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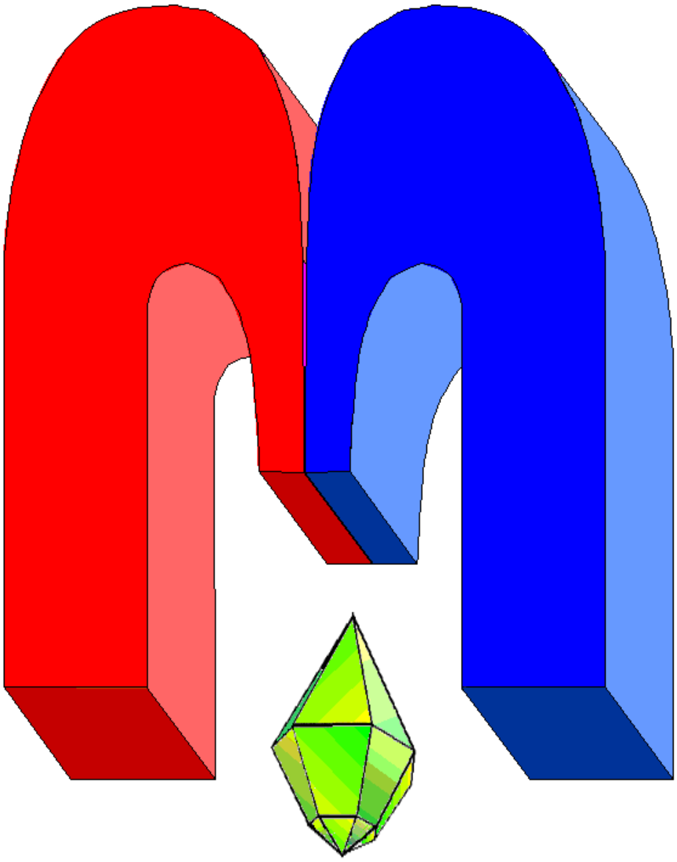

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# Short analytical expressions accounting for the spatial distribution of ligand electrons in the theory of the odd crystal field on rare-earth ions

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Using Gaussian decompositions of the electron potential energy and the $4f$ and $5d$-electron wave functions, we have derived short analytical formulae for calculating the parameters of the odd crystal field on rare-earth ions. Extended charge contributions to the intrinsic parameters $a^{(1)}$, $a^{(2)}$, $a^{(3)}$, $a^{(4)}$, $a^{(5)}$, and $a^{(6)}$ were evaluated using Hartree-Fock wave functions of Pr$^{3+}$-O$^{2-}$ and of Tm$^{3+}$-O$^{2-}$ pairs.

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**Keywords:** crystal filed theory, rare earth ions, electron density

## 1. Introduction

An odd crystal field mixes the states of the ground $4f^n$ electron configuration and excited configuration of opposite parity $4f^{n-1}5d$, thereby inducing electric dipole transitions between terms and multiplets of rare-earth ions in non-centrosymmetric crystals. The first theoretical framework for calculating relative transition intensities between different multiplets, using second-order perturbation theory, was established by Judd [1] and Ofelt [2]. The formulae derived by Judd and Ofelt were tested extensively on a wide range of compounds (see reviews [3,4]). The theory employs three adjustable parameters $\Omega_2$, $\Omega_4$ and $\Omega_6$. However, it was found that to accurately describe the relative intensities of intermultiplet transitions, the $\Omega_2$ parameter sometimes must be treated as negative contrary to the original formulae [1] and [2] which required it to be strictly positive. This discrepancy was resolved in the works of Kornienko et al. [5, 6] who incorporated third-order perturbation theory to account for the mixing of $4f^n$ and $4f^{n-1}5d$ configurations induced by odd crystal fields.

Furthermore, the question of physical interpretation for the odd crystal field parameters arises naturally. Initial estimates of these parameters were made using the point charge model [1]. Beyond laser transition theory, odd field effects have also been investigated through magnetic resonance techniques [7,8]. Notably, it has been demonstrated that in second-order perturbation theory, the odd crystal field additionally induces renormalization of even crystal field parameters [9, 10]. Attempts were made to improve calculations of odd crystal field parameters within the point charge model by incorporating field-induced electric dipole and quadrupole moments on lattice ions under external electric fields. Numerous compounds were analyzed using this approach [11].

