

STUDY OF THE ABSORPTION SPECTRA OF THE Fe^{2+} AND K_2FeF_4 SYSTEMS

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Abstract: The d-orbital energy level splitting of free Fe^{2+} ions under electrostatic and spin-orbit interactions leads to d-electron rearrangement and the formation of different energy states, which may result in the occurrence of electron jumps between different energy levels. When Fe^{2+} is doped with K_2FeF_4 , the combination of electrons in the Fe^{2+} d-orbitals changes, and accordingly new d-d absorption spectra are generated. In this thesis, from the crystal field theory, the center field approximation method, crystal field matrix meta-algorithm and electron spin-orbit interaction matrix meta-algorithm are used in the study to establish the Hamiltonian quantities of the system and to calculate the fine spectra of the system. Diagonalizing the full energy matrix can yield the Fe^{2+} d-d absorption spectra, and by analyzing the experimental EPR zero-field splitting (ZFS) parameters Dq , B , C , and Z and combining them with the full energy matrix, the energy values of the Fe^{2+} energy levels can be derived, and the results of this study show that the theoretical values conform well to the experimental values. My research data can provide some theoretical references for the study of the spectra of crystal doped Fe^{2+} ions. However, there are also experimental data that have not been derived, and it is expected that they can be supplemented and improved in the future.

Keywords: D-d absorption spectroscopy; EPR parameter; Crystal field theory

1 INTRODUCTION

In recent years, complex crystals of transition metal ions have great prospects for many applications, and these crystals are often widely used as good optoelectronic materials and nonlinear optical materials, etc. Especially when transition metals are doped in semiconductors in trace amounts, its optical and magnetic properties change dramatically, so the theoretical and experimental study of electron paramagnetic resonance (EPR) of transition metals has been a hot spot in the field of crystal fields. The crystal field theory has been tightly integrated with spectroscopy and EPR techniques, which has led to further investigation of the optical and magnetic properties of doped transition metal ion crystals [1]. Hamiltonian of the cubic system in the absence of an external magnetic field: $H = H^{ee}(B, C) + V^{A_1}(D_q) + H^{so}(\zeta)$. According to quantum mechanics, the full energy matrix elements are obtained, each of which is a function of Dq , B , C , ζ . The Hamiltonian coefficients Dq , B , C , ζ are obtained by experimental fitting, so that the eigenvalues of the Hamiltonian quantities can be obtained, and the absorption spectra of Fe^{2+} can be obtained by jumping between energy levels [2]. The central field approximation, full energy matrix method and theories related to crystal fields are adopted in the process of investigating the case of free Fe^{2+} under electrostatic and spin-orbit effects, where the splitting of its d-orbital energy levels leads to the rearrangement of the d-electrons and the formation of different energy states, which may lead to the occurrence of the leaps of the electrons between the different energy levels. Under the center-field approximation, following the symmetry of the group O_h to form the standard d-orbitals in the text, we then arrive at the fact that for the d_6 electronic grouping state there should be 210 energy levels if there is no simplicial merger. The free Fe^{2+} ion has six electrons in the d-orbital, and its Hamiltonian consists of two terms: the electrostatic interaction term between the electrons and the spin-orbit interaction term of the electrons. Using the previous single-electron wave function we can construct 210 basis functions for the d_6 system, each of which is a combinatorial form of the determinant wave function [3].

This paper is a series of systematic studies of 3d energy levels and 3d ions in crystals, where in many crystals the ground state is a spin=2 orbital, for which it exhibits a large zero-field splitting (ZFS). In the last decades, most theoretical studies of the ZFS of 3d energy levels and 3d ions in crystals have been based on the D approximation, i.e., considering only the contribution of the high-spin state D of these ions to the ZFS and neglecting the low-spin state L ($L=DG$), however, spin-orbit (SO) and spin-spin (SS) interactions have triggered the validity of the D approximation to make the energy of the L much larger than that of the D state, the spin triplet state's contribution to ZFS may be small. This is significant for understanding the microscopic mechanism of crystal doping and may further provide a favorable theoretical basis for material designers.

