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EFFECTIVE INTERATOMIC FORCES FROM ONE-PARTICLE CRYSTAL FIELD PARAMETERS

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1. INTRODUCTION

In a recent paper[1], which will be quoted henceforth as I, the one-particle crystal field experienced by f electrons of magnetic ions within crystals has been derived under the general assumption of arbitrary (possibly noncentral, as, e.g., in the co covalent crystals) effective interatomic forces.

In the present paper, assuming central one-particle effective interatomic forces (a hypothesis which is known to hold, e.g., for metallic systems), we first push a step further the argument of I and derive, in Section 2, more explicit expression for the coefficients of the crystal field occurring both in cubic and hexagonal compounds. The simplicity of Stevens' standard expression for the crystal field coefficients, $A_{mn} < r^m >$ [2-4], is shown to be preserved with, however, the terms of the product specifically renormalized by the non-Coulombian interaction. Then, inverting the argument, we show, in Section 3, that the experimental knowledge of the crystal field coefficients enables us to get valuable insight into the spatial behaviour of the one-particle forces that govern the interaction between the magnetic electrons and the crystal lattice within monocrystalline samples.

The general procedure of Section 3 is applied, in Section 4, to the magnetic Sm^{3+} ion in $SmCo_5$. Amongst the data previously proposed in the literature for the crystal field coefficients in $SmCo_5$ [5-7], those of de Wijn et al.[6] can be markedly better fitted within our one-particle model than the others. Therefrom, we infer that the effective one-particle interatomic forces in $SmCo_5$ are of the Born type, in agreement with the general quantum picture of the effective interatomic forces in solids (see ref.[8] for a comprehensive survey). This result is at variance with the assessement[5] that a simple Coulombian model would be able to account for the crystal field effects in $SmCo_5$.

2. CRYSTAL FIELD COEFFICIENTS FOR CENTRAL INTERATOMIC FORCES

As usual, we choose the origin of the system of coordinates at the nucleus of the magnetic ion to which the considered f electron belongs, denote by $\vec{r} = (x, y, z) = (kr, \ell r, mr)$, the position vector of this electron and by $\vec{R}_j = (X_j, Y_j, Z_j) = (K_j R_j, L_j R_j, M_j R_j)$, the position vector of the point charge standing for the j-th neighbouring ion, j=1,2, ...

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In I.S. units, the effective one-particle potential at $\vec{r}$ due to the j-th ion is given by $(Q_j/4\pi\epsilon_0)v(\vec{R}_j-\vec{r})$, where Q_j is the effective point charge of the ion and $v(\vec{R}_j-\vec{r})$ describes the spatial behaviour of the interaction. Allowing full generality for the spatial behaviour of the function $v(\vec{R}_j-\vec{r})$ and supposing that the potential due to all the surrounding lattice ions is obtained as a superposition of individual contributions, expressions have been derived in I for the one-particle crystal field Hamiltonians in the case of cubic and hexagonal crystals. Let us observe that every potential function $v(\vec{R})$ can be separated into two parts,

$$v(\vec{R}) = v_c(R) + v_{n.c.}(\vec{R}),$$

where $v_c(R) \equiv v_0(|\vec{R}|)$ denotes the central part of the interaction, while $v_{n.c.}(\vec{R})$, its noncentral part. When discussing crystal field effects, in the literature it has been assumed that $v(\vec{R})$ reduces to its central part, $v_c(R)$, (see, e.g., ref.[3] ref.[9] (chapter 1) and ref.[10]). Such a hypothesis reasonably holds for all but the covalent crystals. It is therefore worthwhile to see whether the results reported in I could be further simplified for central forces. It happens that the expressions of the crystal field coefficients can be worked out further to become simpler and more manageable from the point of view of the numerical evaluation. For simplicity, the index c specifying the central part of $v(\vec{R})$ will be henceforth dropped.

