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Atomic Parameters for the $4f^{N-1}5d$ Configurations of Nd^{3+} and Er^{3+} Ions in Crystals

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Matrix elements of spin–orbit interaction, nephelauxetic parameters β_k ($k = 2, 4, 6$), and radial expectation values $\langle r^k \rangle_{4f}$ have been evaluated semi-empirically for the excited configurations $4f^{N-1}5d$ of the Nd^{3+} and Er^{3+} ions doped in crystals. It comprise the crystals as CaF_2, $LiYF_4$, YPO_4, $Y_3Al_5O_{12}$, Cs_2NaYF_6, $Cs_2NaErCl_6$, and K_3YF_6. The $\langle r^k \rangle_{4f}$ values have been determined by the dielectric screening model. The obtained results were compared with those for the ground $4f^N$ configurations of the same ions. It has been concluded that the wave functions of the $4f^{N-1}$ core electrons are more extended than those reported in theoretical studies.

topics: Ln(3+) ions, $4f^{N-1}5d$ configurations, atomic parameters

1. Introduction

The four basic configurations of the trivalent lanthanide ions (Ln^{3+}) are $4f^N$, $4f^{N-1}$5d, $4f^{N-1}$6s, and $4f^{N-1}$6p, with $4f^N$ being the lowest, and $4f^{N-1}5d$ — the first excited configuration ($N = 1$–14). The energy levels within the $4f^N$ and $4f^{N-1}5d$ configurations are spread over hundreds of thousands cm^{-1} [1]. The first excited configurations are rather complex since the number of levels in $4f^2 5d$ of Nd^{3+} ions is 107, while this for $4f^{10}5d$ of Er^{3+} ions is 977 [1]. Throughout the text, Ln^{3+} designates lanthanide ions in the crystals and Ln IV — free lanthanide ions.

There exists an increasing research interest in the $4f^{N-1}5d$ configurations, mainly due to the applications of Ln^{3+} ions in vacuum ultraviolet phosphors [2]. For $4f^{N-1}5d$ the direct Coulomb parameters are $F^k(4f,4f)$, with $k = 2,\ 4, 6$, $F^2(4f,5d)$, and $F^4(4f,5d)$, while the exchange Coulomb parameters are $G^k(4f,5d)$ with $k = 1,\ 3, 5$ [2]. The experimental determinations of the energy levels of the free ions Ln IV (Ln = Nd, Er, Tm, Yb) including the corresponding $4f^N$ ground configurations, as well as the excited configurations $4f^{N-1}5d$, have been performed by Wyart's group [3–7]. The lowest terms of the $4f^2 5d$ configuration of Nd IV found in these studies have been $(^3H)^2H$ at 70817 cm^{-1}, and for Er IV, these are $d(^5I)^6H$ in the *LS* scheme or $(^5I_8)$ (8.3/2) in *JJ*-coupling, at 73426.4 cm^{-1}. Though complementary, the ground configurations $4f^3$ (Nd^{3+}) and $4f^{11}$ (Er^{3+}) differ by the magnitude of spin–orbit interaction and of *J*-mixing, which effects prevail at the end of the lanthanide series [8].

We have previously calculated the matrix elements of spin–orbit interaction (SOI) for the lowest level in the ground $4f^N$ configurations of the Ln^{3+} ions in crystals, namely Ce^{3+} [9], Pm^{3+} and Ho^{3+} [10], Er^{3+} [11], Tm^{3+} [12], Yb^{3+} [13], as well as of certain free ions Ln IV (Ln = Pr, Nd, Er, Tm, Yb) [14].

The radial expectation values $\langle r^k \rangle_{4f}$ in the ground configurations $4f^N$ were used to determine the crystal-field parameters in the point-charge electrostatic description [15] for the calculations of the Slater parameters shifts ΔF_k in the dielectric screening model [16, 17]. Importantly, $\langle r^k \rangle_{4f}$ for the ground states in the $4f^N$ electronic configurations known from atomic-structure studies have recently been compared [18]. However, for the radial expectation values $\langle r^k \rangle_{4f}$ and $\langle r^k \rangle_{5d}$ of the excited configurations $4f^{N-1}5d$ of Ln^{3+} ions, the information is scarce and may be exemplified by the atomic structure computations [2, 19] or by the difference $\langle r^2\rangle_{5d} - \langle r^2\rangle_{4f}$ used in semi-empirical determinations of contributions from two-electron interactions [20, 21]. Corresponding estimates related to $4f^{N-1}5d$ of Ln^{3+} ions in crystals are lacking.

