

4582/81

IC/81/167  
INTERNAL REPORT  
(Limited Distribution)

International Atomic Energy Agency  
and  
United Nations Educational Scientific and Cultural Organization  
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

LOCAL FIELDS IN IONIC CRYSTALS\*

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ABSTRACT

Local fields arising from the electronic distortion in perfect ionic crystals are described in terms of multipolar excitations. Field factors for the alkali halides and chalcogenide ions are found to differ significantly from the Lorentz value of  $4\pi/3$ , the correction size following an exponential dependence on the difference in ionic radii. Local fields are only slightly modified by these corrections however, and together with the Clausius-Mossotti relation may be regarded as accurate to within 2% if the Lorentz value is adopted.

MIRAMARE - TRIESTE

August 1981

\* To be submitted for publication.

+ Work supported by Fondo de Investigaciones de la Universidad Católica de Chile.

I. INTRODUCTION

Improvements over the past years in the methods for calculating properties of many electron systems have stimulated a first principles approach to obtaining the polarizability of ions in ionic crystals<sup>1-2</sup>. These quantities are quite sensitive to the shape of the electron distribution and their calculation requires a careful account of details in the effective potential as well as numerical accuracy. Once polarizabilities are obtained the standard test is to compare them with semi empirical values extracted from optical data through the use of the Clausius-Mossotti relation<sup>3-4</sup>. One finds that calculated values yield indices of refraction that differ by as much as 30% from experiment. The question then arises of whether it is the Clausius-Mossotti relation that induces to error, or whether the theoretical polarizabilities need further improvement.

The validity of the Clausius-Mossotti relation in crystals has been previously questioned by several authors<sup>5-10</sup>. In fact a rigorous proof of it is still lacking, save for the simplest model in which the linear response to an external field is accounted for by pure dipole polarization of individual ions. The perturbation field at an ion site is then the external field plus a reaction component that is the same at all sites. This model ignores the finite extent of the ion as well as its ability to react to the external field through higher order polarization. If one goes beyond the dipole approximation however, the local perturbing field at a cation site is different from that at an anion site. This was pointed out first in an earlier paper where as a solvable model a lattice of conducting spheres in an external field is considered. In this model the local field factors weighting the strength of the reaction field at a given site differ significantly from the point dipole value of  $4\pi/3$  when the radii of the spheres in the two different sublattices are unequal<sup>7</sup>. Simple dipole-octupole coupling in true ions yields the same result<sup>8</sup>. The overlapping of charge distributions in neighbouring cells also modifies the local field factors although the effect seems to be small in highly ionic compounds where the overlap is itself small<sup>9-11</sup>.

In this paper we derive an expression for the static local field factors arising from electronic distortion that is exact provided that the ion response can be represented by localized multipolar excitations. Based on numerical results for the alkali halide and chalcogenide crystals we argue that the local field at an ion site, be it a cation or an anion, is modified only slightly

by multipolar corrections higher than dipole. This results in an accuracy of more than 2% for the Clausius-Mossotti relation. We regard this as a proof of the latter for this class of crystals.

## II. THE LOCAL FIELD FACTORS

We consider two interpenetrating sublattices of anions and cations labelled A and C respectively, in an external field E in the z-direction which is assumed to be a main crystal axis. The perturbing potential in the cell centred at the origin has the form

$$V = -Er \cos\theta + \sum_j' \phi_j \quad (1)$$

Here  $\phi_j$  arises from the distortion in the charge distribution at cell j and the prime in the sum indicates that the cell at the origin is to be omitted. As a result the electronic charge is redistributed in the latter in such a way that it acquires selfconsistently the same distortion in like-cells that give rise to (1). The perturbing potential induces a dipole moment at the central cell but it also excites higher order polarizabilities since it is very non uniform in this cell. This means that the multipole moment of order l,m of an ion, say, of type  $\sigma$

$$q_{lm}^\sigma = \int \rho_\sigma(\vec{r}) Y_l^m(\theta, \varphi) r^l d\vec{r} \quad (2)$$

is in general non zero. Here  $\rho_\sigma$  is the charge density of the ion which we assume well localized so that the integral extends over a well-defined cell that contains the ion entirely and none of the neighbours charge. If instead of ions one speaks of cells, this model is still true, only that the moments (2) would not be as easily obtained from a first principles calculation. Using a multipolar expansion for the field in the cell centred at the origin one then arrives at the following expression for the reaction field contained in (1) (Appendix),

$$\sum_j^{(A)} \phi_j = \sum_{LM} \sum_{l'm'} (-1)^{l+m'} B_{LM, l'm'}^{A, \sigma'} q_{l'm'}^{\sigma'} Y_L^M(\theta, \varphi) r^L$$

