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OF Br^{80} AND $\text{Br}^{80\text{m}}$**

Berkeley, California

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HYPERFINE STRUCTURE AND NUCLEAR MOMENTS
OF Br^{80} AND Br^{80m}

Matthew B. White, Edgar Lipworth, and Seymour Alpert

October 14, 1963

Hyperfine Structure and Nuclear Moments
of Br^{80} and $\text{Br}^{80\text{m}}$ (*)

Matthew B. White,[†] Edgar Lipworth,[‡] and Seymour Alpert[§]

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ABSTRACT

The hyperfine-structure-interaction constants have been measured in the ground states of 18-min Br^{80} and 4.5-h $\text{Br}^{80\text{m}}$. The method used was that of atomic-beam radio-frequency spectroscopy with radioactive detection. The results are: $|a(\text{Br}^{80})| = 323.9(4)$ Mc/sec, $|b(\text{Br}^{80})| = 227.62(10)$ Mc/sec with $\frac{b}{a} < 0$; and $a(\text{Br}^{80\text{m}}) = 166.05(2)$ Mc/sec and $b(\text{Br}^{80\text{m}}) = -874.9(2)$ Mc/sec. The magnetic-dipole and electric-quadrupole moments of these isotopes were calculated from the measured interaction constants and known nuclear data for the stable Br isotopes; these moments are: $|\mu_I(\text{Br}^{80})| = 0.5138(6)$ nm, $|Q(\text{Br}^{80})| = 0.199(8)$ barn, $Q/\mu_I > 0$; $\mu_I(\text{Br}^{80\text{m}}) = 1.3170(6)$ nm $Q(\text{Br}^{80\text{m}}) = 0.76(3)$ barn. The μ_I 's are corrected for diamagnetic shielding and the Q 's are corrected for core polarization effects.

INTRODUCTION

The nuclei Br^{76} and Se^{75} possess large quadrupole moments, which might lead one to suspect the existence of incipient collective effects in this region of the periodic table.¹ The work described in this paper was initiated to further explore this possibility. Additionally, the isomeric relationship existing between Br^{80m} and Br^{80} is an attractive feature which invites comparison of the nuclear moments of these two isotopes.

EXPERIMENTAL METHOD

The experimental method used was standard atomic-beam magnetic-resonance spectroscopy with radioactive detection. The "flop-in" atomic-beam apparatus, and its allied equipment, was essentially the same as that used for previous work and has been described in detail by Garvin et al.² The main modification was the incorporation of a new "C" magnet with very accurately aligned pole tips. The uniformity of the C field was thus considerably improved; in the case of the K^{39} resonances used for magnetic-field calibration purposes, line widths at half maximum intensity remained around 40 kc for all fields from 0 to 500 G. This represents an improvement in accuracy over the original apparatus of about a factor of 50 at 500 G.

The Br^{80} and Br^{80m} were produced by bombarding 3- to 4-g lots of KBr crystals with thermal neutrons. Bombardment times ranged from 15 min to 4 h depending on the neutron flux used. Although the 18-min Br^{80} , which was produced directly by neutron bombardment, quickly decayed away, the decay of Br^{80m} to Br^{80} provided a continuous supply of this isotope, once secular equilibrium was attained. In this way, atomic beams containing an appreciable percentage of Br^{80} could be produced for periods of time ranging from 5 to 8 h.

Elemental bromine was obtained from the target material and dissociated into an atomic beam using the same chemical procedures and discharge tube described by Lipworth et al.⁴ The atoms were collected on freshly flamed platinum foils, which, though exhibiting only 80% of the collection efficiency of silver surfaces used earlier, were more uniform and consistent in their behavior.

THEORY

The general theory needed for the determination of spins, hyperfine structures, and nuclear moments of free atoms by the method of atomic-beam radio-frequency spectroscopy is given detailed discussion in two review articles,^{3,4} and application of the method to the particular case of bromine isotopes is fully treated by Garvin et al.⁵ Therefore, only the results of the theory that are necessary for an understanding of the measurements reported below are given here. The meanings of the various symbols are quite standard and are the same as those adopted by Garvin et al.

The Hamiltonian (in units of Mc/sec) is

$$\mathcal{H} = a \underline{I} \cdot \underline{J} + b \frac{3(\underline{I} \cdot \underline{J})^2 + 3/2 \underline{I} \cdot \underline{J} - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)} - g_J \frac{\mu_0 H}{h} J_z - g_I \frac{\mu_0 H}{h} I_z, \quad (1)$$

where

$$(\underline{I} \cdot \underline{J}) = 1/2 [F(F+1) - J(J+1) - I(I+1)],$$

a is the magnetic-dipole-interaction constant, and b is the electric-quadrupole-interaction constant.