The aims of the present study related to the excited $4f^{N-1}5d$ configurations of the Nd^{3+} and Er^{3+} ions in certain crystals are the following: (i) evaluate the matrix elements of SOI; (ii) determine the nephelauxetic parameters β^k, with $k = 2, 4, 6$; (iii) calculate semi-empirically the radial expectation values $\langle r^k\rangle_{4f}$ of the $4f^{N-1}$ core electrons in ions in the same crystals.

2. Method

The $4f^{N-1}$ and $5d$ electrons of the $4f^{N-1}5d$ configurations will be treated separately, as follows. It has been assumed that the parameters of the $4f^{N-1}$ core (designated with ff) are similar to the parameters for the configurations $4f^N$ [2]. The elements of the matrix A of SOI, depending on the quantum numbers M, were calculated by the products of the doubly-reduced matrix elements (DRME), i.e., double-bar $V^{(11)}$ and $6j$-symbols according to the Wigner–Eckart theorem, for an energy level labeled as $^{2S+1}L_J$ [22–24]. Thus,

$$A_{nl} = \left\langle nl^{\nu}\alpha LSJM \middle| \zeta_{nl} \sum_{i-1}^{N} \boldsymbol{l_i}\cdot\boldsymbol{s_i} \middle| nl^{\nu}\alpha' L'S'J'M' \right\rangle =$$

$$\zeta_{nl}\left(-1\right)^{J+L+S'}\sqrt{l\left(l+1\right)\left(2l+1\right)}\begin{Bmatrix} L & L' & 1 \\ S' & S & J \end{Bmatrix}\langle nl^{\nu}\alpha LS||V^{(11)}||nl^{\nu}\alpha' L'S'\rangle, \qquad (1)$$

where nl^{ν} designates $4f^{N-1}$ or $5d^1$ (i.e., $5d$), the subscripts nl denote $4f$ or $5d$, $l = 3$ stands for f electrons, and α and α' are unspecified quantum numbers. The notations $\langle JM|$ and $|J'M\rangle$ are related to the initial and final states, respectively. For a single $5d$ electron [23], one has

$$\langle l^1 ls||V^{(11)}||l^1\, ls\rangle = \sqrt{\tfrac{3}{2}}. \qquad (2)$$

The $4f^{10}$ core electrons of the excited configuration $4f^{10}5d$ in the Er^{3+} ion are complementary to $4f^4$ with respect to the filled shell $4f^{14}$. The matrix elements of $4f^{14-N}$ and $4f^N$ are interrelated by means of the seniority numbers v and v'. With the term $v = v' = 1$ [22, 23],

$$\langle f^{14-N}vLS||V^{(11)}||f^{14-N}v'L'S'\rangle =$$

$$-\left(-1\right)^{\frac{1}{2}(v-v')+1}\,\langle f^N vLS||V^{(11)}||f^N v'L'S'\rangle. \qquad (3)$$

The sign of $V^{(11)}$ in the matrix elements A_{nl} for $4f^{14-N}$ depends on the sign of $4f^N$ as given by the following expression [23]

$$\langle f^{14-N}vLS||V^{(11)}||f^{14-N}v'L'S'\rangle =$$

$$\frac{2l+1-N}{2l+1-v}\,\langle f^N\alpha LS||V^{(11)}||f^N\alpha' L'S'\rangle. \qquad (4)$$

The above equations (1)–(4) pertain only to wave functions preserving the total spin quantum number S via the delta function $\delta\left(S,S'\right) = 1$.

No attempts have been made to assess the effect in coupling schemes other than LS in order to preserve the coupling schemes used in [3–5] as compatible for both Ln IV ions. Contributions from the next excited configurations $4f^{N-1}6s$ have not been considered since for both Ln IV ions the average energies of the same configurations are about 30×10^3 cm^{-1} higher than those of $4f^{N-1}5d$ [3–5].