For definiteness we have taken the site at the origin to be of A-type. Since we are dealing with two sublattices that polarize differently a summation index  $\sigma'$  that can be either A or C has been included. The coefficients B are purely geometric and their explicit form is given in the Appendix.

Because the perturbing potential depends on the moments, the charge distortion itself will depend on the multipole polarization. This turns (2) into a set of relations between the  $q_{lm}^\sigma$ . For low enough fields first order perturbation theory yields the expression

$$q_{lm}^A = e \sum_{g,i}^{(A)} \frac{\langle i | V^A | g \rangle \langle g | Y_l^m r^l | i \rangle + \langle i | Y_l^m r^l | g \rangle \langle g | V^A | i \rangle}{\epsilon_g - \epsilon_i}$$

where matrix elements and energies refer to an unperturbed A-ion and the contribution of all ground state orbitals has been made explicit through a summation over the index g. To obtain the relation between the moments we have introduced the potential (1) referred to an A-cell,  $V^A$ . For closed shell ions only the  $L = l, M = m$  term in the spherical harmonics expansion of the potential contributes<sup>12</sup>, and one gets

$$q_{lm}^A = \alpha_{lm}^A \left[ \sqrt{\frac{4\pi}{3}} \delta_{l,1} \delta_{m,0} - \sum_{l'm'} (-1)^{l+m'} B_{lm, l'm'}^{A, \sigma'} q_{l'm'}^{\sigma'} \right] \quad (3)$$

where the multipole polarizability of the A-ion comes out as an overall factor and is given by

$$\alpha_{lm}^A = e^2 \sum_{g,i}^{(A)} \frac{|\langle i | Y_{\ell}^m r^{\ell} | g \rangle|^2 + |\langle i | Y_{\ell}^{-m} r^{\ell} | g \rangle|^2}{\epsilon_i - \epsilon_g} \quad (4)$$

We note that this definition for the polarizability has been taken here for convenience of notation and that there are factors involved in relating it to other definitions. For instance, for the usual dipole polarizability  $\alpha_d$  defined as the ratio of the dipole moment to the uniform component of the local field one has  $\alpha_d = \frac{4\pi}{3} \alpha_{10}$ . The quantity in parenthesis in (3) is the local field component effective in exciting the  $\ell, m$  - pole moment and must not be confused with the complete perturbing field. Thus, for dipole polarization it includes the uniform component of the field only whereas for higher order polarization it includes derivatives of the electric field with respect to spatial coordinates. Eq. (3) constitutes a set of non-homogeneous linear equations that can be easily solved by iteration. One obtains in this way for the dipole moment in the direction of the external field  $p^A = (4\pi/3)^{1/2} \alpha_{10}^A$ .

$$p^A = \alpha_d^A \left\{ E + \frac{3}{4\pi} \sum_{\sigma} \frac{1}{n_{\sigma}} \left[ B_{10,10}^{A,\sigma} - \sum_{\ell',m',\sigma'} B_{10,\ell',m'}^{A,\sigma'} (-1)^{\ell'+m'} \alpha_{\ell',m'}^{\sigma'} B_{\ell',m',10}^{\sigma',\sigma} + \sum_{\ell',m',\sigma'} B_{10,\ell',m'}^{A,\sigma'} (-1)^{\ell'+m'} \alpha_{\ell',m'}^{\sigma'} B_{\ell',m',\ell'',m''}^{\sigma',\sigma''} (-1)^{\ell'+m''} \alpha_{\ell'',m''}^{\sigma''} B_{\ell'',m'',10}^{\sigma'',\sigma} \dots \right] P^{\sigma} \right\} \quad (5)$$