If it is assumed that the ${}^2P_{3/2}$ ground state of Br arises from a pure $4s^2 4p^5$ configuration and that this ground state represents a case of pure L-S coupling,⁶ then the hyperfine-interaction constants are given (in units of Mc/sec) by the expressions^{5,7}

$$a = \frac{\mu_0^2}{h \times 10^6} \frac{\mu_I}{I} \frac{m}{M} \frac{2L(L+1)}{J(J+1)} \mathcal{F}(J, Z_i) \left\langle \frac{1}{r^3} \right\rangle \quad (2)$$

and

$$b = - \frac{e^2 Q}{h \times 10^6} \frac{2J-1}{2J+2} \mathcal{R}(L, J, Z_i) \left\langle \frac{1}{r^3} \right\rangle . \quad (3)$$

For two isotopes x and y we have, from Eq. (2),

$$\mu_I(x) = \mu_I(y) \frac{a(x)}{a(y)} \frac{I(x)}{I(y)} . \quad (4)$$

This equation can be used to calculate the unknown nuclear moment μ_I of an isotope from its "a" value, provided the μ_I and "a" value of another isotope of the element is available. This equation is valid under the assumption that the hyperfine anomaly can be ignored and would thus be expected to hold quite accurately⁶ for the ${}^2P_{3/2}$ state of Br. Alternatively, an explicit expression for μ_I can be obtained by eliminating the unknown $\left\langle \frac{1}{r^3} \right\rangle$ term from Eq. (2) if we use an expression given by Casimir⁷ for the fine-structure separation (in units of cm^{-1}). We then have

$$\delta = \frac{\mu_0^2}{hc} Z_i^2 (2L+1) \mathcal{C}(L, Z_i) \left\langle \frac{1}{r^3} \right\rangle , \quad (5)$$

where Z_i is the "effective charge" that the valence "hole" experiences while inside the electron core; Z_i can be estimated from optical spectroscopic data with an accuracy of about 5%. By solving Eq. (5) for $\left\langle \frac{1}{r^3} \right\rangle$ and by substituting the result into Eq. (2) yields (in units of the nuclear magneton)

$$\mu_I = I \frac{M}{m} \frac{a \times 10^6}{c} z_i \frac{J(J+1)(2L+1)}{2L(L+1)} \mathcal{H}/\mathcal{F} \quad (6)$$

To obtain an expression for Q involving only directly measurable quantities, either Eq. (2) or Eq. (5) can be used to eliminate the $\langle 1/r^3 \rangle$ term from Eq. (3). The use of Eq. (2) gives

$$Q = -4 \frac{m}{M} \frac{\mu_I}{I} \frac{\mu_0^2}{e^2} \mathcal{H}/\mathcal{R} \frac{L(L+1)}{J(2J-1)} b/a \quad (7)$$

DATA AND RESULTS

The hyperfine-interaction constants a and b were determined for Br^{80} and Br^{80m} by measuring the frequencies of 15 rf resonances for each isotope at magnetic fields ranging from 5.57 to 504.33 G. The "observable" flop-in transitions studied are shown in the schematic energy-level diagrams of Figs. 1 and 2 for Br^{80} and Br^{80m} , respectively. These diagrams, which show the correspondence between high- and low-field transitions, are drawn under the assumption that μ_I is positive and that the hyperfine levels exhibit normal ordering for both Br^{80} and Br^{80m} . In constructing the diagrams, we made use of the known nuclear spins $I(\text{Br}^{80}) = 1$ and $I(\text{Br}^{80m}) = 5$. Observable transitions (i. e., those for which m_J changes to $-m_J$ in the high-field limit) within the $F = I + J$ hyperfine level are designated by α , while those within the $F = I + J - 1$ level are labeled β . The resonance data were analyzed by using an improved version of the computer program described by Garvin et al.,⁵ which was modified for use on the IBM 7090 digital computer.

Figures 3 and 4 show some typical intermediate-field resonance curves traced out for Br^{80} and Br^{80m} , respectively. For both isotopes Tables I and II give: (a) a list of all frequencies at which resonances were observed, together with the uncertainties in these frequencies and the corresponding fields and

field uncertainties; (b) the best values of a and b obtained by the least-squares fit; (c) the frequency residuals using these values of a and b ; and (d) χ^2 (a quantity that measures the "goodness of fit.")

Only a and b were allowed to vary during the data-fitting process because of the high accuracy with which g_J and g_I^1 are known⁶ for Br^{79} and Br^{81} .

In Table I the values of a , b , χ^2 , and the frequency residuals are given where we assume both $g_I^1 > 0$ and $g_I^1 < 0$. Although the normal ordering of levels assumed in Fig. 1 is apparently verified, no conclusion can be drawn from the data collected concerning the sign of g_I^1 . Therefore, by taking the average of the results for these two cases and by doubling the errors quoted in Table I to give a 95% chance that the actual values lie inside our error limits, we have as the final results for Br^{80} ,

$$|a(\text{Br}^{80})| = 323.9 \pm 0.4 \text{ Mc/sec,}$$

and

$$|b(\text{Br}^{80})| = 227.62 \pm 0.10 \text{ Mc/sec,}$$

where $b/a < 0$. By using these results and the solution of Eq. (1) at $H=0$, one obtains for Br^{80} the zero-field hyperfine-structure separations

