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CHARGE PENETRATION EFFECTS IN RARE-EARTH CRYSTAL FIELDS.(U)
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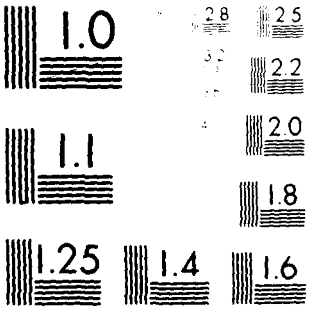

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SECURITY CLASSIFICATION OF THIS PAGE (*When Data Entered*)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER HDL-TR-1990 — 2. GOVT ACCESSION NO. AD A117494	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (*and Subtitle*) Charge Penetration Effects in Rare-Earth Crystal Fields	5. TYPE OF REPORT & PERIOD COVERED Technical Report 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(*s*) Cylde A. Morrison	8. CONTRACT OR GRANT NUMBER(*s*)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Harry Diamond Laboratories 2800 Powder Mill Road Adelphi, MD 20783	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Program Ele: 6.11.10.2
11. CONTROLLING OFFICE NAME AND ADDRESS U.S. Army Materiel Development and Readiness Command Alexandria, VA 22333	12. REPORT DATE June 1982 13. NUMBER OF PAGES 31
14. MONITORING AGENCY NAME & ADDRESS(*if different from Controlling Office*)	15. SECURITY CLASS. (*of this report*) UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (*of this Report*)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (*of the abstract entered in Block 20, if different from Report*)

18. SUPPLEMENTARY NOTES

DRCMS Code: 611102.31B.00.11
HDL Project: 319232
DA Project: 1L161102A31B

19. KEY WORDS (*Continue on reverse side if necessary and identify by block number*)

Crystal field
Shielding
Overlap
Rare-earth ions
Charge penetration
Ligand effects

20. ABSTRACT (*Continue on reverse side if necessary and identify by block number*)

Corrections are given to the multipolar components, A_{nm}, of the crystal field at a rare-earth ion site in a solid. These corrections are caused by the penetration of an electron on the rare-earth ion into the charge distribution of the ligand. A semiclassical description of the ligand charge distribution is used in the analysis, and the results are cast into a form so that the total charge on a ligand and the extent of the charge distribution can be treated as parameters.

CONTENTS

APPENDICES

FIGURES

1. INTRODUCTION

An earlier report[1] attempts to reconcile the multipolar lattice sums, A_{nm}, of various structures to the phenomenological crystal field parameters, B_{nm}, for a number of rare-earth ions. In the theory that was used, three parameters were introduced. For calcium tungstate, the three parameters introduced were τ, the outward expansion of the radial wave functions from the Hartree-Fock value; q, the effective charge on the oxygen ion; and η, an effective position of the oxygen with respect to the tungsten site chosen such as to reproduce the lowest of the $(WO_4)^{-2}$ complex when viewed from a distance large compared with the W-O distance. This model, when used with appropriate shielding factors,[2-5] gave excellent results for calcium tungstate. Later improvements[6] in the three-parameter theory gave better results for calcium tungstate. For other host materials such as YVO_4, the same procedure does not give satisfactory results.

Therefore, it was decided to investigate the possibility of a correction due to the penetration of the rare-earth electrons into the charge distribution on the ligands. The exchange of rare-earth electrons with the electrons on the ligands was ignored in the investi-

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[1] *Richard P. Leavitt, Clyde A. Morrison, and Donald E. Wortman, Rare Earth Ion-Host Crystal Interactions, 3. Three-Parameter Theory of Crystal Fields, Harry Diamond Laboratories HDL-TR-1673 (June 1975).*

[2] *R. M. Sternheimer, Phys. Rev., 84 (1951), 244.*

[3] *R. E. Watson and A. J. Freeman, Phys. Rev., 135 (1964), A1209.*

[4] *D. Sengupta and J. O. Artman, Phys. Rev., B1 (1970), 2986.*

[5] *P. Erdös and J. H. Kang, Phys. Rev., B6 (1972), 3393.*

[6] *Clyde A. Morrison, Nick Karayianis, and Donald E. Wortman, Rare-Earth Ion-Host Lattice Interactions, 4. Predicting Spectra and Intensities of Lanthanides in Crystals, Harry Diamond Laboratories HDL-TR-1816 (June 1977).*

gation. The effects of charge penetration were previously calculated,[7] but the method followed did not leave any parameters that could be used to fit the experimental data; thus, this method is not suitable for our purposes.