Let us consider first the case of cubic crystals, for which the effective one-particle crystal field Hamiltonian of a magnetic f electron reads

$$H_{cf}(\vec{r}) = A_4(r)p_4(k,\ell,m) + A_6(r)p_6(k,\ell,m), \qquad (1)$$

with the coefficients $A_4(r)$ and $A_6(r)$ given respectively by the equations (20a) and (20b) of I. For central interatomic forces, these expressions simplify to

$$A_m(r) = \frac{e}{4\pi\epsilon_0} \sum_{q=0}^{\infty} \frac{\langle r^{m+2q}\rangle}{(m+2q)!} c_{m+2q,m} \sum_j Q_j p_m(K_j, L_j, M_j)F_{q,m}(R_j), \qquad (2)$$

$m=4, 6$.

In (1) and (2), the meaning of the functions p_4 and p_6 is that given by Hutchings[3], namely,

$$p_4(a,\beta,\gamma) = a^4 + \beta^4 + \gamma^4 - 3/5, \qquad (3a)$$

$$p_6(a,\beta,\gamma) = a^6 + \beta^6 + \gamma^6 + (15/4)(a^4\beta^2 + \beta^4\gamma^2 + \gamma^4a^2 +$$

$$+ a^2\beta^4 + \beta^2\gamma^4 + \gamma^2a^4) - 15/14 . \qquad (3b)$$

In equation (2),

$$F_{0,4} = v^{IV} - 6R_j^{-1}v^{III} + 15R_j^{-2}v^{II} - 15R_j^{-3}v^I, \qquad (4a)$$

$$F_{0,6} = v_j^{VI} - 15R_j^{-1}v^V + 105R_j^{-2}v^{IV} + 420R_j^{-3}v^{III} + 945R_j^{-4}v^{II} - 945R_j^{-5}v^I, \qquad (4b)$$

while for $q=1,2,\ldots$, the quantities $F_{q,m}$ are found by recurrence from:

$$F_{q,m} = F_{q-1,m}^{II} + 2R_j^{-1}F_{q-1,m}^I - m(m+1)R_j^{-2}F_{q-1,m} . \qquad (4c)$$

For the sake of simplicity, in eqs. (4a)-(4c), the argument R_j of the functions $F_{q,m}$ and of the potential v has been omitted. Here and in what follows, upper Roman numerals or upper Arabic numerals enclosed in parantheses are alternative notations for the derivatives with respect to R_j.

Let us consider next the case of hexagonal structures, for which the effective one-particle crystal field Hamiltonian reads

$$H_{cf}(\vec{r}) = A_{20}(r)p_{20}(k,\ell,m) + A_{40}(r)p_{40}(k,\ell,m) +$$

$$+ A_{60}(r)p_{60}(k,\ell,m) + A_{66}(r)p_{66}(k,\ell,m), \qquad (5)$$

with the coefficients $A_{20}(r)$, $A_{40}(r)$, $A_{60}(r)$, $A_{66}(r)$ given by the equations (30a)-(30b) of I. For central interatomic forces, these coefficients simplify to

$$A_{mn}(r) = \frac{e}{4\pi\epsilon_0} \sum_{q=0}^{\infty} \frac{\langle r^{m+2q}\rangle}{(m+2q)!} c_{m+2q,m}^n \sum_j Q_j p_{mn}(K_j, L_j, M_j)F_{q,m}(R_j), \qquad (6)$$

where the pairs (m,n) are those entering equation (5).

In (5) and (6), the functions p_{mn} denote unnormalized tesseral harmonics, given respectively by (see ref.[3])

$$p_{20}(a,\beta,\gamma) = 3\gamma^2 - 1, \qquad (7a)$$

$$p_{40}(a,\beta,\gamma) = 35\gamma^4 - 30\gamma^2 + 3, \qquad (7b)$$

$$p_{60}(a,\beta,\gamma) = 231\gamma^6 - 315\gamma^4 + 105\gamma^2 - 5, \qquad (7c)$$

$$p_{66}(a,\beta,\gamma) = a^6 - 15a^4\beta^2 + 15a^2\beta^4 - \beta^6 . \qquad (7d)$$

In equation (6), the meaning of the functions $F_{q,4}(R_j)$ and $F_{q,6}(R_j)$ is that given in equations (4). Further, omitting the argument R_j, we have:

$$F_{0,2} = v^{II} - R_j^{-1} v^I \tag{8}$$

while for $q = 1, 2, \ldots$ the functions $F_{q,2}$ are found from equation (4c) provided $m = 2$.

