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Effect of Electron-Shell Rearrangement Due to K Capture on the Intermediate-State Reorientation of Oriented Nuclei

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The effect of electron-shell deexcitation following electron-capture decay on the intermediate-state reorientation of oriented nuclei is studied by considering various final electron-shell configurations of the daughter atom. It is known that these configurations are reached in a time interval much shorter than the lifetime of the intermediate state. The reorientation, affected mainly by the hyperfine interaction of the nucleus with the atomic electrons in the new configurations, is calculated using a technique previously described by Daniels and Misra. The numerical results indicate that this model is capable of explaining the observed reorientations following K-capture decay of Sm^{145} and Co^{57} in a double-nitrate lattice, and of Sm^{145} in a neodymium ethyl sulfate lattice.

I. INTRODUCTION

The interest in the physical picture behind the reorientation of oriented nuclei is rapidly growing. This problem becomes inportant when the anisotropy of the angular distribution of γ radiation from an ensemble of oriented nuclei is measured in order to determine, among other quantities, the spin and parity of a nuclear level. In the past it has not been possible to determine conclusively the mechanisms responsible for the observed reorientations. This has been due partly to the lack of sufficient experimental data and partly to the uncertainties in the measured values of reorientation. The latter uncertainties are due mainly to the uncertainty in the mixing ratios of the various multipole radiations, to the perturbation of the original nuclear orientation by internal fields, and to temperature inhomogeneities and uncertainties. However, as further data become available and as experimental techniques are improved, the mechanisms responsible for reorientation are becoming better understood. The recent revision of the low-temperature scale and the availability of more precise data (for example, data for Sm^{145} consistent with two different imbedding lattices[1]) have provided the motivation for the present theoretical investigation.

Reorientation of oriented nuclei has been treated in detail by Daniels and Misra[2] on the basis of a static interaction being the sole effective mechanism in the intermediate state (static model). They concluded that the static model could not explain all known cases and that other mechanisms must be sought. Apart from the static interaction, two

possible dynamic mechanisms, namely, the nuclear recoil experienced when a β particle is emitted and the electron-shell deexcitation following K capture, have been pointed out.[3] The first mechanism, the effect of nuclear recoil on reorientation, has been investigated recently.[4] It was found in Ref. 4 that the nuclear recoil may become an important mechanism for reorientation under suitable conditions for cases involving β-particle emission. As regards the second mechanism, experiments have been performed from time to time to search for reorientation following electron-capture decay; no convincing evidence for this effect has been presented to date.

It is the purpose of this paper to study in detail the reorientation for the K-capture cases. The model used has been specifically applied to the cases of Sm^{145} and Co^{57}, both of which have sufficient experimental data available[1,5] to allow a check on the validity of the model. During the K-capture process the electron shell is disturbed most severely. What happens to the electron shell is briefly as follows.[6] After the capture of the K electron, the resultant hole remains in the K shell for an interval of the order of 10^{-16} sec for a medium weight atom. During another interval of the order of 10^{-14} sec, the K, L, and M shells are filled, leaving five vacancies in the outermost shell. During the same interval, Auger electrons and x rays are emitted. The filling of the outermost shell and settling down to the configuration of the daughter atom may take a period of time anywhere from 10^{-12} to 10^{-8} sec, depending on the nature of the chemistry of the environment. The electronic shell thus readjusts to a new configuration following K capture.

This configuration may not be unique to the atom; rather, many charged states may result depending on the number of Auger electrons and on the probability of ionization.[7] The likelihood is that the final configurations of the electron shell after decay will be those having fewer electrons than the parent ion. It is extremely difficult to calculate these final configurations theoretically since it would require exact knowledge of transition probabilities for all possible Auger processes and x-ray transitions, which in turn depend on the appropriate electronic wave functions.[8] We shall therefore assume in our model that the final electron-shell configurations of the daughter atom are those immediately to the left of the parent atom in the periodic table. With these final electron configurations characterizing the intermediate state, the hyperfine interaction of the nucleus with the atomic electrons is essentially changed. This change is reflected as a modification of the initial orientation parameters.

Some of the general theories of reorientation will be reviewed in Sec. II. In Sec. III the spin Hamiltonians for the various daughter configurations are discussed, and in Sec. IV a discussion of the results obtained on the basis of our model and the resulting conclusions will be presented and compared with the experimental data.

