Hyperfine shifts of x-ray levels excited by internal conversion

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A theoretical description is given of the hyperfine shift of x-ray (and conversion) lines excited in the process of internal conversion in any sufficiently deep shell of an atom and subsequent deexcitation by an electromagnetic cascade. General expressions are obtained for the magnetic dipole and electric quadrupole shifts of x-ray levels of an atom excited in this process in the case of conversion transitions of arbitrary (including mixed) multipolarity. It is shown that electromagnetic transitions transfer information on hyperfine shifts from an initial excited level of an atom to the next one, and so on all the way out to the outermost shells of the atom.

1. INTRODUCTION

The hyperfine splitting of x-ray levels of an atom because of the interaction between the magnetic moment of the nucleus and the current in an outer (K, L) shell of an atom with one vacancy was predicted by Breit[1] back in 1930. Forty years passed before this effect was observed[2,3] in high-precision experiments, carried out using a crystal diffraction spectrometer, and it was manifested as broadening of K_{α_1} x-ray fluorescence lines of Eu and Sb.

The effect is difficult to observe because the splitting of the K level is small compared with its width, so that a K line which appears as a result of photoexcitation is only slightly broadened, whereas the center of gravity of the line is not shifted. The magnitude of the observed broadening is several orders of magnitude less than the hyperfine splitting.[2,3]

It was shown in 1977–8 that in the case of K capture[4] and internal conversion[5] there may be a nonstatistical (in contrast to the photoexcitation case[2,3]) population of components of the hyperfine structure of a K level of the final atom. As a result, a K x-ray line is shifted relative to a fluorescence line by an amount of the order of the hyperfine splitting (~ 100 meV/n.m. in the rare-earth element range). Such a shift can be measured quite simply using crystal diffraction spectrometers with an error of a few percent,[4–6] which provides new opportunites for determination of the magnetic moments of the nuclear states practically irrespective of the lifetime. It is found[5] that similar shifts occur also in the case of electron conversion (and also Auger) lines so that the spectrum of conversion electrons also carries information on the magnetic moments of nuclear levels.

In the simplest cases, such as allowed K capture or K conversion accompanied by a change in the nuclear spin by unity (on condition that the escaping neutrino or electron has zero orbital momentum), a nonstatistical population appears as a result of the law of conservation of the angular momentum. An atom is then excited in one specific state of the hyperfine structure.[4,5]

Expressions for the K-line shifts which accompany conversion transitions of arbitrary multipolarity (see Ref. 7) were obtained in Ref. 6 and were used there, together with the measured (in the same investigation) shift of the K_{α_1} line of ^{133}Ba excited by an $M4$ transition, to determine the hitherto unknown magnetic moment of the 12.3-keV excited state of the ^{133}Ba nucleus.

Attention is drawn in Refs. 6 and 8 to the considerable contribution that interference terms can make to the hyperfine shifts of an x-ray line excited by electron capture and conversion of mixed multipolarity. It is then in principle possible to determine (supplementing the familiar correlation methods) the ratios of amplitudes of different multipolarity, including the signs if the moment of the final state of the nucleus is known.

The various aspects of this topic are discussed in Refs. 9–13. In particular, it is shown in Ref. 11 that the electric quadrupole interaction can similarly lead to shifts of a $L_{\rm III}$ level excited by L conversion and that the magnitude of this shift should be sufficient to determine the electric quadrupole moment of the nucleus with the aid of a crystal diffraction spectrometer.

Relativistic Hartree–Fock calculations are reported in the literature[12,13] and tables are given of the magnetic dipole and electric quadrupole hyperfine constants of the K and $L_{\rm I\text{-}III}$ levels for all the nuclei with the atomic numbers from $Z = 10$ to 100. These calculations are very precise because of the extreme simplicity of the atomic system (an atom with one hole in the K or L shell), which is an advantage of this method compared with the available methods for the determination of nuclear moments in external fields or from the optical hyperfine structure.

The present paper will provide a theory of the hyperfine shift of x-ray levels ($n_i j_i \varkappa_i$) excited both directly as a result of internal conversion in an arbitrary ($n_0 j_0 \varkappa_0$) shell of an atom, and by subsequent deexcitation involving an x-ray cascade:

$$n_0 j_0 \varkappa_0 \xrightarrow{X_1} n_1 j_1 \varkappa_1 \xrightarrow{X_2} n_2 j_2 \varkappa_2 \ldots .$$

We shall obtain expressions for hyperfine shifts of x-ray and conversion lines that accompany conversion transitions of arbitrary multipolarity.