In the expressions (2) and (6) of the crystal field coefficients, e denotes the electron charge, $\langle r^{m+2q} \rangle$ denotes the radial matrix element of r^{m+2q}, while $c_{m+2q,m}$ and $c_{m+2q,m}^n$ are numerical coefficients which have been detailed in I.

Equations (2) and (6) show that, for central forces, each ionic contribution to a given crystal field coefficient factorizes into two parts: a symmetry determined part, $p_m(K_j, L_j, M_j)$ in (2), $p_{mn}(K_j, L_j, M_j)$ in (6) (which is precisely of the same functional form as the corresponding electronic term that enters the crystal field Hamiltonian), and an interaction determined part, $F_{q,m}(R_j)$, which depends on the strength of the interatomic forces and on the order m of the given harmonics, but is independent of symmetry (the same $F_{q,4}$ occurs both in $A_4(r)$, eq. (2), and in $A_{40}(r)$, eq. (6), while the same $F_{q,6}$ occurs in the coefficients $A_6(r)$, $A_{60}(r)$, and $A_{66}(r)$).

If the potential $v(R)$ is written in the form

$$v(R) = w(R)/R, \tag{9}$$

then compact expressions are found for the functions $F_{q,m}$, $m = 2, 4, 6$; $q = 0, 1, 2, \ldots$, namely,

$$F_{q,2} = R_j^{-1} w^{(q+2)} - 3R_j^{-2} w^{(q+1)} + 3R_j^{-3} w^{(q)}, \tag{10a}$$

$$F_{q,4} = R_j^{-1} w^{(q+4)} - 10 R_j^{-2} w^{(q+3)} + 45 R_j^{-3} w^{(q+2)} -$$
$$- 105 R_j^{-4} w^{(q+1)} + 105 R_j^{-5} w^{(q)}, \tag{10b}$$

$$F_{q,6} = R_j^{-1} w^{(q+6)} - 21 R_j^{-2} w^{(q+5)} + 210 R_j^{-3} w^{(q+4)} - 1260 R_j^{-4} w^{(q+3)} +$$
$$+ 4725 R_j^{-5} w^{(q+2)} - 10395 R_j^{-6} w^{(q+1)} +$$
$$+ 10395 R_j^{-7} w^{(q)}, \tag{10c}$$

which are natural generalization of the results previously obtained for screened Coulomb potentials [11,12].

In the standard Coulomb case, the quantities $F_{q,m}(R_j)$ vanish identically for $q = 1, 2, \ldots$, and the crystal field coefficients are obtained in the form of the well-known product $A_{mn} \langle r^m \rangle$ which constituted the widely used Stevens' notation (refs. [2,4,10] etc.). It is interesting to note that our results, eqs. (2) and (6) resectively, can be brought to a form which is similar to that of Stevens with, however, the two terms of the product renormalized by the non-Coulombian interaction.

Let us denote:

$$G_{q,m} = \frac{e}{4\pi\epsilon_0} \frac{c_{m+2q,m}}{(m+2q)!} \sum_j Q_j \, p_m(K_j, L_j, M_j) F_{q,m}(R_j) \tag{11}$$

$m = 4, 6$; $q = 0, 1, 2, \ldots$.

Then equation (2) can be written in the form:

$$A_m(r) = G_{0,m} \langle \widetilde{r^m} \rangle, \qquad m = 4, 6. \tag{12}$$

where the quantities

$$\langle \widetilde{r^m} \rangle = \langle r^m \rangle + \sum_{q=1}^{\infty} \langle r^{m+2q} \rangle \, G_{q,m}/G_{0,m}, \tag{13}$$

can be regarded as <u>renormalized radial matrix elements</u> for cubic structures.