where  $n_{\sigma}$  is the density of species  $\sigma$  and  $P^{\sigma}$  is the macroscopic polarization of the same species. The prime in the summations indicate that terms with  $\ell' = 1, m' = 0$ , etc., are to be excluded. As expected the induced polarization gives rise to terms in the local field that are proportional to each sublattice dipole polarization and our expression gives an explicit form for the corresponding local field factors weighting the contribution of each sublattice. It is convenient to rewrite these factors in the more compact form

$$L_{z\sigma} = -\frac{1}{n_{\sigma} \alpha_d^z} \left( \frac{T}{1+T} \right)_{10,10}^{z,\sigma} \quad (6a)$$

where we have adopted the formal notation

$$\left( \frac{T}{1+T} \right)_{10,10}^{z,\sigma} = T_{10,10}^{z,\sigma} - \sum_{\ell',m',\sigma'} T_{10,\ell',m'}^{z,\sigma'} T_{\ell',m',10}^{\sigma',\sigma} + \sum_{\ell',m',\sigma'} T_{10,\ell',m'}^{z,\sigma'} T_{\ell',m',\ell'',m''}^{\sigma',\sigma''} T_{\ell'',m'',10}^{\sigma'',\sigma} \dots \quad (6b)$$

where

$$T_{LM,L'M'}^{A,\nu} = (-1)^{L+M} B_{LM,L'M'}^{A,\nu} \alpha_{LM}^A$$

The physical interpretation of our result then follows easily. The uniform external field is only capable of exciting the dipole polarizability of the closed shell ions. Once it is established however, the point like dipole moments that form at each site produce a non uniform electric field within the ionic cell. This field is capable of exciting higher order multipole moments which themselves modify the local perturbing field. A full self consistent evaluation of these effects therefore involves a coupling of multipoles to all orders as exhibited in (6b). The  $T_{LM,L'M'}^{A,\nu}$  represents the effect of the  $L, M$  multipole at anion of type  $\mu$ , on the moment of order  $L', M'$  at a  $\nu$ -ion. Thus  $T_{10,10}^{A,C}$  for example displays the direct action of the dipole polarization of sublattice A on the dipole moment of ions in sublattice C. This is the first term in the series (6b) and its contribution to the local field factor is the usual Lorentz value of  $4\pi/3$  that leads to the CM relation (Appendix). The second term in (6b) gives the action of the dipole moment at sublattice  $\tau$  on that at sublattice  $\sigma$  through intermediate higher order polarization of both sublattices, as indicated by the sum over  $\ell', m'$  and  $\sigma'$ . The third term represents the action through <sup>twice</sup> intermediate higher order polarization, and so on.

One can easily verify the symmetry of the local field factors under exchange of indices as required by thermodynamic arguments<sup>10</sup>. It suffices to show it for the general term in the expansion (6b) with the aid of the symmetry property with respect to exchange of indices in the factors (Appendix), Eq. (4), and the fact that the indices  $m'$ ,  $m''$ , etc. cover an equal range of positive and negative integers.

### III. NUMERICAL RESULTS

The alkali-halide and chalcogenide crystals are highly ionic to a varying degree and they provide good systems in which to test the relative importance of correction terms arising from polarization higher than dipole. Earlier work on a lattice of conducting spheres allowed the consideration of arbitrarily high multipole excitations<sup>7</sup>. For real systems however polarizabilities have been reported up to octupole only, so we are limited to this order in evaluating the local field factors. Using free ion values for the octupole polarizability Mahan has reported values for the first order correction<sup>8</sup>. We here use crystal polarizabilities<sup>13</sup> and include higher order corrections involving the octupole moment.

We have calculated the B coefficients appearing in the expansion (6) for the local field factors in the NaCl crystal structure. In centrosymmetric lattices all coefficients of even L or L' and M or M' not a multiple of 4 vanish. The dipole polarization thus does not couple with multipoles of such orders and the leading corrections come from the excitation of the octupole moment. For crystals of the CsCl structure the results are similar and are not worth reporting here.

