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Electron-nuclear-double-resonance investigations of $[\mathrm{Li}]^0$ and $[\mathrm{Na}]^0$ centers in MgO, CaO, and SrO†

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Electron-nuclear-double-resonance (ENDOR) measurements of the $[\mathrm{Li}]^0$ and $[\mathrm{Na}]^0$ centers in the alkaline-earth oxides, MgO, CaO, and SrO, are reported. These centers, formed by the trapping of holes generated by ionizing radiation at 77 K, are not stable at room temperature. The investigation established that the symmetry of these trapped-hole centers is exactly axial along a $\langle 100\rangle$ direction and that the monovalent alkali impurity ion occupies a substitutional cation site. The spin-Hamiltonian parameters obtained show that the isotropic and anisotropic portions of the magnetic hyperfine tensor have opposite signs for all six systems. Interpretation of the latter as pure dipolar implies that there is outward relaxation of the axial oxygens upon the introduction of the smaller lithium ion but negligible relaxation in the case of the larger sodium ion. Conclusive evidence for hopping of the positive hole between the six nearest oxygen neighbors at temperatures as low as 1.5 K was seen in the ENDOR spectra. The electric field gradients appear to be correlated with the ion positions in a manner which can be reasonably understood on the basis of a simple point charge and dipole model.

INTRODUCTION

Ionizing radiation in the alkaline-earth oxides can result in a large variety of trapped-hole centers.[1] These oxides have the rock-salt structure, and the trapped-hole centers usually exhibit tetragonal symmetry about the crystal $\langle 100\rangle$ axes. Such trapped-hole centers associated with alkali impurities have previously been reported,[2-6] and they have been studied mainly through the use of electron-paramagnetic-resonance (EPR) techniques. The hyperfine structure resulting from the presence of the alkali nucleus contains definite information about the hole wave functions. However, before definite conclusions can be made, more precision than is usually acquired with the EPR technique is necessary to obtain values of the hyperfine parameters.

We report here an electron-nuclear-double-resonance (ENDOR) investigation of two of these centers, the $[\mathrm{Li}]^0$ and $[\mathrm{Na}]^0$, in the three hosts MgO, CaO, and SrO. This ENDOR work emphasizes that the symmetry of these centers is indeed axial and that the monovalent alkali resides at the cation vacancy site in the lattice as was indicated in earlier EPR studies.[2-5] It also provides accurate values and signs for the hyperfine and quadrupole interaction constants. Evidence that the positive hole is not completely localized (hopping), even at 1.5 K, is also presented.

EXPERIMENTAL

All of the ENDOR measurements were performed at liquid-helium temperatures employing a standard X-band superheterodyne EPR spectrometer with a detachable rectangular TE_{102} cavity. A 1.25-mm slot in the cavity wall permitted entry of the radio-frequency magnetic field produced by a coil wound around the outside of the cavity. The samples used in this study were similar to those used in previous investigations[4,5] and were glued in the cavity at room temperature. The entire cavity was then immersed in liquid nitrogen and irradiated for periods of about 2 h in a $^{60}\mathrm{Co}$ γ-ray source whose intensity was approximately 5×10^5 R/h. The cold cavity was then replaced in the spectrometer and into the double dewar system for subsequent liquid-helium transfer without any intervening warming above 77 K. This procedure was necessary because of the low thermal stability of some of these centers; it also permitted careful alignment of the crystal in the cavity at room temperature prior to the irradiation at 77 K.

RESULTS AND DISCUSSION

The spin Hamiltonian appropriate to the present situation is

$$H=\mu_B\vec{\mathrm{H}}\cdot\overleftrightarrow{\mathrm{g}}\cdot\vec{\mathrm{S}}+\vec{\mathrm{I}}\circ\overleftrightarrow{\mathrm{A}}\circ\vec{\mathrm{S}}+\vec{\mathrm{I}}\circ\overleftrightarrow{\mathrm{P}}\circ\vec{\mathrm{I}}-g_N\mu_N\vec{\mathrm{H}}\cdot\vec{\mathrm{I}}\,, \tag{1}$$