2 DOCTRINAL

2.1 $d^1(O_h)$ System Standard Base-standard D-track

Under the central field approximation, the one-electron solution of the fixed-state Schrödinger equation is

$$R_{nl}(r)Y_{lm}(\theta\varphi)$$

When $l = 2$, five standard d-orbitals are formed according to the symmetry of the group Oh as follows [4]:

$$\begin{aligned}
 d_1 = \theta = d_{z^2} &= R_d Z_{20}^c = R_d \frac{1}{\sqrt{2\pi}} \sqrt{\frac{5}{8}} (3 \cos^2 \theta - 1) \sim 3z^2 - r^2 \\
 d_2 = \varepsilon = d_{x^2-y^2} &= R_d Z_{22}^c = R_d \frac{1}{\sqrt{\pi}} \sqrt{\frac{15}{16}} \sin^2 \theta \cos 2\theta \sim \sqrt{3}(x^2 - y^2) \\
 d_3 = \xi = d_{yz} &= R_d Z_{21}^s = R_d \frac{1}{\sqrt{\pi}} \sqrt{\frac{15}{4}} \sin \theta \cos \theta \sin \varphi \sim yz \\
 d_4 = \eta = d_{xz} &= R_d Z_{21}^c = R_d \frac{1}{\sqrt{\pi}} \sqrt{\frac{15}{4}} \sin \theta \cos \theta \cos \varphi \sim xz \\
 d_5 = \zeta = d_{xy} &= R_d Z_{22}^s = R_d \frac{1}{\sqrt{\pi}} \sqrt{\frac{15}{16}} \sin^2 \theta \sin 2\varphi \sim xy
 \end{aligned} \tag{1}$$

The tracks are divided into two groups as follows

$$\left. \begin{array}{l} \theta = d_{z^2} \\ \varepsilon = d_{x^2-y^2} \end{array} \right\} \text{Genus eg,} \quad \left. \begin{array}{l} \xi = d_{yz} \\ \eta = d_{zx} \\ \zeta = d_{xy} \end{array} \right\} \text{Genus t2g} \tag{2}$$

constitute the standard d-orbitals of the incommensurable representations Eg and T2g, respectively, giving 10 spin d-orbitals when the spins are accounted for:

$$\begin{array}{c} \theta, \varepsilon, \xi, \eta, \zeta, \\ \bar{\theta}, \bar{\varepsilon}, \bar{\xi}, \bar{\eta}, \bar{\zeta} \end{array}$$

where the first five orbitals spin up and the last five spin down. The Slater function is a normalized determinant of order m consisting of any m distinct d-orbitals dk_1, dk_2, \dots, dk_m , abbreviated as $|dk_1 dk_2 \dots dk_m|$. It satisfies the antisymmetry requirement of the Bubbleley principle. In the d-orbit expression, R_d stands for $R_{n^2}(r)$; $Z_{20}^c, Z_{22}^c, Z_{21}^s, Z_{21}^c, Z_{22}^s$ is a real spherical harmonic function consisting of $Y_{2m}(\theta, \varphi)$ [5];

$$\begin{aligned}
 Z_{20}^c &= Y_{20} \\
 Z_{22}^c &= \frac{1}{\sqrt{2}}(Y_{22} + Y_{2-2}) & Z_{21}^s &= \frac{1}{\sqrt{2}}(Y_{21} + Y_{2-1}) \\
 Z_{21}^c &= -\frac{1}{\sqrt{2}}(Y_{21} - Y_{2-1}) & Z_{22}^s &= -\frac{1}{\sqrt{2}}(Y_{21} - Y_{2-1})
 \end{aligned} \tag{3}$$

These real spherical harmonic functions satisfy the following relations:

$$\begin{aligned}
 Z_{l0}^s &= 0 \\
 \langle Z_{l\alpha} | Z_{l'\alpha'} \rangle &= \delta_{ll'} \delta_{\alpha\alpha'}
 \end{aligned} \tag{4}$$

2.2 $d^4(O_h)$ Derivation of the Standard Basis Functions of the System

A strong-field group state is a cubic field group state defined by m t-electrons and n e-electrons, denoted $t_2^m e^n$. The cubic crystal field energies of all states belonging to a strong-field group state are simply merged:

$$E(t_2^m e^n) = mE(t_{2g}) + nE(e_g) \tag{5}$$

These groupings are divided into subgroups by electrostatic interactions between the dN electrons, and each subgroup has a certain spin S belonging to a certain irreducible representation Γ of Oh. The totality of the states of a subgroup is called a strong-field spectral term $S\Gamma$, or denoted $2S+1 \Gamma$.