2. EXPRESSIONS FOR THE HYPERFINE STRUCTURE OF X-RAY LEVELS; EXCITATION OF FLUORESCENCE

A shift of the center of gravity of an x-ray level $nj\varkappa$ split by the hyperfine interaction depends on the method of excitation (G) of this level and is described by the expression

$$\delta E^{(G)}_{nj\varkappa} = \sum_F R^{(G)}_{F(nj\varkappa)} \Delta E^F_{nj\varkappa}, \tag{1}$$

where $R^{(G)}_{F(nj\varkappa)}$ is the relative probability of excitation in a process G (i.e., the population) of a hyperfine component of

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the level $nj\varkappa$ characterized by the total angular momentum **F** of the atom (**F** = **I** + **j**, where **I** is the nuclear spin) and $\Delta E^F_{nj\varkappa}$ is the energy shift of this component, relative to the unperturbed position of the level $nj\varkappa$, caused by the hyperfine interaction.

We can represent the quantity $\Delta E^F_{nj\varkappa}$ conveniently in the form[13]

$$\Delta E^F_{nj\varkappa}=\sum_\lambda \Delta E^F_{nj\varkappa}(\lambda)=\Delta E^F_{nj\varkappa}(\mu 1)+\Delta E^F_{nj\varkappa}(Q2), \quad (2)$$

where $\lambda = 1$ corresponds to the magnetic dipole hyperfine interaction ($\mu 1$) and $\lambda = 2$ corresponds to the electric quadrukole ($Q2$) hyperfine interaction; here,

$$\Delta E^F_{nj\varkappa}(\lambda)=A^{(\lambda)}_{Ijn\varkappa}(-1)^{F+I+j}\begin{Bmatrix} F & I & j \\ \lambda & j & I \end{Bmatrix}, \quad (3)$$

where {...} is the $6j$ Wigner symbol.[14]

It is usual to employ expressions given in Refs. 15–17:

$$\Delta E^F_{nj\varkappa}(\mu 1)=a_{nj\varkappa}(\mathbf{Ij})_F\equiv a_{nj\varkappa}c_F/2, \quad (4)$$

$$\Delta E^F_{nj\varkappa}(Q2)=\Delta_{nj\varkappa}+b_{nj\varkappa}c_F(c_F+1)\equiv {}^1/_6 b_{nj\varkappa}Y_2(IFj) \quad (5)$$

where

$$c_F=F(F+1)-I(I+1)-j(j+1)\equiv 2(\mathbf{Ij})_F,$$

$$a_{nj\varkappa}=\frac{2e\mu_N g\varkappa}{j(j+1)}\int f_r g_r\,dr, \qquad b_{nj\varkappa}=\frac{3e^2Q}{16}\,\frac{B_{nj\varkappa}}{j(j+1)I(2I-1)},$$

$$\Delta_{nj\varkappa}=-\frac{e^2Q}{4}\,\frac{I+1}{2I-1}B_{nj\varkappa}, \qquad B_{nj\varkappa}=\int (f_r^2+g_r^2)\frac{dr}{r}.$$

The constants $A^{(\lambda)}_{Ijn\varkappa}$ are related to the constants $a_{nj\varkappa}$ and $b_{nj\varkappa}$ as follows[13]:

$$A^{(\mu 1)}_{Ijn\varkappa}=a_{nj\varkappa}[I(I+1)(2I+1)j(j+1)(2j+1)]^{1/2}, \quad (6)$$

$$A^{(Q2)}_{Ijn\varkappa}={}^2/_3 b_{nj\varkappa}[I(I+1)(2I+3)(4I^2-1) \times j(j+1)(2j+3)(4j^2-1)]^{1/2}. \quad (7)$$

Here, μ_N is the nuclear magneton; g is the gyromagnetic ratio; the expression $\mu = \mu_N g\mathbf{I}$ gives the magnetic moment of the nucleus; Q is the quadrupole moment of the nucleus; f_r and g_r are the radial parts of the Dirac wave functions describing excitation of an atomic state $nj\varkappa$ [n is the principal quantum number, j is the total momentum of the electron shell, $\varkappa = (l-j)(2j+1)$, and l is the orbital momentum]. The ratio $a_{nj\varkappa}/g$ for the $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, and also $b_{2p_{3/2}}$ states with $I(2I-1)/Q$ are tabulated in Ref. 13.

In the case of photoexcitation (γ) we have $R^{(\gamma)}_{F(nj\varkappa)} \propto (2F+1)$ (statistical excitation). In this case we find that $\delta E^{(\gamma)}_{nj\varkappa} = 0$, which follows from the properties of the $6j$ Wigner symbol occurring in Eq. (3) and is governed by the tensor properties of the hyperfine interaction operators. This circumstance (together with the smallness of the broadening) allows us to use x-ray fluorescence lines as the reference standards.[2-10]

3. HYPERFINE SHIFT OF AN X-RAY LEVEL EXCITED BY A CONVERSION TRANSITION

We shall calculate the populations $R^{(e)}_{F(nj\varkappa)}$ of the hyperfine structure components F of the final state $nj\varkappa$ of an atom excited in the course of internal conversion.