where all the symbols have their usual significance. In principle, the symmetry axes of the $\overleftrightarrow{\mathrm{g}}$, $\overleftrightarrow{\mathrm{A}}$, and $\overleftrightarrow{\mathrm{P}}$ tensors may differ, but this is not the case for all of the six systems considered here. The maximum and minimum hyperfine and quadrupole splittings occur at $\theta=0^\circ$ and $\theta=90^\circ$, requiring that all three tensors have the same symmetry axes. Furthermore, the accurate coincidence of the two $\theta=90^\circ$ ENDOR spectra, when the magnetic field is along a crystal $\langle 100\rangle$ direction, establishes that the symmetry is axial. The Hamiltonian therefore reduces to

$$H=\mu_B[g_{\parallel}H_zS_z+g_{\perp}(H_xS_x+H_yS_y)]+AI_zS_z$$
$$+B(I_xS_x+I_yS_y)+P[I_z^2-\tfrac{1}{3}I(I+1)]-g_N\mu_N\vec{\mathrm{H}}\cdot\vec{\mathrm{I}}\,. \tag{2}$$

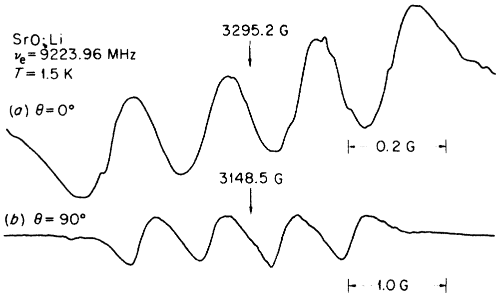

FIG. 1. EPR spectra of the $[\mathrm{Li}]^0$ center in SrO with $\vec{H}$ parallel and perpendicular to the defect axis.

Both Na^{23} (100% natural abundance) and Li^7 (93% abundance) have nuclear spins of $\frac{3}{2}$, therefore, there are six transitions corresponding to $\Delta M_S = 0$ and $\Delta M_I = \pm 1$ for each of the six systems. All of these transitions have been observed, and a least-squares computer program was employed to evaluate the spin-Hamiltonian parameters, using only the data obtained with the magnetic field parallel and perpendicular to the defect axis.

In each of the six cases, the accuracy of crystal alignment was checked for several different mountings of the samples by locating the extrema of the EPR and ENDOR transitions as a function of angle. The exact coincidence of the ENDOR transitions for the two equivalent $\theta = 90°$ sites with $\vec{H} \parallel \langle 100 \rangle$ confirmed that the symmetry is precisely tetragonal. Relative signs were determined from both the angular variation of the ENDOR spectra and the appearance (or nonappearance) of ENDOR transitions on particular EPR lines.

The EPR spectrum of the $[\mathrm{Li}]^0$ center in SrO, shown in Fig. 1, illustrates the narrow absorption lines observed with all the crystals used in the present study. In the earlier work[3] on SrO : $[\mathrm{Li}]^0$, the lines were broader, and resolution of the individual hyperfine components could not be achieved at $\theta = 0°$. However, owing to even smaller magnetic hyperfine interactions, similar resolution of the four EPR lines at $\theta = 0°$ for the $[\mathrm{Li}]^0$ center in both MgO and CaO still could not be achieved. Figure 2 shows the ENDOR signals obtained while saturating the unresolved single $\theta = 0°$ EPR absorption line of the $[\mathrm{Li}]^0$ center in MgO. All six ENDOR responses can be seen clearly, and the "crossover" that occurs for a small angular variation shows that the parallel and perpendicular components of the hyperfine tensor are opposite in sign. The variations in intensities of individual ENDOR responses obtained from the saturation of both sides of the unresolved $\theta = 0°$ EPR line of the $[\mathrm{Li}]^0$ center in CaO are illustrated in Fig. 3. The relative signs of the spin-Hamiltonian parameters were deduced in the cases of unresolved EPR lines from the

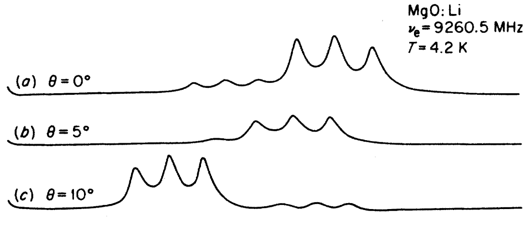

FIG. 2. ENDOR spectra of the $[\mathrm{Li}]^0$ center in MgO showing the crossover of the transitions as the applied magnetic field was rotated away from the defect axis.