Similarly, if we denote

$$G_{q,mn} = \frac{e}{4\pi\epsilon_0} \frac{c_{m+2q,m}^n}{(m+2q)} \sum_j Q_j \, p_{mn}(K_j, L_j, M_j) F_{q,m}(R_j) \tag{14}$$

the equation (6) can be written in the form

$$A_{mn}(r) = G_{0,mn} \langle \widetilde{r^m} \rangle_n, \qquad (m,n) = (2,0), (4,0), (6,0), (6,6). \tag{15}$$

where

$$\langle \widetilde{r^m} \rangle_n = \langle r^m \rangle + \sum_{q=1}^{\infty} \langle r^{m+2q} \rangle \, G_{q,mn}/G_{0,mn}, \tag{16}$$

are renormalized radial matrix elements in the case of hexagonal structures.

3. EFFECTIVE INTERACTOMIC FORCES FROM CRYSTAL FIELD DATA

The usual interpretation of the experimental data concerning the crystal field splittings of the one-electron levels of the incompletely filled f shells simply attributes to the crystal field coefficients the role of some conventional fit parameters [13,4,9]. To give a theoretical interpretation to these coefficients, most of the research reports published in the last years (see, e.g., Refs. [8-18] of I, as well as the recent authoritative reviews by de Wijn et al. [6] and by Kirchmayer et al. [14]) still compare the experimental data with the predictions of the electrostatic charge model although strong arguments have been previously furnished by Newman and co-workers on the inadequacy of this model (see Newman [10] and references quoted therein).

The results derived in the previous section show that the crystal field Hamiltonian explicitly contains, through the functions $F_{q,m}(R_j)$ entering the crystal field coefficients, the effective one-particle potential that governs the interatomic interactions. This suggests <u>the use of the experimental crystal field data to get information on the effective interatomic forces within crystals.</u>

Solutions have to be given first to the following preliminary points: (i) ensure knowledge of the radial matrix elements $<r^{2p}>$, $p=1,2,\ldots$, for the magnetic ion of interest; (ii) ensure knowledge of the effective point charges Q_j for the given crystal lattice; (iii) solve the technical difficulties associated to the evaluation of the lattice sums ((11) and/or (14)).

(i) Reliable theoretical values for the radial matrix elements $<r^2>$, $<r^4>$ and $<r^6>$, which cover practically all the di- and trivalent rare-earth ions of interest have been recently reported by Freeman and Desclaux[15]. If in the equations (13) and (16), a cut-off of the q sums, at

$$q_{max} = 3 - m/2 , \qquad (17)$$

is introduced, then the already tabulated values of reference[15] suffice to calculate the renormalized radial matrix elements. For many crystals containing rare-earth ions, the experimental values of the crystal field coefficients significantly decrease in the sequence of the increasing order of the electronic harmonics. Taking into account the exponential convergence of the q sums in the equations (13) and (16), we conclude that there are crystalline compounds for which the use of the cut-off (17) should not introduce errors larger than a few percent in the theoretical estimates.

(ii) As discussed in the papers by Chetal and Sarode [16,17], it is the Pauling method [18,19], which yields an adequate measure for the effective point charges that are to replace the spatially extended ions of the crystal. Accurate Pauling charges have been reported for several RCo_5 (R= rare-earth metal) compounds [17].

(iii) In equations (11) and (14), the lattice sums are obtained by point-by-point summation over all the lattice sites. We can write generically,

$$\delta = \sum_j \mathcal{F}_j = \lim_{n \to \infty} \delta_n , \qquad (18)$$

$$\delta_n = \sum_{j \in \mathcal{C}_n} \mathcal{F}_j , \quad \mathcal{C}_1 \subset \mathcal{C}_2 \subset \ldots \subset \mathcal{C}_n \subset \ldots \qquad (19)$$

Convergence of $\{\delta_n\}$ in (18) towards physically correct results, irrespective of the spatial decay of the summands $\mathcal{F}_j$ in (19),

is automatically ensured if and only if the volumes in the sequence $\{\mathcal{C}_n\}$ are similarily related to the elementary cell of the Bravais lattice associated to the given crystal structure.