The strong-field spectral term wavefunction can be coupled into the strong-field spectral term wavefunction of the general grouping according to the following equation $t_2^m e^n$ [6]:

$$\begin{aligned}
 &|t_2^m(S_1 \Gamma_1) e^n(S_2 \Gamma_2), S \Gamma M \gamma\rangle \\
 &= \sum_{M_1 M_2} \langle S_1 S_2 M_1 M_2 | S M \rangle \sum_{\gamma_1 \gamma_2} \langle \Gamma_1 \Gamma_2 \gamma_1 \gamma_2 | \Gamma \gamma \rangle \\
 &\quad \cdot |t_2^m(S_1 \Gamma_1 M_1 \gamma_1)\rangle \otimes |e^n(S_2 \Gamma_2 M_2 \gamma_2)\rangle
 \end{aligned} \tag{6}$$

included among these

$$\langle S_1 S_2 M_1 M_2 | SM \rangle = \left\{ \frac{(S+M)!(S-M)!(S_1-M_1)!(S_2-M_2)!(S_1+S_2-S)!(2S+1)}{(S_1+M_1)!(S_2+M_2)!(S_1-S_2+S)!(S_2-S_1+S)!(S_1+S_2+S+1)!} \right\}^{1/2} \quad (7)$$

$$\times \delta(M, M_1 + M_2) \sum_r (-1)^{S_1+r-M_1} \frac{(S_1+M_1+r)!(S_2+S-r-M_1)!}{r!(S-M-r)!(S_1-M_1-r)!(S_2-S+M_1+r)!}$$

The "direct multiplication" method yields a Slater function of order m+n from an m-order and an n-order Slater function in the following way:

$$\left| d_{k_1} d_{k_2} \cdots d_{k_m} \right| \otimes \left| d_{p_1} d_{p_2} \cdots d_{p_n} \right| = \left| d_{k_1} d_{k_2} \cdots d_{k_m} d_{p_1} d_{p_2} \cdots d_{p_n} \right| \quad (8)$$

thereby automatically satisfying the antisymmetrization requirement. We agree that t-electron comes first and e-electron comes second.

The number of strong-field spectral term wavefunctions $\Psi = |t_2^m(S_1 \Gamma_1) e^n(S_2 \Gamma_2), S \Gamma M \gamma\rangle$ corresponding to the d⁶(O_h) system is 210.

3 CALCULATION OF MATRIX ELEMENTS

3.1 Computation of Electrostatic Matrix Elements

3.1.1 Two theorems related to the computation of electrostatic matrix elements

1. orthogonality theorem for invariant operator matrix elements
2. Wigner-Eckart theorem

Assuming that $|\alpha j m\rangle$ denotes a common eigenstate of (J², J_z) and T_q^k is an irreducible tensor operator, one has

$$\langle \alpha' j' m' | T_q^k | \alpha j m \rangle = \langle j m k q | j' m' \rangle \frac{1}{\sqrt{2j'+1}} \langle \alpha' j' || T^k || \alpha j \rangle \quad (9)$$

3.1.2 The diagonal elements of the electrostatic matrix are

$$V_{ii} = \langle \varphi_i | \hat{V} | \varphi_i \rangle = \sum_{k < \lambda}^N [J(k, \lambda) - K(k, \lambda)] \quad (10)$$

included among these

Coulomb integral (math.): $J(k, \lambda) = J(d_k^i, d_\lambda^i) = \langle d_k^i d_\lambda^i | V | d_k^i d_\lambda^i \rangle = (d_k^i d_k^i; d_\lambda^i d_\lambda^i)$

Exchange Points: $K(k, \lambda) = K(d_k^i, d_\lambda^i) = \langle d_\lambda^i d_k^i | V | d_k^i d_\lambda^i \rangle = (d_\lambda^i d_k^i; d_k^i d_\lambda^i)$

3.1.3 Non-diagonal elements of electrostatic matrices

1. If φ_i and φ_j differ in only one orbit, for example $d_k^i \neq d_k^j$, The rest of the correspondences are the same, then

$$V_{ij} = \sum_{\lambda (\neq k)}^N [(d_k^i d_k^j; d_\lambda^i d_\lambda^i) - (d_k^i d_\lambda^j; d_k^j d_\lambda^i)] \quad (11)$$