2. THEORY

The charge distribution, $\rho(r_i)$, surrounding the ligand ion is chosen to be spherically symmetric and of the form

$$\rho\left(r_i\right) = N r_i^2 e^{-\gamma r_1} \quad , \tag{1}$$

where $N = \gamma^5 Q/96\pi$ and Q is the effective charge on the ligand. Such a charge density is expected for hydrogenic wave functions representing the six 2p electrons or for both the 2s and 2p electrons using five Slater-type orbitals.[8]

We let $\vec{R}$ be the position of the nucleus of a ligand ion measured from the rare-earth nucleus and $\vec{r}$ be the position of the rare-earth electron. Also, we let $\vec{r}_1$ be the position of the volume element of charge $\rho(r_1)\, d\tau_1$ from the oxygen nucleus. Then the electric potential at the rare-earth electron at $\vec{r}$ due to this element of charge is

$$d\phi = \frac{\rho\left(r_1\right)\, d\tau_1}{\left|\vec{R}_1 + \vec{r}_1\right|} \quad , \tag{2}$$

where

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[7] *A. K. Raychaudhuri and D. K. Ray, Proc. Phys. Soc.,* <u>*90*</u> *(1967), 839.*

[8] *J. C. Slater, Phys. Rev.,* <u>*36*</u> *(1930), 57.*

$$\vec{R}_1 = \vec{R} - \vec{r} \quad ,$$

$$d\tau_1 = r_1^2 \; dr_1 \; d\Omega_1 \quad ,$$

and

$$d\Omega_1 = \sin\,\theta_1 \; d\theta_1 \; d\phi_1 \quad .$$

Before integrating equation (2), it is convenient to expand $|\vec{R}_1 + \vec{r}_1|$ in spherical harmonics so that

$$\frac{1}{\left|\vec{R}_1 + \vec{r}_1\right|} = \sum_{\ell m} \frac{4\pi}{2\ell + 1} \, (-1)^{\ell} \left[\frac{r_1^{\ell}}{R_1^{\ell+1}}\right] Y_{\ell m}^{*}\left(\hat{R}_1\right) Y_{\ell m}\left(\hat{r}_1\right) \tag{3}$$

for $r_1 < R_1$; for $r_1 > R_1$, the factor in brackets becomes $R_1^{\ell}/r_1^{\ell+1}$. Since we assumed that the charge density $\rho(r_1)$ is spherically symmetric, we can integrate over $d\Omega_1$ so that

$$\int_{\Omega_1} \frac{d\Omega_1}{\left|\vec{R}_1 + \vec{r}_1\right|} = \begin{cases} \dfrac{4\pi}{R_1} \quad , & \text{for } R_1 > r_1 \quad , \\[2ex] \dfrac{4\pi}{r_1} \quad , & \text{for } R_1 < r_1 \quad , \end{cases} \tag{4}$$

where we have used the relation

$$\int_{\Omega_1} Y_{\ell m}\left(\hat{r}_1\right) \, d\Omega_1 = \sqrt{4\pi} \; \delta_{\ell 0} \delta_{m0} \quad .$$

The electric potential at the rare-earth electron is then

$$\phi = 4\pi \int_0^{R_1} \frac{\rho\left(r_1\right)}{R_1} r_1^2 \, dr_1 + \int_{R_1}^{\infty} \rho\left(r_1\right) r_1 \, dr_1 \quad , \tag{5}$$

or

$$\phi = \frac{1}{R_1} \int_0^{\infty} 4\pi\rho\left(r_1\right) r_1^2 \, dr_1 - \int_{R_1}^{\infty} 4\pi r_1^2 \rho\left(r_1\right) \, dr_1 \left(\frac{1}{R_1} - \frac{1}{r_1}\right) \quad . \tag{6}$$

