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# Hyperfine Structure of  $^{5}I_{8,7}^{\phantom{5}}$  Atomic States of Dy $^{16\,1,\,16\,3}$  and the Ground-State Nuclear Moments~

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The atomic-beam magnetic-resonance technique has been used to measure the hyperfin structure of the  $4f^{10}6s^2\bar{5}I_{8,7}$  atomic states of Dy $^{161,163}$ . Values of the hyperfine–interaction constants A, B, and C, corrected for hyperfine interactions with other states, are given for both structure of the  $4f^{\prime\prime}6s^{\prime\prime}t_{8,7}$  atomic states of Dy<sup>1617</sup>. Values of the nyperfine-interaction con-<br>stants A, B, and C, corrected for hyperfine interactions with other states, are given for both<br>atomic states of  $= -1.400(3)$ , and, less accurately,  $\mu^{163} = +0.65(6)\mu_{N}$ ,  $Q^{163} = +2.51(30)$  b,  $\mu^{161} = -0.46(5)\mu_{N}$  $Q^{161}$  = + 2. 37(28) b. The electron g factor  $g<sub>J</sub>$  is measured for the atomic states  $4f<sup>10</sup>6s<sup>25</sup>I<sub>6,7,6</sub>$ and also for the lowest  $J=8$  level of  $4f^95d6s^2$  at 7565 cm<sup>-1</sup>. The lifetime of this level cannot be appreciably less than 2 msec, the transit time for the atom in the apparatus.

### I. INTRODUCTION

Ebenhoh, Ehlers, and Ferch' pointed out that the electric-quadrupole moment of the  $Dy^{161}$  nuclear ground state appeared about  $50\%$  larger when determined from the Mössbauer effect<sup>2</sup> than from paramagnetic resonance in salts' (presumably because of difficulties in estimating the electric field gradient at the nucleus). Their atomic-beam magnetic-resonance value, obtained with free atoms, confirmed the Mössbauer result.

The purpose of the present experiment was to extend the atomic-beam experiment<sup>1</sup> on the  $4f^{10}6s^2$ <sup>5</sup> $I_8$ atomic ground state of  $Dy^{161}$  and  $Dy^{163}$  to include measurements of the  $\Delta F = \pm 1$  hfs intervals, and to make corresponding measurements on the  $5I<sub>7</sub>$  metastable state. When hfs measurements are made in only one atomic state, one must postulate details of the state in order to extract values for the magnetic-dipole and electric-quadrupole moments of the nuclear ground state from the observed hfs. As more atomic states are included in the hfs studies, the assumptions about the atomic state become subject to test.

In determining values of the magnetic-dipole mo-In determining values of the magnetic-dipole ments of the  $Dy^{161,163}$  nuclear ground states, it is shown that atomic core polarization is responsible for only about  $1\%$  of the magnetic-dipole hfs. The effects of relativity and the intermediate-coupling composition of the  $^{5\!}I_{8,7}$  states are taken into accoun explicitly, and Sternheimer's estimate of the distortion of the inner electron shells is included in extraction of the nuclear electric-quadrupole moment.

Precision values of the electron g factor  $g<sub>r</sub>$  are also useful in understanding the composition of atomic states and were therefore determined for all states having sufficient population in the atomic beam.

### II. EXPERIMENTAL CONSIDERATIONS

The principles of the atomic-beam magneticresonance technique have been discussed<sup>4</sup> many times in the literature, as has the particular apparatus used for the present experiment.<sup>5</sup> The latter is entirely conventional except that the digital techniques used<sup>6</sup> for handling the data made possible observation of transitions in very weakly populated atomic



FIG. 1. Mass spectrum of the Dy atomic beam after magnetic analysis. Identification of which isotope was responsible for any particular rf transition was greatly simplified by the mass-resolution capability of the detector.

states.

The radio frequency used to induce transitions was produced by generating a signal sweepable from 30 MHz to  $30 + \delta \nu$  MHz in adjustable steps, mixing this with a crystal-locked reference frequency, and then amplifying the sum or difference with a tuned rf amplifier. The sweepable frequency originated in a Hewlett-Packard 1-MHz synthesizer and was added (within the synthesizer) to a crystal-locked 30-MHz signal. Reference frequencies below 1 GHz were obtained from a Solartron precision signal generator, type DO 1001, with the required multipliers and amplifiers; above 1 6Hz, they were obtained from a phase-locked magnetron. Each time the frequency was stepped by one increment, the counts coming from the detector were routed to the next channel of a multichannel sealer. As the sweep was repeated over and over, data could be accumulated until the signal-to-noise ratio for a transition was satisfactory.

The beam of Dy atoms was produced by electronbombardment heating of a Ta oven equipped with a slit 0.015 in. wide and  $\frac{1}{4}$  in. high. A sharp-lipped Ta inner crucible was used inside the oven to limit creep. A second auxiliary oven produced a beam of  $K^{39}$  which was used for calibration of the homogeneous C field.

Observations were made both on the even-even stable isotopes and on the odd-A stable isotopes  $Dy^{161,163}$  The isotope in which a particular transition took place was determined by use of the magnetic mass spectrometer associated with the electronbombardment detector. Figure 1 shows the mass resolution typically used for the principal stable isotopes. While better resolution could undoubtedly have been achieved, that illustrated was found to be

entirely adequate.

The electron  $g$ -factor measurements on even-even isotopes consist in measuring the transition frequency  $\nu$  at several values of the external magnetic field  $H$ , and in addition verifying that they are proportional. For the transition J,  $M_J \rightarrow J$ ,  $M'_J$ , the resonance frequency is

$$
\nu = g_J \mu_0 H/h, \tag{1}
$$

where  $\mu_0$  is the Bohr magneton, and h is Planck's constant. Normally,  $M_J = +1$ ,  $M_J' = -1$ , and the observed transition involves a two-quantum jump. The resonance frequency  $\nu$  was found to be proportional to  $H$ , as expected, for all the present observations (in the even-even isotopes).