2. If only two orbits are different between φ_i and φ_j , for example $d_k^i \neq d_k^j$ and $d_\lambda^i \neq d_\lambda^j$, The rest of the correspondences are the same, then

$$V_{ij} = (d_k^i d_k^j; d_\lambda^i d_\lambda^j) - (d_k^i d_\lambda^j; d_k^j d_\lambda^i) \quad (12)$$

3. If φ_i and φ_j have three or more different orbits, then

$$V_{ij} = 0 \quad (13)$$

4. (ab; cd) is nonzero only if a and b spin in the same direction and c and d also spin in the same direction. where

$$\langle ab | V | cd \rangle \equiv \langle ac; bd \rangle \equiv \langle a(1)b(2) | V(12) | c(1)d(2) \rangle \quad (14)$$

ac and bd are about the 1st and 2nd electrons, respectively. For real d-orbitals:

$$\langle ab; cd \rangle = \langle ba; cd \rangle = \langle ab; dc \rangle = \langle cd; ab \rangle \quad (15)$$

3.2 Calculation of Cubic Crystal Field Matrix Elements

The crystal field potential of the N ligands considered as point charges (coordinates R_p(R_p, θ_p, φ_p)) is

$$V(r, \theta, \varphi) = \sum_{p=1}^N \frac{q_p}{|\vec{R}_p - \vec{r}|} \quad (16)$$

assume

$$V = \sum_{p=1}^N \sum_{k=0}^{\infty} \frac{4\pi q_p}{2k+1} \frac{r_{<}^k}{r_{>}^{k+1}} \sum_{\alpha} Z_{k\alpha}(\theta_p \varphi_p) Z_{k\alpha}(\theta \varphi) \quad (17)$$

In the d-electron problem, only the k=0, 2, 4 terms are meaningful.

The single-electron crystal field potential matrix element can be written as [7]

$$d_{ij} = -eq_0 [P_{ij}(r^2) + Q_{ij}(r^4)] \quad (18)$$

included among these

$$S_{ij} = \beta_{00} C_{00}^{ij} = \beta_{00} \delta_{ij} = \left(\sum_{p=1}^N \frac{1}{R_p} \right) \delta_{ij} \quad (19)$$

$$P_{ij} = \sum_{\alpha} C_{2\alpha}^{ij} \beta_{2\alpha} \quad (20)$$

$$Q_{ij} = \sum_{\alpha} C_{4\alpha}^{ij} \beta_{4\alpha} \quad (21)$$

$$\beta_{k\alpha} = \frac{\sqrt{4\pi}}{2k+1} \sum_{p=1}^N Z_{k\alpha}(\theta_p, \varphi_p) / R_p^{k+1} \quad (22)$$

The crystal field operator is a single-electron operator, and the crystal field matrix elements of the multi-electron system can be reduced to the crystal field matrix elements between determinants, and then to the single-electron crystal field matrix elements, and ultimately to the crystal field coefficients [8].

The crystal field coefficients of an ortho-octahedron are

$$Dq = -eq_0 \frac{\langle r^4 \rangle}{6R^5} \quad (23)$$

The crystal field coefficients of the orthotetrahedron are

$$Dq = \frac{2}{27} \frac{eq_0 \langle r^4 \rangle}{R^5} \quad (24)$$

Then for both of the above cases of cubic symmetry

$$d_{11} = d_{22} = 6Dq \quad d_{33} = d_{44} = d_{55} = -4Dq \quad (25)$$

Thus the cubic crystal field matrix can be calculated in the standard basis functions [9].