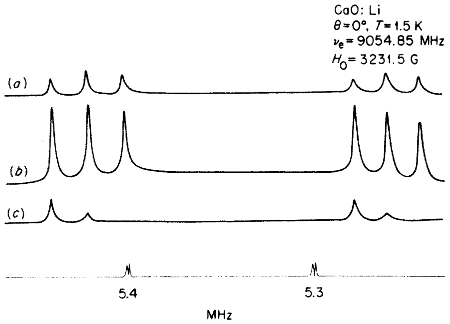

FIG. 3. ENDOR spectra of the $[\mathrm{Li}]^0$ center in CaO with $\vec{H}$ parallel to the defect axis. Trace (b) was taken on the center of the unresolved EPR line, while traces (a) and (c) were taken on the low-field and high-field sides of the EPR line, respectively.

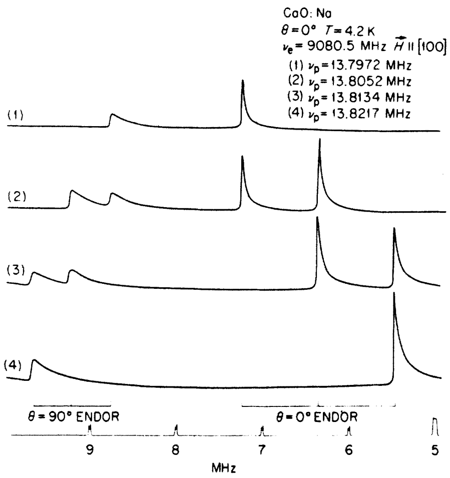

FIG. 4. Portion of ENDOR spectra of the $[\mathrm{Na}]^0$ center in CaO with $\vec{H}$ parallel to the defect axis. Individual traces were taken on different hyperfine lines labeled progressively from 1 (low field) to 4 (high field). Applied magnetic field is specified in terms of proton resonance frequency.

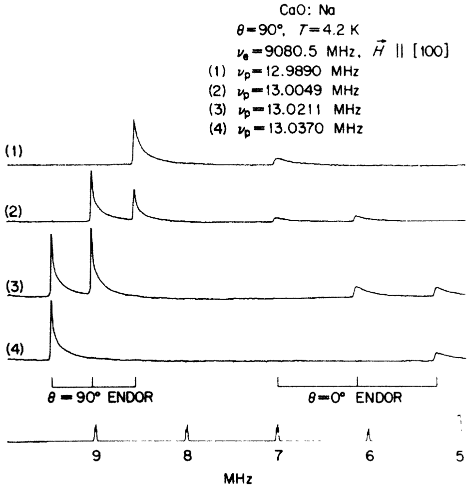

FIG. 5. Portion of ENDOR spectra of the $[Na]^0$ center in CaO with $\vec{H}$ perpendicular to the defect axis. Individual traces were taken on different hyperfine lines labeled progressively from 1 (low field) to 4 (high field). Applied magnetic field is specified in terms of proton resonance frequency.

study of ENDOR intensities in spectra such as that shown in Fig. 3.