$$|\Delta\nu(5/2, 3/2)| = 5/2a + 5/4b = 525.2 \pm 1.2 \text{ Mc/sec}$$

and

$$|\Delta\nu(3/2, 1/2)| = 3/2a - 9/4b = 998.0 \pm 1.0 \text{ Mc/sec.}$$

In Table II, a , b , χ^2 , and the frequency residuals are given for $g_I^1 > 0$ only. That the sign of g_I^1 is positive and that the level ordering is normal for Br^{80m} was established both by trying to fit the data using a negative g_I^1 , and by starting g_I^1 with a negative value and then allowing it to vary freely while fitting the experimental data. In the first case, a value of $\chi^2 = 50.9$ was obtained as compared with $\chi^2 = 4.7$ given in Table II. In the second case, a positive value of g_I^1 consistent with that obtained using Eq. (4) was obtained. Doubling the

errors given in the table, we get for Br^{80m}

$$a(\text{Br}^{80m}) = 166.05 \pm 0.02 \text{ Mc/sec,}$$

$$b(\text{Br}^{80m}) = -87.7 \pm 0.2 \text{ Mc/sec,}$$

and

$$\Delta\nu(13/2, 11/2) = 13/2a + 13/20b = 510.62 \pm 0.25 \text{ Mc/sec}$$

and

$$\Delta\nu(11/2, 9/2) = 11/2a - 5/12b = 1277.80 \pm 0.18 \text{ Mc/sec.}$$

The nuclear magnetic dipole moments are calculated from Eq. (4) by using the a values given above, the a values of the stable Br isotopes measured by King and Jaccarino,⁶ and the corresponding μ_I 's tabulated by Walchli.⁹ When this is done, we obtain

$$|\mu_I(\text{Br}^{80})| = 0.5122(6) \text{ nm (uncorrected for diamagnetic shielding)}$$

and

$$\mu_I(\text{Br}^{80m}) = 1.3131(6) \text{ nm (uncorrected for diamagnetic shielding).}$$

If we multiply by the appropriate diamagnetic shielding factor tabulated by Kopfermann,¹⁰ we obtain the diamagnetically corrected moments

$$|\mu_I(\text{Br}^{80})| = 0.5138(6) \text{ nm (corrected)}$$

and

$$\mu_I(\text{Br}^{80m}) = 1.3170(6) \text{ nm (corrected).}$$

Barns and Smith¹¹ have recommended a value $Z_1 = 31$ for the effective charge seen by the valence hole in Br. When this value and the values of the a 's obtained above are substituted into Eq. (6), one finds

$$|\mu_I(\text{Br}^{80})|_{\text{calculated}} = 0.47 \text{ nm (uncorrected),}$$

and

$$\mu_I(\text{Br}^{80m})_{\text{calculated}} = 1.20 \text{ nm (uncorrected).}$$

These are in reasonable agreement with the preceding uncorrected values.

The nuclear quadrupole moments are obtained from Eq. (7). Use of the results given above, and the appropriate relativistic correction factors tabulated

by Kopfermann,¹⁰ yield

$$|Q(\text{Br}^{80})| = 0.191 \text{ barn (uncorrected)}$$

and

$$Q(\text{Br}^{80m}) = 0.73 \text{ barn (uncorrected).}$$

Multiplication of the above by the factor $C = 1.040$, as suggested by Sternheimer,¹² to account for electron-core polarization effects, gives for the corrected quadrupole moments

$$|Q(\text{Br}^{80})| = 0.199(8) \text{ barn (corrected)}$$

and

$$Q(\text{Br}^{80m}) = 0.76(3) \text{ barn (corrected).}$$

Because of the inaccuracies inherent in corrections of this kind, uncertainties equal to the Sternheimer corrections themselves have been assigned to the final values. Furthermore, even though the algebraic sign of $Q(\text{Br}^{80})$ is not determined by the experimental data, Eqs. (2) and (3), plus the relative signs of $a(\text{Br}^{80})$ and $b(\text{Br}^{80})$ given in Table I, indicate $Q(\text{Br}^{80})/\mu_I(\text{Br}^{80}) > 0$.

DISCUSSION

Both the independent-particle shell model given by Mayer et al.¹³ and the collective model by Bohr et al.,¹⁴ are able to account for the known spins and parities of the Br^{80} and Br^{80m} nuclei, as indicated below. Calculations based on neither nuclear model, however, give good quantitative agreement with the measured nuclear moments. Therefore, just as in the case of Br^{76} discussed by Lipworth et al., Br^{80} and Br^{80m} probably represent transition cases where neither very weak nor very strong coupling of the individual nucleons to the nuclear core exists.

Application of the Shell Model

In view of the fact that Br^{77} , Br^{79} , and Br^{81} all have spins $3/2$, while the last two have positive quadrupole moments,^{6,8} it seems safe to assume that

the proton configuration for Br isotopes is $[(p_{3/2})^3 (f_{5/2})^4]_{3/2}$, as suggested by Mayer and Jensen.¹³

The neutron configurations for Br^{80} and Br^{80m} can be chosen in such a way that (a) the spins are correctly predicted by use of one of the Brennan and Bernstein¹⁵ coupling rules, (b) the neutron configurations are the same as ones previously assigned to even-odd nuclei with valence neutrons lying in the same shell-model sublevel as those of the Br isotopes, (c) the positive parity of Br^{80} and the negative parity of Br^{80m} are properly accounted for,¹⁶ and (d) the relative signs of μ_I and Q for Br^{80} and the absolute signs of μ_I and Q for Br^{80m} are predicted correctly. These criteria lead to the unique shell-model configuration assignments in Table III.

