

Effect of Core Excitation on the Hyperfine Structure of Rubidium

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Perturbations of the ratio of hyperfine coupling constants for the $5P$ levels of rubidium are investigated. The excitation of one $4s$ electron to higher s orbits is most effective in altering the ratio a_1/a_3 , although the effect of $4p$ shell excitation may be perceptible. The fraction of excited $4s$ configuration in the $5P$ state is written in terms of matrix elements of the electrostatic interaction, from which it appears that the sign of the perturbation is in agreement with the discrepancy observed by Senitzky and Rabi.

ANALYSIS of the effect of core excitation on the ratio a_1/a_3 for the $5P$ levels of rubidium was undertaken in an attempt to account for the observation¹ that this ratio is about 14% smaller than would be expected on the basis of the usual theory. Such perturbations of the hyperfine structure in a configuration consisting of a single valence electron in a p orbit have long been known.² For quantitative results it is customary^{3,4} to employ variational methods with Hartree single particle functions to find the amount of excited core wave function to be added to the zero order function. An equally consistent procedure is to solve the problem formally in terms of the radial integrals that arise in the expansion of the electrostatic interaction responsible for the mixing of configurations. For numerical results it is necessary to evaluate these integrals with the Hartree functions, but the initial formal computation is useful for classifying the contributions from various excited states, and the total numerical work is much reduced. Only the formal computation is reported here.

The zero-order rubidium configuration investigated is (in addition to closed K, L, M shells) $(4s)^2(4p)^65p$. The excited core configurations considered were $(4s)^2(4p)^5 \times (5p)^2$, $(4s)^2(4p)^5 5pn p$, $4s(4p)^6 ns 5p$, and $4s(5p)^6 nd 5p$. The first of these is most strongly mixed with the zero order configuration, but in the ratio a_1/a_3 the effect of the first term in the expansion of $1/r_{12}$ cancels, and only terms involving the nondiagonal radial integral $F_2(4p5p; 5p5p)$ survive. (The notation is that of Condon and Shortley.⁵) From an estimate of all the quantities involved, it seems unlikely that the resulting correction could be larger than perhaps 2%. The effect of configurations in which one of the $4p$ electrons is more highly excited also seems too small to account for the observed discrepancy.

The effect of $(4p)^6 4s 5s 5p$ is analogous to that considered by Fermi and Segrè for thallium, and in greater quantitative detail by Koster³ to account for the

hyperfine structure of gallium. To facilitate comparison between the present treatment and that of Koster we use his notation for the coefficients of the excited configuration wave functions. Let $\psi(^3S)$ and $\psi(^1S)$ be the wave functions for the 2P states of the excited configuration for which the parent terms in the $4s5s$ combination are 3S and 1S , respectively. Then

$$\psi = \psi_0 + \alpha_1 \psi(^3S) + \alpha_2 \psi(^1S).$$

In terms of the matrix elements of the electrostatic interaction,

$$\alpha_2 = \sqrt{2} [-F_0(ss') - F_0(sp) + \frac{1}{2}G_1(sp)]/E,$$

$$\alpha_1 = (\frac{3}{2})^{1/2} G_1(sp)/E,$$

where E is the excitation energy and

$$F_0(ss') = e^2 \int_0^\infty \int_0^\infty (1/r_>) R_{4s}(1) R_{5s}(1) R_{4s}^2(2) dr_1 dr_2,$$

$$F_0(sp) = e^2 \int_0^\infty \int_0^\infty (1/r_>) R_{4s}(1) R_{5s}(1) R_{5p}^2(2) dr_1 dr_2,$$

$$G_1(sp) = \frac{e^2}{3} \int_0^\infty \int_0^\infty (r_</r_>) R_{4s}(1) R_{5p}(1) \times R_{5s}(2) R_{5p}(2) dr_1 dr_2.$$

(The phases of the combinations of product functions are chosen to agree with those of Koster; in general it is only necessary to use the same phases for the matrix elements of the electrostatic interaction and those of the magnetic field at the nucleus.) The expressions for the hyperfine coupling constants are just those given by Koster's Eqs. (16). As would be expected, the effect on the hyperfine structure comes primarily from $\psi(^3S)$. The largest term in the correction arises from the nondiagonal matrix element of the magnetic field at the nucleus, $\langle 4s | H_z | 5s \rangle$, which has the factor $G_1(sp)/E$ in its coefficient. The sign of $G_1(sp)$ would therefore determine whether the perturbation serves to increase or to decrease the ratio of the hyperfine structure constants. For rubidium a rough calculation with screened functions does give a negative value for $G_1(sp)$, but numerical integration with Hartree wave functions would be required to answer this question definitely.