The F^k values, with $k = 2, 4, 6$, used in the following equations are known experimental (fitted) ones for a $4f^{N-1}$ electron core and relevant to both the free ions Ln IV and to Ln^{3+} ions in crystals. The nephelauxetic ratios β_k have been obtained by the Slater parameters F^k as follows

$$\beta_k = F^k\left(\mathrm{Ln}^{3+}\right)/F^k\left(\mathrm{Ln\,IV}\right). \qquad (5)$$

The Slater parameters shifts ΔF^k of the title ions in crystals are defined as

$$\Delta F^k = F^k\left(\mathrm{Ln\,IV}\right) - F^k\left(\mathrm{Ln}^{3+}\right). \qquad (6)$$

The radial expectation values $\langle r^k\rangle_{4f}$ of Ln^{3+} in crystals have been determined in this work by means of a transformed formula of the one proposed by Newman [17]

$$\langle r^k\rangle_{4f}\left(\times10^{-10}m\right)^k = \sqrt{\Delta F^k\left(\frac{k}{k+1}+\varepsilon\right)\frac{R^{2k+1}}{C(\varepsilon-1)}}, \qquad (7)$$

where R is the radius of a hole taken by a Ln^{3+} ion in a crystal with optical dielectric constant ε, such that $\varepsilon = n^2$, where n is the index of refraction of the crystal. The coefficient $C = (e^2/(hc))$ Å$=1.1614\times10^5$ cm^{-1} is used to convert units of length Angström [Å] for R and [cm^{-1}] for ΔF^k in $a_0 = 0.5291772$ Å. The radius of the hole in the dielectric has been approximated by the effective ionic radius of the Ln^{3+} ion occupying the substitution site with definite coordination number (CN) in a crystal.

3. Results and discussion

The necessary parameters, i.e., those needed in (1)–(7), for the free ions Nd IV, Er IV, and for the Nd^{3+} or Er^{3+} ions in crystals used in this work are given in Table I. A comparison between the values

TABLE I

The parameters $F^k(ff)$ and spin–orbit coupling constants ζ_{4f}, ζ_{5d} for the $4f^{N-1}5d$ configurations of the free ions Ln IV and Ln^{3+} ions in crystals (in [cm^{-1}]).

Ln IV or Ln^{3+}	$F^2(ff)$	$F^4(ff)$	$F^6(ff)$	ζ_{4f}	ζ_{5d}	Ref.
Nd IV, $4f^25d$	83559	60656	40565	988	1124	[3]
Er IV, $4f^{10}5d$	105750.7	75867.8	53985.1	2548.5	1629.9	[5]
Nd^{3+}:CaF_2	73018	52789	35757	885.3	1216	[25]
Nd^{3+}:LiYF_4	72667	52737	35817	870.1	1216	[26]
Nd^{3+}:YPO_4	71872	51793	35591	876.3	1257	[26]
Nd^{3+}:$\text{Y}_3\text{Al}_5\text{O}_{12}$	70845	51235	34717	876	1132	[27]
Nd^{3+}:K_3YF_6	77399	55956	37902	938.4	1216	[28]
Nd^{3+}:Cs_2NaYF_6	72188	52625	35372	871	1216	[29]
Er^{3+}:CaF_2	103332	71978	57251	2376	1768	[30]
Er^{3+}:LiYF_4	97449	68539	56051	2374	1768	[26]
Er^{3+}:YPO_4	96567	68144	53393	2364	1821	[26]
Er^{3+}:K_3YF_6	103332	71978	57251	2518.6	1768	[28]
$\text{Cs}_2\text{NaErCl}_6$	96717	67374	47541	2363	1346	[31]

TABLE II

Matrix elements A_{nl} of spin–orbit interaction (in [cm^{-1}]) and nephelauxetic parameters β_k for the $4f^{N-1}5d$ configurations of the free ions Ln IV and Ln^{3+} ions in crystals.

