2({}^3A_2)$	5	$-\frac{3}{2\sqrt{10}}d_{45}$	$\frac{d_5 - d_1}{2\sqrt{5}}$	$\frac{1}{2\sqrt{10}}(3d_2 - d_1)$	$-\frac{\sqrt{3}}{2\sqrt{10}}d_{45}$	$-\frac{3\sqrt{3}}{10\sqrt{2}}d_1 - \frac{\sqrt{3}d_2}{10\sqrt{2}}$	$-\frac{d_{45}}{5\sqrt{2}}d_5$
B_1^1	T_1^1	${}^5T_{23}$	$t_2^3({}^3T_1)e^2({}^3A_2)$	6	$-\frac{\sqrt{3}}{2\sqrt{5}}d_{45}$	$\frac{\sqrt{3}}{2\sqrt{10}}d_1 - \frac{d_5}{2\sqrt{6}}d_2$	$\frac{3}{4\sqrt{15}}d_1 + \frac{d_2}{4\sqrt{15}}$	$-\frac{\sqrt{3}}{2\sqrt{5}}d_{45}$	$-\frac{3\sqrt{3}}{10\sqrt{2}}d_1 - \frac{\sqrt{3}d_2}{10\sqrt{2}}$	$-\frac{2d_1 - 3d_2}{3d_5 + d_4 + \frac{2}{3}\zeta}$
A_2^2	A_2^2	5E	$t_2^3({}^4A_2)e$	1	$-\frac{1}{2}(d_3 - d_4)$	$\frac{1}{2}(d_4 - d_3)$	$-\frac{d_5}{\sqrt{15}}$	$-\frac{d_{45}}{\sqrt{3}}$	$-\frac{d_{45}}{\sqrt{6}}$	
A_2^2	E^1	5E	$t_2^3({}^4A_2)e$	2	$\frac{1}{2}(d_4 - d_3)$	$-\frac{1}{2}(d_3 - d_4)$	$\frac{\sqrt{3}}{2}\zeta$	$\frac{d_{45}}{\sqrt{3}}$	$\frac{d_{45}}{\sqrt{6}}$	
A_2^2	E^1	5T_2	$t_2^3({}^3T_1)e^3({}^3A_2)$	3	$-\frac{\sqrt{3}}{2}\zeta$	$-\frac{\sqrt{3}}{2}\zeta$	$-\frac{1}{2}(d_1 + d_2) + d_4 + \frac{1}{2}\zeta$	$\frac{d_1 - d_2}{2\sqrt{3}}$	$\frac{d_2 - d_1}{\sqrt{6}}$	
A_2^2	T_1^1	5E	$t_2^3({}^4A_2)e$	4				$-d_3 + d_4$	$-\frac{1}{2}\sqrt{6}\zeta$	
A_2^2	T_1^1	${}^5T_{22}$	$t_2^3({}^3T_1)e^2({}^3A_2)$	5	$-\frac{d_{45}}{\sqrt{3}}$	$\frac{d_{45}}{\sqrt{3}}$	$\frac{d_1 - d_2}{2\sqrt{3}}$	$-\frac{1}{2}\sqrt{6}\zeta$	$-\frac{1}{2}\sqrt{6}\zeta$	$-\frac{1}{3}\sqrt{3}\zeta$
A_2^2	T_1^1	${}^5T_{25}$	$t_2^3({}^3T_1)e^2({}^3A_2)$	6	$-\frac{d_{45}}{\sqrt{6}}$	$\frac{d_{45}}{\sqrt{6}}$	$\frac{d_2 - d_1}{\sqrt{6}}$	$-\frac{1}{2}\sqrt{3}\zeta$	$\frac{1}{3\sqrt{2}}(d_1 + d_2)$	$-\frac{\zeta}{3}d_5$

†(1) With the substitution of $d_1 \rightarrow -d_2$ and $d_{45} \rightarrow -d_{45}$, the B_1^1 matrix will be changed into B_2^2 matrix.

(2) $6A - 21B + d_1 + d_2 + d_3 + d_5$ has been subtracted from each diagonal element.

(3) For d^6 , the signs of the parameters d_i ($i = 1$ to 5), d_{45} and ζ in the above d_4 matrices should be changed.

(4) For tetrahedral field, one should make $d_i \rightarrow -d_i$ and $d_{45} \rightarrow -d_{45}$.