We have observed a rather startling effect, which is characteristic of all six systems. Upon saturating a $\theta=0°$ EPR absorption line, not only were all the corresponding $\theta=0°$ ENDOR signals obtained, but *also all* the corresponding $\theta=90°$ ENDOR signals as well. Conversely, when saturating a $\theta=90°$ EPR line, all the $\theta=90°$ and all the $\theta=0°$ ENDOR responses were observed. The relative intensities of the additional responses depend on the rf input power. Figures 4 and 5 illustrate a portion of the ENDOR spectra for the $[Na]^0$ center in CaO. Such spectra certainly constitute strong evidence for hopping of the trapped hole among the equivalent oxygen nuclei. Cross relaxation can be ruled out since the linewidths are fractions of a gauss and the separations between the parallel and perpendicular extrema are of the order of 10^2 G; also, no concentration dependence was observed. Multiple spin rearrangement effects, if they existed, would be most potent among the equally spaced hyperfine lines, leading to cross saturation of the EPR lines and nonsequential ENDOR responses as one progressively saturates the hyperfine lines. As Figs. 4 and 5 show, the proper ENDOR responses are progressively seen at both $\theta=0°$ and $90°$. Thus there are no cross-relaxation effects within the hyperfine structure (where small equal spacings exist), and cross relaxation to just a single group of lines separated approximately 100 times farther in field cannot lead to the orthogonal ENDOR spectra shown in Figs. 4 and 5. This hopping occurs at temperatures as low as 1.5 K; ENDOR and also electron-double-resonance methods should provide an effective means of studying the dynamics of hopping at low temperatures.

The spin-Hamiltonian paramters are tabulated in Table I. The nuclear g values for Li and Na were calculated within experimental error to be equivalent to those quoted in the Nuclear Data Tables,[7] and their reported positive values fix the absolute signs of the parameters listed in Table I. All these parameters are in reasonable agreement with those reported earlier,[2–5] with one notable exception (MgO : Na) which will be discussed later. Following Schirmer,[3,8] we decomposed the magnetic hyperfine interaction into its isotropic and anisotropic portions, $A=a+2b$ and $B=a-b(1+\frac{1}{2}\Delta g_\perp)$, where $\Delta g_\perp = g_\perp - 2.00232$. The a and b values are shown in Table II. All six cases exhibit a negative contact interaction, presumably arising from the indirect exchange mechanisms discussed by Schirmer.[9] In the case of Li especially, one can see the decrease in this negative contribution due to expansion of the lattice proceeding from MgO to SrO. If the anisotropic interaction constant b is interpreted as arising only from a classical dipole interaction, we may set $hb=\mu_e\mu_n/(ISR^3)$ and solve for R, the clasical distance between the alkali nucleus and the trapped hole. This average interaction length can be further corrected for the finite extent of the wave function belonging to the trapped hole by means of the relation[3]

$$\frac{1}{\langle R^3\rangle}=\frac{1}{l^3}+\frac{12\langle\rho^2\rangle}{5l^5}\ , \qquad (3)$$

TABLE I. Spin-Hamiltonian parameters for $[Li]^0$ and $[Na]^0$ centers.

	$g_\parallel$	$g_\perp$	A (MHz)	B (MHz	P (MHz)
MgO: $[Li]^0$	2.0049(1)	2.0545(1)	+0.087(1)	−6.912(1)	−0.014(1)
CaO: $[Li]^0$	2.0020(1)	2.0891(1)	+0.161(1)	−3.846(1)	+0.009(1)
SrO: $[Li]^0$	2.0003(1)	2.0934(1)	+0.533(1)	−2.103(1)	+0.013(1)
MgO: $[Na]^0$	2.0057(4)	2.0725(4)	+3.024(2)	−11.259(2)	+0.790(1)
CaO: $[Na]^0$	2.0003(2)	2.1227(2)	−5.390(1)	−11.135(1)	+0.446(1)
SrO: $[Na]^0$	1.9955(4)	2.1454(4)	−5.115(2)	−8.391(2)	+0.245(1)

TABLE II. Decomposition of magnetic hyperfine interaction.

	a (MHz)	b (MHz)	R (Å)	l (for $\rho^2 = 0.48$) (Å)	l (for $\rho^2 = 0.85$) (Å)
MgO: $[\mathrm{Li}]^0$	-4.539	$+2.313$	2.368	2.505	2.588
CaO: $[\mathrm{Li}]^0$	-2.472	$+1.317$	2.858	2.977	3.053
SrO: $[\mathrm{Li}]^0$	-1.198	$+0.866$	3.287	3.393	3.463
MgO: $[\mathrm{Na}]^0$	-6.388	$+4.706$	1.644	1.817	1.908
CaO: $[\mathrm{Na}]^0$	-9.145	$+1.877$	2.234	2.376	2.461
SrO: $[\mathrm{Na}]^0$	-7.248	$+1.067$	2.697	2.821	2.900

where l is the true distance between the alkali nucleus and the O ion and $\langle \rho^2 \rangle$ describes the radial extent of the wave function.