	A_{4f}	$-A_{5d}$	β_2	β_4	β_6
Nd IV, $4f^25d$	−2964	1686	1.00	1.00	1.00
Er IV, $4f^{10}5d$	7645.5	2444.9	1.00	1.00	1.00
Nd^{3+}:LiYF_4	−2610.3	1824	0.8696	0.8694	0.8830
Nd^{3+}:Cs_2NaYF_6	−2613	1824	0.8639	0.8676	0.8720
Nd^{3+}:$\text{Y}_3\text{Al}_5\text{O}_{12}$	−2628	1698	0.8479	0.8447	0.8558
Nd^{3+}:YPO_4	−2628.9	1885.5	0.8601	0.8539	0.8774
Nd^{3+}:CaF_2	−2655.9	1824	0.8738	0.8703	0.8815
Nd^{3+}:K_3YF_6	−2815.2	1824	0.9263	0.9225	0.9344
Er^{3+}:$\text{Cs}_2\text{NaErCl}_6$	7089	3028.5	0.9146	0.8880	0.8806
Er^{3+}:YPO_4	7092	4097.2	0.9132	0.8982	0.9890
Er^{3+}:LiYF_4	7122	3978	0.9215	0.9034	1.0383
Er^{3+}:CaF_2	7128	3978	0.9771	0.9487	1.0605
Er^{3+}:K_3YF_6	7555.8	3978	0.9771	0.9487	1.0605

of $F^k(ff)$ parameters for $4f^{N-1}5d$ calculated in [2] and the experimental ones for Ln IV in Table I reveals that the former are 12% to 30% higher than the latter. For the studied crystals, the corresponding deviations from the experiment are almost double. This fact will be used in the discussion below.

The results of the calculations after applying (1)–(5) are listed in Table II. It should be noted that the quantities following ζ_{4f} on the right-hand side of (1) are equal to -3 for Nd^{3+} or 3 for Er^{3+} ions. For a single $5d$ electron, the corresponding factor is $-3/2$ in both cases. For CaF_2, LiYF_4, and K_3YF_6 doped with Er^{3+} the nephelauxetic parameters $\beta_6 > 1.00$ as the experimental $F^6(ff)$ (Er^{3+}) exceed the experimental $F^6(ff)$ for Er IV.

We have compared the relative variations with respect to the corresponding free ion values of the nephelauxetic parameters β_k with those of the SOI designated as $\eta = A_{4f}(\text{Ln}^{3+})/A_{4f}(\text{Ln IV})$, for both $4f^{N-1}5d$ configurations. The meaning of such a doubly-normalized presentation is that it reveals, via the slope $\Delta\beta_k/\Delta\eta$, the mode of changes in a complete nephelauxetic aspect for both ions doped in crystals. The argument for this treatment is based also on the decrease of the magnitude of $\zeta_{4f}(\text{Ln}^{3+})$ in a crystal relative to the free ion value $\zeta_{4f}(\text{Ln IV})$ [32, 33].

With β_6 for Er(3+) in crystals, the number of points is insufficient (3 out of 5 values are > 1.00) to ascertain the applicability of the model. For that reason, it has not been included in Fig. 1c.