Appendix 2. The energy matrices for Zeeman correction. Where $A_1'(7)$, $A_2'(6)$, $B_1'(6)$ and $B_2'(6)$ are the matrices in Appendix 1. $H_\alpha = 0.466868B_\alpha$.

$$\left[\begin{array}{c|cccccc}
 & H_z & -\frac{H_z}{\sqrt{6}} & \frac{H_z}{\sqrt{3}} & \sqrt{3}H_z & \frac{\sqrt{3}}{\sqrt{10}}H_z & \frac{H_z}{\sqrt{5}} \\
 B_1'(6) & -\frac{H_z}{\sqrt{6}} & -\frac{3H_z}{2} & \sqrt{2}H_z & \frac{H_z}{\sqrt{2}} & -\frac{9}{2\sqrt{5}}H_z & \frac{\sqrt{6}}{\sqrt{5}}H_z \\
 & \frac{H_z}{\sqrt{3}} & \sqrt{2}H_z & \frac{H_z}{2} & -H_z & 0 & -\frac{\sqrt{15}}{2}H_z \\
 & \sqrt{3}H_z & \frac{H_z}{\sqrt{2}} & -H_z & -H_z & -\frac{3}{\sqrt{10}}H_z & -\frac{\sqrt{3}}{\sqrt{5}}H_z \\
 & \frac{\sqrt{3}}{\sqrt{10}}H_z & -\frac{9}{2\sqrt{5}}H_z & 0 & -\frac{3}{\sqrt{10}}H_z & -\frac{7}{2}H_z & 0 \\
 & \frac{H_z}{\sqrt{5}} & \frac{\sqrt{6}}{\sqrt{5}}H_z & -\frac{\sqrt{15}}{2}H_z & -\frac{\sqrt{3}}{\sqrt{5}}H_z & 0 & \frac{3}{2}H_z \\
 \hline
 HC & & & & & & B_2'(6)
 \end{array} \right]$$

$$\left[\begin{array}{c|cccccc}
 & 0 & 0 & 0 & 0 & 2\sqrt{2}H_z & -\frac{2}{\sqrt{5}}H_z & \frac{\sqrt{6}}{\sqrt{5}}H_z \\
 A_2'(6) & 0 & 0 & 0 & 0 & -2\sqrt{2}H_z & -\frac{2}{\sqrt{5}}H_z & \frac{\sqrt{6}}{\sqrt{5}}H_z \\
 & 0 & 0 & 0 & 0 & 0 & \frac{3\sqrt{3}}{\sqrt{5}}H_z & \frac{3\sqrt{2}}{\sqrt{5}}H_z \\
 & 2\sqrt{2}H_z & -\frac{2}{\sqrt{3}}H_z & 2\sqrt{2}H_z & -\frac{4}{\sqrt{6}}H_z & 0 & 0 & 0 \\
 & -\frac{2}{\sqrt{3}}H_z & \sqrt{2}H_z & -\frac{2}{\sqrt{3}}H_z & 3H_z & 0 & 0 & 0 \\
 & -\frac{\sqrt{2}}{\sqrt{3}}H_z & 2H_z & -\frac{\sqrt{2}}{\sqrt{3}}H_z & \frac{2\sqrt{2}}{3}H_z & 0 & 0 & 0 \\
 \hline
 HC & & & & & & & A_1'(7)
 \end{array} \right] \quad H_z = 0.466803B_z$$