The first integral in equation (6) gives the total charge and, since $R_1 \leq r_1$, the integrand of the second integral is always positive. Thus, the potential is always less than that of a point charge located at $\vec{R}_1$. If we let

$$I = \int_{R_1}^{\infty} r_1^2 \rho\left(r_1\right) \, dr_1 \left(\frac{1}{R_1} - \frac{1}{r_1}\right) \tag{7}$$

and use the charge distribution given in equation (1), this becomes

$$I = \frac{N4!}{\gamma^5 R_1} \left(1 + \frac{3}{4} \gamma R_1 + \frac{\gamma^2 R_1^2}{4} + \frac{\gamma^3 R_1^3}{24}\right) e^{-\gamma R_1} \quad , \tag{8}$$

where we have used the easily derivable expression

$$\int_y^{\infty} x^n e^{-\gamma x} \, dx = \frac{n! e^{-\gamma y}}{\gamma^{n+1}} \sum_{\nu=0}^{n} \frac{(\gamma y)^{\nu}}{\nu!} \quad .$$

Further, by differentiating $e^{-\gamma R_1}$ with respect to γ, the result on the right side of equation (8) can be written

$$\frac{1}{R_1}\left(1 + \frac{3}{4}\gamma R_1 + \frac{\gamma^2 R_1^2}{4} + \frac{\gamma^3 R_1^3}{24}\right) e^{-\gamma R_1}$$

$$= 1 - \frac{3}{4}\gamma \frac{d}{d\gamma} + \frac{\gamma^2}{4}\frac{d^2}{d\gamma^2} - \frac{\gamma^3}{24}\frac{d^3}{d\gamma^3}\frac{e^{-\gamma R_1}}{R_1} \tag{9}$$

$$\equiv O(\gamma)\frac{e^{-\gamma R_1}}{R_1} \quad ,$$

and equation (8) becomes

$$I = \frac{Q}{4\pi} O(\gamma)\frac{e^{-\gamma R_1}}{R_1} \quad .$$

The entire expression of equation (6) can be written

$$\phi = Q\left(\frac{1}{R_1} - O(\gamma)\frac{e^{-\gamma R_1}}{R_1}\right) \quad , \tag{10}$$

where $R_1 = |\vec{R} - \vec{r}|$.

It is convenient for later work to expand equation (10) in terms of $C_{nm}(\hat{r})$, defined by

$$C_{nm}(\hat{r}) = \left(\frac{4\pi}{2n+1}\right)^{1/2} Y_{nm}(\hat{r}) \quad ,$$

so that the first term in equation (10) becomes

$$\frac{1}{\left|\vec{R} - \vec{r}\right|} = \sum_{n,m} \frac{r^n}{R^{n+1}} C^*_{nm}\left(\hat{R}\right)C_{nm}\left(\hat{r}\right) \quad , \tag{11}$$

with $r < R$. Similarly,[9]

$$\frac{e^{-\gamma\left|\vec{R} - \vec{r}\right|}}{\left|\vec{R} - \vec{r}\right|} = \sum_{n,m} \frac{2\gamma}{\pi} (2n+1) i_n(\gamma r) k_n(\gamma R) C^*_{nm}\left(\hat{R}\right)C_{nm}\left(\hat{r}\right) \quad , \tag{12}$$

where $R < r$ and $i_n(x)$ and $k_n(x)$ are modified spherical Bessel functions of the first and third kinds, respectively.

If we define

$$A_{nm} \equiv \frac{-eQ}{R^{n+1}} C_{nm}\left(\hat{R}\right)$$

and

$$\Delta_n(r,R) \equiv \frac{R^{n+1}}{r^n} \frac{2(2n+1)}{\pi} O(\gamma)\gamma i_n(\gamma r) k_n(\gamma R) \quad , \tag{13}$$

we can write the potential energy of the electron at r using equation (10) as

$$\begin{aligned} U(r) &= -e\phi(r) \\ &= \sum_{n,m} A^*_{nm}\left[1 - \Delta_n(r,R)\right] r^n C_{nm}\left(\hat{r}\right) \quad , \end{aligned} \tag{14}$$

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[9] *M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, National Bureau of Standards Applied Mathematics Series (1966), 445.*

which shows that, if $\Delta_n(r,R)$ is positive and less than 1, the charge distribution reduces the A_{nm} that would be calculated from a point charge model. Since, as R becomes very large, $k_n(\gamma R)$ decreases as $e^{-\gamma R}$, $\Delta_n(r,R)$ vanishes, and the rare-earth electron "sees" effectively a point charge. Thus, for ions remote from the rare-earth site, a point charge model is sufficient.