II. GENERAL THEORY

Since the final electron configuration is achieved in a time interval much shorter than the half-life of the daughter nucleus, the reorientation is governed predominantly by the change in coherence between electron and nuclear spin states which takes place during the electron-shell turmoil and the time development of the density matrix after the final electron configuration of the daughter atom is achieved. The technique which was developed by Daniels and Misra[2] for the static model can then be used, with the change in the electron shell after decay properly taken into account. According to this technique, which is especially suited to computations on a digital computer, the time-average of the axially symmetric orientation parameters M_r^0, in accordance with the radioactive decay law, is expressed as

$$M_r^0 = \sum_a M_{aa}(0+)\langle a \mid \mathcal{Y}_r^0(\vec{I})\underline{1}(\vec{S}) \mid a\rangle + \sum_{ab,b>a} \frac{2M_{ab}(0+)\langle b \mid \mathcal{Y}_r^0(\vec{I})\underline{1}(\vec{S}) \mid a\rangle}{[1+(E_a-E_b)^2\tau^2/\hbar^2]}\ , \qquad (2.1)$$

where $\mid a\rangle$ and $\mid b\rangle$ are the eigenvectors of the spin Hamiltonian effective in the intermediate state after the final electron-shell configuration has been acquired, with eigenvalues E_a and E_b. $\vec{I}$ and $\vec{S}$ are, respectively, the nuclear and electronic spins, τ is the half-life of the intermediate state, $\hbar$ is Planck's constant divided by 2π, $\mathcal{Y}_r^0(\vec{I})$ is the axially symmetric spherical tensor of rank r in the nuclear spin space, and $\underline{1}(\vec{S})$ is the unit matrix in the electronic spin-space. $M_{ab}(0+)$ are the coefficients in the expansion of $\rho(0+)$, the density matrix after the electron-shell rearrangement has taken place, in terms of the orthonormal basis $\mid a\rangle\langle b \mid$:

$$\rho(0+) = \sum_{ab} M_{ab}(0+) \mid a\rangle\langle b \mid\ . \qquad (2.2)$$

$\rho(0+)$ is obtained (i) by a unitary transformation of $\rho^{(p)}$, the density matrix of the parent state, via a matrix U, which takes into account the change in the angular momentum that takes place during decay,[9] and (ii) by accounting for the phase incoherence that develops between electron and nuclear spin states after decay. We will assume that the electron shell settles down in such a way that the phase coherence between electron and nuclear spin states is completely lost, since there is at present no reason to believe the contrary. In the event that the final electron spin is the same as that of the parent state, two extreme cases are possible:

(a) The electron shell retains the same polariza-

tion as before decay, i.e.,

$$\rho(0+) = \mathrm{Tr}_e(U\rho^{(p)}U^{-1}) \otimes \mathrm{Tr}_n(U\rho^{(p)}U^{-1}), \qquad (2.3)$$

where the subscripts e and n refer to the electronic and nuclear spin-spaces, respectively (incoherent polarized case).

(b) The electron shell is completely depolarized after decay, i.e.,

$$\rho(0+) = \mathrm{Tr}_e(U\rho^{(p)}U^{-1}) \otimes \underline{1}\,(\vec{S})/(2S+1). \qquad (2.4)$$

In the event that the effective electron spin does change after decay only case (b) seems plausible (incoherent depolarized case).

The quantities of experimental interest will be A_2 and Q_2. A_2 represents the expectation value of the operator $\mathcal{Y}_2^0(\vec{I})\,\underline{1}\,(\vec{S})/(2S+1)$ and is thus proportional to the nuclear alignment parameter. Q_2 represents the ratio $A_2(\mathrm{av})/A_2(0+)$, the average referring to either an average over the nuclear lifetime or to the hard core average (obtained by letting $\tau \to \infty$).