However, since the point charge and dipole model exhibits inherent oversimplified, investigations incorporating wave function overlap effects between rare-earth ions and ligands remain highly relevant. While comprehensive quantum mechanical calculations of these overlap effects present significant complexity and have yet to be fully implemented, Malkin proposed a semi-empirical solution through the exchange charge model (ex), which accounts for the overlap between $4f/5d$ electron wave functions and ligand wave functions. The main formulae are presented in review [12]. The model accounts for both types of Coulomb contributions arising from the spatial distribution of ligand electrons. Following Faucher's terminology, these include: the extended charge (ec) contribution [13] and exchange effects. Both contributions can be approximated through overlap integrals.

The calculated relationships between internal parameters of the even crystal field for both types of contributions were previously discussed in [14]. In this work, we present calculation results for the odd crystal field. To our knowledge, such calculations have not been reported previously. These investigations are particularly relevant given recent experimental findings. Notably, in studies of $\mathrm{Er}^{3+}$-activated $\mathrm{LuLiF}_4$ and $\mathrm{YLiF}_4$ crystals [15], measurements of photon echo intensity dependence on magnetic field orientation, magnitude, and direction revealed a memory effect (persisting up to 6 hours), which may be associated with magnetoelectric phenomena. Interference effects between magnetic and electric dipole transitions have been observed in optical and terahertz spectra of crystals containing unfilled $3d$-shells (see, for example, [15–18]). Consequently, advancing the theory of odd crystal fields and by extension, the theory of electric dipole transitions holds significant practical relevance. This extends beyond laser physics to include emerging applications such as optical and terahertz diodes [19].

## 2. Derivation of calculated expressions

An additional important point, which was allowed us to obtain rather simple computational equations is that we use solutions of the Poisson equation as well in the form of expansions over Gaussian orbitals.

We start from superposition model Hamiltonian:

$$H_0 = \sum_{k=1,3,5} \sum_{q=-k}^{k} B_q^{(k)} C_q^{(k)}(\theta, \varphi),$$

where $C_q^{(k)} = \sqrt{\frac{4\pi}{2k+1}} Y_q^k$ are components of the spherical tensors. In the superposition model the crystal field parameters can be written as follows:

$$B_q^{(k)} = \sum_j a^{(k)}(R_j)(-1)^q C_{-q}^{(k)}(\theta_j, \varphi_j).$$

The contributions originated from the spatial distribution of electrons for $a^{(1)}$, $a^{(3)}$, and $a^{(5)}$ can be calculated using by expressions:

$$a^{(k)} = \sum_m (2k+1)(-1)^{3-m} \begin{pmatrix} 3 & k & 2 \\ -m & 0 & m \end{pmatrix} \frac{\langle 4fm|V|5dm\rangle}{(f||C^{(k)}||d)},$$

where $\begin{pmatrix} 3 & k & 2 \\ -m & 0 & m \end{pmatrix}$ are $3j$-symbols, $\langle 4fm|V|5dm\rangle$ are matrix elements of potential energy operator of $4f$ electron, and $(f||C^{(k)}||d)$ are reduced matrix elements of the spherical tensors.

The total potential energy of an electron in the field of a point charge and electron clouds $2s$ and $2p$ of oxygen we will use in the form suggested in [21]. It is obtained by solving the Poisson equation and written as (in atomic units):

$$V(r_b) = -\frac{Ze^2}{r_b} - \frac{e^2}{r_b} \sum p_k e^{-\gamma_k r_b^2}.$$

The entering parameters $p_k$ and $\gamma_k$ for oxygen ion are given in Appendix. The space distribution of $1s$ electron is included in renormalization of effective charge of ligand. Later we will use $Z = -2$ for oxygen ion. Since the $5d$-electron wave functions are more strongly delocalized with respect to the $4f$ functions the integration in all expressions is carried out without the restriction $r < R$. Wave functions of $4f$-electron are described as:

$$R_{4f} = r_a^3 \sum_i C_i \exp\left(-\alpha_i r_a^2\right).$$

Wave functions of $5d$-electron are described as:

$$R_{5d} = r_a^2 \sum_j S_j \exp\left(-\beta_j r_a^2\right).$$

The $C_i$, $S_j$, $\alpha_i$ and $\beta_j$ values of $\mathrm{Pr}^{3+}$ and $\mathrm{Tm}^{3+}$ are collected in Appendix. In our approach the matrix elements of the operator $V$ are written as two-center triple integrals:

$$\langle 4fm|V|5dm\rangle = \iiint\limits_{-\infty}^{\infty} R_{4f} R_{5d} V(r_b) Y_{3m}^{*} Y_{2m} dx_a dy_a dz_a.$$

This matrix elements are useful to separate in two terms

$$\langle 4fm|V|5dm\rangle = \langle 4fm|V(\mathrm{pc})|5dm\rangle + \langle 4fm|V(\mathrm{ec})|5dm\rangle.$$

The first one corresponds to point charge and the second one takes into account the spatial distribution of ligand electrons. For both types of integrals the following transformation is carried out first of all:

$$\frac{1}{r_b} = \frac{1}{2\pi^2} \int\limits_{-\infty}^{\infty} \frac{d\mathbf{q}}{q^2} e^{i(q_x x_b + q_y y_b + q_z z_b)}.$$

and then the new variable $z$ is introduced [22]:

$$z_b = z - \frac{\alpha_{\mathrm{odd}}}{\varkappa} R, \quad z_a = z + \frac{\gamma_k}{\varkappa} R.$$

Some substitutions of variables were included in the calculations

$$\begin{aligned} \alpha_{\mathrm{odd}} &= \alpha_i + \beta_j, \\ \varkappa &= \alpha_{\mathrm{odd}} + \gamma_k, \\ b &= R\left(\gamma_k + \alpha_{\mathrm{odd}} y^2\right). \end{aligned}$$

For simplifying the integrals over the wave vector $q$ variables, the following relation is additionally used:

$$\frac{1}{q^2} e^{-\frac{q^2}{4\varkappa}} = \frac{1}{2\varkappa} \int\limits_0^1 \frac{1}{y^3} e^{-\frac{q^2}{4\varkappa y^2}} dy.$$

As a result, it is possible to obtain calculation formulae in the form of single integrals, which can be easily programmed.

Therefore, final equations for $a^{(1)}$, $a^{(3)}$ and $a^{(5)}$ take form of:

$$a^{(1)}(\text{pc}) = -\int\limits_0^1 \sum_{i,j} \frac{3ZRy^2C_iS_j}{2\alpha_{\text{odd}}^3} e^{-\alpha_{\text{odd}}R^2y^2} \Big(\frac{35}{4}(1-y^2)^2 + 7\alpha_{\text{odd}}R^2y^4(1-y^2) + (\alpha_{\text{odd}}R^2y^4)^2\Big)dy,$$

$$a^{(3)}(\text{pc}) = -\int\limits_0^1 \sum_{i,j} \frac{7ZRy^2C_iS_j}{2\alpha_{\text{odd}}^3} e^{-\alpha_{\text{odd}}R^2y^2} \Big(\frac{9}{2}\alpha_{\text{odd}}R^2y^4(1-y^2) + (\alpha R^2y^4)^2\Big)dy,$$

$$a^{(5)}(\text{pc}) = -\int\limits_0^1 \sum_{i,j} \frac{11ZRy^2C_iS_j}{2\alpha_{\text{odd}}^3} e^{-\alpha_{\text{odd}}R^2y^2} \Big(\alpha_{\text{odd}}R^2y^4\Big)^2 dy,$$

$$a^{(1)}(\text{ec}) = -\int\limits_0^1 \sum_{i,j,k} \frac{3C_iS_jp_k}{2\varkappa^4} b\Big(\frac{35}{4}(1-y^2)^2 + \frac{7b^2}{\varkappa}(1-y^2) + \frac{b^4}{\varkappa^2}\Big) e^{-(\frac{\gamma_k R}{\varkappa}-R)^2\varkappa y^2} e^{-\gamma_k R^2} e^{\frac{\gamma_k^2 R^2}{\varkappa}} dy,$$