Table I shows a few low order coefficients. In order to visualize better the convergence properties of the series (6) we have chosen to display them in terms of a parameter  $b$  that equals half the nearest neighbour distance. Since a polarizability of index L appears always as a factor and is expected to scale as the  $L + 2$  power of the ionic radius, convergence is controlled by the numerical coefficients as tabulated. The numbers are small and we expect that in compounds where the anion and cation radii are similar, that is  $r_A \approx r_C \approx b$ , corrections to the Lorentz factor will be also small, whereas if one ion is much bigger than the other so will be its polarizability and the correction is enhanced.

Our results for the alkali halide and chalcogenide crystals are given in tables II and III, respectively. Entries are in units of the Lorentz value of  $4\pi/3$  so that an entry of 1.00 means no correction at all and 2.00 for instance, a 100% correction. The main contribution comes from the simple octupole coupling contained in the first sum in (6b). Double and triple octupole coupling coming from the second and third sums account for up to 10% and 3% of the total correction, respectively. Inspection shows that field factors are enhanced by the octupole polarization of like ions and somewhat decreased in unlike ions. This comes from the different sign of the geometrical factors involved.

The cation-cation correction is quite large, increasing with anion size. In the alkali halides the largest value is for LiI, a compound that combines the smallest cation with the largest anion. When ion radii are about equal on the other hand, the correction approaches zero. Fig. 1 is a plot of  $L_{CC}$  in units of  $4\pi/3$ , as a function of the difference between cation and anion radii  $\Delta r = r_A - r_C$ , where the Pauling values for the ionic radii have been used. All alkali-halides are found to fall close to the curve

$$L_{CC} = 1.0 + 0.135 e^{1.8(r_A - r_C)} \quad (7)$$

The universal character of this behaviour is a strong indication that the radii difference controls the local field correction. The same fit with opposite sign in the exponent is obeyed by  $L_{AA}$ . For the chalcogenide crystals a similar fit is obtained if the coefficient and exponent in (7) are replaced by 0.3 and 1.7, respectively.

The large relative size of the cation-cation correction arises from the intermediate polarization of the anion sublattice. To lowest order the interaction may be described in terms of the dipole at the cation site exciting the large octupole polarizability of the anion which in turn acts back on the dipole through the local field where the cation sits. Anions and cations are nearest neighbours so the effect is additionally enhanced if the cation is small since its centre then lies close to the anion thus making the interaction back and forth more intensive. The anion-anion correction through polarization of the cation is also favoured by geometry but results in a small correction due to the small polarizability of the latter. Finally, the cation-anion terms are disfavoured by geometry since they involve the intermediacy of a next nearest neighbour.

The  $\sigma = q'$  column in Table I may also be used in evaluating local field corrections in mono-atomic lattices. We have calculated the local field factors for the inert gas crystals and have found a positive correction to the Lorentz value, which is of opposite sign to the result reported for overlapping charge distributions<sup>9</sup>. The correction is however very small amounting to less than 2% in all cases.

#### IV. THE LOCAL FIELDS

Our results shown on Tables II and III are remarkably similar to those previously obtained by use of the very crude model of a lattice of perfectly conducting spheres<sup>7</sup>, the difference for most compounds being just a few percent. This is not fortuitous and is due to the scaling of the quantum mechanical polarizabilities with anion size which is roughly similar to the scaling for conducting spheres. More accurate values for the octupole polarizabilities than those used here would change our numbers somewhat but the essence of our results will remain unaltered.

The local field effective in polarizing sublattice  $\mu$  as obtained from (5) is

$$E_{loc}^A = E + \sum_{\sigma} L_{A\sigma} P^{\sigma} \quad (8)$$

where  $\mu$  and  $\sigma$  can be either A or C. Noting that  $P^{\sigma} = \chi^{\sigma} E_{loc}^{\sigma}$  where  $\chi^{\sigma}$  is the dipole polarizability per unit volume of the  $\sigma$ -ions we may solve (8) to obtain for sublattice A

$$\frac{E_{loc}^A}{E} = \frac{1 - \chi^C (L_{CC} - L_{AC})}{1 - (\chi^A L_{AA} + \chi^C L_{CC}) + \chi^A \chi^C (L_{AA} L_{CC} - L_{AC}^2)} \quad (9)$$