III. APPLICATIONS

A. Sm^{145}

This nucleus has recently been oriented in cerium magnesium nitrate (CMN) and neodymium ethyl sulphate (NES) lattices.[1] It decays by K capture to the 61-keV state of Pm^{145} (half-life 2.6 nsec, spin $\frac{7}{2}$), which further decays to the ground state of Pm^{145} by emission of 61-keV γ rays. The ratio of the attenuation factors of the alignment parameter in the CMN lattice to that in the NES lattice was found to be 0.44. The details of the angular momentum L, carried off during K capture, are not known. The present calculations will be made with assumed L values of 0 and 1 units. The spin Hamiltonians effective in the parent state and in the intermediate state are found to have the form

$$g_{\parallel}\mu_B H_z S_z + A S_z I_z + g_{\perp}\mu_B (H_x S_x + H_y S_y) + B(S_x I_x + S_y I_y)$$

or the form

$$g_{\parallel}\mu_B H_z S_z + A S_z I_z + \Delta_x S_x + \Delta_y S_y;\ \Delta = (\Delta_x^2 + \Delta_y^2)^{1/2}\ .$$

(The form being used in any particular case will be evident from the parameters quoted.) The values of the spin-Hamiltonian parameters for the parent state in the CMN lattice are[1,10,11] $A = 0.04$ cm^{-1}, $B = 0.011$ cm^{-1}, $g_{\parallel} = 0.76$, and $g_{\perp} = 0.40$. For the NES lattice these are[1,10,12] $A = 0.007$ cm^{-1}, $B = 0.028$ cm^{-1}, $g_{\parallel} = 0.596$, and $g_{\perp} = 0.604$. The effective magnetic field due to low-temperature ordering in the CMN lattice at the rare-earth site is represented as $H_x = 67$G, $H_y = H_z = 0$.[13] The effective magnetic field in the NES lattice is axially symmetric and thus does not bring about any reorientation of the axially symmetric orientation parameters.[14] For the electron configuration in the daughter state we consider the configuration appropriate to Pm ($Z = 61$), Nd ($Z = 60$), Pr ($Z = 59$), and Ce ($Z = 58$), since these are the rare-earth atoms appearing to the left of Sm ($Z = 62$) in the periodic table. The parameters of the effective spin Hamiltonians after the daughter ion has assumed these configurations will then be taken to be the values measured experimentally for these neighboring ions, but with their A and B parameters scaled in the ratio of the magnetic moment of the daughter nucleus μ to that of the nucleus of the respective neighboring ion considered. The magnetic moment of the daughter nucleus is not known. We shall assume the values ± 1 and ± 0.1 μ_N for our computations. The magnetic moments of Nd^{147}, Ce^{141}, Sm^{145}, and Pr^{141} are respectively $+5.6$,[15] -0.89,[15] $+0.92$,[1] and $+3.92$ μ_N.[16] Noting now that the effective spin $S = \frac{1}{2}$ for all these configurations, the values of the spin-Hamiltonian parameters for these ions are as follows. (i) Pm^{+++}: The spin Hamiltonian is axially symmetric for both the NES and CMN lattices[17] and therefore no reorientation is expected for this configuration.[14] (ii) Nd^{+++}: For this ion in the CMN lattice $g_{\parallel} = 0.45$, $g_{\perp} = 2.73$, $A = 0.004$ cm^{-1}, and $B = 0.0237$ cm^{-1},[16] for the NES lattice $g_{\parallel} = 3.535$, $g_{\perp} = 2.072$, $A = 0.0289$ cm^{-1}, and $B = 0.0151$ cm^{-1}.[18] (iii) Pr^{+++}: For the CMN lattice $g_{\parallel} = 1.55$, $g_{\perp} = 0$, $A = 0.054$ cm^{-1}, and $\Delta \sim 0$.[10] For the NES lattice $g_{\parallel} = 1.69$, $g_{\perp} < 0.3$, $A = 0.058$ cm^{-1}, and $\Delta = 0.028$ cm^{-1}.[10] (iv) Ce^{+++}: For this ion in the CMN lattice $g_{\parallel} = A = 0$, $g_{\perp} = 1.84$, and $B = -0.0128$ cm^{-1};[16] for the NES lattice $g_{\parallel} = 3.80$, $A = 0.0188$ cm^{-1}, and $g_{\perp} = 0 = B$.[19] There is no reorientation in the latter case due to the axial symmetry of the effective Hamiltonian.[14]

