Journal of Alloys and Compounds 488 (2009) 586–590

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jallcom

$f \leftrightarrow f$ electric dipole transitions; old problems in a new light

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ARTICLE INFO

Article history:
Received 4 June 2008
Received in revised form 9 July 2008
Accepted 5 November 2008
Available online 18 November 2008

In memory of Brian G. Wybourne
(1935–2003).

Keywords:
Spectroscopy of lanthanides
Judd–Ofelt theory
Forbidden transitions
Parametrization of *f*-spectra

ABSTRACT

Very well known difficulties of the theoretical description of the $f \leftrightarrow f$ electric dipole transitions of lanthanides are addressed in the old language of the standard Judd–Ofelt (J–O) theory, which has been widely applied for more than 45 years. New light is shed on a competitive physical mechanism of these transitions, which is presented to complement the existing J–O model. Possible new solutions are given for the old problems of the negative intensity parameters obtained from the adjusting procedure. An alternative scheme for the reproduction of the hypersensitive transitions is discussed and a theoretical description of highly forbidden transitions 0–0 and 0–1 observed for Eu^{3+} and Sm^{2+} ions is presented.

1. Introduction

The problems of the reproduction of the hypersensitive $f \leftrightarrow f$ transitions and of the theoretical description of highly forbidden transitions 0–0 and 0–1 observed for Eu^{3+} and Sm^{2+} ions are strong motivation for the search for a reliable parametrization of *f*-spectra. At the same time, these particular transitions are the best examples of the important application of the spectroscopy of the lanthanide ions doped in various materials as diagnostic and therapeutic tools.

DOTA, EDTA, EDTMP, CDTMP, DTPA, DOTP are the organic chelates that, when coordinated with the Gd ion, are contrast agents used in clinical medicine to enhance NMR signals enabling the diagnosis of pathological changes in various organs of human body. When these systems are chelated with the other members of the lanthanide family, they act as markers of cancerous changes in different tissues. The signals monitoring the presence of a tumor originate from the sensitized luminescence of the lanthanide ion imbedded into the chelate built like a cage. The architecture of the cage is correlated with the kind of the targeted tissue. Although it is possible to verify, using the radiative isotopes of the lanthanides, where a certain system is absorbed the most, still the mechanisms of the energy transfer and of subsequent luminescence are not well understood. Not much is also known about the geometry of various cages. Only recently, due to the results of the DFT calculations, several aspects of the structure of various conformers of the chelates are becoming clearer. This knowledge is crucial for designing new systems that would be characterized by more efficient energy transfer and stronger luminescence enhanced by attaching to the main cage of the chelate the so-called antenna, which harvests the energy from the external beam. Special attention is also directed to the synthesis of such chelates that absorb visible light and emit infra-red radiation, the optimal one due to its penetration depth through biological samples.

The best benchmark for the theoretical investigations devoted to the structural properties of the potential probes are the highly forbidden by the standard selection rules $f \leftrightarrow f$ electric dipole transitions $0 \leftrightarrow 0$ and $0 \leftrightarrow 1$ of Eu^{3+}. Indeed, in the case of several chelates coordinated with the Eu ion there were two lines observed in the emission spectrum assigned to the $^5D_0 \rightarrow {}^7F_0$ transition! This was obvious evidence that at least two conformers of a given cage exist in equilibrium. This expectation based on the spectroscopic properties of a system was only recently confirmed by the numerical analysis of the optimal geometries of DOTA [1], EDTMP [2], CDTMP [3] and DOTP [4].

Thus, not only for the sake of the pure knowledge about the possible theoretical description of the transitions forbidden by the standard Judd–Ofelt selection rules, but also because of their important applications, the old problems of the theory of *f*-spectra are presented here in a new light shed by the results of the recent investigations.