3. DISCUSSION OF AND APPROXIMATIONS TO $\Delta_n(r,R)$

In defining $\Delta_n(r,R)$ by equation (13), the expression

$$O(\gamma)\left[\gamma i_n(\gamma r)k_n(\gamma R)\right]$$

occurs. With a great deal of tedious algebra using $O(\gamma)$ defined by equation (9) and using the differential equations satisfied by $i_n(x)$ and $k_n(x)$, this result is given by

$$O(\gamma)\gamma i_n(\gamma r)k_n(\gamma R) = \frac{(2n+1)y^{n+1}}{2\pi x^n}\Big[F_n(x,y)i_n(x)k_n(y)$$

$$- G_n(x,y)i_{n-1}(x)k_n(y) + H_n(x,y)i_n(x)k_{n-1}(y) \qquad (15)$$

$$-3xyi_{n-1}(x)k_{n-1}(y)\Big] \quad ,$$

with $x = \gamma r$ and $y = \gamma R$. In this derivation, the following were used:

$$i_n' = i_{n-1} - \left(\frac{n+1}{x}\right)i_n \quad ,$$

$$k_n' = -k_{n-1} - \left(\frac{n+1}{y}\right)k_n \quad ,$$

and

$$z^2 w_n'' + 2zw_n' - \left[z^2 + n(n+1)\right]w_n = 0 \quad ,$$

with w_n either i_n or k_n and z given by x or y, respectively. The various functions in equation (15) are defined by

$$\begin{aligned} F_n(x,y) &= \frac{(2n+3)(n+2)(2n+5)}{3} + \frac{4n+9}{6}\left(x^2+y^2\right) \quad , \\ G_n(x,y) &= x\left(\frac{2n^2+11n+18}{3} + \frac{y^2}{2} + \frac{x^2}{6}\right) \quad , \\ H_n(x,y) &= y\left(\frac{2n^2+11n+18}{3} + \frac{x^2}{2} + \frac{y^2}{6}\right) \quad . \end{aligned} \tag{16}$$

The result given in equation (15), which is rigorously correct, is not very desirable. In the theory of crystal fields using the point charge model, the A_{nm} are used in conjunction with shielding factors and appropriate radial wave functions to attempt to fit the phenomenological crystal field parameters, B_{nm}, which are obtained by fitting the crystal field spectra of a given ion by using the hamiltonian

$$H = \sum_{n,m} B_{nm}^{*} C_{nm}\left(\hat{r}\right) \quad . \tag{17}$$

With the inclusion of the factor $\Delta_n(x,y)$ given in the form of equation (15), this combination would be possible, but would be extremely cumbersome. For this reason, we have chosen to replace $\Delta_n(x,y)$ by an approximation for small x (small γr).

Before proceeding, it is convenient to make a few simplifying changes in variables. We let

$$i_n(x) = \frac{2^n x^n n!}{(2n+1)!} R_n \quad ,$$

$$(18)$$

$$k_n(y) = \frac{\pi e^{-y}}{2y^{n+1}} \frac{(2n)!}{2^n n!} q_n \quad ,$$

where

$$R_n = 1 + \frac{x^2}{2(2n+3)} + \frac{x^4}{8(2n+3)(2n+5)} + \ldots \quad ,$$

$$q_0 = 1 \quad ,$$

$$q_1 = 1 + y \quad ,$$

$$q_n = q_{n-1} + \frac{y^2 q_{n-2}}{(2n-1)(2n-3)} \quad .$$

With these changes, $\Delta_n(x,y)$ (eq 15) becomes

$$\begin{aligned}\Delta_n(x,y) = \frac{e^{-y}}{4}\Bigg[& F_n(x,y) q_n R_n - G_n(x,y)\,\frac{2n+1}{x}\, q_n R_{n-1} \\ & + H_n(x,y)\,\frac{y}{2n-1}\, q_{n-1} R_n \\ & -3y^2\,\frac{2n+1}{2n-1}\, q_{n-1} R_{n-1}\Bigg] \;.\end{aligned} \qquad (19)$$