B. Co^{57}

The K-capture decay brings this nucleus (spin $\frac{7}{2}$, magnetic moment 4.65 μ_N) to the 137-keV state of Fe^{57} (spin $\frac{5}{2}$, magnetic moment 0.366 μ_N, half-life 9 nsec). The value of the angular momentum change during decay is predominantly $L = 1$. This nucleus has been oriented by Strohm and Sapp[5] in a cerium zinc nitrate (CZN) lattice, who found an attenuation factor of alignment Q_2 of 0.81 for 123-keV γ's and 0.90 for 137-keV γ's. The most probable value for the ratio of occupation probabilities of the X and Y sites in the CZN lattice is 1.8:1 (this value varies slightly with the method of crystal growing used). At an X site where the local field is $H_x = 150$ G, $H_y = H_z = 0$,[20] the spin-Hamiltonian parameters are $g_{\parallel} = 4.34$, $g_{\perp} = 4.28$, $A = B = 0.0103$ cm^{-1};[20] for the Y site $g_{\parallel} = 7.18$, $g_{\perp} = 2.38$, $A = 0.031\,54$ cm^{-1}, $B \simeq 0$, and the local field there is $\vec{H} = 0$ G.[20] For the daughter state two configurations will be considered. (i) Fe^{++}: A crystal field calculation for this configuration shows that $g_{\perp} = B = 0$,[2] bringing thereby no reorientation.[14] (ii) Fe^{+++}: It has the same electronic structure as Mn^{++}. The spin Hamiltonian for Fe^{+++} has then been assumed

to be that of Mn^{++} for the purpose of the present calculation, namely,

$$g\mu_B \vec{H}\cdot\vec{S} + D[S_z^2 - \tfrac{1}{3}S(S+1)] + A\vec{S}\cdot\vec{I}$$

with the following values of the parameters. $g = 2$ (same as that for Mn^{++}). The value of A for Fe^{+++} has been obtained from that for Mn^{++} by scaling in the ratio of the magnetic moment of 137-keV Fe^{57} and Mn^{55} nuclei [$A(Mn^{++}) = -0.009\ cm^{-1}$ for both X and Y sites]. The value of D for Fe^{+++} in the 137-keV state is not known at present either experimentally or theoretically and there is no obvious way to obtain it from its value for Mn^{++}. Its value depends on the details of the electron-shell configuration. Several values have been assumed for the present calculation, namely, (a) $-0.0215\ cm^{-1}$ for the X site, $-0.0080\ cm^{-1}$ for the Y site (i.e., those for Mn^{+++}), (b) twice the values given in (a), (c) five times the values given in (a), and (d) one-fifth the values given in (a).

IV. DISCUSSION AND CONCLUSIONS

The numerical results are given in Tables I–V. The results for Sm^{145} are included in Tables I–III. Table I contains the results for the NES lattice for cases characterized by $L = 0$, $\mu = \pm 0.1\ \mu_N$ and $L = 0$, $\mu = \pm 1\ \mu_N$; Tables II and III contain results for the CMN lattice for cases characterized by $L = 1$, $\mu = \pm 0.1\ \mu_N$ and $L = 1$, $\mu = \pm 1\ \mu_N$, respectively. Tables IV and V contain the results for Co^{57} in the X and Y sites of the CZN lattice, respectively. The general features of these results are as follows. The values of Q_2 are approximately of the same magnitude at all temperatures for all cases. For Sm^{145}, for both the NES and CMN lattices the values of A_2 are the same for both the incoherent depolarized and incoherent polarized cases, and those of Q_2 are the same for both $L = 0$ and $L = 1$ for each configuration. The values of Q_2 for the various configurations in the NES lattice are 1 for the Ce^{+++}, Pr^{+++}, and Pm^{+++} configurations, ~0.94 for the Nd^{+++} configuration and ~0.88 for the Sm^{+++} configuration for both $L = 0$ and $L = 1$ and for all μ. Moreover, the values of A_2 as well are independent of the sign and magnitude of μ for the NES lattice. Inspection of Eq. (2.1) reveals why, for all these cases, $(E_a - E_b)^2\tau^2/\hbar^2 \gg 1$ so that the contribution from the second term of Eq. (2.1) is negligible; the only contribution comes from the first term (in this case the lifetime averages are the same as the hard core averages). Now, for the NES lattice the effective magnetic field is zero and the parameters A and B are scaled in the ratio of the magnetic moment of the daughter nucleus to that of the nucleus of the particular ion considered. Thus the effective Hamiltonian has the same eigenvectors for all values of μ, leading to an independence of A on μ. The values of A_2 in the CMN lattice are not the same for the two values of $|\mu|$ considered, since $\vec{H} \neq 0$ in the CMN lattice. In this lattice, nevertheless, the values of Q_2 are, except for the Ce^{+++} configuration, the same (for all configurations) when averaged over the nuclear lifetime, as are the hard core values, for both values of $|\mu|$. The values of the ratio $Q_2(CMN)/Q_2(NES)$, to be compared with experiment, are for $\mu = \pm 0.1\ \mu_N$, 1 for the

