$H_1 = 4.1$ mG $H_1 = 13$ mG $H_1 = 29$ mG

85°K

294°K

451°K

668°K

FIG. 3. Line shapes of F^{19} in $CaF_2:Sm^{2+}$ single crystal at different T and H_1.

rowed. This was not observed in the natural crystals.

Although it appears the Sm is responsible for the narrowing, it is not through a change in the static dipole $(I \cdot S)$ interaction because the linewidth of the synthetic and natural crystals are the same at room temperature indicating that the $(I \cdot S)$ contribution is small. The Sm^{3+} probably caused fluorine interstitials. O'Connor and Bostick[6] have shown that Sm^{3+} is charge compensated by an interstitial F^- ion in one of the vacant octahedral holes surrounding a cation site. The high-temperature F^{19} NMR line narrowing is thought to be due to a decrease in the nuclear dipole contribution to the linewidth caused by interstitial diffusion averaging.

For $CaF_2:Sm$ we plotted $\ln \Delta H$ against $(1/kT)$ from the $H_1 = 4.1$ mG curve and from the slope in the high-temperature region calculated an activation energy $E = 0.26$ eV. This is of the order for interstitial diffusion. The accuracy of this calculation could be improved if observations at higher temperature were available.

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Hyperfine Structure of Erbium-169*

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The hyperfine structure of radioactive Er^{169} ($T_{1/2} = 9.4$ days) has been studied in the $^3H_6$ 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/sec, $g_J = -1.16381(5)$, 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 $\langle 1/r^3 \rangle$ value given by Lindgren.

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 $\langle 1/r^3 \rangle$ to the form of the electronic wave function. In order to obtain information concerning the $\langle 1/r^3 \rangle$ 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 $(I = \frac{1}{2})$ and the electronic angular momentum $(J = 6)$.[1] The hyperfine structure of such a

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[1] A. Y. Cabezas, I. Lindgren, and R. Marrus, Phys. Rev. 122, 1796 (1961).
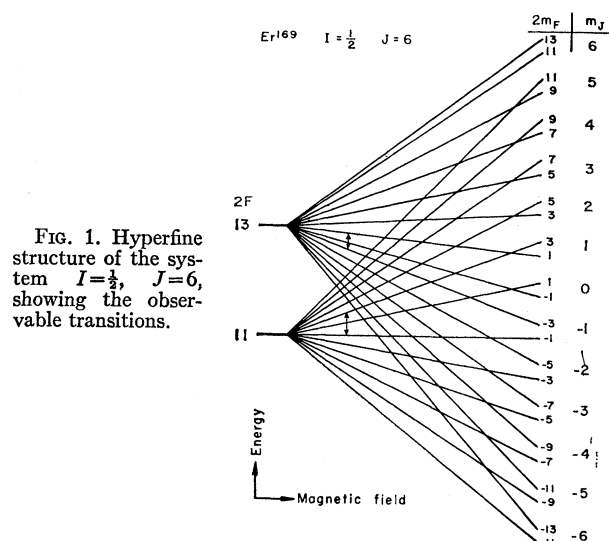
FIG. 1. Hyperfine structure of the system $I=\frac{1}{2}$, $J=6$, showing the observable transitions.

TABLE I. Comparison of the observed frequencies with the frequencies predicted from the Hamiltonian (in Mc/sec) $\mathcal{H}=725.46 I \cdot J+1.1638 \mu_0 J \cdot H-5.55 \times 10^{-4} \mu_0 I \cdot H$.

Field (G)	Predicted frequency (kc/sec)	Observed frequency (kc/sec)	Residual (kc/sec)	Transition
467.595	704 496.5	704 499.0(4.0)	2.5	$F=13/2$
504.329	760 020.2	760 020.0(4.0)	−0.2	$F=13/2$
540.903	815 336.0	815 332.0(4.0)	−4.0	$F=13/2$
540.903	815 336.0	815 336.0(2.4)	0.0	$F=13/2$
613.698	925 539.9	925 533.0(4.0)	−6.9	$F=13/2$
649.962	980 996.1	980 995.0(2.4)	−1.1	$F=13/2$
686.158	1 035 387.7	1 035 388.0(2.4)	0.3	$F=13/2$
722.298	1 090 232.4	1 090 237.0(2.4)	4.6	$F=13/2$
722.298	1 090 232.4	1 090 235.0(4.0)	2.6	$F=13/2$
758.390	1 145 044.8	1 145 044.0(2.4)	−0.8	$F=13/2$
794.442	1 199 836.1	1 199 835.0(2.4)	−1.1	$F=13/2$
196.279	344 409.4	344 411.0(5.6)	1.6	$F=11/2$
317.719	557 484.5	557 480.0(5.6)	−4.5	$F=11/2$
467.595	820 293.9	820 290.0(4.0)	−3.9	$F=11/2$
467.595	820 293.9	820 292.0(8.0)	−1.9	$F=11/2$
504.329	884 665.7	884 666.0(2.4)	0.3	$F=11/2$
540.903	948 736.7	948 735.0(5.6)	−1.7	$F=11/2$
577.351	1 012 564.7	1 012 567.0(2.4)	2.3	$F=11/2$
613.698	1 076 191.7	1 076 190.0(2.4)	−1.7	$F=11/2$
649.962	1 139 648.9	1 139 650.0(2.4)	1.1	$F=11/2$
686.158	1 202 960.0	1 202 959.0(2.4)	−1.0	$F=11/2$
722.298	1 266 142.9	1 266 143.0(2.4)	0.1	$F=11/2$
794.442	1 392 177.4	1 392 180.0(4.0)	2.6	$F=11/2$