3.3 Computation of the Spin-Orbit Matrix Element

3.3.1 Spin-orbit coupling manifolds and standard basis

$d^N(O_h^*)$ Constructive formulae for the standard basis functions of spin-orbit coupled manifolds

$$\begin{aligned} |q_i, S\Gamma\tilde{\Gamma}\beta\Gamma'\gamma'\rangle &= \sum_{\gamma\tilde{\gamma}} |q_i, \check{S}\check{\Gamma}\check{M}\check{\gamma}\rangle |\tilde{\Gamma}\tilde{\gamma}\rangle \langle \tilde{\Gamma}\tilde{\gamma} | \langle q_i, \check{S}\check{\Gamma}\check{M}\check{\gamma} | q_i, S\Gamma\tilde{\Gamma}\beta\Gamma'\gamma'\rangle \\ &= \sum_{\gamma\tilde{\gamma}} |q_i, \check{S}\check{\Gamma}\check{M}\check{\gamma}\rangle |\tilde{\Gamma}\tilde{\gamma}\rangle \langle q_i, \check{S}\check{\Gamma}\check{M}\check{\gamma}\tilde{\Gamma}\tilde{\gamma} | q_i, S\Gamma\tilde{\Gamma}\beta\Gamma'\gamma'\rangle \end{aligned} \quad (26)$$

abbreviated as

$$|q_i, S\Gamma\tilde{\Gamma}\beta\Gamma'\gamma'\rangle = \sum_{\gamma\tilde{\gamma}} \langle \Gamma\gamma\tilde{\Gamma}\tilde{\gamma} | \beta\Gamma'\gamma'\rangle |q_i, \check{S}\check{\Gamma}\check{M}\check{\gamma}\rangle |\tilde{\Gamma}\tilde{\gamma}\rangle \quad (27)$$

3.3.2 Calculation of spin-orbit matrix elements in spin-orbit manifolds

The spin-orbit coupling operator for the N-electron is

$$H_{so} = \sum_k h_{so}(k) = \sum_{\gamma^*=-1}^{+1} V_{\gamma^*-\gamma^*}^{1T_1} (-1)_{1+\gamma^*} \quad (28)$$

included among these

$$\begin{aligned} v_{\gamma^*-\gamma^*}^{1T_1} &= s_{\gamma^*} l_{-\gamma^*} \xi(\Gamma) \\ V_{\gamma^*-\gamma^*}^{1T_1} &= \sum_k v_{\gamma^*-\gamma^*}^{1T_1}(k) \end{aligned} \quad (29)$$

The spin-orbit coupling matrix element between a pair of $S\Gamma\beta$ inside a given $\Gamma'\gamma'$ block is

$$\mathcal{H}_{ij}^{so}(\Gamma', S_1\Gamma_1\beta_1, S_2\Gamma_2\beta_2) = \langle q_i, S_1\Gamma_1\beta_1\Gamma'\gamma' | \mathcal{H}^{so} | q_j, S_2\Gamma_2\beta_2\Gamma'\gamma' \rangle = K' \langle q_i, S_1\Gamma_1 \| V^{1T_1} \| q_j, S_2\Gamma_2 \rangle \quad (30)$$

K' is known as the transfer coefficient.

The spinor matrix element obeys a selection law in the spinor manifold:

$\Gamma_1 \times \Gamma_2$ must contain T_1 (2) $\Delta S = 0, \pm 1$ (3) $\Delta M = 0, \pm 1$

Computation of approximation matrix elements within uncoupled manifolds

$$\begin{aligned} &\langle q_i, S_1\Gamma_1 M_1 \gamma_1 | \mathcal{H}^{so} | q_j, S_2\Gamma_2 M_2 \gamma_2 \rangle \\ &= \langle q_i, S_1\Gamma_1 \| V^{1T_1} \| q_j, S_2\Gamma_2 \rangle \\ &\cdot \sum_{\gamma^*} \frac{\langle S_2 M_2 1 \gamma^* | S_1 M_1 \rangle \langle \Gamma_2 \gamma_2 T_1 - \gamma^* | \Gamma_1 \gamma_1 \rangle}{\sqrt{(2S_1+1) \cdot \lambda(\Gamma_1)}} (-1)^{1+\gamma^*} \end{aligned} \quad (31)$$

4 CALCULATION RESULTS

Theoretical calculations were carried out through a Fortran program, where $B=800\text{cm}^{-1}$, $C=3200\text{cm}^{-1}$, $Z=410\text{cm}^{-1}$, $Dq=0\text{cm}^{-1}$ was taken in the calculations, and the resulting d-d absorption spectra of Fe^{2+} were obtained, as shown in Table 1.