The matrix element of a conversion transition involving excitation of an atom in a specific state F of the hyperfine structure is of the form[6]

$$H_F^e(\varkappa')=[(2F+1)(2j'+1)]^{1/2}\sum_L (-1)^L\begin{Bmatrix} I_0 & I & L \\ j & j' & F \end{Bmatrix} b^{(\tau L)}_{\varkappa'}. \quad (8)$$

Here, I_0 and I are, respectively, the spins of the initial and final states of the nucleus; L is the multipolarity of the transition ($|I-I_0| \leqslant L \leqslant I+I_0$); τ is the type of transition ($\tau = E$ for electrical and $\tau = M$ for magnetic transitions); $\varkappa'$ represents the final state of an emitted electron: $\varkappa' = (l'-j')(2j'+1)$; $j' = l' \pm 1/2$, $j' = |\varkappa'| - 1/2$; l' and j' are the orbital and total momenta of an electron; $b^{(\tau L)}_{\varkappa'}$ is a reduced matrix element of the conversion transition.[6] The population is given by the expression

$$R^{(e)}_{F(nj\varkappa)}=W^{(e)}_{F(nj\varkappa)}\Big/\sum_F W^{(e)}_{F(nj\varkappa)}, \quad (9)$$

where $W^{(e)}_{F(nj\varkappa)}$ is the probability of excitation of the F component of the hyperfine structure of a level $nj\varkappa$ by a conversion transition:

$$W^{(e)}_{F(nj\varkappa)}=\frac{2\pi}{\hbar}\sum_{\varkappa'}|H_F^e(\varkappa')|^2. \quad (10)$$

Consequently, using the properties of the $6j$ symbols,[13] we obtain

$$R^{(e)}_{F(nj\varkappa)}=(2F+1)\sum_{\varkappa',L,L'}(2j'+1)(-1)^{L+L'} \times\begin{Bmatrix} I_0 & I & L \\ j & j' & F \end{Bmatrix}\begin{Bmatrix} I_0 & I & L' \\ j & j' & F \end{Bmatrix} b^{(\tau L)*}_{\varkappa'} b^{(\tau' L')}_{\varkappa'} \times\Big(\sum_{\varkappa',L}\frac{2j'+1}{2L+1}|b^{(\tau L)}_{\varkappa'}|^2\Big)^{-1}. \quad (11)$$

The nonstatistical nature of the population of the components of the hyperfine structure is due to the fact that the fraction on the right-hand side of Eq. (11) differs from unity.

Separating Eq. (1) into two parts in accordance with Eq. (2) and substituting Eqs. (3) and (11), we find that the shift of the center of gravity of an x-ray level $nj\varkappa$ excited by conversion is given by

$$\delta E^{(e)}_{nj\varkappa}=\sum_\lambda \delta E^{(e)}_{nj\varkappa}(\lambda), \quad (12)$$

where

$$\delta E^{(e)}_{nj\varkappa}(\lambda)=(-1)^{I+I_0+\lambda}A^{(\lambda)}_{Ijn\varkappa}\sum_{\varkappa',L,L'}(-1)^{j+j'}(2j'+1) \times\begin{Bmatrix} I_0 & I & L \\ \lambda & L' & I \end{Bmatrix}\begin{Bmatrix} j' & j & L \\ \lambda & L' & j \end{Bmatrix} \times b^{(\tau L)*}_{\varkappa'} b^{(\tau' L')}_{\varkappa'}\Big(\sum_{\varkappa',L}\frac{2j'+1}{2L+1}|b^{(\tau L)}_{\varkappa'}|^2\Big)^{-1}. \quad (13)$$

It should be noted that, in the case of mixed conversion transitions, Eqs. (11) and (13) contain terms corresponding to interference of transitions of different multipolarity (see also Refs. 6 and 8).

4. CONVERSION TRANSITIONS OF SPECIFIC MULTIPOLARITY

In the case of a hyperfine shift of a level $nj\varkappa$ excited by a conversion transition of specific multipolarity, it follows from Eq. (13) that

$$\delta E_{nj\varkappa}^{(e)}(\lambda)=(-1)^{I+I_0+\lambda}A_{Ijn\varkappa}^{(\lambda)}\sum_{\varkappa'}(-1)^{j+j'}(2j'+1)\times\begin{Bmatrix} I_0 & I & L \\ \lambda & L & I\end{Bmatrix}\begin{Bmatrix} j' & j & L \\ \lambda & L & j\end{Bmatrix}|b_{\varkappa'}^{(\tau L)}|^2\times\left(\sum_{\varkappa'}\frac{2j'+1}{2L+1}|b_{\varkappa'}^{(\tau L)}|^2\right)^{-1}. \quad (14)$$

