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HYPERFINE STRUCTURE OF ERBIUM-169

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ABSTRACT

The hyperfine structure of radioactive Er^{169} ($T_{1/2} = 9.4$ days) has been studied in the $^3\text{H}_6$ electronic ground state by the atomic-beam magnetic-resonance method. The apparatus used was of sufficient accuracy to measure the nuclear dipole moment directly through its interaction with the external magnetic field. The results are $A = 725.46(31)$ Mc, $g_J = -1.16381(5)$, and $g_I = +5.55(27) \times 10^{-4}$, where A is the magnetic dipole interaction constant and the electronic and nuclear g factors, g_J and g_I , are given in units of Bohr magnetons. The nuclear magnetic moment inferred from g_I and corrected for diamagnetic shielding is $\mu_I = +0.513(25)$ nm. This value of μ_I is consistent with that obtained from A using the $\langle \frac{1}{r^3} \rangle$ value given by Lindgren.

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INTRODUCTION

About thirty-five nuclear moments in the rare earth region have been determined from paramagnetic-resonance and atomic-beam data. Because of the paucity of direct information about the moments, it has been necessary in most cases to infer their values from the measured interaction constants by means of theoretical calculations involving considerable uncertainty. Much of this uncertainty arises from the sensitivity of $\langle \frac{1}{r^3} \rangle$ to the form of the electronic wave function. In order to obtain information concerning the $\langle \frac{1}{r^3} \rangle$ values we have undertaken to measure, by atomic-beam magnetic resonance, the hyperfine-structure constant, A , and the magnetic moment, μ_I , of Er^{169} .

EXPERIMENTAL METHOD AND RESULTS

Prior work on erbium-169 had determined the ground-state spin ($I = 1/2$) and the electronic angular momentum ($J = 6$).¹ The hyperfine structure of such a system is indicated in Fig. 1, and the energy levels are described by the Breit-Rabi Hamiltonian:

$$\mathcal{H} = A \underline{I} \cdot \underline{J} - g_J \mu_0 \underline{J} \cdot \underline{H} - g_I \mu_0 \underline{I} \cdot \underline{H}$$

The effect of the term in g_I on the erbium transition frequencies is estimated to be a few parts in 10^5 , but is not negligible with an apparatus of sufficient precision. Our ability to determine g_I for erbium rests on the good line width of our apparatus and on the ability to form very stable erbium beams which give highly reproducible data with a good signal-to-noise ratio. A sample resonance curve is shown in Fig. 2.

Data were taken on the two transitions, which may be observed by the flop-in method and which are indicated in Fig. 1. The magnetic field was calibrated by observing the flop-in potassium resonance. It was found that, with this method of calibration, the pulsating magnetic field of the nearby Bevatron caused small frequency shifts. For that reason all our data were obtained when the Bevatron was off.

The best fit to our data was obtained by a least-squares calculation on the IBM 709. The parameters best fitting our data are: $A = 725.46(31)$ Mc, $g_J = -1.16381(5)$ and $g_I = 5.55(27) \times 10^{-4}$, where the error given for A and g_I is twice the standard deviation. Frequencies calculated by use of these parameters are compared with the observed frequencies in Table I. The observed g_I value must be increased by the factor 1.0078 to correct for diamagnetic shielding.² This gives the true nuclear moment $\mu_I = 0.513(25)$ nm.

DISCUSSION OF POSSIBLE ERRORS

We have investigated the possibility of there being contributions to the measured g_I value from other sources than the true nuclear moment. Let us write, for the nuclear moment term, $g_I(1+\alpha) \underline{I} \cdot \underline{H}$, where g_I is the true nuclear g factor and α arises from possible perturbations. The possible contributions to α that we have considered are (a) systematic errors, which cause the true magnetic field to be different from the measured field by an amount proportional to the field (such an error arises, for example, if the field seen by the calibrating isotope differs from that seen by the erbium); (b) Doppler shift; (c) mixing of the fine-structure levels of the 3H term by the hyperfine-structure interaction in such a way as to introduce a pseudo $\underline{I} \cdot \underline{H}$ term in the Hamiltonian.

We have found the first two effects to be completely negligible

(i. e. , $< 10^{-6}$). In addition we have calculated the fine-structure mixing and found the effect to be less than 1% .