$B_1^1(6)$	$2H_x$	$-\frac{\sqrt{2}}{\sqrt{3}}H_x$	$-H_x$	$\frac{H_x}{\sqrt{3}}$	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{\sqrt{10}}$	0	$\frac{H_x}{\sqrt{3}H_x}$	0	$-H_x$	$-\frac{H_x}{\sqrt{2}}$	$\frac{H_x}{2\sqrt{3}}$	$-\frac{H_x}{\sqrt{6}}$	
	$-\frac{\sqrt{2}}{\sqrt{3}}H_x$	H_x	$\frac{H_x}{\sqrt{6}}$	$-\frac{3}{2\sqrt{2}}H_x$	$\frac{H_x}{2}$	$\frac{\sqrt{3}}{2\sqrt{10}}H_x$	0	0	$\frac{H_x}{\sqrt{2}}$	$\frac{9}{2\sqrt{6}}H_x$	$\frac{H_x}{2\sqrt{3}}$	$\frac{9}{6\sqrt{2}}H_x$	$-H_x$	
	$\frac{H_x}{\sqrt{3}}$	$\sqrt{2}H_x$	$\frac{H_x}{2\sqrt{3}}$	$-\frac{H_x}{2}$	$-\frac{H_x}{\sqrt{2}}$	0	$\frac{3\sqrt{5}}{2\sqrt{6}}H_x$	0	$\frac{H_x}{2}$	$\frac{\sqrt{3}}{2}H_x$	$-\frac{H_x}{\sqrt{6}}$	$-\frac{H_x}{2}$	$\frac{H_x}{2\sqrt{2}}$	
	0	0	$-\sqrt{3}H_x$	0	$\frac{H_x}{\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$-2H_x$	$-H_x$	0	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{2}$	$-\frac{H_x}{\sqrt{2}}$	
	0	0	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$\frac{9}{2\sqrt{10}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{7}{2\sqrt{2}}H_x$	0	$\frac{\sqrt{2}}{\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{3\sqrt{3}}{2\sqrt{10}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$-\frac{9}{2\sqrt{10}}H_x$	0	
	0	0	$\frac{3}{2\sqrt{5}}H_x$	$\frac{3\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	0	$-\frac{3}{2\sqrt{2}}H_x$	$-\frac{\sqrt{3}}{\sqrt{5}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{H_x}{\sqrt{5}}$	$\frac{\sqrt{15}}{2\sqrt{2}}H_x$	
	$B_2^1(6)$	$2H_x$	$-\frac{\sqrt{2}}{\sqrt{3}}H_x$	$-H_x$	$\frac{H_x}{\sqrt{3}}$	$-\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{\sqrt{10}}$	0	$\sqrt{3}H_x$	$-H_x$	$-\frac{H_x}{\sqrt{2}}$	$-\frac{H_x}{2\sqrt{3}}$	$\frac{H_x}{\sqrt{6}}$	H_x
		$-\frac{\sqrt{2}}{\sqrt{3}}H_x$	H_x	$\frac{H_x}{\sqrt{6}}$	$-\frac{3}{2\sqrt{2}}H_x$	$\frac{H_x}{2}$	$\frac{\sqrt{3}}{2\sqrt{10}}H_x$	0	0	$\frac{H_x}{\sqrt{2}}$	$\frac{9}{2\sqrt{6}}H_x$	$-\frac{9}{6\sqrt{2}}H_x$	H_x	H_x
		$\frac{H_x}{\sqrt{3}}$	$\sqrt{2}H_x$	$\frac{H_x}{2\sqrt{3}}$	$-\frac{H_x}{2}$	$-\frac{H_x}{\sqrt{2}}$	0	$\frac{\sqrt{15}}{2\sqrt{2}}H_x$	0	$\frac{H_x}{2}$	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{\sqrt{6}}$	H_x	$\frac{H_x}{2\sqrt{2}}$
		0	0	$-\sqrt{3}H_x$	0	$\frac{H_x}{\sqrt{2}}$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$-2H_x$	$-H_x$	0	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{2}$	$\frac{H_x}{\sqrt{2}}$
		0	0	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$\frac{9}{2\sqrt{10}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{7}{2\sqrt{2}}H_x$	0	$\frac{\sqrt{2}}{\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{3\sqrt{3}}{2\sqrt{10}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$-\frac{9}{2\sqrt{10}}H_x$	0
		0	0	$\frac{3}{2\sqrt{5}}H_x$	$\frac{3\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	0	$-\frac{3}{2\sqrt{2}}H_x$	$-\frac{\sqrt{3}}{\sqrt{5}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{H_x}{\sqrt{5}}$	$\frac{\sqrt{15}}{2\sqrt{2}}H_x$
$A_1^1(7)$	0	0	$-\sqrt{3}H_x$	0	$\frac{H_x}{\sqrt{2}}$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$-2H_x$	$-H_x$	0	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{2}$	$\frac{H_x}{\sqrt{2}}$	
	0	0	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$\frac{9}{2\sqrt{10}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{7}{2\sqrt{2}}H_x$	0	$\frac{\sqrt{2}}{\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{3\sqrt{3}}{2\sqrt{10}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$-\frac{9}{2\sqrt{10}}H_x$	0	
	0	0	$\frac{3}{2\sqrt{5}}H_x$	$\frac{3\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	0	$-\frac{3}{2\sqrt{2}}H_x$	$-\frac{\sqrt{3}}{\sqrt{5}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{H_x}{\sqrt{5}}$	$\frac{\sqrt{15}}{2\sqrt{2}}H_x$	
	0	0	$-\sqrt{3}H_x$	0	$\frac{H_x}{\sqrt{2}}$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$-2H_x$	$-H_x$	0	$\frac{\sqrt{3}}{2}H_x$	$\frac{H_x}{2}$	$\frac{H_x}{\sqrt{2}}$	
	0	0	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	$\frac{9}{2\sqrt{10}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{7}{2\sqrt{2}}H_x$	0	$\frac{\sqrt{2}}{\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{3\sqrt{3}}{2\sqrt{10}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$-\frac{9}{2\sqrt{10}}H_x$	0	
	0	0	$\frac{3}{2\sqrt{5}}H_x$	$\frac{3\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{\sqrt{6}}{2\sqrt{5}}H_x$	0	$-\frac{3}{2\sqrt{2}}H_x$	$-\frac{\sqrt{3}}{\sqrt{5}}H_x$	$\frac{\sqrt{3}}{2\sqrt{5}}H_x$	$\frac{3}{2\sqrt{5}}H_x$	$\frac{H_x}{\sqrt{10}}$	$\frac{H_x}{\sqrt{5}}$	$\frac{\sqrt{15}}{2\sqrt{2}}H_x$	
HC	0													
	$A_2^1(6)$													

$$H_x = 0.466803B_x$$

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