TABLE I. The orientation parameter $A_2(=\langle \mathcal{Y}_2^0(\vec{I})\mathcal{Y}_0^0(\vec{S})\rangle)$ for Sm^{145} oriented in NES lattice. The superscript p refers to the parent nucleus Sm^{145}, d refers to the daughter nucleus Pm^{145} immediately after its formation by K-capture decay of Sm^{145}, τ refers to the orientation of the daughter nucleus averaged over its lifetime, and ∞ refers to the hard core value. Note that the same values of A_2 are obtained for both "incoherent polarized" and "incoherent depolarized" cases as well as for μ (the nuclear magnetic moment of the intermediate state) $= \pm 0.1$ and $\pm 1\ \mu_N$.

(i) $L = 0$								
T(°K)	0.02			0.003			0	
$A_2^p (= A_2^d) \times 10$	−1.19			−2.37			−2.73	
Electron-shell configuration after decay	Ce^{+++}, Pr^{+++}, Pm^{+++}			Nd^{+++}			Sm^{+++}	
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0
$A_2^\tau (= A_2^\infty) \times 10$	No reorientation			−1.12	−2.21	−2.51	−1.01	−2.11	−2.46
(ii) $L = 1$								
T(°K)	0.02			0.003			0	
$A_2^p \times 10$	−1.19			−2.37			−2.73	
$A_2^d \times 10$	−0.96			−1.92			−2.21	
Electron-shell configuration after decay	Ce^{+++}, Pr^{+++}, Pm^{+++}			Nd^{+++}			Sm^{+++}	
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0
$A_2^\tau (= A_2^\infty) \times 10$	No reorientation			−0.911	−1.81	−2.08	−0.814	−1.66	−1.94

TABLE II. The orientation parameter A_2 for Sm^{145} oriented in CMN lattice for the case when $\mu = \pm 0.1\ \mu_N$. The same values are obtained for both the signs of μ as well as for both "incoherent polarized" and "incoherent depolarized" cases.

(i) $L=0$												
T(°K)			0.02			0.003			0			
$A_2^p(=A_2^d)\times 10$			2.55			3.77			3.77			
Electron-shell configuration after decay	Pr^{+++}, Pm^{+++}			Ce^{+++}			Nd^{+++}			Sm^{+++}		
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0
$A_2^T(=A_2^\infty)\times 10$ [a]	No reorientation			$A_2^T=0.073$	0.112	0.112	1.46	2.18	2.18	2.50	3.72	3.72
				$A_2^\infty=0.051$	0.076	0.076						
(ii) $L=1$												
T(°K)			0.02			0.003			0			
$A_2^p\times 10$			2.55			3.77			3.77			
$A_2^d\times 10$			2.07			3.05			3.05			
Electron-shell configuration after decay	Pr^{+++}, Pm^{+++}			Ce^{+++}			Nd^{+++}			Sm^{+++}		
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0
$A_2^T(=A_2^\infty)\times 10$ [a]	No reorientation			$A_2^T=.058$	0.087	0.087	1.12	1.74	1.74	2.02	3.00	3.00
				$A_2^\infty=.041$	0.061	0.061						

[a] $A_2^T=A_2^\infty$ unless stated otherwise.