The existence of errors nonlinear in the field would be reflected in the quality of the least-squares fit achieved, and such errors would contribute to the uncertainties quoted for the results.

MAGNETIC MOMENT INFERRED FROM A

The magnetic moment may be obtained from the measured interaction constant by use of the relation

$$\mu_I = -IJA / \langle H_z \rangle J, m_J$$

where $m_J = J$, and $\langle H_z \rangle$, the expectation value of the magnetic field at the nucleus, is given by

$$\langle H_z \rangle = -2\mu_0 \left\langle \frac{1}{r^3} \right\rangle \left\langle \sum_i (\ell_i - s_i - 3r_i \frac{(s_i \cdot r_i)}{r_i^2})_i \right\rangle .$$

If the ground configuration is assumed to be $(4f)^{12}$, states with $J = 6$ arise only from the terms 3H and 1I and the ground-state wave function is of the form $\psi = [1 - a^2]^{1/2} |^3H_6\rangle + a |^1I_6\rangle$. The value of a can be determined by diagonalizing the Coulomb and spin orbit energies for $J = 6$. The Coulomb energy is characterized by three Slater radial integrals, F_2 , F_4 , and F_6 , while the spin-orbit energy is characterized by the parameter a_{4f} . These have been reliably evaluated for erbium by Judd and Lindgren,³ and we use their results. We obtain for a the value -0.094. The contributions to $\langle \Sigma_i \rangle$ come from three terms:

$$\langle \Sigma_i \rangle = (1 - a^2) \langle ^3H_6 | \Sigma_i | ^3H_6 \rangle + 2a \langle ^3H_6 | \Sigma_i | ^1I_6 \rangle + a^2 \langle ^1I_6 | \Sigma_i | ^1I_6 \rangle .$$

The resultant value differs by about 1% from that obtained under the assumption of Russell-Saunders coupling (i. e. , $a = 0$).

There is disagreement in the literature concerning the correct value of $\langle \frac{1}{r^3} \rangle$. Using hydrogenic functions, Bleaney has derived values for

the triply ionized rare earths with an uncertainty of about 5%.⁴ Values have since been obtained by Judd and Lindgren, using modified hydrogenic functions, for both the triply ionized and neutral atoms.^{3, 5} These values differ from Bleaney's by about 15 to 25%, and are also estimated to be uncertain to about 5%. The most recently reported work is that of Freeman and Watson, who have made nonrelativistic Hartree-Fock calculations for rare earth ions.⁶ They report values lying within 5% of Bleaney's, but they conclude that rather substantial uncertainties are to be associated with the moments derived from any theoretical $\langle \frac{1}{r^3} \rangle$ value.

The effect of the admixing of configurations involving unpaired s electrons on the hyperfine fields of triply ionized rare earths has been investigated by Bleaney. He estimates that the correction for all rare earths is small, the maximum being about 6% for terbium. In particular, he quotes a value of $\pm 1.4\%$ for Er^{3+} . Lindgren believes that the effect should be even smaller for neutral rare earth atoms, and assigns it an error of 5% in his calculations.

If Lindgren's $\langle \frac{1}{r^3} \rangle$ value of 9.84 atomic units is used, we obtain $\mu_I = 0.504(50)$ nm for the moment inferred from A. The 10% uncertainty is assigned to cover the effects of configuration mixing and the quoted uncertainty in $\langle \frac{1}{r^3} \rangle$.

CONCLUSIONS

Recently, directly measured nuclear magnetic moments have been reported for Nd^{143} , Tm^{169} , and Yb^{171} .^{7,8,9} These moments are summarized in Table II along with the present result and the values inferred from hyperfine-structure data using the various $\langle \frac{1}{r^3} \rangle$'s. The $\langle \frac{1}{r^3} \rangle$ values of Lindgren appear to give reasonably good agreement with experiment for the heavier lanthanides, while the neodymium result is less conclusive and would seem to favor the work of Freeman and Watson. The good agreement achieved for the heavier lanthanides tends to substantiate the belief that the effects of configuration mixing are small. It should be borne in mind that the erbium result includes a correction for the breakdown in Russell-Saunders coupling.