Further, in (19), the contributions coming from crystalographically equivalent neighbours can be grouped together to yield:

$$\delta_n = \sum_{s \in V_n} \nu_s \mathcal{F}_s , \qquad (20)$$

where the "reduced" volume V_n contains only crystallographically unequivalent neighbours of the given magnetic ion, and ν_s denotes the number of equivalent neighbours of the ion located at $R_s \in \mathcal{C}_n$. The reduced volume V_n is similarly related to the representation domain of the elementary cell, defined (Cracknell [20], chap. 1) as the smallest region from which the entire cell is generated once by the generators of the symmetry point group of the given crystal structure.

The next point of our discussion of principle concerns the manner of describing the one-particle potential $v(R)$. An approach that is both very simple and efficient, consists (Torrens [8] chap. 4) in choosing some functional dependence which interpolates between known behaviour of $v(R)$ in the limit of very small R and of very large R.

Existing elastic and heat data suggest that, at distances smaller than the lattice constant, the screened Coulomb potential should provide a satisfactory picture for the effective potential, while at larger distances it is the Born potential which is more adequate to this purpose. A mathematical function which meets these requirements is the following parametric representation of $v(R)$:

$$v(R) = \frac{B}{e^{BR} - 1} e^{-CR} , \quad 0 \le B, C < +\infty , \qquad (21)$$

Indeed, if $B=C=0$, then $(Q/4\pi\epsilon_0) v(R) = Q/(4\pi\epsilon_0 R)$, the pure Coulomb case, while if $B=0$, $C >0$, then $(Q/4\pi\epsilon_0) v(R) = Qe^{-CR}/(4\pi\epsilon_0 R)$, the screened Coulomb case. Moreover, if $R \to 0$, $(Q/4\pi\epsilon_0) v(R) \to Qe^{-CR}/(4\pi\epsilon_0 R)$, the screened Coulomb potential, while if $R \to +\infty$, $(Q/4\pi\epsilon_0) v(R) \to B Q e^{-(B+C)R}/(4\pi\epsilon_0)$, the Born potential.

Equation (21) represents a Brinkman-2 type potential (Torrens [8, p.68], Brinkman [21]), modified so as to show correct physical behaviour at every available value of the parameters in the pair (B,C).

Let $A_{mn}^T (B,C)$ be, at given B and C values, a set of crystal field coefficients calculated from Eqs. (12) or (15), accor-

ding to the procedure discussed above, and let A_{mn}^E be a set of experimental data for these coefficients. We construct the deviation in the least squares sense,

$$\chi^2(B, C) = \sum_{m,n} [A_{mn}^T(B, C) - A_{mn}^E]^2 , \qquad (22)$$

and define the "physical parameters" of the potential (21), B_0 and C_0 respectively, to be that point of the (B, C) plane at which

$$\chi^2(B_0, C_0) = \min_{B,C} \{\chi^2(B, C) \mid 0 \le B, C < +\infty \} . \qquad (23)$$

This problem is strongly non-linear, therefore it is useless to try to locate the point (B_0, C_0) from the condition of vanishing the first variation of $\chi^2(B, C)$. The solution is obtained only numerically via successive evaluations of $\chi^2(B, C)$. A study of the behaviour of the function $\chi^2(B, C)$ in the (B, C) plane shows that, in general, two isolated valleys of minima exist which are separated by a high ridge. This property gives us the possibility of define economical paths towards the local minima at every valley, consisting in the location of a particular point of that valley and then of the minimum along it. A comparison of the two minima provides the physical parameters B_0, C_0.

4. CRYSTAL FIELD COEFFICIENTS AND THE EFFECTIVE INTERATOMIC POTENTIAL IN $SmCo_5$

The crystal field investigations of the last decade have been characterized by extensive studies of the various rare earth (R) –transition metal (T) intermetallic compounds. Among the RT_5 compounds, $SmCo_5$ received particular attention, motivated bot both by its interesting physical properties and the important permanent magnet applications.