$$a^{(3)}(\text{ec}) = -\int\limits_0^1 \sum_{i,j} \frac{7C_iS_jp_k}{2\varkappa^4} b^3\Big(\frac{9}{2\varkappa}(1-y^2) + \frac{b^2}{\varkappa^2}\Big) e^{-(\frac{\gamma_k R}{\varkappa}-R)^2\varkappa y^2} e^{-\gamma_k R^2} e^{\frac{\gamma_k^2 R^2}{\varkappa}} dy,$$

$$a^{(5)}(\text{ec}) = -\int\limits_0^1 \sum_{i,j} \frac{11C_iS_jp_k}{2\varkappa^6} b^5 e^{-(\frac{\gamma_k R}{\varkappa}-R)^2\varkappa y^2} e^{-\gamma_k R^2} e^{\frac{\gamma_k^2 R^2}{\varkappa}} dy.$$

## 3. Calculation results

We calculated two variants for point charge contributions, extended and exchange charge contributions in even crystal field theory on $\text{Pr}^{3+}$ and $\text{Tm}^{3+}$ ions, using formula from work [14]. The results are presented in Fig. 1. Contribution to the crystal field parameters from point charges was calculated using the expression:

$$a_1^{(k)}(\text{pc}) = -\frac{Ze^2\langle r^k\rangle}{R^{k+1}},$$

where $R$ is the distance between ions, $Z$ is the effective ligand charge in the units of $|e|$, $\langle r^k\rangle$ are the average values calculated on radial wave function of $4f$-electron. They can be found in Abragam-Bleaney book [20]. Contributions originated from spatial distribution of electron can be calculated as follows:

$$a^{(2)}(\text{pc}) = -\frac{5}{8}Z\sum_{i,j}\frac{C_iC_j}{\alpha_{\text{even}}^4}\int\limits_0^1 e^{-\alpha_{\text{even}}R^2y^2}\Big[63R^2\alpha_{\text{even}}y^4(1-y^2)^2$$
$$+36R^4\alpha_{\text{even}}^2y^8(1-y^2) + 4(R^2\alpha_{\text{even}}y^4)^3\Big]dy,$$

$$a^{(2)}(\text{ec}) = -\frac{5}{8}\sum_{i,j,k}\frac{C_iC_jp_k}{\xi^4}e^{-\gamma_k R^2}e^{\frac{\gamma_k^2R^2}{\xi}}\int\limits_0^1 e^{-R^2(\frac{\gamma_k}{\xi}-1)^2\xi y^2}\Big[\frac{63}{\xi}R^2(1-y^2)^2[\gamma_k-(\gamma_k-\xi)y^2]^2$$
$$+\frac{36}{\xi^2}R^4(1-y^2)[\gamma_k-(\gamma_k-\xi)y^2]^4 + \frac{4}{\xi^3}R^6[\gamma_k-(\gamma_k-\xi)y^2]^6\Big]dy,$$

$$a^{(4)}(\text{pc}) = -\frac{9}{4}Z\sum_{i,j}\frac{C_iC_j}{\alpha_{\text{even}}^4}\int\limits_0^1 e^{-\alpha_{\text{even}}R^2y^2}\Big[11R^4\alpha_{\text{even}}^2y^8(1-y^2) + 2(R^2\alpha_{\text{even}}y^4)^3\Big]dy,$$