and a similar expression for sublattice C. Use of a set of polarizabilities such as the TKS values<sup>3</sup> and the local field factors in tables II and III allows then an evaluation of the size of the multipolar corrections to the Lorentz field. We get for all cases a correction of less than 2%. To see how this comes about we may expand (9) in a power series in the quantities  $\chi$ . These

are small and we may keep just the leading terms, which yield for sublattice A

$$\frac{E_{loc}^A}{E} \approx \left( \frac{E_{loc}^A}{E} \right)_0 \left[ 1 + \frac{l_{CC} \chi^C + l_{AC} \chi^A}{1 - \frac{4\pi}{3} (\chi^A + \chi^C)} \right], \quad (10)$$

with the corresponding expression for sublattice C. The first factor is the Lorentz field ratio that results from setting in (9)  $L_{\mu\nu} = 4\pi/3$ , and the quantities  $l_{\mu\nu} = L_{\mu\nu} - \frac{4\pi}{3}$  are the multipolar corrections to the local field factors. We have seen in Sec. III that these are largest for the cation-cation coupling and for a cation small compared to the companion anion. But the smaller the cation, the smaller its polarizability so that the large value of  $l_{CC}$  is counteracted by a small factor  $\chi^C$ . This compensating feature is responsible for the very small effect on the local field of the multipolar correction. Unless one is interested in an accuracy of better than 2% it is therefore safe to ignore these corrections in highly ionic perfect crystals. The same statement holds for the Clausius-Mossotti relation, that is a direct consequence of (9) if all field factors are given the Lorentz value of  $4\pi/3$ .

#### ACKNOWLEDGEMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste where this work was completed.

The potential at a point  $\vec{r} = (r, \theta, \varphi)$  in the cell centred at the origin due to the charge distribution at cell-j may be expanded in terms of multipoles in the form

$$V_j = \sum_{l'm'} \frac{4\pi}{2l'+1} \frac{Y_{l'm'}(\vec{\theta}_j, \vec{\varphi}_j)}{R_j^{l'+1}} q_{l'm'}^j$$

where  $\vec{r} - \vec{R}_j = (R_j, \vec{\theta}_j, \vec{\varphi}_j)$ ,  $\vec{R}_j$  being the lattice vector at site j. To uncouple the coordinates of the two vectors we use the identity

$$\frac{Y_{l'm'}(\vec{\theta}_j, \vec{\varphi}_j)}{R_j^{l'+1}} = (-1)^{l'+m'} \sqrt{\frac{2l'+1}{4\pi(l'+m')!(l'-m')!}} \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^{m'} \frac{1}{\partial z^{l'-m'}} \frac{1}{|\vec{r} - \vec{R}_j|}$$

expand the inverse distance using spherical harmonics and with the aid of the further identities

$$\frac{\partial^n}{\partial z^n} Y_l^m(\theta, \varphi) r^l = \sqrt{\frac{2l+1}{2l-2n+1} \frac{(l+m)! (l-m)!}{(l+m-n)! (l-m-n)!}} Y_{l-n}^m(\theta, \varphi) r^{l-n}$$

valid for  $l \geq n$ ,  $|m| \leq l-n$  and

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^p Y_l^m(\theta, \varphi) r^l = \sqrt{\frac{2l+1}{2l-2p+1} \frac{(l-m)!}{(l-m-2p)!}} Y_{l-p}^{m+p}(\theta, \varphi) r^{l-p}$$

valid for  $l \geq p$ ,  $-l \leq m \leq l-2p$  we obtain

$$V_j = \sum_{2m} \sum_{l'm'} (-1)^{l'+m'} \sqrt{\frac{(4\pi)^3}{(2l+1)(2l'+1)(2l-2l'+1)} \frac{(l+m)! (l-m)!}{(l'+m')!(l-l'+m+m')!(l'-m')!(l-l'-m-m')!}}$$

$$\times \frac{Y_l^m(\theta_j, \varphi_j)}{R_j^{l+1}} q_{l'm'}^j Y_{l-l'}^{m+m'}(\theta, \varphi) r^{l-l'}$$