Table 1 D-d Absorption Spectra of Fe^{2+}

energy level	J	Theoretical data(cm ⁻¹)	Experimental data(cm ⁻¹)
3d ⁶	4	0.00	0.000
3d ⁶	3	436.20	422.478
3d ⁶	2	738.90	721.891
3d ⁶	1	932.40	915.202
3d ⁶	0	1027.30	1010.188
3d ⁶	6	20051.10	20043.808
3d ⁶	5	20300.80	20266.731
3d ⁶	4	20481.90	20433.095
3d ⁶	2	21857.20	21930.043
3d ⁶	5	24558.80	25365.580
3d ⁶	4	24904.60	25760.185
3d ⁶	3	25142.40	25942.025
3d ⁶	6	30356.20	30216.503
3d ⁶	4	30886.40	31893.814
3d ⁶	2	40999.80	39783.966

Analyzing Table 1, we can see that the calculated results are basically consistent with the experimental results, and at the same time, we also see that certain energy level errors are relatively large, which may be due to the fact that the above three covariates are derived from fitting with the experiments, and a certain amount of error inevitably exists in the fitting.

Changing the value of Dq, the theoretical calculations were carried out again, and six different sets of data were taken in the calculations B=800cm⁻¹, C=3200cm⁻¹, Z=410cm⁻¹, Dq (cm⁻¹) thus obtaining six sets of absorption spectra, and some of the intercepted data are shown in Table 2.

Table 2 D-d Absorption Spectra of Fe²⁺ for Different Values of Dq

J	Dq=1000	Dq=900	Dq=800	Dq=700	Dq=600	Dq=500
1	0.000	0.000	0.000	0.000	0.000	0.000
1/2	184.501	185.406	185.764	185.551	184.658	182.829
1	200.146	200.758	201.121	201.221	200.999	200.306
0	450.276	453.111	454.320	453.932	451.685	446.902
1	483.480	485.850	487.443	488.318	488.427	487.578
1	505.833	508.196	510.205	511.984	513.628	515.219
0	6855.508	8513.547	8312.435	7314.898	6317.368	5320.061
1	8362.446	9280.636	8313.630	7317.505	6321.654	5326.529
1/2	8393.687	9305.514	8314.797	7320.085	6325.908	5332.940
1	8735.593	9309.666	8317.432	7324.056	6331.572	5340.926
0	9272.042	9310.437	8319.858	7327.920	6337.133	5348.791
1/2	10302.680	9310.482	9949.888	11095.306	11985.258	12858.947
1	10304.180	9313.359	10193.232	11127.496	12018.115	12892.485
1	10304.291	9317.063	10224.885	11137.045	12166.827	13111.188
1	10305.575	9655.897	10567.058	11469.026	12357.996	13228.810
0	10306.700	10421.200	11772.905	13348.132	14619.337	15151.458

5 CONCLUSION

The three research methods used in this thesis are the center-field approximation, the crystal-field matrix meta-algorithm, and the electron spin-orbit interaction matrix meta-algorithm. Under the center-field approximation, a one-electron solution to the Schrödinger equation is obtained, which gives 10 d orbitals when $l = 2$. This leads to the introduction of the number of strong-field spectral term wavefunctions for this system, which is 210, i.e., there are 210 values of energy in the 3d energy level of the Fe²⁺ and K₂FeF₄ system. In this experiment, we reduce the problem of constructing the electrostatic matrix to calculating the electrostatic matrix elements between the determinant wave functions. The crystal field matrix elements of the multielectronic system can be reduced to the crystal field matrix elements between the determinants and thus to the single-electron crystal field matrix elements, and ultimately to the crystal field coefficients. In this way we can easily calculate the cubic crystal field matrix in the standard basis functions. From the standard basis functions, we obtain the basis functions in the spin-orbit coupling manifold, which in turn leads to the spin-orbit coupling matrix elements. In order to make a clear comparison, we take the energy of the first energy level to be zero, which does not affect the results. By comparing the experimental data with the calculated results, some theoretical values are in very good agreement with the experimental values, but some data differ from the experimental results, which is a result of the lack of precision in the fitting of B, C, and Dq. My research data can provide a certain basis for future spectroscopic research, and at the same time, there are some data that I have not been able to derive, and I expect that they can be supplemented and improved in the future.

COMPETING INTERESTS

The authors have no relevant financial or non-financial interests to disclose.

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