Pr^{+++} and Pm^{+++} configurations, 0.20 for the Ce^{+++} configuration, 0.61 for the Nd^{+++} configuration, and 1.04 for the Sm^{+++} configuration. For $\mu = \pm 1\ \mu_N$ these values are 1, 0.74, 0.87, and 1.04, respectively. For Co^{57}, there should be no reorientation ($Q_2 = 1$) when the electron-shell configuration after decay is that of the Fe^{++} ion (see Sec. III). For the various cases of the Fe^{+++} configuration the values of Q_2, to be compared with experiment, calculated on the basis of occupation probabilities of 1.8 and 1 for the X and Y site, respectively, are 0.55 at $\frac{1}{157}$ °K and 0.86 at 0 °K for case (a), 0.52 at $\frac{1}{157}$ °K and 0.57 at 0 °K for case (b), 0.51 at $\frac{1}{157}$ °K and 0.33 at 0 °K for case (c), and 0.23 at $\frac{1}{157}$ °K and −0.23 at 0 °K for case (d).

There are various factors of uncertainty in the present calculation which lead one not to expect full correspondence with the actual picture of reorientation. For Sm^{145} these factors are as follows. (i) A theoretical estimate of Q_2 can be made with accuracy only when a knowledge of the configurational mixture after decay is available. Our results indicate that the value of Q_2 is extremely sensitive to the particular mixture of configurations considered.

TABLE III. The orientation parameter A_2 for Sm^{145} oriented in CMN lattice for the case when $\mu = \pm 1\mu_N$. The same values are obtained for both the signs of μ as well as for both "incoherent polarized" and "incoherent depolarized" cases.

(i) $L=0$												
T(°K)			0.02			0.003			0			
$A_2^p(=A_2^d)\times 10$			2.55			3.77			3.77			
Electron-shell configuration after decay	Pr^{+++}, Pm^{+++}			Ce^{+++}			Nd^{+++}			Sm^{+++}		
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0
$A_2^T(=A_2^\infty)\times 10$	No reorientation			1.88	2.77	2.77	2.07	2.99	2.99	2.51	3.73	3.73
(ii) $L=1$												
T(°K)			0.02			0.003			0			
$A_2^p\times 10$			2.55			3.77			3.77			
$A_2^d\times 10$			2.07			3.05			3.05			
Electron-shell configuration after decay	Pr^{+++}, Pm^{+++}			Ce^{+++}			Nd^{+++}			Sm^{+++}		
T(°K)	0.02	0.003	0	0.02	0.003	0	0.02	0.003	0	0.2	0.003	0
$A_2^T(=A_2^\infty)\times 10$	No reorientation			1.52	2.26	2.26	1.70	2.49	2.49	2.03	3.01	3.01

TABLE IV. The orientation parameter A_2 for Co^{57} oriented in CZN in the X site and decaying to Fe^{57} by K capture. Case (a) refers to the configuration of the electron shell being the same as that of Mn^{++}; the same spin-Hamiltonian parameters as those of Mn^{++} but the parameter A scaled in the ratio of magnetic moment of Fe^{57} nucleus to that of the Mn^{55} nucleus. Cases (b)–(d) refer to the same spin-Hamiltonian parameters as (a) but the parameter D being, respectively, twice, five times, and one-fifth that for case (a).

T(°K)	$A_2^p \times 10$	$A_2^d \times 10$
$\frac{1}{157}$	−0.597	−0.603
0	−1.84	−1.86

T(°K)	Configuration	$A_2^T \times 10^2$	$A_2^\infty \times 10^2$
$\frac{1}{157}$	a	−2.12	−2.12
	b	−3.12	−3.13
	c	−3.23	−3.24
	d	−2.02	−2.02
0	a	−8.18	−8.18
	b	−9.45	−9.45
	c	−10.3	−10.3
	d	−7.02	−7.03

TABLE V. The orientation parameter A_2 for Co^{57} oriented in CZN in the Y site (for a description of the various cases see Table IV).

T(°K)	$A_2^p \times 10$	$A_2^d \times 10$
$\frac{1}{157}$	3.72	3.76
0	3.82	3.86

T(°K)	Configuration	$A_2^T \times 10$	$A_2^\infty \times 10$
$\frac{1}{157}$	a	1.86	1.86
	b	1.94	1.94
	c	1.96	1.96
	d	0.974	0.974
0	a	1.91	1.91
	b	1.99	1.99
	c	2.02	2.02
	d	1.00	1.00

For example, for $\mu = \pm 0.1 \mu_N$, in a pure Ce^{+++} configuration, in the decay of Sm^{145} in the CMN lattice, Q_2 is as small at 0.20. However, there is no information yet available on which particular configurations are attained after K capture. The ones considered in this paper seem to be the most plausible. (ii) The magnetic moment of the intermediate nuclear state is not known. From Tables I–III it is seen that Q_2 is sensitive to the values of μ. In case of Co^{57}, the uncertain factors are (i) the occupation probabilities of the X and Y sites in the CZN lattice, and (ii) the probabilities of reaching the Fe^{++}, Fe^{+++}, ..., configurations after decay.