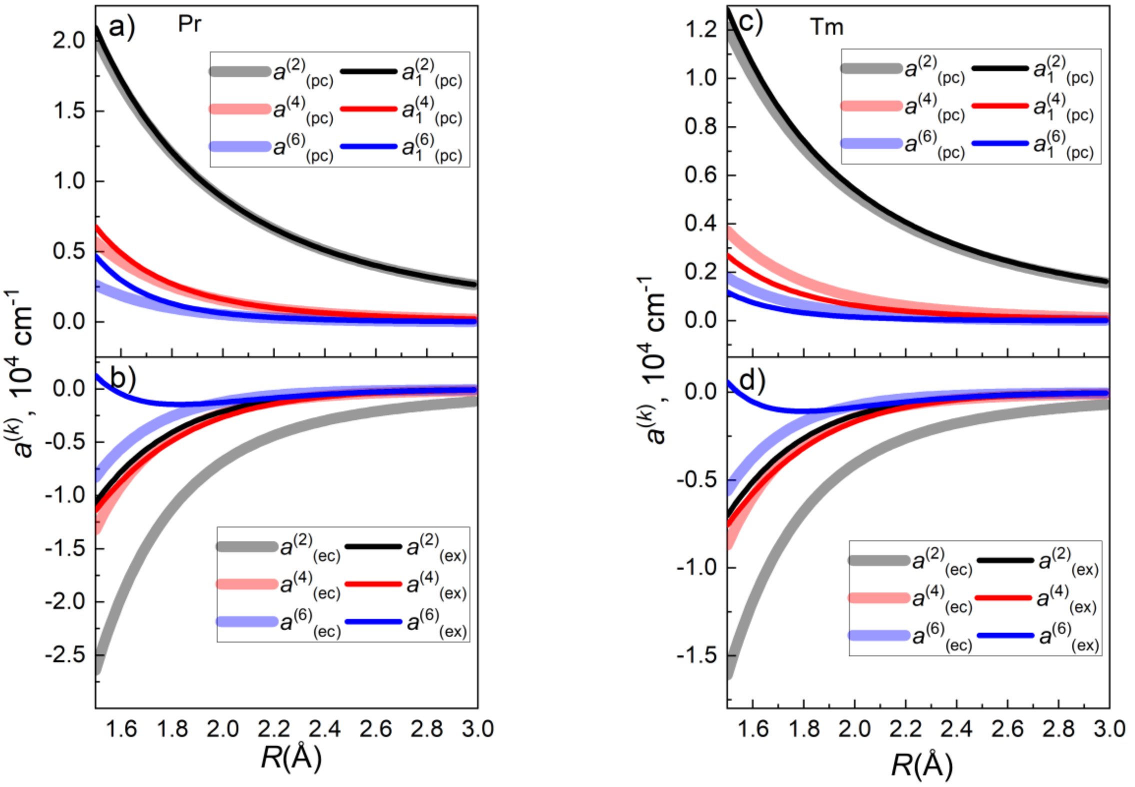

**Figure 1.** Calculated values of $a^{(k)}(k=2,4,6)$ as functions of internuclear distances. The respective results for the Pr-O and Tm-O are a) and c) two variants for point charge contributions $a^{(k)}$ values, b) and d) extended (ec) and exchange (ex) contributions

$$a^{(4)}(\mathrm{ec}) = -\frac{9}{4}\sum_{i,j,k}\frac{C_iC_jp_k}{\xi^4}e^{-\gamma_k R^2}e^{\frac{\gamma_k^2R^2}{\xi}}\int\limits_0^1 e^{-R^2(\frac{\gamma_k}{\xi}-1)^2\xi y^2}\Big[\frac{11}{\xi^2}R^4(1-y^2)[\gamma_k-(\gamma_k-\xi)y^2]^4 + \frac{2}{\xi^3}R^6[\gamma_k-(\gamma_k-\xi)y^2]^6\Big]dy,$$

$$a^{(6)}(\mathrm{pc}) = -\frac{13}{2}Z\sum_{i,j}\frac{C_iC_j}{\alpha_{\mathrm{even}}^4}\int\limits_0^1 e^{-\alpha_{\mathrm{even}}R^2y^2}(R^2\alpha_{\mathrm{even}}y^4)^3dy,$$

$$a^{(6)}(\mathrm{ec}) = -\frac{13}{2}\sum_{i,j,k}\frac{C_iC_jp_k}{\xi^4}e^{-\gamma_k R^2}e^{\frac{\gamma_k^2R^2}{\xi}}\int\limits_0^1 e^{-R^2(\frac{\gamma_k}{\xi}-1)^2\xi y^2}\frac{R^6}{\xi^3}[\gamma_k-(\gamma_k-\xi)y^2]^6dy,$$

where $\alpha_{\mathrm{even}} = \alpha_i + \alpha_j$, $\xi = \alpha_{\mathrm{even}} + \gamma_k$. The expressions for calculating contribution from the exchange charges are given in [14]. Calculated values of $a^{(k)}(k=2,4,6)$ as functions of internuclear distances are presented in Fig. 1. It is demonstrated that extended contribitions have much in common with those expected in the semi-empirical model of exchange charges.