We can simplify Eq. (14) significantly using explicit expressions for the $6j$ symbols[14]:

$$\begin{Bmatrix} j & j_2 & j_1 \\ \varkappa & j_1 & j_2\end{Bmatrix}=(-1)^{\varkappa+j+j_1+j_2}\left[\frac{(2j_1-\varkappa)!(2j_2-\varkappa)!}{(2j_1+\varkappa+1)!(2j_2+\varkappa+1)!}\right]^{1/2}\times Y_\varkappa(j_1jj_2). \quad (15)$$

The quantity $Y_\varkappa$ is described by the recurrence relationships of Ref. 14 . In particular, for $\varkappa=1$ or 2, we have

$$Y_1(j_1jj_2)=-4(\mathbf{j}_1\mathbf{j}_2)_j\equiv-2c_j, \quad (16)$$

$$Y_2(j_1jj_2)=6c_j(c_j+1)-8j_1(j_1+1)j_2(j_2+1), \quad (17)$$

where

$$c_j=j(j+1)-j_1(j_1+1)-j_2(j_2+1)\equiv2(\mathbf{j}_1\mathbf{j}_2)_j. \quad (18)$$

The relationship between Eqs. (3), (4), and (5) follows from Eqs. (15)–(17).

Substituting Eq. (16) into Eq. (14) and using Eq. (6), we find that the magnetic hyperfine shift can be written in the following transparent form:

$$\delta E_{nj\varkappa}^{(e)}(\mu1)=-a_{nj\varkappa}\frac{(\mathbf{IL})_{I_0}\overline{(\mathbf{Lj})_{j'}}}{L(L+1)}, \quad (19)$$

where $\overline{(\mathbf{Lj})_{j'}}$ is the average (over the final states j' of the emitted electron) value of the scalar product:

$$\overline{(\mathbf{Lj})_{j'}}=\sum_{\varkappa'}(2j'+1)|b_{\varkappa'}^{(\tau L)}|^2(\mathbf{Lj})_{j'}\left(\sum_{\varkappa'}(2j'+1)|b_{\varkappa'}^{(\tau L)}|^2\right)^{-1}. \quad (20)$$

Similarly, in the case of an electric quadrupole shift, we obtain

$$\delta E_{nj\varkappa}^{(e)}(Q2)=\frac{1}{24}b_{nj\varkappa}\frac{Y_2(LI_0I)\overline{Y_2(Lj'j)}}{L(L+1)(2L+3)(4L^2-1)}, \quad (21)$$

where

$$\overline{Y_2(Lj'j)}=\sum_{\varkappa'}(2j'+1)|b_{\varkappa'}^{(\tau L)}|^2Y_2(Lj'j)\times\left(\sum_{\varkappa'}(2j'+1)|b_{\varkappa'}^{(\tau L)}|^2\right)^{-1}. \quad (22)$$

The values of the averages given by Eqs. (20) and (22) differ from zero not only in the case of a nonstatistical distribution of conversion electrons between j', i.e., not only when the quantitites $|b_{\varkappa'}^{(\tau L)}|^2$ differ from one another. Therefore, the nonstatistical nature of population of the hyperfine components of an x-ray level excited by a conversion transition of specific multipolarity is automatically related to the nonstatistical distribution of the emitted electrons in accordance with j'.

A set of permissible values of $\varkappa'$ (and, therefore, of j') is governed by the selection rules for conversion (see, for example, Ref. 18):

$$ML\text{-transitions}\begin{cases}|j-L|\leqslant j'\leqslant j+L,\\ |\bar{l}-L|\leqslant l'\leqslant \bar{l}+L,\\ l+l'+L-\text{ is odd,}\end{cases} \quad (23)$$

where $\bar{l}=-\varkappa$ for $\varkappa<0$ and $\bar{l}=\varkappa-1$ for $\varkappa>0$; we also find that

$$EL\text{-transitions}\begin{cases}|j-L|\leqslant j'\leqslant j+L,\\ |l-L|\leqslant l'\leqslant l+L,\\ l+l'+L-\text{ is even,}\end{cases} \quad (24)$$

We now consider some examples.

a. Hyperfine shifts of $ns_{1/2}$ ($j=1/2$, $l=0$, $\bar{l}=1$, $\varkappa=-1$) and $np_{1/2}$ ($j=1/2$, $l=1$, $\bar{l}=0$, $\varkappa=1$) levels