In this form, it is apparent from equations (16) and (19) that $\Delta_n(x,y)$ is a function of x^2 and, further, the limit $x = 0$, $y = 0$ gives $\Delta_n(0,0) = 1$. For small x, the following expansion for $\Delta_n(x,y)$ can be obtained:

$$\Delta_n(x,y) = \Delta_n(0,y) + x^2\Delta_n'(0,y) + x^4\Delta_n''(0,y) \quad , \qquad (20)$$

where

$$\Delta_n(0,y) = \frac{e^{-y}}{4}\left\{\left[\frac{1}{4} + \frac{3-n}{3}\,y^2\right] q_n + \frac{y^2}{3(2n-1)}\left(2n^2 - 7n + 9 + \frac{y^2}{2}\right) q_{n-1}\right\} \quad ,$$

$$\Delta_n'(0,y) = \frac{y^2 e^{-y}}{24(2n+3)}\left\{-nq_n + \left[n + \frac{y^2}{2(2n-1)}\right] q_{n-1}\right\} \quad ,$$

$$\Delta_n''(0,y) = \frac{y^2 e^{-y}}{96(2n+3)(2n+5)}\left\{-(n+3)q_n + \frac{1}{2n-1}\left[(n+1)(2n+3) + \frac{y^2}{2}\right] q_{n-1}\right\} \quad .$$

The first term in $\Delta_n(x,y)$ from equation (20) is, in principle, only host dependent as $y = \gamma R$ and γ is dependent on the ligand ion, whereas R is the distance, which in the absence of local distortion is characteristic of the host material. The other two terms in equation (20) are dependent on the particular rare-earth ion through the factors x^2 and x^4. From equation (14), we see that the total radial dependence of the term containing $\Delta_n(x,y)$ is of the form $r^n\Delta_n(x,y)$ and, with $x = \gamma r$, for the equivalent electrons, we can write

$$\langle r^n \Delta_n(x,y)\rangle = \langle r^n\rangle \Delta_n(0,y) + \gamma^2 \langle r^{n+2}\rangle \Delta_n'(0,y) + \gamma^4 \langle r^{n+4}\rangle \Delta_n''(0,y) \quad , \tag{21}$$

where $\langle r^k\rangle$ is the expectation value of r^k for the rare-earth electrons. Frequently, Hartree-Fock wave functions modified in some manner are used to calculate these expectation values. However, the unmodified Hartree-Fock functions may be sufficiently accurate to allow us to write equation (21) as

$$\langle r^n \Delta_n(x,y)\rangle = \langle r^n\rangle \left[\Delta_n(0,y) + \gamma^2 \lambda_2(n) \Delta_n'(0,y) + \gamma^4 \lambda_4(n) \Delta_n''(0,y)\right] \quad , \tag{22}$$

where

$$\lambda_2(n) = \langle r^{n+2}\rangle / \langle r^n\rangle \quad ,$$

$$\lambda_4(n) = \langle r^{n+4}\rangle / \langle r^n\rangle \quad ,$$

with the $\lambda_2(n)$ and $\lambda_4(n)$ calculated once and for all for each rare-earth ion by using Hartree-Fock wave functions. The modifications of these functions could then be employed in the $\langle r^n\rangle$. The functions $\lambda_2(n)$ and $\lambda_4(n)$ were calculated for a number of rare-earth ions, and the results for Nd^{3+} and Er^{3+} are given in appendix A.

4. ESTIMATION OF γ and R

In theory, the functions $\Delta_n(0,y)$, $\Delta_n'(0,y)$, and $\Delta_n''(0,y)$ are dependent only on the host lattice through γ, which describes the size of the ligand charge distribution, and the distance, R, from the rare-earth site to the nearest ligand. It would be advantageous to have these quantities tabulated for a range of values of γ and R centered at some typical values. A rough estimate of γ for oxygen can be obtained by using the charge distribution given by equation (1) to calculate the average value of r by

$$\bar{r} = \frac{\int r\rho \, d\tau}{Q} = \frac{5}{\gamma} ,$$

and if we let $\bar{r}$ be the ionic radius of oxygen, which is approximately 140 nm, we obtain

$$\gamma \simeq 3.57/\text{Å} .$$

A second estimate of γ for oxygen can be obtained by using rules given by Slater[8] for deriving the exponential factors in the wave functions for the $2p^6$ (also the $2s^2$) of oxygen to obtain a value

$$\gamma \simeq 3.86/\text{Å} ,$$

where this value of γ is twice that given by Slater's rule since the charge distribution is proportional to the square of the wave function. To obtain an estimate of typical values of R, the x-ray data

