Electronic g Factors of the p^2 Configuration in Ge I and Sn I*

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Electronic g factors have been obtained by the atomic-beam magnetic-resonance technique for all $J\neq 0$ states arising from the p^2 electronic configuration in Ge I and Sn I. The results for the $^1D_2$, $^3P_2$, and $^3P_1$ states for Ge are 1.00639(8), 1.49458(9), 1.50111(7); and for Sn they are 1.05230(8), 1.44878(9), and 1.50110(7), respectively. The results are compared with intermediate-coupling calculations.

I. INTRODUCTION

THE normal electronic configuration of the group-IV elements C, Si, Ge, Sn, and Pb is ns^2np^2. Of the terms which can arise from this configuration ($^1S_0$,$^1D_2$,$^3P_{0,1,2}$) the $^1D_2$ and $^3P_{1,2}$ have measurable g factors. The present investigation was intended to make these measurements for Ge and Sn.

The experiment was performed with an atomic-beam magnetic-resonance apparatus equipped with an electron-bombardment universal detector. The stable, even-even isotopes (which amount to 92% in normal Ge and 83% in normal Sn) were used for the measurements. The Boltzmann distribution of atoms in the atomic beam provided sufficient population of the metastable $^1D_2$ and $^3P_{1,2}$ states. The g factors are obtained relative to $g_J(\mathrm{Ag};\,^2S_{1/2})$. The results are compared with the theory, and interesting evidence of the spin-orbit mixing of the $^1D_2$ and $^3P_2$ states is presented.

II. PROCEDURE

The atomic-beam magnetic-resonance apparatus and its associated electron-bombardment universal detector used in the present experiment have been described at some length previously,[1] as have the general principles of the Rabi-Zacharias,[2–4] technique.

A single graphite oven was used for all of the runs on Ge and Sn and also for the intercalibration of each element with Ag. The oven was normally reloaded with chunks of Ge or Sn each morning and then heated by electron bombardment until a beam was observed with the universal detector. The inhomogeneous magnetic fields were normally left on, and the oven was positioned laterally to maximize the intensity of the undeflected beam, most of which consisted of atoms in the $^3P_0$ ground state. A central obstacle was then positioned in order to reduce this contribution to the background counting rate. The homogeneous C field was then set and the applied rf frequency varied until resonances could be observed.

The experiment consisted of two parts: (1) the use of a beam of pure Ge (or Sn) for measurement of ratios of g factors of different states in the same element, and (2) the use of a beam from an oven loaded with both Ge (or Sn) and Ag for absolute calibration of one or more Ge (or Sn) g factors against the known g value of Ag.[5]

The resonance frequency for the state i is just the spacing of adjacent Zeeman states divided by Planck's constant h,

$$\nu(i)=g_J(i)\mu_0 H,$$

where $\nu(i)$ is in Mc/sec, H is the intensity of the homogeneous field in gauss, $\mu_0=1.399677$ Mc/G, and $g_J(i)$ is the g factor for the state i. In the first part of the experiment, the C field was held constant by observing the $^3P_1$ resonance (which lies highest in frequency and is strongest for both Ge and Sn) and the radio frequency was swept through the region of the resonance for the state being examined. Such a measurement for state i then gives

$$g_J(i)/g_J(^3P_1)=\nu(i)/\nu(^3P_1).$$

The resonance frequencies of the $^1D_2$ and $^3P_2$ states were measured relative to that of the $^3P_1$ state for both Ge and Sn at a number of values of the field in order to establish the linearity of the frequency-field relationship. (Other resonances, corresponding to hyperfine transitions in the odd isotopes Ge^{73}, Sn^{117}, and Sn^{119} in both the $^3P_1$ and $^3P_2$ atomic states were also observed, and their nonlinearity has lead to measurements[6] of their hyperfine interaction constants. This work will be published when completed.)

When these ratios of the g factors had been measured with sufficient precision, the oven was loaded with a mixture of Ge and Ag (or Sn and Ag), and the field measured absolutely by use of the Ag resonances as standards. The $(F,\ m_F\leftrightarrow F',\ m_{F'})=(1,\ 0\leftrightarrow 1,\ -1)$ transition was observed in both Ag^{107} and Ag^{109}, and the former was used for calibrating the C-field intensity. With the field held steady in this way, the frequencies of the $^3P_1$ and $^3P_2$ states in Ge, and of the $^3P_1$ state in Sn were measured. When observing

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[1] W. J. Childs, L. S. Goodman, and D. von Ehrenstein, Phys. Rev. **132**, 2128 (1963).
[2] I. I. Rabi, J. R. Zacharias, S. Millman, and P. Kusch, Phys. Rev. **53**, 318 (1938).
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[4] W. J. Childs, L. S. Goodman, and L. J. Kieffer, Phys. Rev. **120**, 2138 (1960).
[5] G. S. Hayne and H. G. Robinson, Bull. Am. Phys. Soc. **5**, 411 (1960).
[6] W. J. Childs and L. S. Goodman (to be published).