X - ray studies established that the monocrystalline $SmCo_5$ structure is of the $CaCu_5$ type with the lattice constants[22]:

$$a = 0.4997 \text{ nm}, \quad c = 0.3978 \text{ nm}, \qquad (24)$$

The Sm^{3+} ions occupy sites of point symmetry 6/mmm, while the Co ions are distributed between two unequivalent crystallographic sites, trigonal and icosahedral.

The effective Pauling charges which are to replace the bare charges of the Sm and Co ions in a point charge calculation have been determined by Sarode and Chetal[17] from X-ray data to be, respectively,

$$Q_{Sm} = +2.13|e| \quad \text{and} \quad Q_{Co} = -0.41|e|, \qquad (25)$$

where $|e|$ is the absolute value of the electron charge. The value Q_{Co} in (25) represents an average over the trigonal and icosa-

hedral Co sites in the $SmCo_5$ lattice. Although the non-equivalence of these positions should result in some difference between the Co effective charges at the two sites, it was not possible to establish a measure for this difference from X-ray data [17].

The radial integrals for the Sm^{3+} ion are [15]:

$$\langle r^2 \rangle = 0.9743 a_0^2, \quad \langle r^4 \rangle = 2.260 a_0^4, \quad \langle r^6 \rangle = 10.55 a_0^6, \qquad (26)$$

where $a_0 = 5.29177 \times 10^{-11}$ m, is the Bohr radius.

In order to solve the least squares problem (23), we need reference values for the one-particle crystal field coefficients at the Sm^{3+} sites in $SmCo_5$. We have at our disposal three sets of such data:

Sankar et al.[5] have obtained:

$$A_{20}^E / k_B = -420°K, \qquad A_{40}^E / k_B = -25°K,$$
$$A_{60}^E / k_B = +1°K, \qquad A_{66}^E / k_B = +6°K, \qquad (27a)$$

where k_B denotes the Boltzmann constant.

De Wijn, van Diepen and Buschow[6] have used:

$$A_{20}^E / k_B = -200°K, \qquad A_{40}^E / k_B = 0,$$

$$A_{60}^E / k_B = 0°K, \qquad A_{66}^E / k_B = 0°K \qquad (27b)$$

Finally, Bouncherle et al.[7] inferred from their measurements
$$A_{20}^E / k_B = -200°K, \qquad A_{40}^E / k_B = 0°K ,$$
$$A_{60}^E / k_B = +50°K, \qquad A_{66}^E / k_B = 0°K, \qquad (27c)$$

with an uncertainty of $\pm 50°K$ in the data.

Starting with every of the sets (27a)-(27c) as the experimental one for the crystal field coefficients, the least squares problem (23) has been solved. The obtained results are collected in Tables I-III.

Table I shows that, equation (27a) on one side, and equations (27b) and (27c) on the other side, lead to completely different predictions for the spatial behaviour of the effective interatomic potential (21). Thus, the set (27a) is consistent with the screened Coulomb potential

$$v(R) = e^{-C_0 R}/R, \quad C_0 = 5.780/a, \qquad (28a)$$

while both the sets (27b) and (27c) lead to the prediction that the effective potential should be of the Born type,

$$v(R) \approx B_0 e^{-B_0 R}, \quad B_0 = 11.725/a, \qquad (28b)$$

where a is the lattice constant given in equation (24).

In fact, the crystal field coefficients (27a) have been evaluated in [6] as theoretical coefficients under the following hypotheses:(a) the potential is purely Coulombian; (b) nearest neighbours contribution only is retained; (c) $Q_{Sm} = +3|e|$, , $Q_{Co} = 0$. The hypothesis $Q_{Co} = 0$ has been adopted because [23]

Table 1

Parameters of the Brinkman-2 potential (21) and minimal χ^2 values for the three sets of experimental data, equations (27a)-(27c)

Experimental set	$B_0 a$ *	$C_0 a$ *	$\chi^2(B_0, C_0)/k^2$ ($^\circ$K)
(27a)	0.000	5.780	355.230
(27b)	11.725	0.000	7.455
(27c)	11.724	0.000	2449.87

* The products $B_0 a$ and $C_0 a$ are dimensionless; a denotes the lattice constant, Eq. (24).