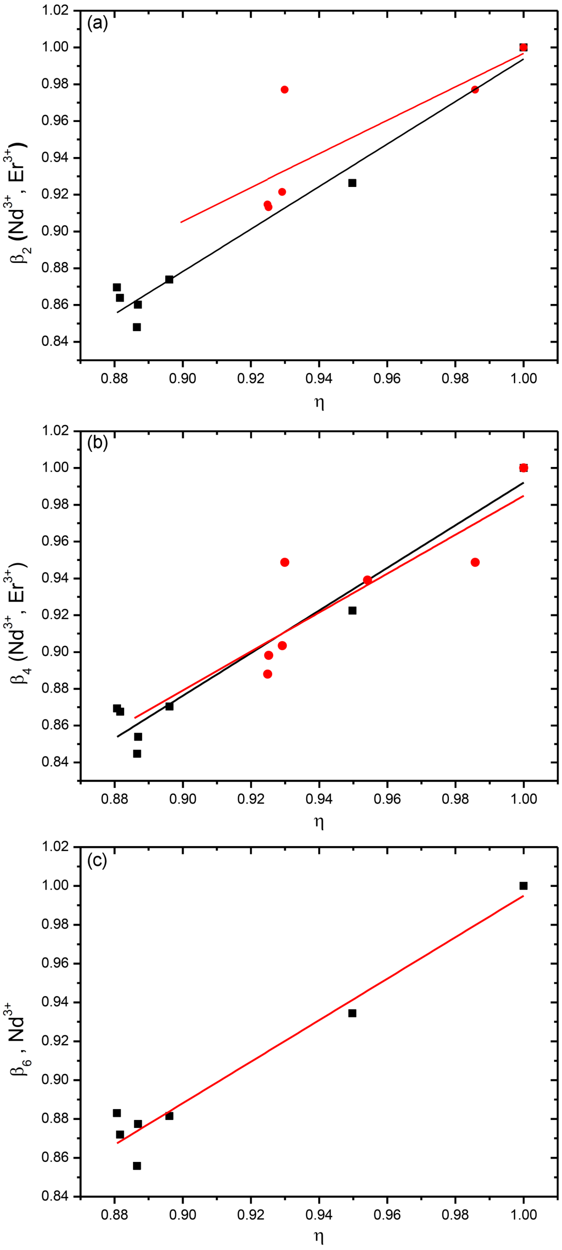

Fig. 1. Nephelauxetic parameters β_k vs ratios of matrix elements of SOI $\eta = A_{4f}(\mathrm{Ln}^{3+})/A_{4f}(\mathrm{Ln\,IV})$ for $4f^{N-1}5d$ configurations of Nd^{3+} (lower lines) and Er^{3+} ions in crystals: (a) β_2, (b) β_4, (c) β_6, for Nd^{3+} only.

TABLE III

Optical dielectric constants ε of some crystals.

Crystal	ε	Ref.
CaF_2	2.056	[34]
$LiYF_4$	2.15	[35]
YPO_4	2.96	[36]
$Y_3Al_5O_{12}$	3.345	[35]
Cs_2NaYF_6	2.25	[37]
Cs_2NaYCl_6	2.85	[38]
K_3YF_6	1.97	[39]