As we said, neither of these configurations leads to accurate predictions of the nuclear moments. Calculations using "effective nucleon-gyromagnetic ratios" give the results shown in Table III. These possess the correct algebraic signs but are quantitatively far from the experimentally measured values.

Some known data pertaining to the odd-odd isotopes of Br as well as data¹⁶ pertaining to related even-odd isotopes of Se are given in Table IV. The results for Br^{76} and Br^{82} were obtained by Green et al.^{1,5} and the neutron configurations for these isotopes were also assigned by these authors. For Br^{76} , Br^{82} , and Br^{80} , the relative signs of μ_I and Q have been well established but the actual signs given in Table IV, although the most likely on the basis of the data, are not definitely known. From this table the correspondences between a given Se isotope and the Br isotope that has the same neutron configuration is quite clear. Two points are particularly noteworthy of mention:

(a) There is apparently a one-to-one correspondence in the order of neutron-level filling in Se and in Br. This indicates, as predicted by the shell model,¹³ that the presence of the odd-proton configuration has little effect on the neutron configuration.

(b) The difference in the signs of the magnetic moments (or at least the relative signs of μ_I and Q) of Br^{76} and Br^{80} , which at first sight seems surprising because of other similarities between these isotopes [e. g., $I(\text{Br}^{76}) = I(\text{Br}^{80})$; $|\mu(\text{Br}^{76})| \approx |\mu(\text{Br}^{80})|$; $|Q(\text{Br}^{76})| \approx |Q(\text{Br}^{80})|$], is reflected by a similar difference between Se^{75} and Se^{77} and is apparently due to radically different neutron configurations.

Also, the systematic trends in Table IV seem to support the configuration assignments and signs of nuclear moments given above for Br^{80} and Br^{80m} as well as those given for the other Br isotopes by other authors. In particular, the positive signs of μ_I and Q for Br^{82} seem very likely in view of the similarity exhibited between this isotope and Br^{80m} .

Application of the Collective Model

Even though the mass number of Br^{80} and Br^{80m} lies far outside the range where collective aspects of nuclear motion would be expected to be important,¹⁴ the possibility that collective effects might be significant is indicated by the low shell-model quadrupole-moment estimates in Table III, and by the apparent collective nature of the Br^{76} nucleus.¹

To decide upon collective-model configuration assignments for Br^{80} and Br^{80m} , one must derive appropriate values of the nuclear-deformation parameter δ from the measured quadrupole moments. In this way, one obtains $\delta(\text{Br}^{80}) = 0.24$ and $\delta(\text{Br}^{80m}) = 0.12$. That these values are so different probably reflects the inadequacy of a strong-coupling approximation.

Unique collective-model configurations emerge for both Br^{80} and Br^{80m} , if we take any value in the range $0.1 < \delta < 0.3$ as a possible value of δ and impose, on acceptable configurations, the conditions that the values (a) are plausible on the basis of the Nilsson-level filling diagrams,¹⁴ (b) give the correct spin values when the Gallagher and Moszkowski coupling rules are used,¹⁷ (c) give the

correct nuclear parities, and (d) account correctly for the relative signs of μ_I and Q for Br^{80} and the absolute signs of μ_I and Q for Br^{80m} . These configurations are given in Table III and are the same as those previously assigned by Gallagher and Moszkowski without knowledge of the nuclear moments. Calculations based on these configurations for any value of δ in the range mentioned above lead to μ_I values comparable in accuracy to those resulting from shell-model calculations.

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FOOTNOTES AND REFERENCES

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Table I. Br⁸⁰ resonance data and final results.

	<u>$g_I^1 > 0$</u>			<u>$g_I^1 < 0$</u>			
	$a = 323.77(8) \text{ Mc/sec}$ $b = -227.63(3) \text{ Mc/sec}$	}	$\chi^2 = 2.2$	$a = -324.01(8) \text{ Mc/sec}$ $b = 227.60(3) \text{ Mc/sec}$	}	$\chi^2 = 2.1$	
	Average of $g_I^1 > 0$ and $g_I^1 < 0$						
	$ a = 323.9(2) \text{ Mc/sec}$ $ b = 227.62(5) \text{ Mc/sec}$						
	}						
	$b/a < 0$						
Type of Resonance	ν_K (Mc/sec)	H (G)	ΔH (G)	ν_{Br} (Mc/sec)	$\Delta \nu_{Br}$ (Mc/sec)	Residuals (Mc/sec)	
						$g_I^1 > 0$	$g_I^1 < 0$
a	4.0	5.567	0.005	6.275	0.060	0.015	0.014
a	16.0	20.75	0.01	23.650	0.067	0.057	0.051
a	25.0	30.92	0.01	35.400	0.067	-0.010	-0.018
a	50.0	55.19	0.01	64.338	0.015	0.013	0.001
a	100.0	93.04	0.01	111.450	0.015	0.004	-0.011
β	4.0	5.567	0.005	7.620	0.067	-0.001	-0.002
β	16.0	20.75	0.01	28.400	0.083	-0.032	-0.037
β	25.0	30.92	0.01	42.400	0.033	0.003	-0.004
β	50.0	55.19	0.01	75.938	0.015	0.007	-0.005
β	100.0	93.04	0.01	129.145	0.015	0.005	-0.013
a	200.0	149.71	0.01	186.555	0.015	0.008	-0.002
a	400.0	238.621	0.008	314.238	0.020	-0.005	0.003
β	200.0	149.71	0.01	212.010	0.020	0.010	-0.014
β	400.0	238.621	0.008	352.270	0.020	0.015	-0.009
β	1100.0	504.329	0.007	834.740	0.015	-0.004	0.003