Table 2

Theoretical crystal field coefficients at Sm^{3+} site in $SmCo_5$ as given by equation (15), with the parameters of the Brinkman 2 potential (21) given in Table 1.

Experimental set	A_{20}^T/k_B ($^\circ$K)	A_{40}^T/k_B ($^\circ$K)	A_{60}^T/k_B ($^\circ$K)	A_{66}^T/k_B ($^\circ$K)
(27a)	-420.32	-7.47	0.71	-0.91
(27b)	-199.91	-2.55	0.58	-0.78
(27c)	-200.00	-2.55	0.58	-0.78

the model would had otherwise contradict the experimental evidence for an easy magnetization axis of the ferromagnetic phase along the crystallographic c-axis; (d) Burns corrections [24] are introduced to account for the shielding of the 4f electrons from the crystalline environment.

Further, several alternative values have been tested and it was then concluded that the set (27a) provides the best data for the crystal field coefficients.

Our results, equation (28a), does not support the simplifying assumptions (a)-(c), while the assumption (d) is unnecessary to a general crystal field calculation. Table 2 shows that, in the set (27a), the cofficients A_{40} and $\overline{A_{66}}$ are exceedingly large in magnitude, the latter carrying also a wrong sign.

As for the sets (27b) and (27c), the latter leads to an enormous minimal χ^2. We conclude therefore that the reference value of the coefficient A_{60} in (27c) should be in error in a proportion of about 100%. While using the set (27b), de Wijn, van Diepen, and Buschow [8,25] asserted that from their experimental data it cannot be confirmed or excluded the existence of small nonzero higher order coefficients. The results summarized in Table 2 show that these coefficients are different from zero with, however, very small values. (Thus, A_{40}, which is the largest among them, is about two orders of magnitude smaller than A_{20}).

The last point of our discussion concerns the results given in Table 3. These show that the non-Coulombian character of the effective interatomic interactions leads to a renormalization of the radial matrix elements, equation (16), which seriously alters the bare radial matrix elements (26).

A comparison of the relative magnitudes of the two correction terms which enter the expression of $<r^2>$ shows that the first correction brings the overhelming part to the renormalization. This result provides an a posteriori proof for the use of the cut-off (17) in (16).

Table 3

Renormalization factors, $\widetilde{<r^m>}/<r^m>$, for the radial matrix elements, Eq. (16), in the case of the Brinkman-2 potential (21) with the parameters determined as in Table 1

Experimental set	$\widetilde{<r^2>}/<r^2>$	$\widetilde{<r^4>}/<r^4>$
(27a)	1.065	1.080
(27b)	1.178	1.278
(27c)	1.178	1.277

In conclusion, a method was given for the derivation of the effective interatomic forces in crystals starting with crystal field data. In turn, the obtained results allow us to decide upon the consistency of existing crystal field data.

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Адам С., Адам Г., Корчовей А.   E17-82-422
Эффективные межатомные силы из одначастичных параметров кристаллического поля

На основе полученных теоретических представлений для коэффициентов кристаллического поля развит подход к определению пространственной зависимости эффективных межатомных сил в кристаллах. Предлагаемый метод использован в случае иона Sm^{3+} в $SmCo_5$. Данный подход позволяет определить, как вид эффективного межатомного потенциала, так и самосогласованность экспериментальных данных.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Adam S., Adam Gh., Corciovei A.   E17-82-422
Effective Interatomic Forces from One-Particle Crystal Field Parameters

Theoretical results are obtained for the crystal field coefficients which enable us to develop an approach to the use of the crystal field data for the derivation of information on the effective interatomic forces in crystals. The method is applied to the magnetic Sm^{3+} ion in $SmCo_5$, and it is shown to provide valuable results both for the effective interatomic potential and for the consistency of various sets of crystal field parameters previously proposed in the literature.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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