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doi:10.1016/j.jallcom.2008.11.044

2. Standard Judd–Ofelt theory

The standard Judd–Ofelt theory [5,6] of $f \leftrightarrow f$ electric dipole transitions is based on the Rayleigh-Schrödinger perturbation theory applied for the following Hamiltonian,

$$H = H_0 + \lambda(PV_{CF}Q + QV_{CF}P) \tag{1}$$

where H_0 describes the system within the single configuration approximation and free ionic system approximation. Thus, P is spanned by the eigenfunctions Ψ_i^0 of H_0 of the ground electron configuration $4f^N$ of the lanthanide ion. Its orthogonal complement $Q = 1 - P$ is built of the projection operators originating from the singly excited configurations $4f^{N-1}n'\ell'$ (all the operators regarded here are single particle objects, and therefore the doubly excited configurations do not contribute). In this approach the electric dipole transitions are regarded as forced by the perturbing influence of the inter-shell interactions via the crystal field potential V_{CF} defined as

$$V_{CF} = \sum_{tp} B_p^t \sum_i r_i^t C_p^{(t)}(\vartheta_i \varphi_i) \tag{2}$$

with structural parameters (crystal field parameters) B_p^t.

The transition amplitude is defined by the matrix element of the radiation operator $D_\rho^{(1)}$ of the form

$$D_\rho^{(1)} = \sum_i r_i C_\rho^{(1)}(\vartheta_i \varphi_i) \tag{3}$$

Due to the parity considerations the electric dipole transition amplitude vanishes when evaluated with the eigenfunctions of H_0 (all states are of the same parity). The first non-vanishing contributions to the transition amplitude are of the second order, and they are determined by the matrix elements of $D^{(1)}$ with the functions expanded up to the first order corrections

$$\Phi_i = \Psi_i^0 + \lambda \Psi_i^1 \tag{4}$$

where

$$\Psi_i^{(1)} = \sum_k \frac{\langle \Psi_k^0 | QV_{\mathrm{cryst}}P | \Psi_i^0 \rangle}{E_i^0 - E_k^0} \Psi_k^0 \tag{5}$$

From the whole expansion of the crystal field potential in Eq. (2), only the interactions via its odd part are effective in forcing the electric dipole transitions (parity considerations). Following Judd and Ofelt it is assumed that the energy levels of distinct configurations might be regarded as degenerate *in relation* to the large energy distance between the ground configuration $4f^N$ and all the excited ones. Therefore it is possible to perform *the partial closure* and derive the transition amplitude in its effective operator form

$$\Gamma_{\text{J–O}}^\rho = 2(-1)^\rho \sum_t^{\text{odd}} \sum_p B_p^t \sum_\lambda^{\text{even}} \sum_{\ell'}^{\text{even}} (-1)^p [\lambda]^{1/2} \begin{pmatrix} 1 & t & \lambda \\ \rho & p & -(\rho+p) \end{pmatrix} A_t^\lambda(\ell') R_{\text{JO}}^t(\ell') \langle 4f^N \Psi_f^0 | U_{\rho+p}^{(\lambda)} | 4f^N \Psi_i^0 \rangle \tag{6}$$

where the angular term is defined as

$$A_t^\lambda(\ell') = [\lambda]^{1/2} \begin{Bmatrix} t & \lambda & 1 \\ f & \ell' & f \end{Bmatrix} < f \| C^{(1)} \| \ell' \rangle \langle \ell' \| C^{(t)} \| f \rangle \tag{7}$$

and, as a factor, it has the same value for all the lanthanide ions.

The radial integrals of the original Judd–Ofelt theory have the form

$$R_{\text{JO}}^t(\ell') = \sum_{n'} \frac{\langle 4f | r | n'\ell' \rangle \langle n'\ell' | r^t | 4f \rangle}{(\epsilon_{4f} - \epsilon_{n'\ell'})}$$

and when expressed in the terms of the perturbed functions [7], they are represented by a single integral, namely

$$R_{\text{JO}}^t(\ell') = \langle \varrho^t(4f \to \ell') | r | 4f \rangle \tag{8}$$

where $|4f\rangle \equiv P_{4f}$. The perturbed functions $\varrho^t(4f \to \ell') \equiv \varrho^t(r; 4f \to \ell')$ contain all the first-order corrections caused by the single excitations from the $4f$ shell to one-electron state of $n'\ell'$ symmetry taken into account via the crystal field potential. Indeed, each $\varrho^t(4f \to \ell')$ is a linear combination of the terms

$$\varrho^t(4f \to \ell') = \sum_{n'} \frac{\langle 4f | r^t | n'\ell' \rangle}{(\varepsilon_{4f} - \varepsilon_{n'\ell'})} P_{n'\ell'}(r)$$

Note that due to the perturbed function approach the sum of the original Judd–Ofelt radial integrals over the complete radial basis sets of one electron excited functions of ℓ' symmetry is replaced by a single integral with new functions that contain this very troublesome summation inside their definition (see Ref. [7]).