Table II. $\text{Br}^{80\text{m}}$ resonance data and final results

$$g_I > 0$$

$$\left. \begin{array}{l} a = 166.047(9) \text{ Mc/sec} \\ b = -874.9(1) \text{ Mc/sec} \end{array} \right\} \chi^2 = 4.7$$

Type of resonance	ν_K (Mc/sec)	H (G)	ΔH (G)	ν_{Br} (Mc/sec)	$\Delta \nu_{\text{Br}}$ (Mc/sec)	Residual (Mc/sec)
α	4.0	5.57	0.03	2.400	0.025	-0.029
α	8.0	10.87	0.03	4.800	0.020	0.000
α	16.0	20.75	0.05	9.400	0.025	0.016
α	32.0	38.24	0.03	18.000	0.020	-0.007
α	70.0	71.63	0.01	36.375	0.015	0.006
β	8.0	10.87	0.03	2.700	0.020	0.003
β	16.0	20.75	0.05	5.200	0.025	0.039
β	32.0	38.24	0.02	9.550	0.015	-0.001
β	70.0	71.63	0.01	18.150	0.015	-0.006
β	100.0	93.044	0.009	23.950	0.012	-0.005
α	200.0	149.714	0.008	88.838	0.023	0.013
α	400.0	238.62	0.01	161.710	0.010	-0.002
β	200.0	149.71	0.01	41.235	0.015	-0.001
β	399.988	238.62	0.02	77.277	0.010	0.009
β	1100.0	504.329	0.007	284.610	0.015	-0.002

Table III. Theoretical configuration and moments for Br⁸⁰ and Br^{80m}.

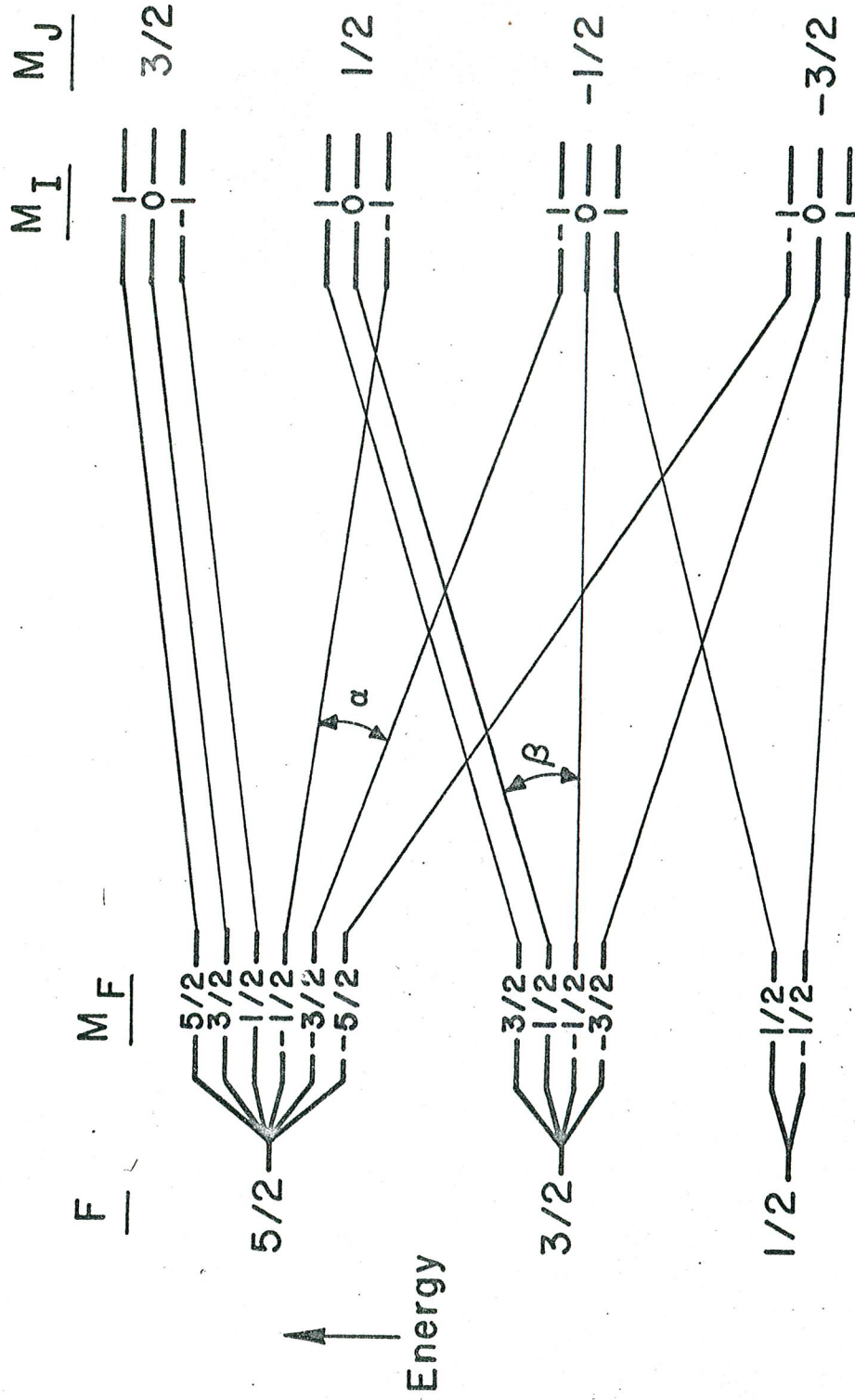
Model	Nuclide	Configuration		μ_I (nm)		Q (barns)	
		Proton	Neutron	Calc.	Meas.	Calc.	Meas.
Shell	Br ⁸⁰	$[(p_{3/2})^3(f_{5/2})^4]_{3/2}$	$[(p_{1/2})^1(g_{9/2})^6]_{1/2}$	1.84	0.51	0.93	0.20
	Br ^{80m}	$[(p_{3/2})^3(f_{5/2})^4]_{3/2}$	$[(p_{1/2})^0(g_{9/2})^7]_{7/2}$	1.20	1.32	0.20	0.76
Collective	Br ⁸⁰	$ 301 + \rangle$	$ 301 - \rangle$				
	Br ^{80m}	$ 301 + \rangle$	$ 413 + \rangle$				