Assuming that the wave function is a free O^- $2p_z$ orbital function, the values of $\langle \rho^2 \rangle$ used by Schirmer were 0.85 Å^2, obtained from a Hartree-Fock function, and 0.48 Å^2 from a Slater function. The use of such a free-ion orbital is an approximation in the crystal environment. All previous work indicates that the ground states of these and similar trapped-hole centers are localized and presumably can be represented by $2p_z$ orbitals. The values of l for these two possible choices of $\langle \rho^2 \rangle$ were calculated and are shown in Table II along with the uncorrected R values for all six systems. In the absence of any definitive information about the radial extent of the trapped-hole wave function, we adopt the average values $\bar{l} = \frac{1}{2}(l_{0.85} + l_{0.48})$ as representing a realistic estimate of the dipolar interaction distance. The R values constitute a lower limit for the distances, and comparison with the corrected $\bar{l}$ values obtained from the $\langle \rho^2 \rangle$ shows the finite extent of the orbital to have an appreciable effect at these small separations. The normal anion-cation lattice distance $\frac{1}{2} a_0$ is 2.107, 2.408, and 2.580 Å for MgO, CaO, and SrO, respectively. Since the R values for the three Li cases are all larger than $\frac{1}{2} a_0$, considerable outward relaxation for the light Li ion is implied.

No such consistent trend of outward relaxation occurs for the larger Na^+ ion in the three hosts. Indeed, in the case of SrO, the Na^+ ion is smaller than the Sr^{++} ion it replaces, and an outward relaxation corresponding to $\bar{l} - \frac{1}{2} a_0 \sim 0.3$ Å is noted. For CaO, where the ionic sizes of Na^+ and Ca^{++} are approximately equal, the disparity between the $\bar{l}$ and $\frac{1}{2} a_0$ values is negligible; this observation is in distinct contrast to MgO : Li, even though the substitutional Li^+ is also of comparable radius to that of the Mg^{++}. For the Na^+ ion in the MgO matrix, however, an unusual feature is observed: the small $\bar{l}$ value ($< \frac{1}{2} a_0$) implies a large overlap between the wave functions of the trapped hole and the Na^+.

The positional information obtained from the dipolar interactions of all six systems can be correlated on the assumption that the Li^+ and Na^+ ions are in contact with the O^{2-} core on the side opposite the O^- ion. The contact radii for Li^+-O^{2-} and Na^+-O^{2-} are $\alpha = 2.00$ and 2.35 Å, respectively.[10] The total axial distance between the O^- and O^{2-} ions, as represented by $d = \bar{l} + \alpha$, describes the degree of axial relaxation. The results are tabulated in Table III and the d values are plotted against the lattice constant a_0 in Fig. 6. Linear relationships for the $[\mathrm{Li}]^0$ and $[\mathrm{Na}]^0$ centers are obtained. In fact, for the $[\mathrm{Na}]^0$ center, $d \approx a_0$ for all three hosts, implying no appreciable axial relaxation. The lack

TABLE III. Axial O^--O^{--} distance and electric field gradient.

	$d = \bar{l} + \alpha$ (Å)	$z = \bar{l} - \frac{1}{2} d$ (Å)	$\frac{1}{2}\bar{l}^3[q(\mathrm{expt})]$	$\frac{1}{2}\bar{l}^3[q(\mathrm{pol})]$
MgO: $[\mathrm{Li}]^0$	4.547	0.2735	$+0.3322$	-0.5493
CaO: $[\mathrm{Li}]^0$	5.015	0.5075	-0.3542	-1.4806
SrO: $[\mathrm{Li}]^0$	5.428	0.7140	-0.7520	-2.0204
MgO: $[\mathrm{Na}]^0$	4.213	-0.2435	$+2.1197$	-0.6188
CaO: $[\mathrm{Na}]^0$	4.769	0.0345	$+2.5902$	-0.5341
SrO: $[\mathrm{Na}]^0$	5.211	0.2555	$+2.3540$	-0.5766