Since the atomic beam was populated thermally, the number of atoms available for transitions in excited atomic states was much less than for the ground state. Table I lists the relative Boltzmann factors for the four lowest levels of DyI. The relative intensities expected for transitions between individual magnetic substates depends, in addition, on the isotopic abundance and on  $I$ . rf power level and angular-momentum considerations also affect the relative transition probabilities. While 20 sec or less of data accumulation yielded a good signalto-noise ratio for the  $^{5}I_{8}$  ground state, nearly 1 h was required for aeeeptable signal-to-noise in the levels at about  $7000 \text{ cm}^{-1}$ .

For the odd-A isotopes  $Dy^{161,163}$ , the nuclear spin  $I = \frac{5}{2}$  couples with the J of the atomic state to produce the hyperfine levels  $F = J + \frac{5}{2}$ ,  $J + \frac{3}{2}$ , ...,  $|J - \frac{5}{2}|$ . The  $(2F + 1)$ -fold degeneracy of each of these zerofield hyperfine states is removed by the application of an external magnetic field  $H$ . The Hamiltonian for the system, with the assumption that the atomic state is perfectly isolated, may be written<sup>7</sup>

$$
\mathcal{K} = \mathcal{K}_{\text{hfs}} + \mathcal{K}_{z} \quad , \tag{2}
$$

in which

$$
\mathcal{K}_{\text{hfs}} = hA\,\mathbf{\tilde{1}}\cdot\mathbf{\tilde{J}}+hB\,\frac{\frac{3}{2}\mathbf{\tilde{1}}\cdot\mathbf{\tilde{J}}\,(2\mathbf{\tilde{I}}\cdot\mathbf{\tilde{J}}+1)-I\,(I+1)J\,(J+1)}{2I\,(2I-1)J\,(2J-1)}
$$

TABLE I. Classification, excitation energies, and relative Boltzmann factors (at 1260 °C) for the lowestfour atomic states of Dy. The Boltzmann factors give a crude indication of the relative intensity which may be expected, for a given Dy isotope, for an rf transition between individual magnetic substates.





FIG. 2. The double-quantum  $(\frac{11}{2}, \frac{7}{2} \rightarrow \frac{11}{2}, \frac{3}{2})$  transition in the  $^{5}I_{8}$  atomic ground state of  $\mathrm{Dy}^{163}$  as observed at  $H= 70$  G. The data-accumulation time was greatly lengthened (to about 15 min) for this run over that normally used in order to permit the much weaker  $\frac{1}{2}+\frac{7}{2}+\frac{3}{2}$ ,  $\frac{3}{2}$ transition in the  ${}^{5}I_{7}$  metastable atomic state of the same isotope to "grow in. " The signal-to-noise ratio for this transition could have been improved by further counting. The Boltzmann factors for the two states (at the effective temperature 1260'C) differ as can be seen in Table I by a factor of 48; other factors also affect the observed signal strength, of course.

$$
+ \frac{hC}{I(I-1)(2I-1)J(J-1)(2J-1)} \frac{5}{4} \{8(\mathbf{\tilde{i}} \cdot \mathbf{\tilde{j}})^3
$$
  
+ 16(\mathbf{\tilde{i}} \cdot \mathbf{\tilde{j}})^2 + \frac{8}{5} (\mathbf{\tilde{i}} \cdot \mathbf{\tilde{j}}) [-3I(I+1)J(J+1) + I(I+1)  
+ J(J+1) + 3] - 4I(I+1)J(J+1) \}, \qquad (3)  
= \mu\_0 H(g\_J J\_z + g\_I I\_z) , \qquad (4)

$$
\mathcal{K}_z = \mu_0 H(g_J J_z + g_I I_z) \tag{4}
$$

where the Hamiltonians for the hyperfine and Zeeman interactions are written separately. In these expressions,  $I$  and  $J$  are the nuclear spin and the total electron angular momentum, respectively,  $I_z$ and  $J_z$  are their projections on the field axis,  $A$ , 8, and <sup>C</sup> are the magnetic-dipole, electric-quadrupole, and magnetic-octupole hyperfine-interaction constants, respectively, and  $g_I$  and  $g_I$  are the electron and nuclear  $g$  factors.

A computer program using this Hamiltonian varied the quantities  $A$ ,  $B$ ,  $C$ , and  $g<sub>J</sub>$  to produce a best

least-squares fit to all the measured transition frequencies for each atomic state of each isotope. These fits were relatively insensitive to  $g_I$ , which was considered known.

Figure 2 shows, at the left, the appearance of the Figure 2 shows, at the left, the appearance of t<br>double-quantum transition  $(\frac{11}{2}, \frac{7}{2} \leftrightarrow \frac{11}{2}, \frac{3}{2})$  in the  $^{5}I_{\varepsilon}$ atomic ground state of Dy<sup>163</sup> at  $H = 70$  G. For this run, the data-collection time was extended far beyond that required for the ground state in order to allow the  $\frac{9}{2}$ ,  $\frac{7}{2}$   $\rightarrow \frac{9}{2}$ ,  $\frac{3}{2}$  transition in the excited  $5I_7$ atomic state of the same isotope to "grow in. " Figure 3 illustrates the appearance of the  $\Delta F = \pm 1$  tranure 3 illustrates the appearance of the  $\Delta F = \pm 1$  transition  $(\frac{11}{2}, -\frac{1}{2} \leftrightarrow \frac{13}{2}, -\frac{3}{2})$  in the  $^5I_7$  atomic state of  $Dy^{161}$  at 1 G after about 20 min of data collection. Table II lists all the observations on Dy. The final column of the table gives the difference between the observed resonance frequencies and those calculated from the Hamiltonian of Eq. (2) for the best-fit values (listed in Table IV) of the parameters  $A, B, C$ , and  $g_J$ . Corrections ( $\leq 0.007$  MHz), small compared to the experimental uncertainties, were applied to the frequencies calculated from Eq. (2) to take account of hyperfine and Zeeman interactions with nearby atomic states.