TABLE I. Excitation energies (Ref. 7) and Boltzmann factors for terms arising from the p^2 configuration in Ge I and Sn I

Atomic state	Ge I Excitation energy (cm^{-1})	Ge I $\exp(-\Delta E/kT)$	Sn I Excitation energy (cm^{-1})	Sn I $\exp(-\Delta E/kT)$
$^3P_0$	0.00	1.00	0.0	1.00
$^3P_1$	557.10	0.64	1691.8	0.22
$^3P_2$	1409.90	0.32	3427.7	0.047
$^1D_2$	7125.26	0.003	8613.0	0.0005
$^1S_0$	16367.14	very small	17162.6	very small

Ge(Sn) and Ag peaks alternately, the high voltage through which the ions were accelerated prior to mass analysis was switched back and forth between that required for Ge(Sn) and that for Ag. During operation with the Ge–Ag beam, the oven temperature was reduced somewhat to conserve the Ag.

With the ion source in operation, the vacuum in the vicinity of the detector was about $2\text{–}3\times10^{-8}$ mm Hg, and the background counting rate was about 6×10^5 sec^{-1}. The signal strength for the $^3P_{1,2}$ states was about 10^6 sec^{-1}, although in most cases this was reduced by factors of up to 50 in order to make certain of sharp, well-shaped resonance peaks. The counting rate of the $^1D_2$ state, which lies about 8000 cm^{-1} above the ground state in both Ge and Sn, was on the order of 10^3 sec^{-1}. The full width at one-half maximum for all the peaks observed was 25–45 kc/sec.

The precision attainable was limited by the fact that the resonances became widened and distorted in shape when the field was raised much above 100 G, even when the rf power was greatly reduced below that required for maximum signal strength.

III. THEORY

The ground-state electronic configuration for Ge I and Sn I is p^2. In Russell-Saunders coupling, this configuration gives rise to the terms $^1S_0$, $^1D_2$, and $^3P_{0,1,2}$, of which the $^3P_0$ lies lowest. The excitation energies of the states are given[7] in Table I. All of the excited states (of the p^2 configuration) are metastable, and some population of each is expected in the atomic beam. The relative signal strength expected from each is given by the Boltzmann factor; these are also given in Table I.

It is well known that the positions of these levels are distorted by the spin-orbit interaction; hence, intermediate-coupling calculations are required to fit the observed energy levels. The degree of intermediate coupling required is given by the ratio $x=\zeta/F_2$, where ζ measures the strength of the spin-orbit interaction and F_2 that of the repulsive electrostatic interaction. Thus, x is 0 for Russell-Saunders coupling (R.S.) and increases as jj coupling is approached.

The energies of the p^2 states in intermediate coupling are obtained by diagonalizing the matrix of the spin-orbit and electrostatic interactions. (The submatrix for $J=2$ is given below.) The expressions obtained[8] for the excitation energies are

$$E(^1S_0)-E(^3P_0)=F_2(2A),$$
$$E(^1D_2)-E(^3P_0)=F_2(-\tfrac{9}{2}+(3x/4)+A+B),$$
$$E(^3P_2)-E(^3P_0)=F_2(-\tfrac{9}{2}+(3x/4)+A-B),$$
$$E(^3P_1)-E(^3P_0)=F_2(-(15/2)+A),$$

where

$$x=\zeta/F_2,$$
$$A=\left(\frac{225}{4}+\frac{15}{2}x+\frac{9}{4}x^2\right)^{1/2},$$
$$B=\left(9-\frac{3}{2}x+\frac{9}{16}x^2\right)^{1/2}.$$

With four energy differences to be matched to the experimental values given in Table I, a number of different criteria can be used to optimize the values of the parameters ζ and F_2. Condon and Shortley,[8] for example, fit the first splitting and the mean of the next two exactly. We have found the least-squares fit to all four energy differences. The values required for the parameters are found to be

Ge I ($4p^2$): $\zeta=904.77$ cm^{-1}, $F_2=1016.11$ cm^{-1},

Sn I ($5p^2$): $\zeta=2171.50$ cm^{-1}, $F_2=920.27$ cm^{-1}.