The value of the Er^{169} moment can be compared to a predicted value of 0.7 based on the Nilsson nuclear wave functions.¹² We have assumed that the 101st neutron is characterized by the state $1/2^- [521]$ with the deformation $\delta = 0.3$.

FOOTNOTES AND REFERENCES

*This work was done under the auspices of the U. S. Atomic Energy Commission.

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Table I. Comparison of the observed frequencies
with the frequencies predicted from the Hamiltonian (in Mc)

$$\mathcal{H} = 725.46 \mathbf{I} \cdot \mathbf{J} + 1.1638 \mu_0 \mathbf{J} \cdot \mathbf{H} - 5.55 \times 10^{-4} \mu_0 \mathbf{I} \cdot \mathbf{H}.$$

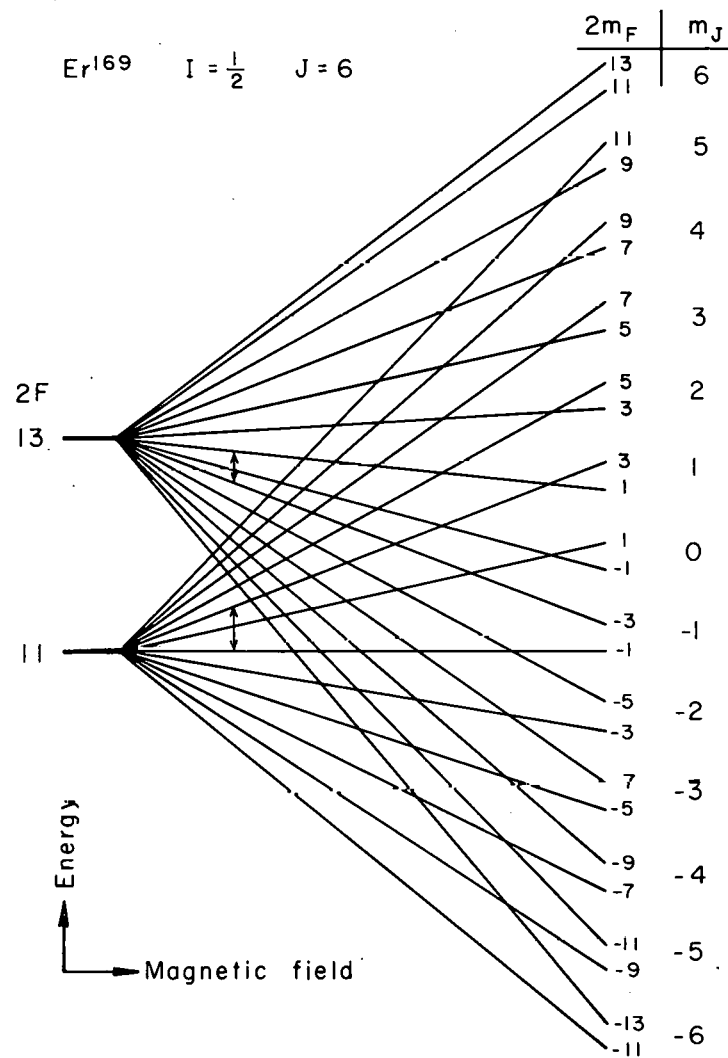
Field (gauss)	Predicted frequency (kc)	Observed frequency (kc)	Residual (kc)	Transition
467.595	704496.5	704499.0(4.0)	2.5	F = 13/2
504.329	760020.2	760020.0(4.0)	-0.2	F = 13/2
540.903	815336.0	815332.0(4.0)	-4.0	F = 13/2
540.903	815336.0	815336.0(2.4)	0.0	F = 13/2
613.698	925539.9	925533.0(4.0)	-6.9	F = 13/2
649.962	980996.1	980995.0(2.4)	-1.1	F = 13/2
686.158	1035387.7	1035388.0(2.4)	0.3	F = 13/2
722.298	1090232.4	1090237.0(2.4)	4.6	F = 13/2
722.298	1090232.4	1090235.0(4.0)	2.6	F = 13/2
758.390	1145044.8	1145044.0(2.4)	-0.8	F = 13/2
794.442	1199836.1	1199835.0(2.4)	-1.1	F = 13/2
196.279	344409.4	344411.0(5.6)	1.6	F = 11/2
317.719	557484.5	557480.0(5.6)	-4.5	F = 11/2
467.595	820293.9	820290.0(4.0)	-3.9	F = 11/2
467.595	820293.9	820292.0(8.0)	-1.9	F = 11/2
504.329	884665.7	884666.0(2.4)	0.3	F = 11/2
540.903	948736.7	948735.0(5.6)	-1.7	F = 11/2
577.351	1012564.7	1012567.0(2.4)	2.3	F = 11/2
613.698	1076191.7	1076190.0(2.4)	-1.7	F = 11/2
649.962	1139648.9	1139650.0(2.4)	1.1	F = 11/2
686.158	1202960.0	1202959.0(2.4)	-1.0	F = 11/2
722.298	1266142.9	1266143.0(2.4)	0.1	F = 11/2
794.442	1392177.4	1392180.0(4.0)	2.6	F = 11/2