The expression for the transition amplitude derived by Judd and Ofelt is the basic one in the theory of f-spectra. In order to evaluate its applicability and usefulness, to discuss its weak and strong points, some questions are answered below.

• *Is it possible to perform ab initio calculations using the expression in* Eq. (6)?

∗ There is no problem with the evaluation of the angular parts of the effective operators defined in Eq. (6);

∗ All the problems with the evaluation of the radial integrals are solved by using the perturbed function approach, and their values for all lanthanide ions, evaluated for the complete radial basis sets of one electron functions are published in Ref. [8];

∗ Unfortunately still it is impossible to perform direct calculations using the effective operators in Eq. (6) because the odd rank crystal field parameters B_p^t are not known, and there is no reliable source of their values available.

• *Would the results of such calculations be reliable, if the odd rank crystal field parameters were known?*

∗ As mentioned, the standard Judd–Ofelt theory is based on the single configuration approximation and therefore the impact of electron correlation is completely ignored. In order to improve this theoretical model the approach has to be based on the double perturbation theory applied for the Hamiltonian

$$H = H_0 + \lambda(PV_{CF}Q + QV_{CF}P) + \mu(PV_{corr}Q + QV_{corr}P) \tag{9}$$

where the second perturbation is the non-central part of the Coulomb interaction and represents correlation effects. As a consequence instead of Eq. (6) the effective operators defined up to the third order have to be included. The numerical analysis of the relative importance of various contributions to the transition amplitude has demonstrated that electron correlation contributions, although of the third order, very often and usually for the heavier ions across the lanthanide series are dominant in comparison to the values of the Judd–Ofelt terms of the second order [9].

3. Semiempirical apporach

The problems with the direct evaluation of the amplitude of $f \leftrightarrow f$ transitions are the reason that the semi-empirical realization of the Judd–Ofelt theory is the most known and commonly used in practice. In this model the transitions are reproduced within the one particle parametrization

$$S^{\mathrm{J-O}}_{f\leftarrow i} = \sum_{\lambda=2,4,6} \Omega_\lambda |\langle \Psi_f || U^{(\lambda)} || \Psi_i \rangle|^2 \tag{10}$$

This means that the intensity of all the transitions in a given system are determined by at most three intensity parameters modulated by the square of the reduced matrix elements of the unit tensor operators between the states involved in the process.

In fact it should be pointed out that there is not much in common with the original Judd–Ofelt theory and the parametrization scheme defined in Eq. (10). Indeed, the expression in Eq. (10) means only that the parametrization of the *f*-spectra is one particle (the Judd–Ofelt effective operators are one particle), that there are three parameters common for all transitions in a given system (without the physical meaning or interpretation), and finally that the parametrization is non-relativistic (as unit tensor operators of the original formulation of the Judd–Ofelt theory). There is neither a physical model nor a physical mechanisms involved in the expression (10), nor any evidence of the approximations of the physical model discussed in the previous section in connection with the original Judd–Ofelt theory. Even there is no any evidence in Eq. (10) that the crystal field potential is the forcing mechanism of the electric dipole $f \leftrightarrow f$ transitions. Just the opposite, the intensity parameters, traditionally called the Judd–Ofelt parameters, represent the perturbing influence of ALL physical mechanisms, which are theoretically described by one particle tensor operators acting within the orbital space. In addition, there is no *a priori* requirement that the intensity parameters HAVE to be positive! Ω_λ is not a square of the coefficient of the tensor operator U in Eq. (6). Each Ω_λ does not represent the second order terms derived from the perturbation approach; Ω_λ's are freely varying parameters without physical interpretation. There is only one case in which the value of Ω_2 is expected to be positive and that is when it determines by itself the intensity of a hypersensitive transition. However, very often in such cases the fitting procedure based on the scheme in (10) gives reasonable reproduction only when the hypersensitive transition is excluded from the adjusted set. The latter problem is solved by the extended parametrization scheme presented below.

4. Electric dipole hyperfine interactions

- *Does any other forcing mechanism of $f \leftrightarrow f$ transitions, except the crystal field potential, exist?*

When the perturbing operator V_{cryst} in Eq. (1) is replaced by the multipole hyperfine interactions V_{EM}, the wave functions of H_0 are modified by the corrections of parity opposite to the parity of the $4f^N$ [10]. This parity condition is satisfied only for the odd part of V_{EM}. As a result, there are non-zero second-order contributions that are of a new origin, and which compete at the second order with the standard Judd–Ofelt terms. Thus, the interactions via V_{EM} represent new mechanism, which forces the electric dipole $f \leftrightarrow f$ transitions.