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[8] *J. C. Slater, Phys. Rev.,* <u>36</u> *(1930), 57.*

on a number of crystals were examined. The smallest distance found was $R \simeq 2.1$ Å (the smallest Yb-O distance in YbP_3O_9), and the largest distance found was near $R = 2.6$ Å (the smallest Ho-O distance in $HoVO_4$). A further check to find a typical range for $y = \gamma R$ was an approximate fitting of the theory to the phenomenological B_{nm}, which gave $y \sim 10$. It was then decided that the functions $\Delta_n(0,y)$, $\Delta'_n(0,y)$, and $\Delta''_n(0,y)$ should be calculated for the range of values $8 \leq y \leq 10$ (fig. 1 to 3). The results for $y = 9.6$, 10, and 10.4 are given in tabular form in appendix B. Several features of these functions are of interest. The function $\Delta_n(0,y)$ (fig. 1) always increases for larger n with y fixed, whereas the function $\Delta'_n(0,y)$ (fig. 2) is larger for intermediate n ($n \sim 4$) for small y, changing when y gets larger. The function $\Delta''_n(0,y)$ (fig. 3) is negative for some values of n for $y < 10.4$ and is positive for larger y. Each correction is of the order of 10^{-2} of the preceding term; for example,

$$\Delta'_n(0,y) \simeq \Delta_n(0,y) \times 10^{-2} \quad .$$

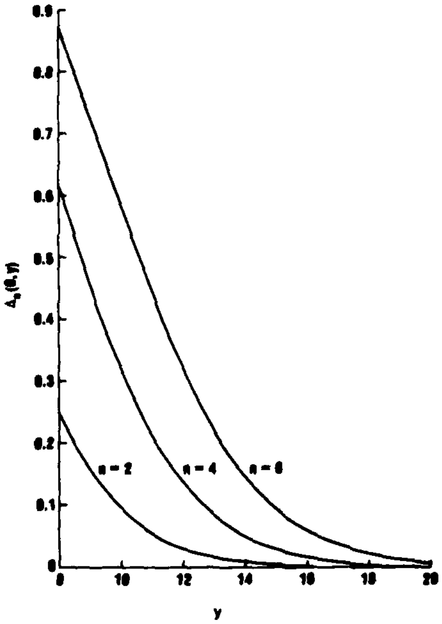


Figure 1. Function $\Delta_n(0,y)$ for $n = 2$, 4, and 6 versus y.

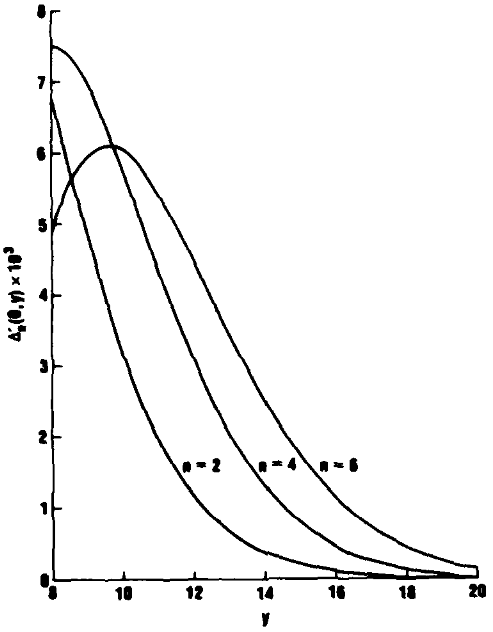
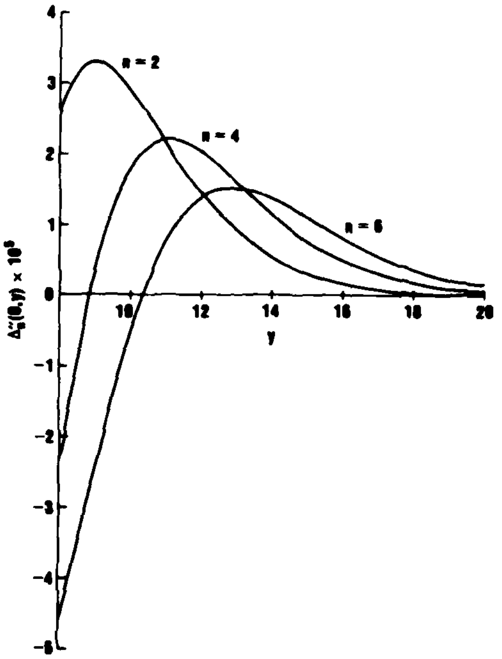


Figure 2. Function $\Delta'_n(0,y)$ for n = 2, 4, and 6 versus y.

Figure 3. Function $\Delta''_n(0,y)$ for n = 2, 4, and 6 versus y.