Table III lists the values of  $g_J$ , the electron g factor, determined from observations in the even-



FIG. 3. The  $\Delta F = \pm 1$  transition  $(\frac{11}{2}, -\frac{1}{2}, -\frac{13}{2}, -\frac{3}{2})$ in the  $^{5}I_{7}$  metastable atomic state of Dy<sup>161</sup> as observed at  $H=1$  G. About 20-min accumulation of dat quired.

d

TABLE II. Resonance frequencies for all transitions observed in the Dy isotopes, as a function of magnetic field strength. The field was calibrated by observing resonances in an auxiliary beam of  $K^{39}$ . Although the calculated frequencies used in obtaining the residuals in the right-hand column include corrections for hyperfine and Zeeman interactions with other atomic states, the corrections were in all cases less than the experimental uncertainty, and thus have little effect on the results.



even isotopes of Dy. Table IV gives the values found for the quantities  $A, B, C,$  and  $g<sub>J</sub>$  from leastsquares fits of the appropriate differences of eigenvalues of Eq. (2) to the observed resonance frequen-

TABLE II. (continued).

Isotope	Atomic state	Transition $(F, M \rightarrow F', M')$	Н (G)	Observed resonance frequency (MHz)	$\nu$ obs $\nu$ calc (kHz)
Dy <sup>162,164</sup>	${}^5I_8$	$(J, MJ \rightarrow J, -MJ)$	100	173.787(10)	3
		$(J, M_J \rightarrow J, -M_J)$	200	347.570(15)	$\overline{2}$
		$(J, MJ \rightarrow J, -MJ)$	200	347.566(12)	$\overline{2}$
	${}^5I_7$	$(J, MI \rightarrow J, -MI)$	10	16,435(15)	10
		$(J, MJ \rightarrow J, -MJ)$	10	16.430(20)	5
		$(J, MI \rightarrow J, -MI)$	100	164.243(20)	- 5
		$(J, M_J \rightarrow J, -M_J)$	200	328,490(20)	$-6$
		$(J, M_J \rightarrow J, -M_J)$	200	328, 498(13)	$\overline{2}$
	${}^5\!I_6$	$(J, M, \longrightarrow J, -M)$	10	15,000(20)	$\overline{2}$
		$(J, MJ \rightarrow J, -MJ)$	100	149, 985 (18)	3
		$(J, Mx \rightarrow J, -Mx)$	200	299, 950 (25)	$-15$
		$(J, MJ \rightarrow J, -MJ)$	200	299, 965(20)	0
		$(J, M_J \rightarrow J, -M_J)$	200	299.970(20)	5
	$4f^95d6s^2$				
	$J=8$	$(J, MJ, -MJ)$	20	37,862(10)	2
	(7565	$(J, MJ \rightarrow J, -MJ)$	100	189.298(16)	3
	$cm^{-1}$ )	$(J, MJ \rightarrow J, -MJ)$	200	378,603(12)	$\overline{2}$

cies. The uncertainties given are two standard deviations. The "uncorrected" values result from fits in which  $\mathcal{R}_{\text{hfs}}$  and  $\mathcal{R}_s$  are given by Eqs. (3) and (4). When the small frequency shifts caused by hfs and Zeeman interactions with other atomic states are allowed for, the "final" values (given at the right in Table IV) result. The procedure for making these corrections has been discussed elsewhere<sup>9</sup>; because they are so small for Dy, they will not be discussed further. The signs given in Table IV for the hfs interaction constants  $A$ ,  $B$ , and  $C$  will be discussed in Sec. IIIE.

### III. ANALYSIS AND COMPARISON WITH THEORY

# A. Eigenvectors for the  $4f^1{}^06s^2{}^5I_{8,7}$  States

The classification and excitation energy is given<sup>10</sup> in Table I for each level of Dy I lying below 8000 cm<sup>-1</sup>. Because no other even-parity levels with  $J$ = 8, 7, 6 lie below 20 000 cm<sup>-1</sup>, the  $^{5}I_{8,7,6}$  levels may be expected to be very near the  $LS$  limit as predicted by Judd and Lindgren<sup>11</sup> and by Conway and Wy-

TABLE III. Summary of  $g_J$  values measured in the even-even isotopes  $Dy^{162,164}$ . The results for the  ${}^{5}I_{8,7}$ states are entirely consistent with the values found by observations in the odd-A isotopes, listed in Table IV. Observations on the even-even isotopes lead to a measurement of  $g_J$ , but not of J itself.

Electron	State	Isotopes	Measured
configuration		used	gs
$4f^{10}6s^2$ $4f^{10}6s^2$ $4f^{10}6s^2$ $4f^95d6s^2$	$^{5\!}I_8$ $^{5}I_{7}$ $^{5}I_{6}$ $J=8$ $(7565 \text{ cm}^{-1})$	$\mathrm{Dy}^{162}$ $Dv^{164}$ $Dy^{162}$ $Dy^{164}$ $\text{Dy}^{162}$ . $Dv^{164}$ $Dv^{162}$ , $Dv^{164}$	1.24160(4) 1.17347(4) 1.07155(5) 1,35246(5)



bourne.<sup>12</sup> The Conway-Wybourne eigenvectors are used for the present analysis because, as discussed in Sec. III B, they are better able to account for the observed  $g<sub>J</sub>$  values. These eigenvectors, calculated before the excitation energies were known, give the purities of the states  $5I_{8,7}$  as 94% and 97%, respectively.

In comparing the observed hyperfine structure of the  ${}^{5}I_{8.7}$  states with the theory, it is convenient to truncate the eigenvectors $12$  to include only the two leading impurities, i.e.,

$$
|^{5}I_{8}^{\prime}\rangle = 0.9710 |^{5}I\rangle - 0.2086 |^{3}K_{2}\rangle + 0.1089 |^{3}K_{1}\rangle + \cdots,
$$
  
(5)  

$$
|^{5}I_{7}^{\prime}\rangle = 0.9871 |^{5}I\rangle - 0.1367 |^{3}K_{2}\rangle + 0.0674 |^{3}K_{1}\rangle + \cdots,
$$

where the subscript on the  ${}^{3}K$  basis states is the same as that employed by Nielson and Koster<sup>13</sup> to distinguish between the two  ${}^3K$  terms of  $f^4$ . These truncated eigenvectors are 99.8% complete.