In this case it follows from the selection rules (23) and (24) that there are two possible states ($i=1$ or 2) of the final electron and the values of j_i', l_i', and $\varkappa_i'$ for these states are given in Table I. Introducing $\rho^{(\tau L)}=|b_{\varkappa_2'}^{(\tau L)}|^2/|b_{\varkappa_1'}^{(\tau L)}|^2$ and bearing in mind that a purely magnetic hyperfine interaction occurs if $j=1/2$, we find that Eq. (19) yields

$$\delta E_{n^1\!/_2\varkappa}^{(e)}=-a_{n^1\!/_2\varkappa}\frac{(\mathbf{IL})_{I_0}(\mathbf{Lj})_{j_1'}}{L(L+1)}\frac{1-\rho^{(\tau L)}}{1+[(L+1)/L]\rho^{(\tau L)}}. \quad (25)$$

This expression reduces to that obtained in Ref. 6 for a K level if we use explicit equations describing the scalar products $(\mathbf{IL})_{I_0}$ and expressing $(\mathbf{Lj})_{j_1'}$ in terms of the hyperfine splitting $\bar{\Delta}_{n1/2\varkappa}$:

$$\bar{\Delta}_{n^1\!/_2\varkappa}\equiv\Delta E_{n^1\!/_2\varkappa}^{F=I+1/2}-\Delta E_{n^1\!/_2\varkappa}^{F=I-1/2}=\frac{2I+1}{2}a_{n^1\!/_2\varkappa}. \quad (26)$$

The final expression, identical with that deduced in Ref. 6, is

$$\delta E_{n^1\!/_2\varkappa}^{(e)}=a_{n^1\!/_2\varkappa}\frac{(I_0-I)(I_0+I+1)-L(L+1)}{4L}\frac{1-\rho^{(\tau L)}}{1+[(L+1)/L]\rho^{(\tau L)}}. \quad (27)$$

TABLE I.

	ML conversion in $ns_{1/2}$ EL conversion in $np_{1/2}$		EL conversion in $ns_{1/2}$ ML conversion in $np_{1/2}$	
i	1	2	1	2
j_i'	$L-1/2$	$L+1/2$	$L-1/2$	$L+1/2$
l_i'	$L-1$	$L+1$	L	L
$\varkappa_i'$	$-L$	$L+1$	L	$-(L+1)$

TABLE II.

	ML conversion ($L>1$)				*EL* conversion ($L>1$)			
i	1	2	3	4	1	2	3	4
j_i'	$L-3/2$	$L-1/2$	$L+1/2$	$L+3/2$	$L-3/2$	$L-1/2$	$L+1/2$	$L+3/2$
l_i'	$L-2$	L	L	$L+2$	$L-1$	$L-1$	$L+1$	$L+1$
$\varkappa_i'$	$-(L-1)$	L	$-(L+1)$	$L+2$	$L-1$	$-L$	$L+1$	$-(L+2)$

It should be noted that the hyperfine shift effect is demonstrated most clearly when the value of $\rho^{(\tau L)}$ differs greatly from unity. At moderate transition energies this occurs in the case of $ns_{1/2}$ levels excited by *ML* conversion and for $np_{1/2}$ levels excited by *EL* conversion. In such cases we have $l_1' < l_2'$ (Table I), so that $\rho^{(\tau L)} \ll 1$, and in Eqs. (25) and (27) we can substitute $\rho^{(\tau L)} \approx 0$, which is accurate to within 10% right up to transition energies ≈ 0.5 MeV (Ref. 6).

b. Hyperfine shifts of $np_{3/2}$ levels ($j=3/2$, $l=1$, $\bar{l}=2$, $\varkappa=-2$)

In the case $L>1$ the rules represented by Eqs. (23) and (24) give four possible values of $\varkappa_i'$ ($i=1,2,3,4$) and the corresponding values of j_i' and l_i', which are listed in Table II. Table III gives the values of $2j_i'+1$, $(\mathbf{Lj})_{j_i'}$, and $Y_2(Lj_i'3/2)$ for all the permissible values of j_i'.

Introducing

$$\rho_i^{(\tau L)} = |b_{\varkappa_i'}^{(\tau L)}|^2/|b_{\varkappa_1'}^{(\tau L)}|^2, \quad \rho_1^{(\tau L)} \equiv 1, \tag{28}$$

we find that the expressions for the hyperfine shifts of the $np_{3/2}$ levels can be represented conveniently in the form

$$\delta E_{n^3/_2\varkappa}^{(e)}(\mu 1) = \frac{3}{2} a_{n^3/_2\varkappa} \frac{(\mathbf{IL})_{I_0}}{L} \eta_{\mu 1}^{(\tau L)}, \tag{29}$$

$$\delta E_{n^3/_2\varkappa}^{(e)}(Q2) = \frac{1}{2} b_{n^3/_2\varkappa} \frac{Y_2(LI_0I)}{L(4L^2-1)} \eta_{Q2}^{(\tau L)}, \tag{30}$$