5. CONCLUSION

The theory of charge penetration by a rare-earth ion into the charge distribution on a ligand has been developed. The results are cast into a form reminiscent of the Sternheimer shielding factors, σ_n, which relate the observed $A'_{nm}\langle r^n\rangle$ to the lattice sum $A_{nm}\langle r^n\rangle$ in the form

$$A'_{nm}\langle r^n\rangle = A_{nm}\langle r^n\rangle(1 - \sigma_n) . \qquad (23)$$

The corresponding form developed here is

$$A_{nm}\langle r^n\rangle = A_{nm}\langle r^n\rangle\left[1 - \Delta_n(x,y)/\langle r^n\rangle\right] , \qquad (24)$$

with explicit expressions given for the $\Delta_n(x,y)$. The $\Delta_n(x,y)$ is then expanded for small x, and a form convenient for calculation is given.

The results obtained here can be used with the three-parameter theory of crystal fields[1] to obtain crystal field parameters $B_{nm}(\tau;q\eta\gamma)$, which give a better representation of the phenomenological B_{nm} than we obtained previously.

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[1] *Richard P. Leavitt, Clyde A. Morrison, and Donald E. Wortman, Rare Earth Ion-Host Crystal Interactions, 3. Three-Parameter Theory of Crystal Fields, Harry Diamond Laboratories HDL-TR-1673 (June 1975).*

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APPENDIX A.--CALCULATION OF $\lambda_2(n)$ AND $\lambda_4(n)$

APPENDIX A

In equation (22) in the main body of this report, the quantities $\lambda_2(n) = \langle r^{n+2}\rangle/\langle r^n\rangle$ and $\lambda_4(n) = \langle r^{n+4}\rangle/\langle r^n\rangle$ are introduced. These quantities are given in tables A-1 and A-2 for Nd^{3+} and Er^{3+}, respectively. The Hartree-Fock wave functions of Freeman and Watson[1] are used.

TABLE A-1. VALUES OF $\lambda_2(n) = \langle r^{n+2}\rangle/\langle r^n\rangle$ AND $\lambda_4(n) = \langle r^{n+4}\rangle/\langle r^n\rangle$ FOR Nd^{3+}

n	$\lambda_2(n)$ (Å)	$\lambda_4(n)$ (Å)
0	0.28030	0.18831
1	0.43768	0.43987
2	0.67181	0.97107
3	1.00500	1.98782
4	1.44545	3.71583
5	1.97793	6.31501
6	2.57070	9.83261
7	3.19274	14.23983
8	3.82487	19.50188

TABLE A-2. VALUES OF $\lambda_2(n) = \langle r^{n+2}\rangle/\langle r^n\rangle$ AND $\lambda_4(n) = \langle r^{n+4}\rangle/\langle r^n\rangle$ FOR Er^{3+}

n	$\lambda_2(n)$ (Å)	$\lambda_4(n)$ (Å)
0	0.18652	0.08828
1	0.30141	0.21297
2	0.47331	0.46836
3	0.70659	0.91977
4	0.98955	1.60912
5	1.30171	2.54414
6	1.62611	3.71580
7	1.95446	5.11960
8	2.28508	6.76357

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[1] *A. J. Freeman and R. E. Watson, Phys. Rev.,* *__127__* *(1962), 2058.*

APPENDIX B.--FUNCTIONS $\Delta_n(0,y)$, $\Delta_n'(0,y)$, AND $\Delta_n''(0,y)$

APPENDIX B

In equations (22) and (23) in the main body of this report, the functions $\Delta_n(0,y)$, $\Delta'_n(0,y)$, and $\Delta''_n(0,y)$ are introduced and depend on the spread of the wave function, γ, of the ligand and the distance, R, to the ligand through $y = \gamma R$. In the main body, it is shown that a value of $y \simeq 10$ is representative for oxide compounds. These three quantities are given for y = 9.6, 10.0, and 10.4 in tables B-1, B-2, and B-3, respectively.