#### B. Comparison of Experimental and Theoretical Values of  $g_I$

As may be seen from a comparison of Tables III and IV, the values obtained for  $g_J$  in the states  ${}^{5}I_{8,7}$  are independent, within experimental error, of which isotope is used for the measurement. The  $g_J$  values given in Table V combine the information of Tables III and IV for the  $^{5}I_{8,7,6}$  states. The calculated  $g$  values of Conway and Wybourne<sup>12</sup> are closer to the experimental values than are those of Judd and Lindgren.<sup>11</sup> Although Conway and Wybourne's values include the relativistic and diamagnetic correction only for the case of the  ${}^{5}I_{8}$  ground state, the corresponding corrections for the  $^{5}I_{7,6}$ 

states may be taken from the calculation of Judd and Lindgren. Table V compares the experimental values with those calculated by Conway and Wybourne after including the effects of these corrections. It can be seen that the difference between the observed and calculated values is extremely small for the  ${}^{5}I_{8,7}$  states. The larger difference for the  ${}^{5}I_{6}$  state may indicate that the  ${}^{5}I_{6}$  eigenvector is less accurate than those for  $^{5}I_{8,7}$ .

Table III also lists the observed  $g_J$  value for a fourth very weakly populated state. The identification of this state as the level classified  $4f^95d6s^2$ .  $J = 8$  at 7565 cm<sup>-1</sup> by Conway<sup>10</sup> depends on (a) its observed intensity relative to that of the others and (b) the very close correspondence between the measured value  $g_J = 1.35246(5)$  and the value obtained optically by Conway.<sup>10</sup> The value of  $J$  is not determined in the present work on even-even isotopes. The lifetime of this state cannot be appreciably shorter than the 2-msec mean transit time for Dy atoms to traverse the atomic-beam apparatus. No calculations for the  $g<sub>J</sub>$  value of this state have been made.

# C. Hyperfine Interaction

Hyperfine-interaction constants  $A$  and  $B$  have been measured for two atomic states, and it is of interest to compare them with theory. Examination of the Hamiltonian of Eq. (3) shows, however, that it treats  $A$  and  $B$  for any state simply as empirical parameters. A more fundamental approach to the theory of the hyperfine interaction is therefore required if one desires to correlate the observed values of the hyperfine-interaction constants with the structure of the atomic and nuclear states involved.

It has been shown<sup>14</sup> that for atoms with only one partially filled electron shell  $nl$  containing N equivalent electrons, the magnetic-dipole hyperfine interaction is characterized by the Hamiltonian

$$
\mathcal{K}_{\text{hfs}}\left(M\,1\right) = \sum_{i=1}^{N} \left[a^{01}\vec{1}_{i} - 10^{1/2}a^{12}(\vec{s} \times \vec{C}^{(2)})_{i}^{(1)} + a^{10}\vec{s}_{i}\right] \cdot \vec{1} \tag{6}
$$

TABLE V. Values of  $g_J$  for the  $4f^{10}6s^2\,5I_{8,7,6}$  states of Dy I. The observed values (second column) are compared with the values calculated by Conway and Wybourne (Ref. 12) in the fourth column, and with the  $LS$  limit in the right-hand column. Each of the theoretical values has been corrected for relativistic and diamagnetic effects. The correction for  ${}^{5}I_{8}$  was made in Ref. 12, and that for  ${}^5\!I_{7,\,6}$  is made by applying the calculated corrections of Ref. 11 to the uncorrected values of Ref. 12.

Atomic	Value of $g_J$			
state		Observed Calculated		$g \, g^{obs} - g \, g^{calc} g \, g^{obs} - g_J(LS)$
	1,24160(3)	1.24144	0.00016	$-0.00898$
$\frac{5I_8}{5I_7}$	1.17346(3)	1.17335	0.00011	$-0.00553$
$^{5}I_{6}$	1,07155(5)	1.07092	0.00063	$-0.00004$

$$
a_{n l} = 2 \mu_{\beta} \mu_{N} \left( \mu_{I} / I \right) \left\langle r^{-3} \right\rangle_{n l} \tag{7}
$$

in the nonrelativistic limit. Here,  $\mu_{\beta}$  and  $\mu_N$  are the Bohr and nuclear magnetons, respectively, and  $\mu_I$  is the nuclear magnetic-dipole moment. Under the same assumptions,  $a^{10}$  approaches zero. Configuration interaction does not normally introduc much difference between  $a^{01}$  and  $a^{12}$ , but it does lead (principally through those types of configuration interaction more commonly referred to as "core polarization") to a nonzero value for  $a^{10}$ . Values of  $a^{01}/a_{n1}$ ,  $a^{12}/a_{n1}$ , and  $a^{10}/a_{n1}$  due to relativistic effects alone may be calculated approximately asshown in the appendix of Ref. 9, in which the required relativistic radial integrals are approximated by the Casimir factors.