where the first sum runs for  $l \geq l'$  and  $|m+m'| \leq l-l'$ . When performing the summation over j only two species of multipole moments need be considered which may be accounted for by means of an index  $\sigma'$  which stands for A (anion site) or C (cation site). Replacing  $l$  by  $l+2'$  and  $m$  by  $m-m'$  we obtain for the multipolar field at a site  $\sigma$

$$\sum_j^{(\sigma)} V_j = \sum_{2m} \sum_{l'm'\sigma'} (-1)^{l'+m'} B_{lm, l'm'}^{\sigma, \sigma'} q_{l'm'}^{\sigma'} Y_l^m(\theta, \varphi) r^l$$

with

$$B_{lm, l'm'}^{\sigma, \sigma'} = \sqrt{\frac{(4\pi)^3}{(2l+1)(2l'+1)(2l+2l'+1)} \frac{(l+l'+m-m')!(l+l'-m+m')!}{(l'+m')!(l+m')!(l'-m')!(l-m)!}}$$

$$\times \sum_{j \in \sigma'}^{(\sigma)} \frac{Y_{l-l'}^{m-m'}(\theta_j, \varphi_j)}{R_j^{l+l'+1}}$$

where the lattice sum runs over sites in sublattice  $\sigma'$  and the origin is at a site of type  $\sigma$ . It can be easily checked that this coefficient is symmetric with respect to an exchange of primed and unprimed indices provided the signs of  $m$  and  $m'$  are changed. For the case  $l = l' = 1$ ,  $m = m' = 0$  the formula gives

$$B_{10,10}^{\sigma,\sigma'} = \frac{4\pi}{3} \sum_{j \in \sigma'} \frac{3 \cos^2 \theta_j - 1}{R_j^3} \\ = \left(\frac{4\pi}{3}\right)^2 n_{\sigma'} \quad ,$$

since the lattice sum is the usual field at the origin due to a lattice of point dipoles of unit strength and density  $n_{\sigma'}$ .<sup>14</sup>

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13. See Ref. 2. Those polarizabilities not found here were obtained by suitable use of the inverse lattice constant dependence of the polarizability of anions in their different compounds.
14. See for example R. Plonsey and R.E. Collin, Principles and Applications of Electromagnetic Fields (Mc-Graw Hill, New York, 1961).

TABLE I. Coefficients  $B_{LM,L'M'}^{\sigma,\sigma'}$  for the NaCl structure.  $b$  is one quarter of the lattice constant.

L	M	L'	M'	$\sigma = \sigma'$	$\sigma \neq \sigma'$
1	0	1	0	$(4\pi/3)^2 n$	$(4\pi/3)^2 n$
3	0	1	0	$-0.079/b^5$	$1.146/b^5$
3	0	3	0	$-0.058/b^7$	$0.219/b^7$
5	0	1	0	$-0.021/b^7$	$0.080/b^7$
5	4	1	0	$0.016/b^7$	$0.061/b^7$
7	0	1	0	$0.005/b^9$	$0.030/b^9$

TABLE II. Local field factors for the alkali halides that crystalize in the NaCl structure. Entries are in units of  $\frac{4\pi}{3}$ . C and A refer to the cation and anion, respectively.