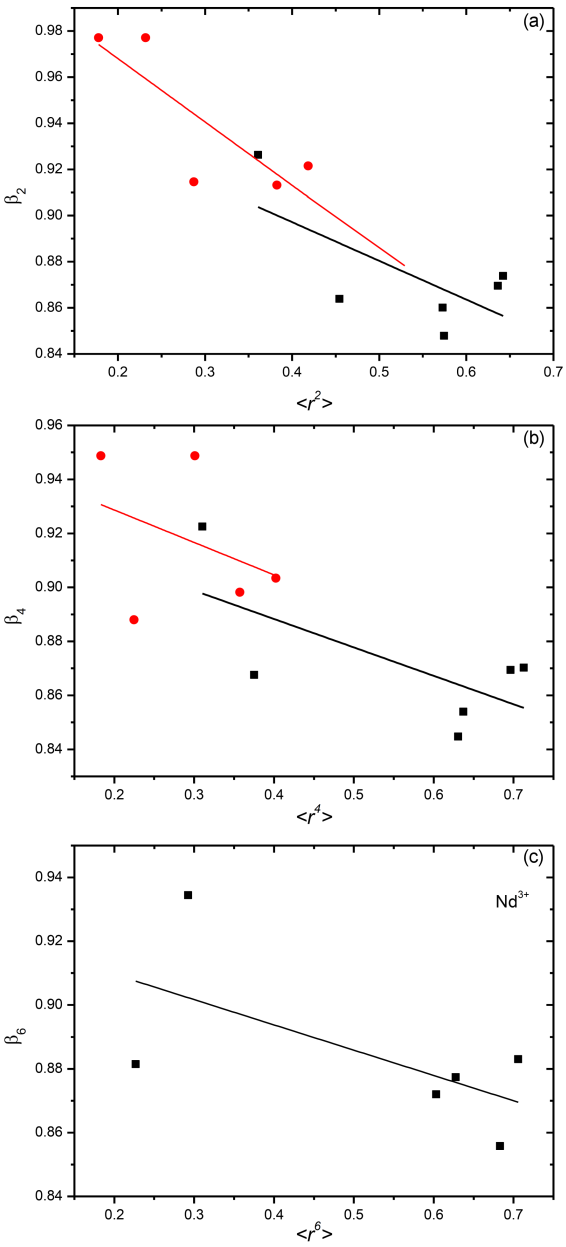

Fig. 2. Nephelauxetic parameters β_k vs radial expectation values $\langle r^k_{4f}\rangle$ for $4f^35d$ configuration of Nd^{3+} (lower lines) and $4f^{10}5d$ of Er^{3+} ions in crystals (a) β_2, (b) β_4, (c) β_6, for Nd^{3+} only.

According to the definitions of the nephelauxetic effect (parameters (5) and (6) and the subsequent dielectric screening model (7)), $\beta_k < 1.00$ and $\Delta F^k < 0$. However, rare exceptions to these restrictions of the physical model may be easily found in the literature for almost every set for each Ln^{3+} ions (with N = 2–12) in crystals, when $\beta_k > 1.00$ and $\Delta F^k < 0$. This pertains most often to the sixth-rank parameters and presents a definite disadvantage of the model. A more precise treatment would require equal approximations in the fitting procedures, i.e., one and the same number and type of atomic parameters included in the fits.

TABLE IV

Radial integrals $\langle r_{4f}^k \rangle$ 10^{-10k} [m^k] of $4f^{N-1}$ core electrons in the $4f^{N-1}5d$ configurations of Ln^{3+} in crystals evaluated in this work by the dielectric screening model. The values with references pertain to the ground $4f^N$ configurations.

Ion:crystal	$\langle r^2 \rangle_{4f}$ ($\times 10^{-20}$) m^2	$\langle r^4 \rangle_{4f}$ ($\times 10^{-40}$) m^4	$\langle r^6 \rangle_{4f}$ ($\times 10^{-60}$) m^6
Nd^{3+}:LiYF$_4$	0.6362	0.6964	0.6830
$4f^3$, Nd^{3+}:LiYF$_4$ [40]^a	0.6109	0.6784	0.7444
Nd^{3+}:CaF$_2$	0.6422	0.7128	0.7059
Nd^{3+}:YPO$_4$	0.5728	0.6372	0.6033
Nd^{3+}:Y$_3$Al$_5$O$_{12}$	0.5745	0.6306	0.6275
Nd^{3+}:Cs$_2$NaYF$_6$	0.4544	0.3751	0.2924
$4f^3$, Nd^{3+}:Cs$_2$NaYCl$_6$ [41]^a	0.4062	0.3812	0.2796
Nd^{3+}:K$_3$YF$_6$	0.3610	0.3104	0.2267
$4f^3$, Nd^{3+} [42]^b	0.3467	0.3070	0.5685
$4f^3$, Nd^{3+} [43]^b	0.3422	0.3039	0.5736
Er^{3+}:CaF$_2$	0.2317	0.3010	–
Er^{3+}:LiYF$_4$	0.4184	0.4023	–
$4f^{11}$, Er^{3+}:LiYF$_4$ [44]^a	0.4061	0.2411	–
Er^{3+}:YPO$_4$	0.3825	0.3572	0.1000
Er^{3+}:K$_3$YF$_6$	0.1778	0.1831	–
Er^{3+}:Cs$_2$NaErCl$_6$	0.2873	0.2248	0.1563
$4f^{11}$, Er^{3+} [42]^b	0.2167	0.1298	0.1765
$4f^{11}$, Er^{3+} [43]^b	0.2165	0.1315	0.1851

^{a} — $\langle r_{4f}^k \rangle_{4f}$ calculated semi-empirically in this work with experimental F^k in Refs., ^{b} — $\langle r_{4f}^k \rangle_{4f}$ theoretical values in studies with relativistic $4f^N$ wave functions in Refs.