Table IV. Some known data pertaining to odd-odd isotopes of Br and to even-odd isotopes of Se.

Neutron configuration	Even-odd nuclide	I	μ_I		Odd-odd nuclide	I	μ_I	
			(nm)	Q (barns)			(nm)	Q (barns)
$[(f_{5/2})^5]_{5/2}$	Se ⁷⁵	5/2	(0)	+1.1	Br ⁷⁶	1	(-0.55)	(+0.27)
$[(p_{1/2})^1(g_{9/2})^4]_{1/2}$	Se ⁷⁷	1/2	+0.53	<0.002	Br ⁸⁰	1	(+0.51)	(+0.20)
$[(g_{9/2})^7]_{7/2}$	Se ⁷⁹	7/2	-1.02	+0.9	Br ^{80m}	5	+1.32	+0.76
$[(g_{9/2})^7]_{7/2}$	Se ⁷⁹	7/2	-1.02	+0.9	Br ⁸²	5	(+1.63)	(+0.76)

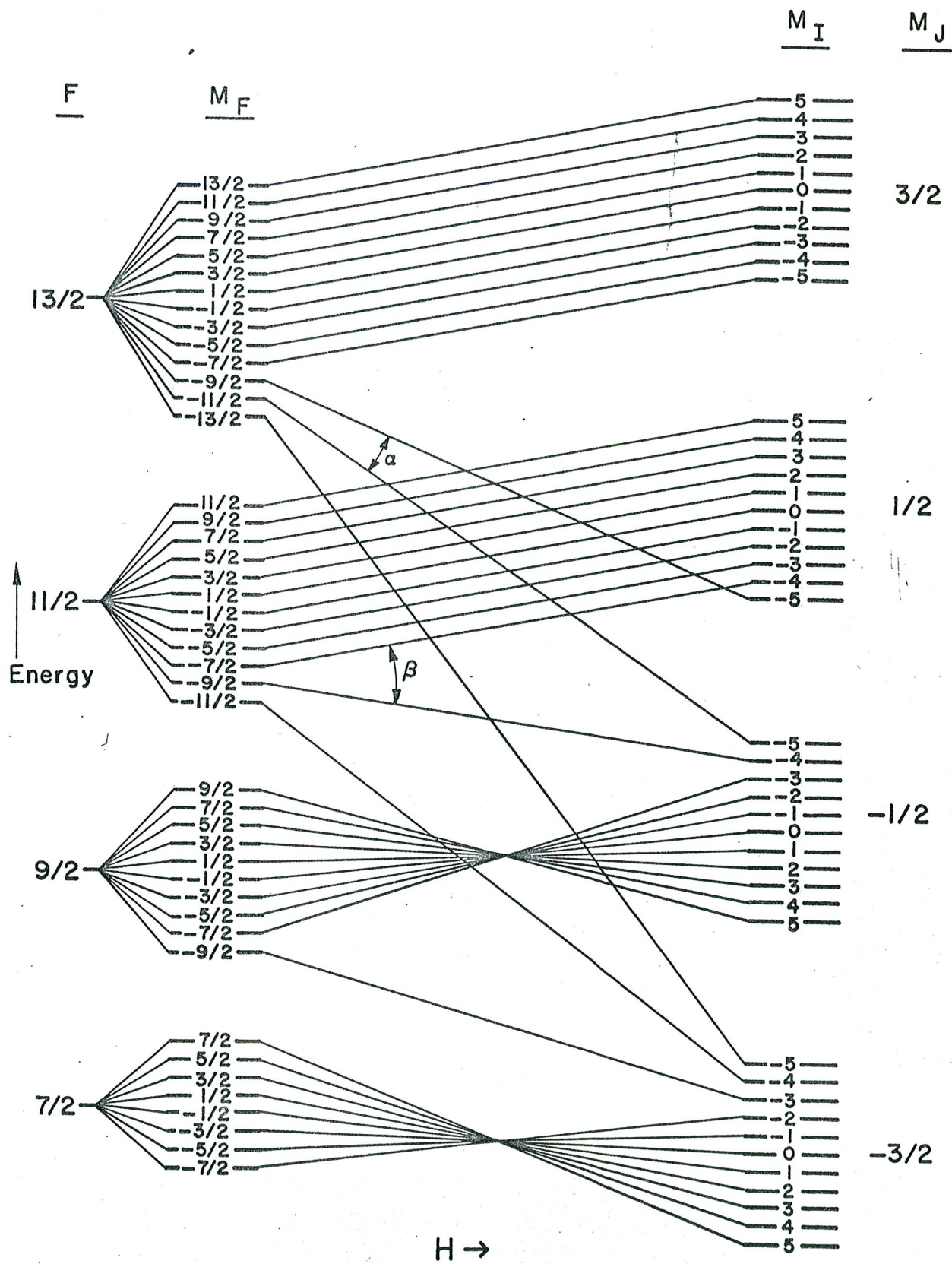
Figure Legends

- Fig. 1. Schematic energy-level diagram for Br^{80} ; $I = 1$, $J = 3/2$.
- Fig. 2. Schematic energy-level diagram for Br^{80m} ; $I = 5$, $J = 3/2$.
- Fig. 3. Intermediate-field resonance curves for Br^{80} .
- Fig. 4. Intermediate-field resonance curves for Br^{80m} .



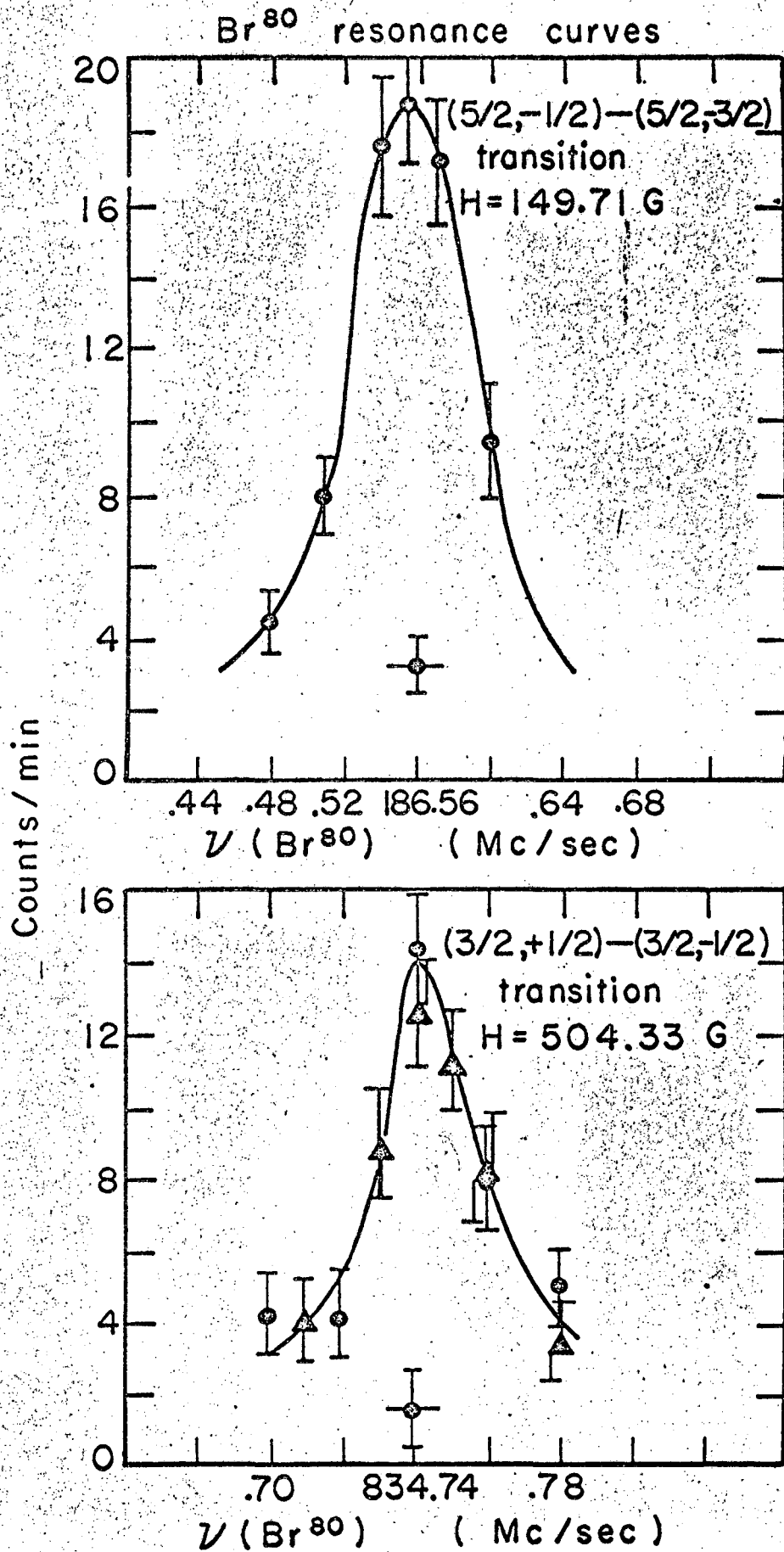
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Fig. 1.