The distortion from the spherical symmetry of a nucleus with the spin $I > 0$ is described by the electrostatic interactions between the electron and nucleon charge densities, which, in the terms of the multipole expansion, have the following tensorial form,

$$V_{EM} = \sum_k \frac{r_n^k}{r_e^{k+1}} (\mathbf{C}_e^{(k)} \cdot \mathbf{C}_n^{(k)}) \tag{11}$$

When the energy is evaluated within the single configuration approximation, k in the expansion above is even, and the remaining contributions for k odd vanish. If the inter-shell electric multipole hyperfine interactions are analyzed, there are non-zero contributions to the transition amplitude for k odd in Eq. (11).

It is straightforward to find within the framework of the basic assumptions and approximations of the standard Judd–Ofelt theory that these new second-order one-particle effective operators have the following form,

$$^2\Gamma^\rho_{EM} = 2(-1)^\rho \sum_k^{\mathrm{odd}} \sum_q M_q^k \sum_{\ell'}^{\mathrm{even}} \sum_\lambda^{\mathrm{even}} [\lambda]^{1/2} \begin{pmatrix} 1 & k & \lambda \\ \rho & q & -(\rho+q) \end{pmatrix} A_k^\lambda(\ell') R_{\mathrm{JO}}^{-k-1}(\ell') \langle 4f^N \Psi_f^0 | U^{(\lambda)}_{\rho+q} | 4f^N \Psi_i^0 \rangle \tag{12}$$

where the angular factors are defined by Eq. (7), the radial integral is presented in Eq. (8) and M_q^k is the matrix element of the nuclear multipole moment.

The tensorial structure of these effective operators is almost the same as those of the standard Judd–Ofelt effective operators from Eq. (7). Note that λ in Eq. (12) is also even, and the selection rules for the non-vanishing contributions are the same; only the odd rank crystal field parameters B_p^t of Eq. (7) are replaced in Eq. (12) by M_q^1, and the physical origin in both cases is different. At the same time, since the transition amplitude is not determined any more by the odd rank crystal field parameters, it is possible to perform direct calculations.

The second order Judd–Ofelt effective operators represent the electrostatic interactions caused by the distortion of the spherical symmetry of a free ion by its environment represented by the crystal field potential. The new second order terms originate from the electrostatic interactions that are the consequence of the distortion of a spherical symmetry of a nucleus caused by its closest environment created by the surrounding electrons.

- *Is the parametrization scheme of the f-spectra changed when the hyperfine interactions are taken into account?*

The tensorial structure of the hyperfine originated terms contributing to the transition amplitude indicates that all these contributions are also included within the standard parametrization scheme of Judd and Ofelt

$$S_{f\leftarrow i} = \sum_{\lambda=2,4,6} \Omega'_\lambda |\langle \Psi_f || U^{(\lambda)} || \Psi_i \rangle|^2$$

where the intensity parameters are only formally distinguished from those in expression (10). Indeed, when the values of Ω_λ's are evaluated from the fitting procedure, as mentioned above, they as freely adjusted parameters represent ALL physical mechanisms taken into account at all orders of the perturbation expansion.

Thus, the intensity parameters represent the interplay between two forcing mechanism of the $f \leftrightarrow f$ electric dipole transitions: the crystal field potential and electric dipole hyperfine interaction. In the particular case of $\lambda = 2$, the term which determines the intensity of the hypersensitive transition Ω_2 contains the contributions from Eq. (6) for $t = 1$, and from Eq. (12) for $k = 1$. However, there are also such examples for which the hypersensitive transitions are observed in spite of the fact that there are no terms for $t = 1$ in the expansion of the crystal field potential. Since the hyperfine mechanism is independent of the crystallographic symmetry of the system, it is concluded that for such systems the electric dipole hyperfine interactions are the sole mechanism which is responsible for the hypersensitivity of some electric dipole transitions.

5. Relativistic parametrization of *f*-spectra

- *Is it possible to reproduce ALL electric dipole $f \leftrightarrow f$ transitions using the one particle non-relativistic parametrization scheme of* Eq. (10)?