Even with this choice of parameters, the fit is far from perfect, and is, in fact, 8 times as bad for the Sn as for the Ge. The impossibility of obtaining a "good" fit is interpreted as evidence of configuration interaction. Measurements of the magnetic-dipole hyperfine-interaction constants a in the $^3P_1$ state of odd-A Ge and Sn isotopes give further evidence of the importance of configuration interaction. In the absence of such an interaction, $|a(^3P_1)|$ should be 0, but it is found experimentally to be about 87 Mc/sec in Ge^{71},[9] 553 Mc/sec in Sn^{117},[6] and 579 Mc/sec in Sn^{119}.[6]

In the absence of configuration interaction, the g factors expected for the $^3P_{1,2}$ and $^1D_2$ states can be readily calculated. Because of the nature of the spin-orbit interaction, only states of the same J may interact, and thus the g factor of the $^3P_1$ state should be the

[7] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Std. Circ. 467 (U. S. Government Printing Office, Washington 25, D. C., August 1962), Vols. II, III.

[8] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1935), pp. 268–275.

[9] W. J. Childs and L. S. Goodman, Phys. Rev. **131**, 245 (1963).

TABLE II. Calculated intermediate-coupling g factors for the $p^2(^1D_2,^3P_2)$ metastable states of Ge I and Sn I.

Intermediate-coupling g factors	Ge I	Sn I
g_J(calc.) $^1D_2$	1.00619	1.04455
g_J(calc.) $^3P_2$	1.49495	1.45660

Russell-Saunders value of 1.50116. The two $J=2$ states, however, may mix with a resultant perturbation of their g factors. The values expected for pure Russell-Saunders coupling are

$$g_J(^1D_2)=1,$$
$$g_J(^3P_{2,1})=1.50116.$$

The matrix of the repulsive electrostatic and spin-orbit interactions is[8]

	$^1D_2$	$^3P_2$
$^1D_2$	F_2	$\zeta\frac{\sqrt{2}}{2}$
$^3P_2$	$\zeta\frac{\sqrt{2}}{2}$	$\frac{1}{2}\zeta-5F_2$.

The components a and b of the eigenvectors for the two states may be evaluated for the optimum values of ζ and F_2 given above. The results are found to be

	Ge I	Sn I
$\|a\|$	0.99379	0.95451
$\|b\|$	0.11124	0.29817.

The intermediate-coupling values of the g factors are then computed from the relations

$$g_J(^1D_2)=a^2(1.00000)+b^2(1.50116),$$
$$g_J(^3P_2)=a^2(1.50116)+b^2(1.00000),$$

where the numbers in parentheses are the Russell-Saunders values of the g factors. These equations lead to the results given in Table II.

IV. RESULTS AND CONCLUSIONS

Rough values for the g factors are known from spectroscopic data for all the states discussed in this report.[7] In addition, atomic-beam measurements have been made on the $^3P_1$ and $^3P_2$ states of Ge I.[9,10] These results are, within experimental error, in agreement with the present results. No precise measurements have been available previously for any of the g factors for Sn or for the $^1D_2$ state of Ge. The present experimental

TABLE III. Observations of transitions in Ge. The values given for the magnetic field H are determined from the Ag^{107}-Ge intercalibration run at 104.652 G. Numbers in parentheses give the uncertainty in the last figure.

H (G)	Calibration element	Calibration state	Calibration frequency (Mc/sec)	Isotope under study	State	Observed frequency (Mc/sec)
9.999	Ge	$^3P_1$	21.008(5)	Ge	$^1D_2$	14.078(10)
49.993	Ge	$^3P_1$	105.039(5)	Ge	$^3P_2$	104.586(7)
49.993	Ge	$^3P_1$	105.039(5)	Ge	$^1D_2$	70.420(7)
99.988	Ge	$^3P_1$	210.082(5)	Ge	$^3P_2$	209.170(8)
99.988	Ge	$^3P_1$	210.082(5)	Ge	$^1D_2$	140.845(9)
104.652	Ag^{107}	$F=1$	159.125(5)	Ge	$^3P_1$	219.881(8)
104.652	Ag^{107}	$F=1$	159.125(5)	Ge	$^3P_2$	218.925(9)
104.652	Ag^{107}	$F=1$	159.125(5)	Ag^{109}	$F=1$	157.480(7)

TABLE IV. Observations of transitions in Sn. The values given for the magnetic field H are determined from the Ag^{107}-Sn intercalibration run at 104.652 G. The numbers in parentheses give the uncertainty in the last figure.