TABLE B-1. FUNCTIONS $\Delta_n(0,y)$, $\Delta'_n(0,y)$, AND $\Delta''_n(0,y)$ FOR y = 9.6

n	$\Delta_n(0,y)$	$\Delta'_n(0,y)$	$\Delta''_n(0,y)$
1	3.7795(-2)	1.8975(-3)	2.5413(-5)
2	1.1450(-1)	3.7665(-3)	3.1391(-5)
3	2.3108(-1)	5.3584(-3)	2.6028(-5)
4	3.6993(-1)	6.2777(-3)	1.3800(-5)
5	5.1102(-1)	6.4717(-3)	-5.3134(-8)
6	6.3959(-1)	6.0987(-3)	-1.1995(-5)

Note: Numbers in parentheses are powers of 10.

TABLE B-2. FUNCTIONS $\Delta_n(0,y)$, $\Delta'_n(0,y)$, AND $\Delta''_n(0,y)$ FOR y = 10

n	$\Delta_n(0,y)$	$\Delta'_n(0,y)$	$\Delta''_n(0,y)$
1	2.9253(-2)	1.5133(-3)	2.1619(-5)
2	9.2308(-2)	3.1528(-3)	2.9026(-5)
3	1.9320(-1)	2.7006(-5)	2.7006(-5)
4	3.1931(-1)	1.8079(-5)	1.8079(-5)
5	4.5343(-1)	6.3338(-6)	6.3338(-6)
6	5.8099(-1)	-4.9131(-6)	-4.9131(-6)

Note: Numbers in parentheses are powers of 10.

TABLE B-3. FUNCTIONS $\Delta_n(0,y)$, $\Delta'_n(0,y)$, AND $\Delta''_n(0,y)$ FOR $y = 10.4$

n	$\Delta_n(0,y)$	$\Delta'_n(0,y)$	$\Delta''_n(0,y)$
1	2.2532(-2)	1.1981(-3)	1.8104(-5)
2	7.3957(-2)	2.6136(-3)	2.6144(-5)
3	1.6035(-1)	4.0634(-3)	2.6664(-5)
4	2.7343(-1)	2.0692(-5)	5.1755(-3)
5	3.9900(-1)	5.7737(-3)	1.1199(-5)
6	5.2339(-1)	1.0883(-6)	5.8660(-3)

Note: Numbers in parentheses are powers of 10.

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CHARGE PENETRATION EFFECTS IN RARE-EARTH CRYSTAL FIELDS.

ABSTRACT

(U) THE THEORY OF CHARGE PENETRATION BY A RARE-EARTH ION INTO THE CHARGE DI
THE RESULTS ARE CAST INTO A FORM REMINISCENT OF THE STERNHEIMER SHIELDING FA
A PRIME NM<R TO THE NTH POWER> TO THE LATTICE SUM A NM<R TO THE NTH POWER> I
= A PRIME NM <R TO THE NTH POWER >(1 - SIGMA N). THE CORRESPONDING FORM DEVE
R > = A PRIME NM <R TO THE NTH POWER > (1 - DEKTA N(X,Y)/<R TO THE NTH POWER
DELTA N(X,Y). THE DELTA N(X,Y) IS THEN EXPANDED FOR SMALL X, AND A FORM CONV
S OBTAINED HERE CAN BE USED WITH THE THREE-PARAMETER THEORY OF CRYSTAL FIELD
U ;QN GAMMA, WHICH GIVE A BETTER REPRESENTATION OF THE PHENOMENOLOGICAL BNM

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POWER TO THE LATTICE
  USE CRYSTAL LATTICES
    POWER

RARE-EARTH ION
  USE IONS
    RARE EARTH

PHRASES NOT FOUND DURING LEXICAL DICTIONARY

FIELDS.

EARTH ION INTO THE CHARGE DISTRIBUTION ON A LIGAND HAS BEEN DEVELOPED.
THE STERNHEIMER SHIELDING FACTORS, SIGMA N, WHICH RELATE THE OBSERVED
M A NM<R TO THE NTH POWER> IN THE FORM A PRIME NM<R TO THE NTH POWER >
THE CORRESPONDING FORM DEVELOPED HERE IS A PRIME NM <R TO THE NTH POWE
A N(X,Y)/<R TO THE NTH POWER>) WITH EXPLICIT EXPRESSIONS GIVEN FOR THE
FOR SMALL X, AND A FORM CONVENIENT FOR CALCULATION IS GIVEN. THE RESULT
ETER THEORY OF CRYSTAL FIELDS TO OBTAIN CRYSTAL FIELD PARAMETERS BNM TA
OF THE PHENOMENOLOGICAL BNM THAN WE OBTAINED PREVIOUSLY. (AUTHOR)

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RARE EARTH COMPOUNDS

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