When $\Psi_f \equiv {}^7F_0$ in Eq. (10), only the transitions to the levels assigned by $J = 2, 4, 6$ are allowed by the selection rules of the standard Judd–Ofelt parametrization scheme. This means that in the particular case of *Eu* ion, all the transitions $J = 0 \leftrightarrow J' = 0, 1, 3, \ldots,$ odd are forbidden, although they are observed and indeed very important, as mentioned in the Introduction. There is also a problem with the reproduction of the hypersensitive transitions using the scheme in Eq. (10). In fact, very often the fitting procedure performed for the set of the allowed transitions which includes the hypersensitive ones (for example ${}^5D_0 \to {}^7F_2$ for Eu ion) gives rather poor reproduction of the measurements. In all these cases the Judd–Ofelt parametrization scheme is not adequate.

It is a common belief that in order to improve the quality of the reproduction of the spectra it is enough to enlarge the number of the intensity parameters. The results of the numerical analysis [11,12], supported by earlier work of Auzel [13], demonstrated however that this is not the case when the semi-empirical procedure is applied for *f*-electron spectra. The extension of the scheme in Eq. (10) by the odd-rank intensity parameters, while alleviating the selection rules for the transitions from $J = 0$ to the levels with $J = odd$, still does not lead to better reproduction. This means that not only the number of the adjusted parameters is crucial but the physical model from which the parametrization scheme originates.

The Judd–Ofelt parametrization scheme is non-relativistic as demonstrated by the fact that the unit tensor operators U in the matrix elements modulating the intensity parameters act only within the orbital space. In this way, even if the fitting procedure is applied, from all possible physical mechanisms contributing to the transition amplitude those of a relativistic nature are excluded. Indeed, the intensity parameters Ω_λ do not contain the impact of spin–orbit and hyperfine magnetic interactions, for example [14–17]. The relativistic formulation of the intensity theory of the $f \leftrightarrow f$ transitions [18,19] led to the conclusion that the original operators $U^{(\lambda)}$ in the parametrization scheme should be replaced by the double tensor operators that act within the spin–orbital space. This is why, instead of Eq. (10), a new extended and physically enriched scheme has been proposed [11,12]

$$S^{\text{rel}}_{f\leftarrow i} = \sum_{\lambda}\sum_{\kappa k} \Omega^{\kappa k}_{\lambda} |\langle \Psi_f | W^{(\kappa k)\lambda} | \Psi_i \rangle|^2. \tag{13}$$

The number of the parameters is simultanously enlarged, and therefore the fitting procedure now requires richer experimental data. In fact the number of parameters is limited by the condition that the sum of the ranks $\kappa + k + \lambda$ has to be *even* to preserve the hermiticity of the effective operators determining the intensity.

- *Is the new parametrization scheme applicable for ALL $f \leftrightarrow f$ transitions?*

The relativistic parametrization scheme allows one to perform the fitting procedure for *all* $f \leftrightarrow f$ transitions, including those forbidden by the non-relativistic approach. Even the transition $0 \leftrightarrow 0$ observed in *Eu*, which is not tractable theoretically by all the previous parameterizations, is very well reproduced by the expression in Eq. (13). Indeed, when $J_f = J_i = 0$ the only consequence is that $\lambda = 0$, which means that $\kappa = k$, and the parameter $\Omega^{(11)}_0$ determines the intensity of this transition. In addition, the fitting procedure performed in accordance with the relativistic scheme gives much better reproduction of other transitions, including those allowed by the Judd–Ofelt selection rules, the hypersensitive ones, and also transitions determined by the effective operators with rank $\lambda =$ odd.

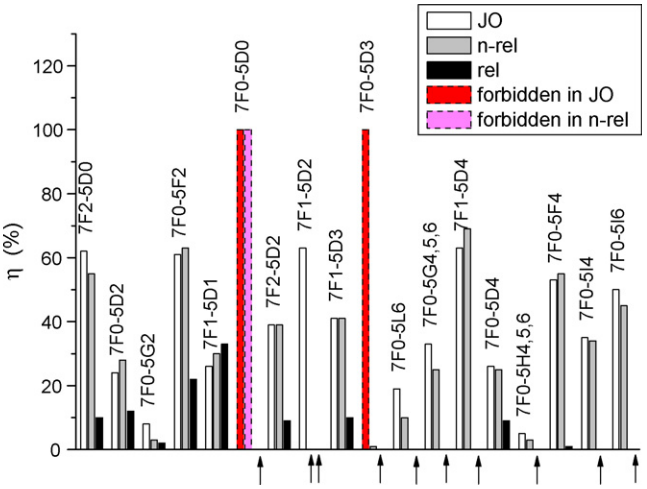

Fig. 1. Relative errors of reproduction of the intensity of $f \leftrightarrow f$ transitions observed in the Eu^{3+} ion in an acetate crystal [11,20].