H (G)	Calibration element	Calibration state	Calibration frequency (Mc/sec)	Isotope under study	State	Observed frequency (Mc/sec)
1.035	Sn	$^3P_1$	2.175(5)	Sn	$^3P_2$	2.103(9)
1.000	Sn	$^3P_1$	2.102(5)	Sn	$^1D_2$	1.481(9)
10.004	Sn	$^3P_1$	21.020(5)	Sn	$^1D_2$	14.731(11)
15.008	Sn	$^3P_1$	31.533(5)	Sn	$^3P_2$	30.439(6)
38.647	Sn	$^3P_1$	81.200(5)	Sn	$^1D_2$	56.925(7)
73.606	Sn	$^3P_1$	154.650(5)	Sn	$^1D_2$	108.413(5)
104.701	Sn	$^3P_1$	219.982(5)	Sn	$^3P_2$	212.315(7)
104.652	Ag^{107}	$F=1$	159.125(5)	Sn	$^3P_1$	219.879(8)
104.652	Ag^{107}	$F=1$	159.125(5)	Ag^{109}	$F=1$	157.481(7)

[10] I. Bender, thesis, Erstes Physikalisches Institut, University of Heidelberg (unpublished).

TABLE V. Present results for the g factors of $J\neq 0$ states in the p^2 configuration of Ge I and Sn I. The figures in parentheses give the uncertainty in the last figure. The departure of the experimental values from those predicted from Russell-Saunders coupling are also given. The equal and opposite perturbation of the g factors in the $J=2$ states is evident.

	Ge I		Sn I	
Atomic state	Measured g factor	$g_{exp}-g_{RS}$	Measured g factor	$g_{exp}-g_{RS}$
$^1D_2$	1.00639(8)	+0.00639(8)	1.05230(8)	+0.05230(8)
$^3P_2$	1.49458(9)	−0.00658(9)	1.44878(9)	−0.05238(9)
$^3P_1$	1.50111(7)	−0.00005(7)	1.50110(7)	−0.00006(7)

observations on Ge and Sn are listed in Tables III and IV, respectively. The present results are given in Table V, along with the departure of the measured values from the Russell-Saunders limits. These results are relative to[5]

$$g_J(\mathrm{Ag};\,^2S_{1/2})=2.002333(20).$$

It is immediately seen that the g factors found for the $^3P_1$ state in Ge and Sn agree with the Russell-Saunders values within experimental uncertainty. In addition, it is seen that the g factors of the $J=2$ states are highly perturbed, and the shift of the measured values from the Russell-Saunders limits for the two states are equal and opposite within experimental error, for both Ge and Sn. The shift is much larger for Sn, which is known to be further from Russell-Saunders coupling, than for Ge.

Table VI gives the differences between the measured g factors for the $J=2$ states and the values calculated from intermediate coupling. The calculation has accounted for about 96% of the shift in Ge, and 85% of that in Sn. This order of agreement, however, is not considered good; rather it is an indication of the importance of other effects. Because of the large size of the remaining discrepancy (6 parts in 10^3 for Sn), it is most likely to be caused by configuration interaction. Other evidence of such interactions has been given above.

TABLE VI. The differences between the experimental g factors and those calculated in intermediate coupling for the $p^2(^1D_2,^3P_2)$ states of Ge I and Sn I.

	Ge I	Sn I
$g_J(\mathrm{exp})-g_J(\mathrm{calc})\ ^1D_2$	+0.00020(8)	+0.00775(8)
$g_J(\mathrm{exp})-g_J(\mathrm{calc})\ ^3P_2$	−0.00037(9)	−0.00782(9)

In addition to the absolute values given above for the measured g factors, ratios of the g factors for the different states can be quoted. These results, which are independent of the Ag intercalibration, are

$$\frac{g_J(\mathrm{Ge};\,^3P_2)}{g_J(\mathrm{Ge};\,^3P_1)}=0.995656(45),$$

$$\frac{g_J(\mathrm{Ge};\,^1D_2)}{g_J(\mathrm{Ge};\,^3P_1)}=0.670429(46),$$

$$\frac{g_J(\mathrm{Sn};\,^3P_2)}{g_J(\mathrm{Sn};\,^3P_1)}=0.965147(39),$$

$$\frac{g_J(\mathrm{Sn};\,^1D_2)}{g_J(\mathrm{Sn};\,^3P_1)}=0.701022(42).$$

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