Table II. Measured nuclear magnetic moments compared with those obtained from hyperfine-structure data using the $\langle \frac{1}{r^3} \rangle$ values of Bleaney, Lindgren, and Freeman and Watson.^{10, 11} (All in units of nuclear magnetons.)

	$\left[\text{Nd}^{143} \right] 3+$	Er^{169}	Tm^{169}	$\left[\text{Yb}^{171} \right] 3+$
Bleaney	-0.99	--	--	0.41
Lindgren	-1.26	0.504	-0.24	0.49
Freeman and Watson	-1.02	--	--	0.43
Measured	-1.076 (60)	0.513 (25)	-0.229 (3)	0.4930 (4)
References	7	--	8	9, 11

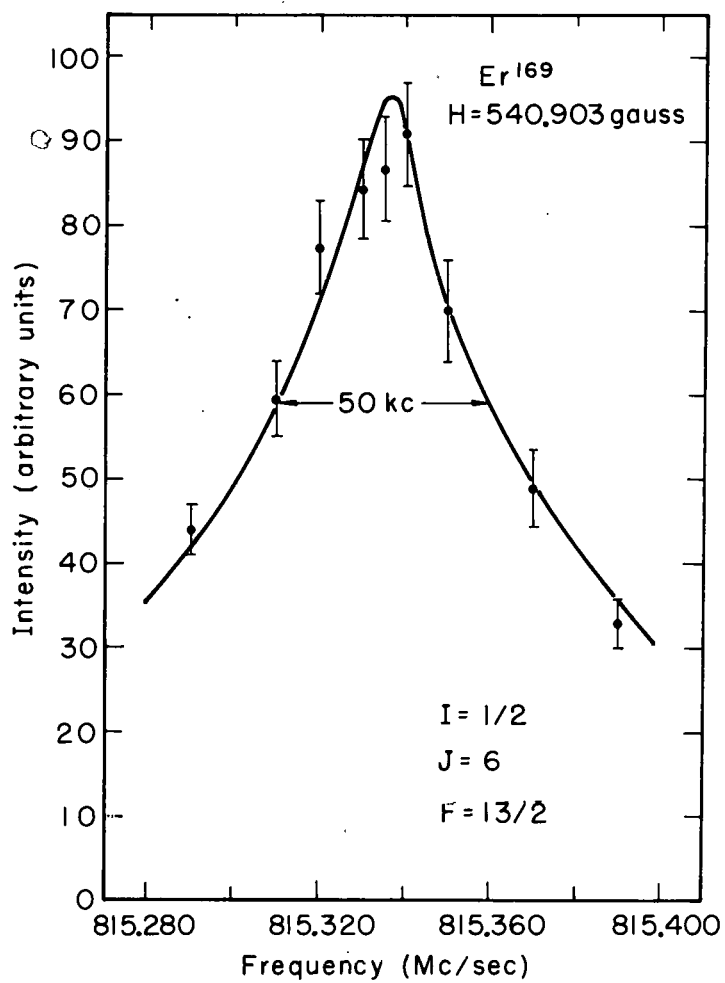
FIGURE LEGENDS

1. Hyperfine structure of the system $I = 1/2$, $J = 6$, showing the observable transitions.
2. Sample resonance in the $F = 13/2$ level.



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Fig. 1.



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Fig. 2.

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