For the odd crystal field theory on $\mathrm{Pr}^{3+}$ and $\mathrm{Tm}^{3+}$ ions, the calculation results are presented in Fig. 2. The functions $R(5d)$ were taken from the work [23] and their representation as a sum of Gaussian orbitals was performed by Anikeenok [24]. The parameters of those decompositions are given in the Appendix (in Table 1 and 2). Parameters of the solution of Poisson equation corresponding to the total electron density of $2s$- and $2p$-electrons of the oxygen ion $\mathrm{O}^{2-}$ are presented in Table 3.

Using Gaussian decompositions of the potential energy of electrons and wave functions of

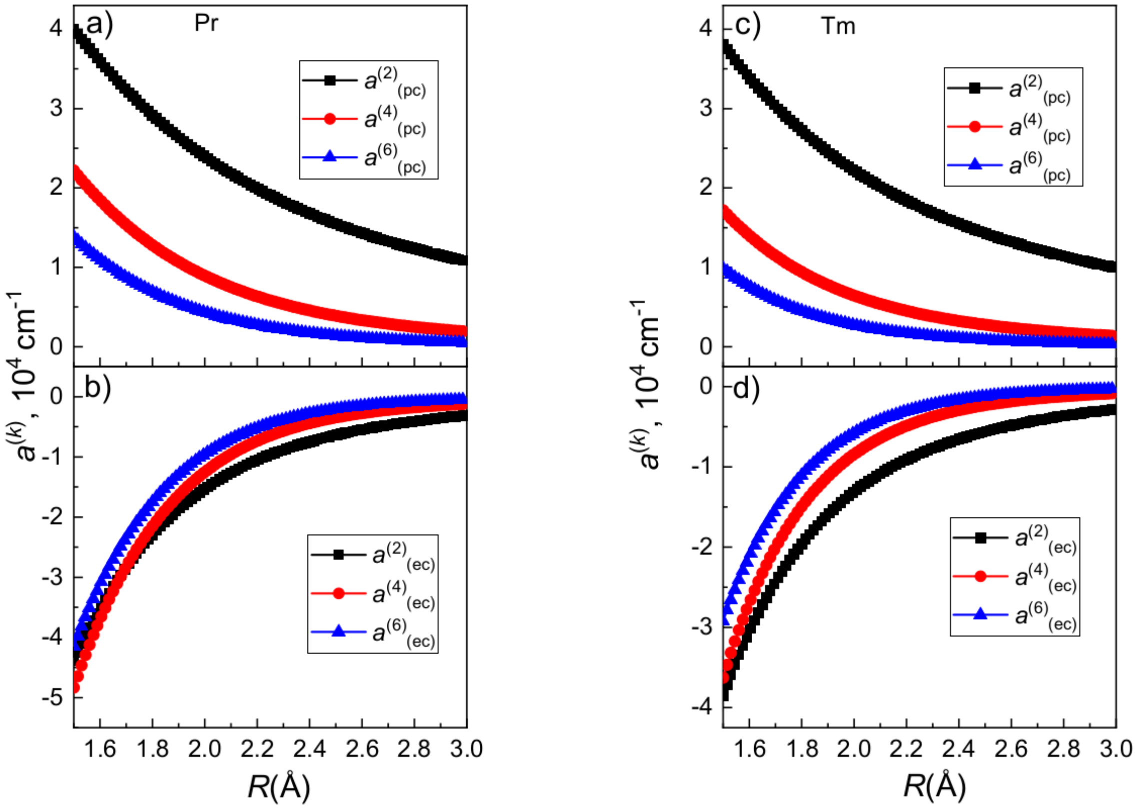

**Figure 2.** Calculated values of $a^{(k)}(k = 1, 3, 5)$ as functions of internuclear distances. The respective results for the Pr-O and Tm-O are a) and c) for point charge contributions $a^{(k)}$ values, b) and d) extended contributions (ec)

the $4f$ and $5d$ electrons, short analytical formulae for calculating the parameters of the odd crystal field on rare-earth ions have been derived. Extended charge contributions to the intrinsic parameters $a^{(1)}$, $a^{(3)}$, and $a^{(5)}$ have been carried out on the Hartree-Fock wave functions of $\mathrm{Pr}^{3+}$-$\mathrm{O}^{2-}$ and of $\mathrm{Tm}^{3+}$-$\mathrm{O}^{2-}$ pairs.