The results are seen in Fig. 1a–c. It is evident that both nephelauxetic parameters change almost evenly since the slopes are close to 1. It is noteworthy that the dependence for β_6 for Er^{3+} in crystals has not been presented in Fig. 1c as there are three points for which $\beta_6 > 1.00$ out of five experimental values. The sequence of the points, i.e., of the crystals, for each ion in Fig. 1a–c is the one in Table II. The positions of the free ions Nd IV and Er IV coincide in points with coordinates $(1, 1)$ in Fig. 1. The nephelauxetic parameters β_k for Nd^{3+} ions doped in the listed crystals vary in the sequence $\beta_6 > \beta_2 > \beta_4$ while for the Er^{3+} ions the same ordering of β_k is less pronounced.

For the dielectric screening model, CN $= 8$ of the activator ions Ln^{3+} in all crystals CaF$_2$, LiYF$_4$, YPO$_4$, Y$_3$Al$_5$O$_{12}$, Cs$_2$NaYF$_6$, and Cs$_2$NaErCl$_6$, except for K$_3$YF$_6$ where CN $= 6$. The effective ionic radii R (given in [m] or [Å]) for CN $= 8$ is $R = 1.12$ for Nd^{3+} and $R = 1.00$ for Er^{3+} ions, while for CN $= 6$, $R = 0.98$ and $R = 0.89$, respectively [34]. The dielectric constants of some crystals are given in Table III.

The mean values $\rangle r^k \rangle_{4f}$ of $4f^{N-1}$ core electrons of the title Ln^{3+} ions in crystals have been compared in Table IV with values related to the ground $4f^N$ configurations, calculated semi-empirically in this work through experimental Slater parameters F^k and those known from theoretical studies involving relativistic $4f^N$ wave functions. Estimates for $4f^N$ and $4f^{N-1}$ in $4f^{N-1}5d$ in both cases reveal that the latter are slightly higher than the former, i.e., the $4f^{N-1}$ core electrons wave functions are more extended. It is noteworthy that for the scarcity of specific data about the $4f^{N-1}5d$ configurations of Ln^{3+} ions, the number of points is restricted, especially in the sixth-rank parameters of Er^{3+} ions diluted in crystals.

Although the Cowan's code implies pseudorelativistic $4f$ wave functions [45], the values reported in [2] corresponding to $\langle r_{4f}^k \rangle$ for $4f^{N-1}5d$ are in turn higher than the results from relativistic computations in [42, 43]. We have plotted each rank of the nephelauxetic parameters β_k vs the respective rank of radial expectation values $\langle r_{4f}^k \rangle_{4f}$ for the first excited configuration $4f^{N-1}5d$ of the title ions in crystals. It is evident in Fig. 2a–c that the values of the latter increase with the decrease of the former. This fact is close to the introduction of a bonding parameter b as a measure of the interpenetration of the $4f^{N-1}$ wave function of the Ln^{3+} ion with that of the ligand in a two-center bonding via the relationship

$$b = \frac{1}{2}\left(1 - \bar{\beta}_k\right), \qquad (8)$$

where $\bar{\beta}_k$ is a mean nephelauxetic parameter.

4. Conclusions

Matrix elements $A_{4f}(\mathrm{Ln}^{3+})$ and $A_{4f}(\mathrm{Ln\,IV})$ of SOI, nephelauxetic parameters β_k, and radial expectation values $\langle r^k\rangle_{4f}$ have been determined for the $4f^{N-1}$ core electrons in $4f^{N-1}5d$ configurations of Nd^{3+} and Er^{3+}ions in certain crystals. It has been found that the ratios of spin–orbit coupling parameters and those of the nephelauxetic effect vary in nearly the same manner since the slope $(\Delta\beta_k/\Delta\eta) \approx 1$, where $\eta = A_{4f}(\mathrm{Ln}^{3+})/A_{4f}(\mathrm{Ln\,IV})$. The radial expectation values $\langle r^k\rangle_{4f}(ff)$ for $4f^{N-1}5d$ configurations have been determined in the present study by the dielectric screening model and compared with $\langle r^k\rangle_{4f}$ for the $4f^N$ ground configurations of the same lanthanide ions. It has been concluded that the radial wave functions of the $4f^{N-1}$ core electrons in $4f^{N-1}5d$ are more extended than those in the respective $4f^N$ configurations.

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