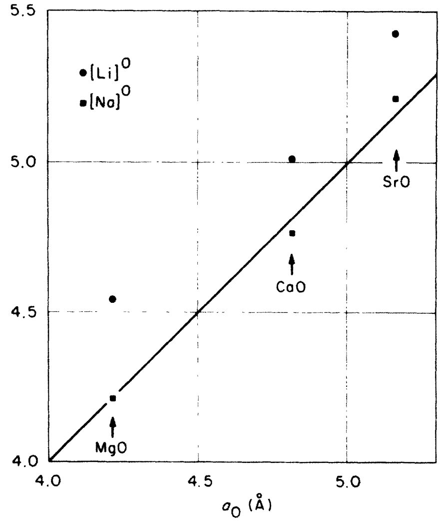

FIG. 6. Graph of O^--O^{--} distance as a function of the lattice constant. Distances were calculated from the dipole interaction and the assumption of ion cores in contact. The solid line represents $d = a_0$.

of axial distortion is rather surprising, particularly in the case of the tight lattice configuration of MgO.

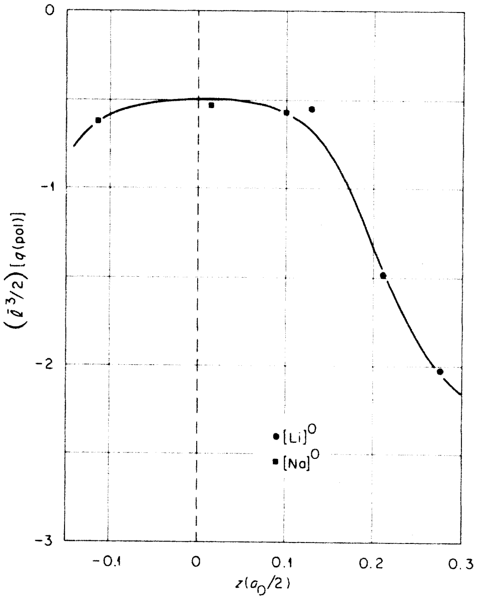

FIG. 7. Polarization contribution to the electric field gradient vs displacement of the ion from the center of the complex. Normalization is indicated in the text.

For the $[\text{Na}]^0$ centers, the present ENDOR work singles out MgO as being different from the other two hosts in that, for this system, the parallel and perpendicular components of the hyperfine tensor, A and B, have opposite signs. This feature is peculiar since identical signs would have resulted in intuitively more acceptable R and $\bar{l}$ values (i.e., no overlap of O^- and Na^+ ionic cores). Indeed the choice of identical signs of A and B in the earlier EPR work,[5] compounded in difficulty by the large experimental P/A ratio in MgO, was made in light of the known ionic core sizes. The ENDOR results permit the determination of the relative signs of the spin-Hamiltonian parameters directly. The seemingly unexpected values of R and $\bar{l}$ may reflect to a certain degree the inadequacy of describing b as purely due to a classical dipole-dipole interaction. It is likely that, however, quantum-mechanical overlap between the O^--Na^+ cores is more important than that for the O^--Li^+ cores, considering that for Na^+, there are additional $2s^2$ and $2p^6$ electrons.

Further information on the lattice distortion is also contained in the electric field gradients which can be extracted from the measured quadrupole interactions P. A simplification can be made if Feuchtwang's results[11] are applied to our data. The measured electric field gradient at the impurity nucleus will contain two contributions,

$$V_{zz}/e = q(\text{expt}) = (1-\gamma_\infty)\,\left|2/\bar{l}^3 + q(\text{pol})\right| , \qquad (4)$$

where the first term is the direct contribution due to the trapped hole and the second term containing $q(\text{pol})$ includes the entire effect of the lattice. The antishielding factors for these two ions are[12] $\gamma_\infty = +0.263$ for Li^+ and $\gamma_\infty = -4.56$ for Na^+. Since the impurity ions are off center and therefore the complex is not cubic, $q(\text{pol})$ includes a direct contribution from the neighboring charges as well as dipolar terms due to the polarizability of the surrounding ion cores (primarily the six-nearest-neighbor oxygens).