The experimental values $[Q_2(\text{CMN})/Q_2(\text{NES}) = 0.44$ for 61-keV γ's obtained in the decay of Sm^{145} [1]; $Q_2(\text{CZN}) = 0.81$ for 123-keV γ's and $Q_2(\text{CZN}) = 0.90$ for the 137-keV γ's obtained in the decay of $Co^{57}]$[5] fall well within the range of our calculated values; probabilities of occurrence of various configurations certainly can be chosen so as to give exact agreement with experiment. We have not attempted to estimate these probabilities. We have also found, in agreement with Ref. 1, that for most cases Q_2(double nitrate) is greater than Q_2(NES). The extent to which our model is applicable can only be ascertained after the various uncertainties have been eliminated. We would suggest that more nuclear orientation experiments involving K-capture decays be performed and efforts made to determine the spin-Hamiltonian parameters of the various resulting electron-shell configurations as well as their probabilities of occurrences.

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Influence of the Dipole-Dipole Coupling on the Specific Heat of Cesium Titanium Alum

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To find the influence of the magnetic dipole-dipole coupling on the specific heat in a fcc lattice, the Hamiltonian was computed in a straightforward way. If one omits the nonring diagrams, the successive terms in $1/kT$ can be obtained from the Fourier transform. We found that the third-order term was different from the results quoted in the literature, both in sign and in magnitude. Some discussion is devoted to the question of what magnetic state will be realized below the critical temperature.

I. INTRODUCTION

Ever since adiabatic cooling was used to obtain lower temperatures, the question about the influence of dipole-dipole coupling has been of interest. This type of interaction is well defined, but its consequences are tedious to evaluate. The problem cannot be sidestepped by considering nearest neighbors only, as was often the custom. The long-range nature of the interaction and its angular dependence make it hard to replace it by some simple approximation. In the 1930's Van Vleck[1] courageously set out to calculate algebraically a number of terms for various cubic lattices. In this calculation he made some simplifications, which although understandable at that time, are no longer necessary. The second-order term in $1/kT$ is relatively simple, but the third- and fourth-order terms required a considerable amount of work. In order to facilitate the computation, the arrangement of dipoles he considered was simple cubic, rather than fcc, for the last two terms. We have made calculations elsewhere[2] for c/a values (c and a are defined in Fig. 1) different from $\sqrt{6}$ (fcc), and found a clear-cut dependence on this parameter. (The simple cubic lattice corresponds to $c/a = \sqrt{\frac{3}{2}}$.) Hence it was considered worth while to repeat the calculations.

To discuss a few more of the technical details of Van Vleck's calculation let me first point out the other simplifications used. In the "triple-bar" terms (compare Fig. 2, diagram 3-2) the sum was taken over the nearest neighbors only, which is indeed a good approximation; moreover, the whole term is of no importance as long as the exchange interaction is small. In the triangular term (diagram 3-1), only isosceles right triangles were used. In the fourth-order calculation, Van Vleck left out the "square" term, since he used nearest neighbors only. We believe that this term gives an important contribution. This term is extremely difficult to obtain algebraically beyond the nearest-neighbor approximation since one is dealing with a ninefold summation: three positions in three dimensions. In our numerical work this difficulty is avoided by using the Fourier transform inside the Brillouin zone.

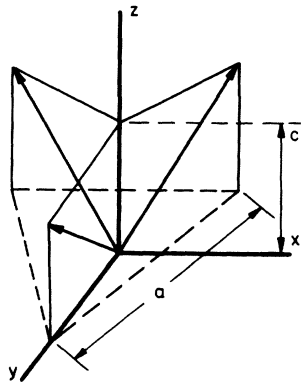

FIG. 1. Choice of primitive lattice vectors $(c/a)^2 = 6$.