The electric-quadrupole interaction can be written,  $^{15}$  in analogy to Eq. (6), as

1O

$$
\mathcal{E}_{\text{hfs}}(E2)
$$
\n
$$
= \frac{r_n^2}{r_e^3} e^2 \vec{C}_n^{(2)} \cdot \sum_{i=1}^N \left[ \left( \frac{2l(l+1)(2l+1)}{(2l-1)(2l+3)} \right)^{1/2} \frac{b^{02}}{b_{n1}} \vec{U}_i^{(02)2} + \left( \frac{3}{10} \right)^{1/2} \frac{b^{13}}{b_{n1}} \vec{U}_i^{(11)2} \right],
$$

where the  $\vec{U}^{(k_s, k_l)K}$  are the unit double tensor operators defined by Sandars and Beck.<sup>14</sup> The electricquadrupole moment Q of the nucleus enters through the relations<sup>14</sup>

$$
e\gamma_n^2 \vec{C}_n^{(2)} = \vec{T}_n^{(2)},
$$
  

$$
\langle II | T_n^{(2)} | II \rangle = \frac{1}{2} eQ.
$$
 (9)

In the nonrelativistic limit,  $b^{\mathsf{02}}$  approaches the value

$$
b_{nl} = e^2 \, Q \left\langle r^{-3} \right\rangle_{nl} \tag{10}
$$

and  $b^{13}$  and  $b^{11}$  approach zero. Relativistic values of  $b^{02}/b_{n1}$ ,  $b^{13}/b_{n1}$ , and  $b^{11}/b_{n1}$  may be obtaine from Eqs. (15) of Ref. 15.

# D. Theoretica1 Expressions for the Hyperfine-Interaction Constants <sup>A</sup> and 8

The expression for the matrix element of  $\mathcal{K}_{\rm nfs}(M1)$ has been given by Childs, <sup>16</sup> and that for  $\mathcal{K}_{\text{hfs}}(E2)$  by Eq. (13) of Ref. 15. If these expressions for the matrix elements between LS basis states of  $l^N$  are compared with Eq. (3) of this paper, expressions for the quantities  $A_J(aSL, a'S'L')$  and  $B_J(aSL, a'S'L')$ can be extracted. These quantities, which may be regarded as the generalized  $A$  or  $B$  values taken between the primed and unprimed  $LS$  states, are

$$
A_J(aSL, a'S'L') = (2 - g_J^*) \delta(aSL, a'S'L')a^{01} + \left(\frac{30(2J+1)}{J(J+1)}\right)^{1/2} \left(\frac{l(l+1)(2l+1)}{(2l-1)(2l+3)}\right)^{1/2}
$$

$$
\times \langle l^N a SL || V^{(12)} || l^N a' S' L' \rangle \begin{cases} S & S' & 1 \\ L & L' & 2 \\ J & J & 1 \end{cases} a^{12} + (g^*_{J} - 1) \delta(aSL, a'S'L') a^{10} \tag{11}
$$

$$
B_{J}(aSL, a'S'L') = \left(\frac{4J(2J+1)(2J-1)}{(J+1)(2J+3)}\right)^{1/2} \left[ (-1)^{S+L'+J} \delta(S, S') \left\{\begin{array}{cc} J & J & 2 \\ L' & L & S \end{array}\right\} \langle l^N aSL || U^{(2)} || l^N a'S'L' \rangle
$$

 $(8)$ 

$$
\times \left( \frac{l(l+1)(2l+1)}{(2l-1)(2l+3)} \right)^{1/2} b^{02} + \left\{ L L' \frac{1}{3} \right\} \langle l^N a S L || V^{(13)} || l^N a' S' L' \rangle b^{13} + \left\{ L L' \frac{1}{J} \right\} \langle l^N a S L || V^{(11)} || l^N a' S' L' \rangle b^{11} \bigg],
$$
\n(12)

where  $g_{J}^{*}$  is the Landé value of the g factor (without the Schwinger correction). If in these expressions we put  $aSL = a'S'L'$ , the result gives the A sions we put  $a3L - a \cdot 3L$ , the result gives<br>or *B* value for the *LS*-limit state  $\frac{1}{s} \frac{1}{s} \frac{1}{s}$ .

If Eqs. (11) and (12) are used together with the eigenvectors of Eqs. (5), one obtains theoretical expressions for the A and B values of the  $4f^{10}6s^2$  ${}^{5}I_{8}$ <sup>'</sup> and  ${}^{5}I_{7}$ <sup>'</sup> states of the Dy atom. [The primes are used, as in Eq. (5), to denote the real state of the atom; the  $LS$  basis states are unprimed. In the atom; the LS basis<br>this way it is found that

$$
A({}^{5}I_{8}^{\prime}) = 0.755582a^{01} - 0.010459a^{12} + 0.242632a^{10},
$$
  

$$
A({}^{5}I_{7}^{\prime}) = 0.823187a^{01} - 0.007692a^{12} + 0.174408a^{10},
$$
 (13)

$$
B({}^{5}I_{8}^{\prime}) = 0.247563b^{02} - 0.042957b^{13} - 0.184908b^{11},
$$
  

$$
B({}^{5}I_{7}^{\prime}) = 0.225710b^{02} + 0.005387b^{13} - 0.137173b^{11},
$$

where the quantities  $a^{k_s, k_l}$  and  $b^{k_s, k_l}$  are as yet unknown. If the effects of configuration interaction are ignored, they may be related to the appropriate relativistic radial integrals according to the theory given by Sandars and Beck.<sup>14</sup> Even without these integrals, the ratios  $a_k^{ks, k_l}/a_{n_l}$  and  $b^{ks, k_l}/b_{n_l}$  may be evaluated (again ignoring configuration-interaction effects) by the procedures of Refs. 9 and 15 in which the Casimir factors<sup>17</sup> are used. When this is done, taking<sup>18</sup>  $Z_{\text{eff}} = Z - 35 = 31$  for the 4f electron shell of Dy, it is found that

$$
A^{\{5\}}_a{}' = 0.749240 a_{4f} ,
$$
  
 
$$
A^{\{5\}}_7{}' = 0.820339 a_{4f} ,
$$
 (15)