where

$$\eta_{\mu 1}^{(\tau L)} = \frac{1-y_{\mu 1}^{(\tau L)}}{1+y_0^{(\tau L)}}, \quad \eta_{Q2}^{(\tau L)} = \frac{1-y_{Q2}^{(\tau L)}}{1+y_0^{(\tau L)}},$$

$$y_{\mu 1}^{(\tau L)} = -\frac{L(L+4)\rho_2^{(\tau L)} - (L-3)(L+1)\rho_3^{(\tau L)} - 3L(L+2)\rho_4^{(\tau L)}}{3(L^2-1)},$$

$$y_{Q2}^{(\tau L)} = \frac{L(L-2)}{L^2-1}\rho_2^{(\tau L)} + \frac{(L+3)(2L-1)}{(L-1)(2L+3)} \times \rho_3^{(\tau L)} - \frac{L(L+2)(2L-1)}{(L^2-1)(2L+3)}\rho_4^{(\tau L)},$$

$$y_0^{(\tau L)} = \frac{L\rho_2^{(\tau L)} + (L+1)\rho_3^{(\tau L)} + (L+2)\rho_4^{(\tau L)}}{L-1}.$$

It should be noted that, as in the preceding example, when the energies of *ML* transitions ($L>1$) are $\lesssim 0.5$ MeV, we can quite accurately assume that $\eta_{\mu 1}^{(\tau L)}\eta_{Q2}^{(\tau L)} \approx 1$. In the case of *EL* transitions considered in the same approximation, we can assume that $\rho_3^{(\tau L)} \approx \rho_4^{(\tau L)} \approx 0$.

The states with $j_i' = L - 3/2$ do not exist for the $M1$ and $E1$ transitions, so that we have to redefine the quantities $\rho_i^{(\tau 1)}$:

$$\rho_i^{(\tau 1)} = |b_{\varkappa_i'}^{(\tau 1)}|^2/|b_{\varkappa_2'}^{(\tau 1)}|^2, \quad \rho_2^{(\tau 1)} \equiv 1. \tag{31}$$

Then,

$$\eta_{\mu 1}^{(\tau 1)} = \frac{1+{}^4/_5\rho_3^{(\tau 1)} - {}^9/_5\rho_4^{(\tau 1)}}{1+2\rho_3^{(\tau 1)}+3\rho_4^{(\tau 1)}}, \tag{32}$$

$$\eta_{Q2}^{(\tau 1)} = \frac{1-{}^8/_5\rho_3^{(\tau 1)} + {}^3/_5\rho_4^{(\tau 1)}}{1+2\rho_3^{(\tau 1)}+3\rho_4^{(\tau 1)}}. \tag{33}$$

In this case at low energies $\eta_{\mu 1}^{(E1)} \approx \eta_{Q2}^{(E1)} \approx 1$ it is important to allow for $\rho_3^{(M1)}$ for the $E1$ and $M1$ transitions.

The amplitudes $b_{\varkappa'}^{(\tau L)}$ for nonanomalous conversion are as follows[19]:

$$b_{\varkappa'}^{(\tau L)} = 2\left[\frac{\alpha E(2L+1)}{2I_0+1}\right]^{1/2} \tilde{a}(\tau L) \frac{M_{\varkappa'}^{(\tau L)}}{(2j'+1)^{1/2}}, \tag{34}$$

where E is the energy of the conversion transition; $\alpha = e^2/\hbar c$; $\tilde{a}(\tau L)$ is the amplitude of a nuclear transition accompanied by the emission of a γ photon; $M_{\varkappa'}^{(\tau L)}$ is a conversion matrix element which is independent of the structure of the nucleus and is defined in such a way that the conversion coefficient for the ith shell is

$$\alpha^i(\tau L) = \sum_{\varkappa'} |M_{\varkappa'}^{(\tau L)}|^2.$$

The amplitude $\tilde{a}(\tau L)$ is related to the probability of γ emission[19] as follows

$$W_\gamma(\tau L) = 8\pi\alpha E|\tilde{a}(\tau L)|^2/\hbar(2I_0+1).$$

It follows from Eq. (34) that in the nonanomalous conversion case, we should have

$$\rho_i^{(\tau L)} = \frac{|b_{\varkappa_i'}^{(\tau L)}|^2}{|b_{\varkappa_0'}^{(\tau L)}|^2} = \frac{2j_0'+1}{2j_i'+1}\frac{|M_{\varkappa_i'}^{(\tau L)}|^2}{|M_{\varkappa_0'}^{(\tau L)}|^2}. \tag{35}$$

TABLE III.