## 4. Conclusion

In the present work, simple analytical expressions are obtained for calculating the parameters of an odd crystalline field, due to the spatial distribution of ligand electrons in compounds with partially filled $f$-shells. They are useful for both rare earth compounds and actinides. Numerical calculations are given on the example of pairs of $\mathrm{Pr}^{3+}$-$\mathrm{O}^{2-}$ and $\mathrm{Tm}^{3+}$-$\mathrm{O}^{2-}$ ions. It is hoped that the calculated dependencies on the metal-ligand distance will contribute to the nature of the formation of odd crystalline fields. These fields mix the states of opposite parity and, as a result, induce electrical dipole transitions between terms and multiplets of $f^n$ configurations. We believe that the obtained formulae will also be useful in studying and predicting various magnetoelectric effects due to interference of magnetic and electric fields in crystals without an inversion center.

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## Appendix

**Table 1.** The values of parameters for the $\mathrm{Pr}^{3+}$ $4f$ and $5d$ wave functions (see Eqs. (5)-(6)) in a.u. [9]

| $C_i(4f)$ | $\alpha_i$ | $S_j(5d)$ | $\beta_j$ |
|---|---|---|---|
| 0.001736 | 0.2 | 0.0079 | 0.089 |
| 0.019626 | 0.388 | 0.155 | 0.234 |
| 0.165342 | 0.75272 | 0.394 | 0.571 |
| 1.352356 | 1.460277 | 0.916 | 1.66 |
| 6.585242 | 2.832937 | $-4.32$ | 2.40 |
| 22.29513 | 5.495898 | $-9.7$ | 6.08 |
| 66.94335 | 10.66204 | 14.6 | 16.5 |
| 131.8784 | 20.68436 | 94 | 35.5 |
| 150.1519 | 40.12766 | 136 | 68 |
| 209.2816 | 77.84766 | 165 | 130 |
| - | - | 270 | 280 |
| - | - | 500 | 1500 |

**Table 2.** The values of parameters for the $\mathrm{Tm}^{3+}$ $4f$ and $5d$ wave functions (see Eqs. (5)-(6)) in a.u. [9]

| $C_i(4f)$ | $\alpha_i$ | $S_j(5d)$ | $\beta_j$ |
|---|---|---|---|
| $1.193802710^{-3}$ | 0.2 | 0.0085 | 0.085 |
| $2.4360152e10^{-2}$ | 0.42 | 0.151 | 0.2813 |
| $2.805697610^{-1}$ | 0.882 | 0.49 | 0.59 |
| 1.9932604 | 1.8522 | 0.75 | 1.65 |
| 9.3469845 | 3.88962 | $-2$ | 3.2 |
| 3.336993710 | 8.168202 | $-17.8$ | 7 |
| 7.432271510 | 17.153224 | 5 | 16.5 |
| $1.121099010^{2}$ | 36.021770 | 30 | 35.5 |
| $1.107032110^{2}$ | 75.645717 | 150 | 60 |
| 8.852034010 | 153.85600 | 250 | 100 |
| - | - | 555 | 300 |

**Table 3.** Parameters of the solution of Poisson equation corresponding to the total electron density of $2s$- and $2p$-electrons of the oxygen ion $O^{2-}$ which were obtained by [21] in a.u.

| $p_k$ | $\gamma_k$ |
|---|---|
| 0.1087 | $7.478010^{3}$ |
| −1.6427 | 5.590910 |
| 0.2428 | $3.952210^{2}$ |
| 2.1133 | 5.641610 |
| 0.8188 | 1.193410 |
| 2.0012 | 3.2214 |
| 2.3481 | 1.1318 |
| 1.2083 | $3.855910^{-1}$ |
| 0.4749 | $9.845110^{-2}$ |
| 0.3254 | $3.317210^{-2}$ |

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