Upon substituting the experimentally determined values of the field gradients, $q(\text{expt})$, for these six cases into Eq. (4), $q(\text{pol})$ values are obtained which may be compared with the positional information from the dipole interaction. The displacement away from the exact center of the complex can be expressed as $z = \bar{l} - \frac{1}{2}d$. Table III shows the normalized $q(\text{expt})$ and $q(\text{pol})$ values, along with the displacements deduced from $\bar{l}$ and α. Figure 7 is a plot of the normalized $q(\text{pol})$ versus the fractional displacement $z/\frac{1}{2}a_0$, for all six cases. The systematic variation and continuity between the results for two ions of quite different γ_∞ suggest that a unified understanding of the origin of $q(\text{pol})$ may be possible on the basis of a fairly simple model involving point-charge and dipole contributions to V_{zz} from the first few shells of ions surrounding the complex.

We have performed a simple illustrative calculation of V_{zz} for all six cases on the assumption that only the 6 nearest-neighbor (nn) O^{2-} and 12 next-nearest-neighbor (nnn) Mg^{2+} ions are important. The Mg^{2+} ion cores were assumed to have negligible polarizability, while O^{2-} cores were taken to have a common polarizability. The dipole moments and the orientations of the O^{2-} cores were determined by the local field provided by the charges of the trapped hole and Li^+ or Na^+ relative to the lattice. As a first approximation, we assume that only the strong axial relaxation is important, so that the geometry is fixed by the magnetic dipolar information, and one adjustable parameter, the O^{2-} polarizability, fits each $q(\text{pol})$. Since the point charges in this model would, in general, make a positive contribution to V_{zz}, the negative $q(\text{pol})$ for all six cases implies a dominant electric dipole contribution. The polarizabilities obtained in this way are quite similar, agreeing to about 15% in four of the cases. The two exceptions are MgO : Li and MgO : Na, suggesting that severe overlap between ions in the small lattice seriously invalidates the model. The electric dipole moments obtained for the O^{2-} in the four cases which agree are remarkably close to a recent estimate by Halliburton *et al.*[13] for a related situation in MgO. On the basis of the quadrupole interaction of the Mg^{2+} adjacent to the trapped hole in the V^- center, they estimated a dipole moment of 0.47 Å as being typical for O^{2-} near a trapped hole, while our results give moments ranging from ~0.5 to ~1.2 Å for the several O^{2-} dipoles within the complex. For example, in the case of CaO : Li, the calculated electric dipole moments are 0.76 Å for the equatorial set, 1.14 Å for the core in contact with the Li^+ ion, and 0.60 Å for the core beneath the trapped hole.

CONCLUDING REMARKS

In principle, such a point-charge and dipole calculation is not necessarily valid since it ignores interactions within the complex. For example, Schirmer[9] has shown that the negative contact interactions exhibited by these centers can result from exchange core polarization due to a significant indirect exchange between the hole wave function and the Li^+ or Na^+ core orbitals through the adjacent nn equatorial O^{2-} ions. This and other treatments of the effects of overlap and finite extent of the ion have tended to concentrate either on the field gradients[14] or on the magnetic hyperfine interactions.[15] But the systematic variation shown in Fig. 7 and the reasonable values of O^{2-} dipole moments, obtained from a simple geometric model calculation of q(pol), suggest that the electric field gradients and magnetic interaction constants, including the negative contact interaction, can be understood on a common basis for these particular centers. Perhaps the cluster approach of Taylor[16] would be a suitable way to obtain a self-consistent understanding of a, b, and V_{zz} for all six cases. Since the value of γ_∞ (= −18.2) for K^+ is so much different[17] from those for Li^+ or Na^+, it will be interesting to see whether the analogous $[K]^0$ centers[6] conform to this same correlation of displacement and q(pol) and have negative contact interactions as well.

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