i	1	2	3	4
$2j_i'+1$	$2(L-1)$	$2L$	$2(L+1)$	$2(L+2)$
$(Lj)_{j_i'}$	$-{}^3/_2(L+1)$	$-{}^1/_2(L+4)$	${}^1/_2(L-3)$	${}^3/_2L$
$Y_2(Lj_i'\,{}^3/_2)$	$12(L+1)(2L+3)$	$-12(L-2)(2L+3)$	$-12(L+3)(2L-1)$	$12L(2L-1)$

The quantities $M_{\varkappa}^{(\tau L)}$ are partly tabulated in Ref. 20 or can be found numerically by means of specialized codes.[21]

5. TRANSFER OF A HYPERFINE SHIFT OF X-RAY LEVELS BY ELECTROMAGNETIC TRANSITIONS

Let us assume that a process G creates a vacancy in one of the inner (K, L,...) shells of an atom, i.e., that a level $n_0j_0\varkappa_0$ is excited. The hole then floats up as a result of electromagnetic $E1$ transitions involving the emission of x-ray photons. We shall calculate the populations $R_{F(nj\varkappa)}^{(r)}$ of the F sublevels of the hyperfine structure of the $nj\varkappa$ level if they are excited by electromagnetic transitions from the sublevels F_0 (characterized by populations $R_{F_0(n_0j_0\varkappa_0)}^{(G)}$) of the $n_0j_0\varkappa_0$ level. The rate of such transitions is given by (see, for example, Ref. 22)

$$w_{n_0j_0\varkappa_0\to nj\varkappa}^{F_0\to F}=w_{tot}(2j_0+1)(2F+1)\left|\begin{Bmatrix} j & F & I\\ F_0 & j_0 & 1\end{Bmatrix}\right|^2, \quad (36)$$

where

$$w_{tot}=\sum_F w_{n_0j_0\varkappa_0\to nj\varkappa}^{F_0\to F}.$$

Then, the population $R_{F(nj\varkappa)}^{(r)}$ is described by

$$R_{F(nj\varkappa)}^{(r)}=\sum_{F_0} R_{F_0(n_0j_0\varkappa_0)}^{(G)}(2j_0+1)(2F+1)\left|\begin{Bmatrix} j & F & I\\ F_0 & j_0 & 1\end{Bmatrix}\right|^2. \quad (37)$$

The shift of the center of gravity of the level $nj\varkappa$ can be described by analogy with Eq. (12):

$$\delta E_{nj\varkappa}^{(r)}=\sum_\lambda \delta E_{nj\varkappa}^{(r)}(\lambda). \quad (38)$$

Calculation of the quantities $\delta E_{nj\varkappa}^{(r)}(\lambda)$ using Eqs. (37) and (3) and the properties of the $6j$ symbols[14] yields the following expression:

$$\delta E_{nj\varkappa}^{(r)}(\lambda)=\sum_{F_0}(2j_0+1)(-1)^{I+j+\lambda+1+F_0}A_{Ijn\varkappa}^{(\lambda)}R_{F_0(n_0j_0\varkappa_0)}^{(G)}$$
$$\times\begin{Bmatrix} F_0 & j_0 & I\\ \lambda & I & j_0\end{Bmatrix}\begin{Bmatrix} 1 & j_0 & j\\ \lambda & j & j_0\end{Bmatrix}. \quad (39)$$

Using Eq. (1), we can represent the final result in the form

$$\delta E_{nj\varkappa}^{(r)}(\lambda)$$
$$=(-1)^{j-j_0+\lambda+1}(2j_0+1)\begin{Bmatrix} 1 & j_0 & j\\ \lambda & j & j_0\end{Bmatrix}\frac{A_{Ijn\varkappa}^{(\lambda)}}{A_{Ij_0n_0\varkappa_0}^{(\lambda)}}\delta E_{n_0j_0\varkappa_0}^{(G)}(\lambda). \quad (40)$$

Expanding the $6j$ symbols in terms of Eqs. (15)–(17) and using Eqs. (6) and (7), we find that

$$\delta E_{nj\varkappa}^{(r)}(\mu 1)=\frac{(\mathbf{j}\mathbf{j}_0)_1}{j_0(j_0+1)}\frac{a_{nj\varkappa}}{a_{n_0j_0\varkappa_0}}\delta E_{n_0j_0\varkappa_0}^{(G)}(\mu 1), \quad (41)$$

$$\delta E_{nj\varkappa}^{(r)}(Q2)=-\frac{Y_2(j1j_0)}{4J(j_0)}\frac{b_{nj\varkappa}}{b_{n_0j_0\varkappa_0}}\delta E_{n_0j_0\varkappa_0}^{(G)}(Q2), \quad (42)$$

where $J(j)=j(j+1)(2j+3)(2j-1)$.