6. Summary

The summary of this discussion is illustrated in Fig. 1, where the quality of the results of numerical calculations are presented for various transitions observed in the Eu^{3+}ion in an acetate crystal [20]. In the figure not the actual values of the intensities of the appropriate transitions are presented, but rather the errors of reproduction defined as follows,

$$\eta = \frac{|P_{\text{exp}} - P_{\text{calc}}|}{P_{\text{exp}}} \times 100\%$$

where P_{calc} denotes the value of the intensity of a particular transition evaluated within the Judd–Ofelt scheme ($S^{\text{J–O}}_{f\leftarrow i}$, Eq. (10)), within non-relativistic scheme which is the Judd–Ofelt approach extended by the odd rank intensity parameters, $S^{\text{nrel}}_{f\leftarrow i}$, and finally within the relativistic scheme ($S^{\text{rel}}_{f\leftarrow i}$, Eq. (13)).

The arrows below the horizontal axis point out the perfect reproduction of the measured intensity ($\eta = 0$). The white bars represent the quality of the standard Judd–Ofelt scheme, the gray color describes the values of η obtained for the non-relativistic scheme in which the odd rank intensity parameters are included, and finally, the black bars show the accuracy of the reproduction when the relativistic scheme is applied. The other bars in the Fig. 1. denote the transitions which are forbidden by the Judd–Ofelt and non-relativistic schemes (error of reproduction of 100%). One of these forbidden transitions, ${}^7F_0 \to {}^5D_3$, becomes allowed by the selection rules of the non-relativistic scheme, while ${}^7F_0 \to {}^5D_0$ is still forbidden; it becomes allowed only within the relativistic scheme.

The results of the fitting procedure of the standard Judd–Ofelt scheme are improved when the extended model is applied, however still there is a rather large discrepancy between the calculated and measured intensities. In the case of all transitions included in the semi-empirical procedure there is visible improvement of the quality of the reproduction based on the relativistic scheme. Note that for the first time the intensity of the unusual and highly forbidden transition ${}^7F_0 \to {}^5D_0$ is reproduced via the fitting procedure, and this is achieved by applying the relativistic scheme of parametrization. In fact this is the only parametrization scheme in which all transitions of a given system are described by the very same semi-empirical approach.

In addition, it should be pointed out that the parameter Ω^{11}_0, which is responsible for the $0 \to 0$ transition, represents the impact due to the $J-J$ mixing and the spin–orbit interaction (indeed, the spin–orbit interaction is represented by the unit double tensor operator $w^{(11)0}$). These are the contributions, which have been evaluated by Downer and Burdick [15,16], Tanaka and Kushida [21] in their direct calculations of the intensity of ${}^7F_0 \rightarrow {}^5D_0$ transition enhanced by the intensity of the transition ${}^7F_0 \rightarrow {}^5D_2$ by means of the "borrowing of intensity" mechanism suggested by Wybourne in 1967 ([8], page 213 and references there); all these contributions are disregarded by the Judd–Ofelt and also non-relativistic parametrization schemes as a result of the limitation of the unit tensor operators U, which act only within the orbital space. This means that extension of the effective operators to the spin-orbital space gives a unique possibility to account for all the interactions, which have been included previously in *ab initio*-type calculations mentioned above. These pioneering calculations and their results are a strong motivation for extension of the parametrization scheme of *f*-spectra by all those interactions, which are represented by double tensor operators.

Although Fig. 1 shows remarkable improvement of the results of the fitting procedure based on the relativistic scheme applied for the particular example of the Eu^{3+} in an acetate crystal, more general conclusions about the effectiveness and accuracy of the relativistic scheme require further numerical analysis. At this point of the discussion the main achievement of this preliminary investigations is the fact that all the transitions, those allowed and also forbidden by the standard scheme, are reproduced by the same semi-empirical approach.

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