B( Is) =0. 250531b«, 

$$
B({}^{5}I_{7}^{\prime})=0.229887b_{4f},
$$

where  $a_{4f}$  and  $b_{4f}$  are defined by Eqs. (7) and (10). These expressions take account of intermediate coupling and of relativistic effects, but ignore the effects of configuration interaction. Equations (16) will be changed by the presence of configuration interaction only to the extent that the value used for  $b_{4f}$  may be slightly altered. In the magnetic-dipole hyperfine interaction, the principal form of configuration interaction is core polarization, and it is known<sup>19</sup> that it may be represented for each basis state by a term  $P(\overline{I} \cdot \overline{S})$  in the Hamiltonian. Since this term has precisely the tensor form of the last term of the dipole Hamiltonian, the effects of core polarization on the  ${}^{5}I_{8}{}'$  and  ${}^{5}I_{7}{}'$  states in intermediate coupling may be taken into account by adding to Eq. (15) a term having the same  $J$  dependence as the last term in Eq.  $(13)$ . We may then write

$$
A^{\{5_I\}}_s{}'
$$
 = 0. 749240 $a_{4f}$  + 0. 242632P,  

$$
A^{\{5_I\}}_t{}'
$$
 = 0. 820339 $a_{4f}$  + 0. 174408P, (17)

where P is proportional to  $\mu_I/I$  and to the spin density at the nucleus. The quantity  $P$  is usually very much less than  $a_{4f}$  for  $4f$  electrons. It may be mentioned that the coefficients appearing in the final expressions for the A and B values [Eqs. (16) and  $(17)$  are within 6% of those that would have been found if the impurities of Eqs. (5) and relativity had been ignored (i.e., in the nonrelativist  $LS$  limit).

#### E. Signs of the Hyperfine-Interaction Constants

Since it is expected that  $P \ll a_{4f}$ , it follows from Eqs. (17) and (7) that the signs of the  $A$  values for the  ${}^{5}I_{8}$  and  ${}^{5}I_{7}$  states will be the same as the sign of  $a_{4f}$  and consequently the same as that of  $\mu_{I}$  for the isotope considered. Similarly, from Eqs. (16) and  $(10)$ , the signs of the B values of both states should be the same as that of  $b_{4f}$  and of Q. Since  $\mu_I(Dy^{161})$  $(0.6, \mu_I(Dy^{163}) > 0, \frac{Q(Dy^{161}) > 0}{P_I(Dy^{163}) > 0, \frac{Q(Dy^{163}) > 0}{P_I(Dy^{163}) > 0, \frac{Q(Dy^{163})}{P_I(Dy^{163}) > 0, \frac{Q(Dy^{163})}{P_I(Dy^{163$ is expected that  $A(Dy^{163})$ ,  $B(Dy^{163})$ , and  $B(Dy^{161})$  will be positive, and that  $A(Dy^{161})$  will be negative. Experimentally, it is found that  $A/B < 0$  for  $Dy^{161}$  and  $A/B > 0$  for Dy<sup>163</sup> as expected. For these reasons, it is assumed that  $A(Dy^{161}) < 0$  and  $A(Dy^{163}) > 0$ ; these signs were not measured.

#### F. Experimental Values of the Hyperfine-Interaction Constants  $A$ ,  $B$ , and  $C$

The final experimental values of the magneticdipole, electric-quadrupole, and magnetic-octupole hyperfine-interaction constants  $A$ ,  $B$ , and  $C$  are given on the right-hand side in Table IV for the  ${}^{5}I_{8}$  and  ${}^{5}I_{7}$ hyperfine-interaction constants A, B, and C are given<br>on the right-hand side in Table IV for the  ${}^{5}I_{8}$  and  ${}^{5}I_{7}$ <br>atomic states of Dy<sup>161,163</sup>. Various ratios formed from the dipole and quadrupole constants are displayed in Table VI. The upper section shows that the  $A$  and  $B$  values measured for the two atomic states are in the same ratio (within experimental error) for both isotopes. The lower section shows that the values measured for the two isotopes are in the same ratio (within experimental error) for

TABLE VI. Comparison of ratios of observed A values and of observed  $B$  values. The upper section shows that the ratios of values for the two atomic states are the same (within experimental error) for both isotopes. The lower section shows that the ratios of values for the two isotopes are the same (within experimental error) for both atomic states. The uncertainties quoted are for two standard deviations.

Ratio	$Dy^{161}$	$\mathrm{Dy}^{163}$
$A\,({}^5I_8)/A\,({}^5I_7)$	0.91674(2)	0.91674(2)
$B({}^5\!I_8)/B({}^5\!I_7)$	1.08105(8)	1,08105(7)
Ratio	$^{5}I_{8}$	$^{5}I_{7}$
$A({\rm Dy}^{163})/A({\rm Dy}^{161})$	$-1,40026(3)$	$-1,40026(3)$
$B({\rm Dy}^{163})/B({\rm Dy}^{161})$	1,056 15(6)	1,05614(9)

both atomic states. The uncertainties assigned to the ratios in Table VI follow from those of Table IV, i.e., they are based on two standard deviation for each measured value of  $A$  or  $B$ .

If the nuclear moments were exactly proportional to the hyperfine-interaction constants, i. e. , if there were no hyperfine anomaly, then the ratios in the lower section of Table VI would also be the ratios between the nuclear moments of the isotopes. Although it is usual to regard the hyperfine anomaly as vanishing for  $f$  electrons, the situation is complicated by polarization of the inner electron shells by the 4f electrons and by the extent to which nuclei of different size and shape  $(Dy^{161}$  and  $Dy^{163})$ see these polarizations differently. The ratios of the nuclear moments will be discussed further below.

The magnetic-octupole hyperfine-interaction constant C is given in Table IV for both the  $^{5\!}I_8$  and the  $I_7$  states of Dy<sup>161,163</sup> All are zero to within experimental error. As has been mentioned above, the effects of hyperfine interactions with other atomic states, which can give rise to pseudo-octupole interactions, have been explicitly taken into account; such effects were found to be very small.