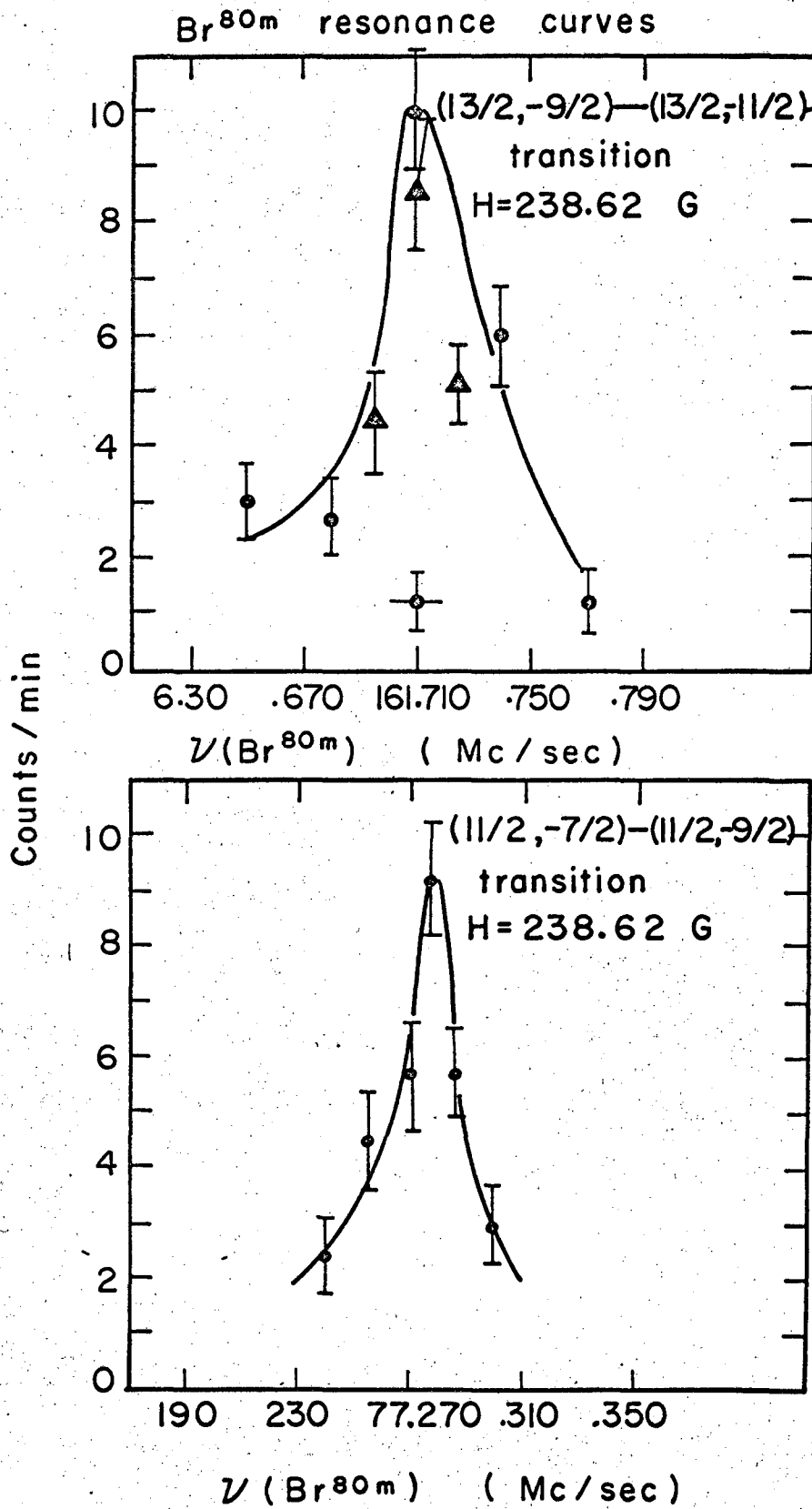
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Fig. 2.



MU-27183

Fig. 3.



MU-27182

Fig. 4.

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