It follows from Eqs. (41) and (42) that in the case of an electromagnetic transition from a level shifted because of the nonstatistical population of the hyperfine components (for example, as a result of excitation by conversion or electron capture), the final level and, consequently, all the other levels in a cascade are shifted and this shift is governed by that of the initial level. It means that information on the multipole moment of a nucleus and on the properties of a nuclear transition, which is carried by the hyperfine shift of the initial level, is transferred to the outermost shells of an atom. Therefore, multipole moments of nuclei can, in principle, be determined—irrespective of their lifetimes (or other nuclear characteristics)—from shifts of the centers of gravity of any lines (or any hyperfine multiplets if these are allowed) belonging to an electromagnetic cascade which accompanies any process that leads to a nonstatistical population of hyperfine components of an excited state of an atom.

Moreover, the transfer of hyperfine shifts from highly excited to lower levels leads to an additional x-ray line shift. The hyperfine shift of an X_1 x-ray line as a result of excitation by the process G of a level $n_0j_0\varkappa_0$ and an electromagnetic transition $n_0j_0\varkappa_0\to nj_1\varkappa_1$ is given by

$$\delta E_{X_1}^{(G)}=\sum_\lambda \delta E_{X_1}^{(G)}(\lambda), \quad (43)$$

where

$$\delta E_{X_1}^{(G)}(\lambda)=\delta E_{\alpha_0}^{(G)}(\lambda)-\delta E_{\alpha_1}^{(r)}(\lambda),\quad \alpha=nj\varkappa. \quad (44)$$

Substituting Eqs. (41) and (42) into Eq. (44), we obtain

$$\delta E_{X_1}^{(G)}(\mu 1)=\left[1-\frac{(\mathbf{j}_0\mathbf{j}_1)_1}{j_0(j_0+1)}\frac{a_{\alpha_1}}{a_{\alpha_0}}\right]\delta E_{\alpha_0}^{(G)}(\mu 1), \quad (45)$$

$$\delta E_{X_1}^{(G)}(Q2)=\left[1+\frac{Y_2(j_11j_0)}{4J(j_0)}\frac{b_{\alpha_1}}{b_{\alpha_0}}\right]\delta E_{\alpha_0}^{(G)}(Q2). \quad (46)$$

The shift of the next X_2 line ($\alpha_1\to\alpha_2$) is

$$\delta E_{X_2}^{(r)}=\delta E_{\alpha_1}^{(r)}-\delta E_{\alpha_2}^{(r)}, \quad (47)$$

where

$$\delta E_{X_2}^{(r)}(\mu 1)=\left[1-\frac{(\mathbf{j}_2\mathbf{j}_1)_1}{j_1(j_1+1)}\frac{a_{\alpha_2}}{a_{\alpha_1}}\right]\frac{(\mathbf{j}_1\mathbf{j}_0)_1}{j_0(j_0+1)}\frac{a_{\alpha_1}}{a_{\alpha_0}}\delta E_{\alpha_0}^{(G)}(\mu 1), \quad (48)$$

$$\delta E_{X_2}^{(r)}(Q2)=-\left[1+\frac{Y_2(j_21j_1)}{4J(j_1)}\frac{b_{\alpha_2}}{b_{\alpha_1}}\right]\frac{Y_2(j_11j_0)}{4J(j_0)}\frac{b_{\alpha_1}}{b_{\alpha_0}}\delta E_{\alpha_0}^{(G)}(Q2). \quad (49)$$

Similar expressions are readily obtained for the other lines in the cascade. It should be pointed out that although the additional shifts of the lines due to the lower levels are small because $a_{\alpha_n}\ll a_{\alpha_{n-1}}$, and $b_{\alpha_n}\ll b_{\alpha_{n-1}}$, they must be allowed for in determination of the nuclear characteristics from precision measurements of the hyperfine shifts of x-ray lines.

6. CONCLUSIONS

The main difficulty limiting the use of x-ray crystal diffraction spectrometers in measurements of the nuclear moments is the need to distinguish precisely that x-ray line which accompanies the investigated nuclear transition. Therefore, experiments have been carried out only on nuclei exhibiting the simplest decay schemes.[4-10] It is difficult to use the coincidence method because of the low luminosity of crystal diffraction spectrometers. The use of a semiconductor spectrometer in an x-ray arm[23] creates problems associated with its much poorer energy resolution and relatively unsatisfactory time characteristics, so that a strong background of random coincidences is created.

These difficulties are eliminated in a natural manner if we determine precisely the energies of electron conversion lines which undergo the same (but opposite) shifts as x-ray levels. The precision of determination of the electron energies is at present approximately an order of magnitude less than that required in such experiments,[23] but such a precision is not unattainable. The solution of the problem of determination of hyperfine energy shifts of conversion lines using a high-resolution beta spectrometer[23,24] would widen considerably the prospects of the method.

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