#### G. Comparison of Theoretical and Experimental Hyperfine-Interaction Constants

In Sec. IIID, theoretical expressions were developed for the magnetic-dipole and electric-quadrupole hyperfine-interaction constants  $A$  and  $B$  in terms of the quantities  $a_{4f}$ , P, and  $b_{4f}$ . Experimental values for the same constants have also been given {Table IV). ln fitting the theoretical expressions to the measured values, "experimental" values are found for the quantities  $a_{4f}$ , P, and  $b_{4f}$ which may then be used, along with their definitions [Eqs. (7) and (10)), to evaluate the nuclear moments. Since  $a_{4f}$ ,  $b_{4f}$ , and P are expected to be proportional to the nuclear moments, different values will result for the two isotopes.

If the expressions for the magnetic-dipole hfs constants  $A$  of Eq. (17) are equated to the final experimental values at the right in Table IV, it is found that for a perfect fit

$$
a_{4f} \text{ (Dy}^{161)} = -153.450(9) \text{ MHz}, \tag{18}
$$

$$
P(Dy^{161}) = -5.195(33) \text{ MHz},
$$

$$
a_{4f} \text{ (Dy}^{163)} = +214.872(9) \text{ MHz},
$$
  
\n
$$
P(\text{Dy}^{163}) = +7.277(33) \text{ MHz}.
$$
 (19)

From these numbers it follows that

$$
a_{4f} \left( \text{Dy}^{163} \right) / a_{4f} \left( \text{Dy}^{161} \right) = -1.40027(10), \tag{20}
$$

$$
P(Dy^{163})/P(Dy^{161}) = -1.401(11). \tag{21}
$$

To the extent that the  $A$  values are proportional

to the nuclear dipole moments  $\mu_I$ , the two numbers on the right-hand sides of Eqs. {20) and (21) should be the same, and should be the ratio of the values of  $\mu_I$  for the isotopes Dy<sup>161,163</sup>. The values of P are not well determined because, as can be seen from substituting Eqs.  $(18)$  and  $(19)$  into  $(17)$ , only about 1% of A arises from the core-polarization contribution. Thus, if our treatment of the magnitude of core-polarization effects (the principal source of any hyperfine anomaly) is even crudely correct, it should be possible to give the ratio of  $\mu_I(Dy^{163}) / \mu_I(Dy^{161})$  to about 0.2%; i.e., from Eq.  $(20)$ ,

$$
\mu_I \left( \text{Dy}^{163} \right) / \mu_I \left( \text{Dy}^{161} \right) = -1.400(3). \tag{22}
$$

For the electric-quadrupole hyperfine interaction, one may equate the theoretical expressions for  $B$ [Eqs. (16)] to the final experimental values of Table IV. Since we have two equations in one unknown  $(b_{4f})$  for each isotope, there is a check on our selfconsistency and we obtain

$$
b_{4f}(Dy^{163}, {}^{5}I_{8}) = +4602 \text{ MHz},
$$
  
\n
$$
b_{4f}(Dy^{163}, {}^{5}I_{7}) = +4639 \text{ MHz},
$$
  
\n
$$
b_{4f}(Dy^{161}, {}^{5}I_{8}) = +4357 \text{ MHz},
$$
  
\n
$$
b_{4f}(Dy^{161}, {}^{5}I_{7}) = +4392 \text{ MHz}.
$$
  
\n(24)

The results are thus self-consistent to within  $0.8\%$ , and we may take the average as

$$
b_{4f} \text{(Dy}^{163)} = +4620(20) \text{ MHz},
$$
  
\n
$$
b_{4f} \text{(Dy}^{161)} = +4375(20) \text{ MHz}.
$$
 (25)

From Table VI, the ratio of the value of the  $B$ factor (in either the  $^{5}I_8$  or  $^{5}I_7$  atomic states) for the two isotopes is

$$
B(Dy^{163})/B(Dy^{161}) = +1.05615
$$
 (26)

with an uncertainty of less than 0. 01%. The ratio of the nuclear ground-state electric-quadrupole moments  $Q(Dy^{163})/Q(Dy^{161})$  should have the same value. The extent to which the ratio of the  $Q$ 's differs from that of the  $B$ 's may be regarded as a quadrupole hyperfine anomaly. Any such anomaly should be small.

#### H. Dipole and Quadrupole Moments of the Dy<sup>161,163</sup> Nuclear Ground States

An accurate value of the ratio between the nuclea dipole moments of the two isotopes  $Dy^{161,163}$  was givn the nuclear<br><sup>1,163</sup> was given in Eq. (22), and the ratio between the quadrupole moments should have the value given in Eq. (26), subject to correction for a possible quadrupole hyperfine anomaly.

It is also possible to evaluate the ratio between the dipole and quadrupole moment for each nucleus

$$
b_{n\,l} = e^2 \, Q' \, \langle r^{-3} \rangle_{n\,l} \quad , \tag{27}
$$

where a prime is placed on  $Q$  to indicate that what is involved is the apparent electric-quadrupole moment  $Q'$ , uncorrected for any possible shielding or antishielding due to distortions of inner shells. Sternheimer<sup>20</sup> expresses the relation between the true and apparent moments  $Q$  and  $Q'$ , respectively, as

$$
Q = Q'/(1 - R_{4f}) \t\t(28)
$$

and his estimate $^{21}$  of  $R_{n\,l}$  (the atomic shielding factor) for the 4f electron shell is

$$
R_{4f} = +0.1 \pm 0.05,
$$
 (29)

so that

$$
Q = (1, 11 \pm 0, 07) Q' . \tag{30}
$$

From Eqs. (7) and (27), we have

$$
\frac{Q}{\mu_I} = \frac{2\mu_B\mu_N}{e^2I} \frac{1}{1 - R_{4f}} \frac{\langle r^{-3}\rangle_{4f}^D}{\langle r^{-3}\rangle_{4f}^Q} \frac{b_{4f}}{a_{4f}} \quad , \tag{31}
$$

where  $I = \frac{5}{2}$  for both Dy<sup>161</sup> and Dy<sup>163</sup>, <sup>8</sup> and super scripts D and Q have been placed on  $\langle r^{-3} \rangle_{4f}$  to indicate whether it arises from the dipole or quadrupole hfs interaction. To the extent that (a) the Casimir factors used in taking account of both dipole and quadrupole relativistic effects are accurate, (b) that the dipole core polarization has been properly taken into account, and (c) that we take account of quadrupole inner-shell distortions by Eq. (28), the quantities  $\langle r^{-3}\rangle^D_{4f}$  and  $\langle r^{-3}\rangle^Q_{4f}$  should be the same. We may then write