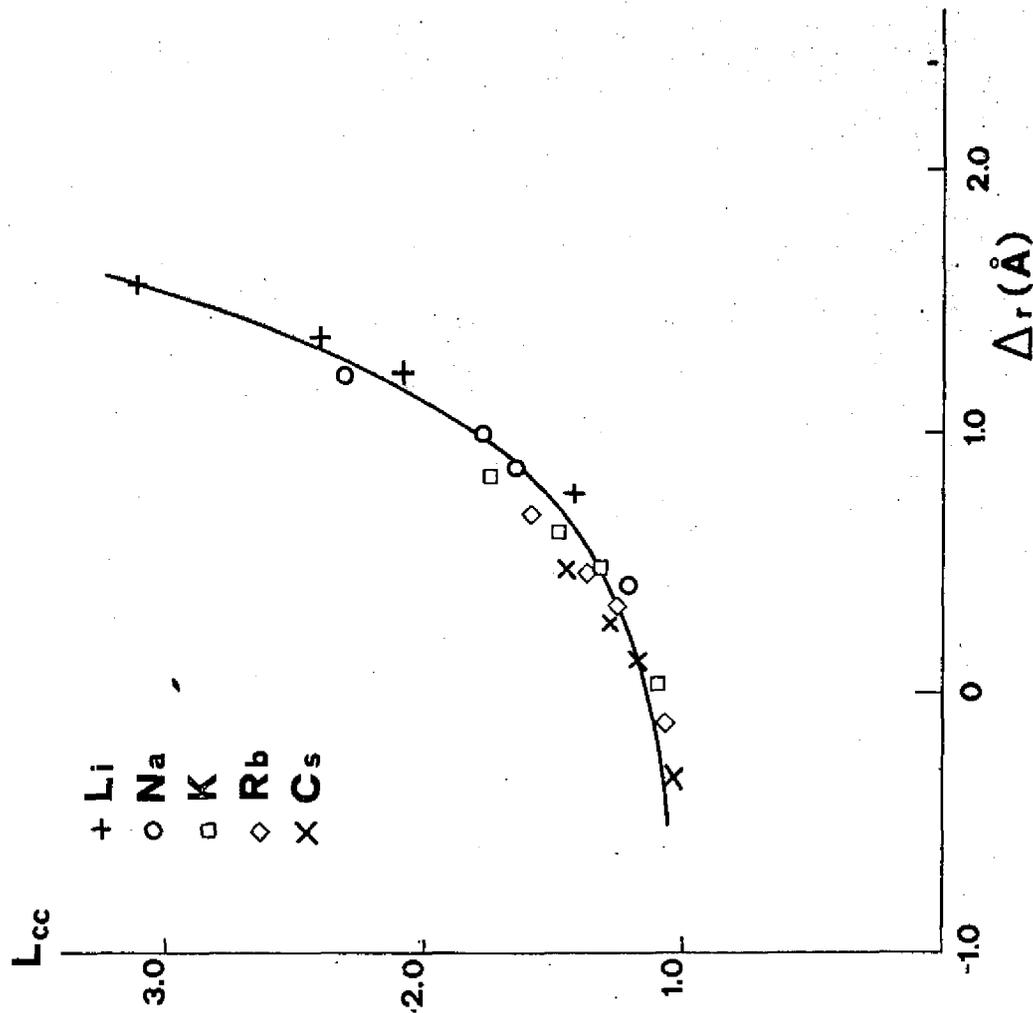
	$L_{CC}$	$L_{AA}$	$L_{AC}$
LiF	1.42	1.00	0.97
LiCl	2.07	1.00	0.93
LiBr	2.40	1.01	0.91
LiI	3.11	1.01	0.87
NaF	1.20	1.01	0.99
NaCl	1.64	1.01	0.96
NaBr	1.87	1.01	0.94
NaI	2.30	1.01	0.92
KF	1.09	1.07	0.99
KCl	1.32	1.02	0.97
KBr	1.47	1.02	0.96
KI	1.75	1.01	0.95
RbF	1.07	1.15	0.98
RbCl	1.25	1.05	0.98
RbBr	1.37	1.04	0.97
RbI	1.59	1.03	0.96
CsF	1.04	1.32	0.97
CsCl	1.17	1.11	0.98
CsBr	1.28	1.10	0.97
CsI	1.45	1.06	0.96

TABLE III. Local field factors for chalcogenide ions. Entries are as in Table II.

	$L_{CC}$	$L_{AA}$	$L_{AC}$
MgO	1.92	1.01	0.94
MgS	3.50	1.01	0.83
MgSe	4.07	1.01	0.79
CaO	1.61	1.05	0.95
CaS	2.54	1.02	0.89
CaSe	2.95	1.02	0.86
SrO	1.44	1.11	0.95
SrS	2.14	1.04	0.91
SrSe	2.45	1.04	0.89
BaO	1.33	1.27	0.94
BaS	1.83	1.10	0.92
BaSe	2.09	1.08	0.90

FIGURE CAPTION

Dependence of the cation-cation local field factor on the difference in ionic radii of the anion and cation,  $\Delta r = r_A - r_C$ .  $L_{CC}$  is in units of  $\frac{4\pi}{3}$ . The line follows Eq. (7).



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