system is indicated in Fig. 1, and the energy levels are described by the Breit-Rabi Hamiltonian:

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

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/sec, $g_J=-1.16381(5)$, and $g_I=5.55(27)\times10^{-4}$, 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, $g_I(1+\alpha)I \cdot H$, where g_I is the

[2] W. E. Lamb, Phys. Rev. **60**, 817 (1941).

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 $I \cdot H$ term in the Hamiltonian.

We have found the first two effects to be completely negligible (i.e., $<10^{-6}$). In addition, we have calculated
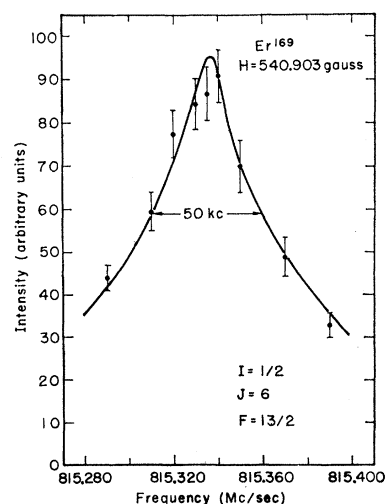

FIG. 2. Sample resonance in the $F=13/2$ level.

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 $\langle \mathbf{H} \rangle$, the expectation value of the magnetic field at the nucleus, is given by

$$\langle \mathbf{H} \rangle = -2\mu_0 \left\langle \frac{1}{r^3} \right\rangle \left\langle \sum_i \left(1 - \mathbf{s} - 3\mathbf{r}\frac{(\mathbf{s} \cdot \mathbf{r})}{r^2} \right)_i \right\rangle.$$

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 $\psi = [1-\alpha^2]^{1/2}|^3H_6\rangle + \alpha|^1I_6\rangle$. The value of α 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 α the value -0.094. The contributions to $\langle \sum_i \rangle$ come from three terms,

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

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

There is disagreement in the literature concerning the correct value of $\langle 1/r^3 \rangle$. Using hydrogenic functions, Bleaney had 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 $\langle 1/r^3 \rangle$ 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 $\pm1.4\%$ 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 $\langle 1/r^3 \rangle$ 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 $\langle 1/r^3 \rangle$.

CONCLUSIONS

Recently, directly measured nuclear magnetic moments have been reported for Nd^{143}, Tm^{169}, and Yb^{171}.[7-9] These moments are summarized in Table II along

TABLE II. Measured nuclear magnetic moments compared with those obtained from hyperfine-structure data using the $\langle 1/r^3 \rangle$ values of Bleaney, Lindgren, and Freeman and Watson.[a] (All in units of nuclear magnetons.)

	$(Nd^{143})^{3+}$	Er^{169}	Tm^{169}	$(Yb^{171})^{3+}$
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

[a] See Refs. 10 and 11.

with the present result and the values inferred from hyperfine-structure data using the various[10,11] $\langle 1/r^3 \rangle$'s. The $\langle 1/r^3 \rangle$ 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 $\frac{1}{2}-$ [521] with the deformation $\delta=0.3$.

[3] B. R. Judd and I. Lindgren, Phys. Rev. 122, 1802 (1961).
[4] B. Bleaney, Proc. Phys. Soc. (London) A68, 937 (1955).
[5] I. Lindgren, Nucl. Phys. 32, 151 (1962).
[6] A. J. Freeman and R. E. Watson, Phys. Rev. 127, 2058 (1962).

[7] D. Halford, Phys. Rev. 127, 1940 (1962).
[8] G. J. Ritter, Phys. Rev. 128, 2238 (1962).
[9] A. C. Gossard, V. Jaccarino, and J. H. Wernick, Bull. Am. Phys. Soc. 7, 482 (1962).
[10] The Nd^{143} inferences are based on Halford's hyperfine-structure result $g_n\langle 1/r^3 \rangle = (-11.88\pm0.12)\times10^{24}$ cm^{-3}.
[11] W. Low, Phys. Rev. 118, 1608 (1960). The Yb^{171} moments usually found in the literature are based on an earlier, less accurate, hyperfine-structure result [A. H. Cooke and J. G. Park, Proc. Phys. Soc. (London) A69, 282 (1956)]. The various inferred moments appear also to be inconsistent.
[12] S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 29, No. 16 (1955).