$$
\frac{Q}{\mu_I} = (1, 11 \pm 0, 07) \frac{2\mu_B \mu_N}{e^2 I} \frac{b_{4f}}{a_{4f}} , \qquad (32)
$$

where the factor  $(1.11\pm0.07)$  is the Sternheimer correction. When the values of Eqs. (18), (19), and  $(25)$  are used, we obtain

$$
(Q/\mu_I)(Dy^{163}) = +3.9 \pm 0.2 b/\mu_N ,
$$
  
(Q/\mu\_I)(Dy^{161}) = -5.1 \pm 0.3 b/\mu\_N . (33)

Evaluation of the nuclear moments themselves from the observed values of the hyperfine-interaction constants is a more difficult problem. From the equations above,

$$
\mu_I = a_{4f} \frac{I}{2 \mu_\beta \mu_N} \frac{1}{\langle r^{-3} \rangle_{4f}} \quad , \tag{34}
$$

$$
Q = b_{4f} \frac{1}{e^{2}(1 - R_{4f})} \frac{1}{\langle r^{-3} \rangle_{4f}} \quad . \tag{35}
$$

The problem is thus reduced to the evaluation of  $\langle r^{-3} \rangle_{4f}$ . This quantity has been calculated<sup>22</sup> from three different sets of Hartree-Fock radial wave

functions with the results  $\langle r^{-3} \rangle_{4f} = 9.8, 9.9,$  and 10. 5 a. u. Although these values deviate from the average of 10.1 a.u. by only about  $\pm 4\%$ , the wave functions used were obtained from the single-configuration Hartree-Fock approach in each case. This method often appears to overestimate expectation values of radial integrals by  $10-30\%$ , presumably because it ignores the time the atom spends in other configurations.

Bleaney<sup>23</sup> has attempted to evaluate  $\langle r^{-3} \rangle_{4f}$  by examining the entire  $4f$  shell at once, using the available data from all sources. By comparing dipole hfs measurements in tripositive ions with measured values of  $\mu_I$  for those nuclei for which such measurements have been made, he has obtained an empirical curve for  $\langle r^{-3} \rangle_{4f}$  for all neutral 4f atoms. In this way, he obtains for Dy<sub>I</sub> the result

$$
\langle r^{-3} \rangle_{4f} = 8.70 \pm 0.17 \text{ a.u.}, \qquad (36)
$$

which is  $14\%$  below the average of the single-configuration Hartree-Pock results. If one uses this value in Eq. (34), one obtains

$$
\mu_I (Dy^{163}) = + 0.647(65) \mu_N ,\n\mu_I (Dy^{161}) = - 0.462(46) \mu_N .
$$
\n(37)

The uncertainty assigned here is  $10\%$ , although if the  $2\%$  uncertainty Bleaney assigns to his value of  $\langle r^{-3} \rangle_{4f}$  is accepted, then the uncertainty in Eqs. (37) is also 2%. These values of  $\mu_I$  are in good agreement with those given by Bleaney and by Munck, <sup>24</sup> as well as with those found by atomic-beam studies by Ebenhoh et  $al$ <sup>1</sup>. Similarly, from Eq. (35), we have

$$
Q(Dy^{163}) = +2.51(30) \text{ b},
$$
  
 
$$
Q(Dy^{161}) = +2.37(28) \text{ b},
$$
 (38)

where the uncertainty is increased to  $12\%$  to take account of the additional  $6\%$  uncertainty in the Sternheimer correction  $[Eq. (30)]$ . These values are in agreement with those of Ref. 1, but are about 65% larger than those extracted by Bleaney<sup>23</sup> from electron-spin resonance of paramagnetic salts.

#### IV. SUMMARY AND CONCLUSIONS

The eigenvectors of Eqs. (5), developed by Conway and Wybourne<sup>12</sup> appear to be in reasonable agreement with the observed  $g<sub>J</sub>$  values and hyperfine-interaction constants  $A$  and  $B$ , although the availability of data on more states of the  $5<sup>I</sup>$  multiplet would make possible a much more sensitive test. Core polarization is shown to make a relatively unimportant contribution to the dipole hfs.

Although various ratios between the nuclear moments of  $Dy^{161}$  and  $Dy^{163}$  can be evaluated from the hfs, uncertainty in our knowledge of  $\langle r^{-3} \rangle_{4f}$  precludes assignment of precise absolute values for the moments. It is planned, in a future experiment, to measure the nuclear magnetic-dipole moments of 'Dy<sup>161,163</sup> directly through the nuclear Zeeman interaction. The nuclear electric-quadrupole moments could then be evaluated to within about  $\pm 6\%$  from Eq. (33).

\*%'ork performed under the auspices of the U. S. Atomic Energy Commission.

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# PHYSICAL REVIEW A VOLUME 2, NUMBER 5

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# Calculations of  $3S-10S$  States of He<sup>†</sup>

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Nonrelativistic energies and mass-polarization shifts of 3S-10S states of He were calculated with 40- to 80-term Rayleigh-Ritz expansions in  $r_1$ ,  $r_2$ , and  $r_{12}$ . Pekeris's calculated values of relativistic shifts were used in making comparisons with experimental values. Except for  $8<sup>1</sup>S$ , the calculated ionization energies are less than the experimental values (in agreement with variational principle) by amounts ranging from  $0.01 \text{ cm}^{-1}$  upward

# INTRODUCTION

Low-lying 8 states of two-electron atoms have been calculated to very high precision, especially

by Pekeris<sup>1, 2</sup> and by Schwartz, <sup>3</sup> by use of extensive Rayleigh-Ritz calculations, in which the electron correlation is accounted for by inclusion of