¹ B. Senitzky and I. I. Rabi, preceding paper [Phys. Rev. **103**, 315 (1956)].

² E. Fermi and E. Segrè, Rend. della R. Accademia d'Italia **4**, 18 (1933); also Z. Physik **82**, 729 (1933).

³ G. F. Koster, Phys. Rev. **86**, 148 (1952).

⁴ R. Sternheimer, Phys. Rev. **86**, 316 (1952).

⁵ E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1935), Sec. 8.

Reasonable estimates for the other parameters indicate that the effect of the admixture of excited s electron configurations could account for a major fraction of the discrepancy observed by Senitzky and Rabi. Formally, configurations in which a $4s$ electron is excited to any higher s orbit contribute in the same way. Although it might be expected that the series would converge rapidly for high excitation, a systematic investigation of excited states would be desirable.

Somewhat analogous terms arise from the admixture of configurations $4snd5p$, and for $4s4d5p$ the excitation energy is not much larger than that for $4s5s5p$. The

effect of these terms is small, however, for two reasons: the matrix elements of the electrostatic interaction are reduced because of angular interference, and the non-diagonal term in H_z is small.

The relative importance of perturbations due to $s \rightarrow s'$ excitation, even when the excitation energy is large, suggests that the quasi-empirical quantitative calculations of Schwartz⁶ for gallium may be extended to the p states of the alkalis. It is possible, however, that p -shell excitation plays a perceptible role in the hyperfine structure of alkali spectra.

⁶ C. Schwartz, Phys. Rev. **99**, 1035 (1955).

Mass Spectrometrically Determined Independent Yields of I^{128} , I^{130} , Br^{80} , and Br^{82} for U^{233} , U^{235} , and Pu^{239} Fission

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The primary yields of the shielded nuclei I^{128} and I^{130} have been accurately determined for the thermal neutron fission of U^{233} , U^{235} , and Pu^{239} . This has been done by the measurement of their stable daughters Xe^{128} and Xe^{130} using sensitive mass spectrometric techniques. The values of these primary yields show marked deviations from those predicted by the present theories of charge distribution. This discrepancy can be explained if the effect of the 50 proton shell is taken into account in the evaluation of the most probable initial nuclear charge Z_p for mass numbers 128 and 130. This can be done by postulating a most probable charge which will yield the greatest energy release in the fission process.

Also the primary yields of Br^{80} and Br^{82} were determined by means of their daughters Kr^{80} and Kr^{82} for the thermal fission of U^{233} and U^{235} and for the fast fission of Pu^{239} . The yields of these nuclei for fast neutron fission were ~ 100 times those for thermal fission, indicating a shift in the charge distribution curve with neutron energy.

INTRODUCTION

FOR a complete understanding of the fission process it is necessary to know both the charge and mass distribution of the fission fragments. Fission yield studies to date have been concerned mainly with mass distribution, the total or cumulative yield for a given mass being determined by radiochemical or mass spectrometric techniques. In this work the mass spectrometer measurements are less prone to contamination errors and are therefore the most reliable. The question of the distribution of charge for a given mass involves primary or independent yields of the fission fragments. In view of the short half-lives of most of these fragments, primary yield measurements are very difficult. Further, since all the primary yield data obtained to date¹⁻³ have

been obtained radiochemically, the contamination errors are in most cases quite large. A number of accurate primary yield values have now been obtained using very sensitive mass spectrometric techniques. The results of these measurements are reported in this paper.

The fission process can be represented by the equation

$$M(A, Z) + M(1, 0) \rightarrow M^*(A+1, Z) \rightarrow M(A_1, Z_1) + M(A_2, Z_2) + \nu M(1, 0) + \gamma + Q,$$

where $M(A, Z)$ is the mass of the fissioning nucleus, $M(A_1, Z_1)$ and $M(A_2, Z_2)$ are the masses of the primary fission fragments, and ν the total number of prompt neutrons released. γ is the electromagnetic energy released at the instant of fission and Q is the kinetic energy of the fragments and the neutrons released. Since the neutron to proton ratio of the fissioning nucleus is considerably higher than that corresponding to stability in the fission product region, the primary fission products are unstable and achieve nuclear stability through a series of β^- disintegrations. Therefore two types of fission yields can be defined:

(a) The total or cumulative yield Y of a given mass chain, defined as the percentage of fission acts giving the mass number in question.

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¹ Glendenin, Coryell, and Edwards, *Radiochemical Studies: The Fission Products*, edited by C. D. Coryell and N. Sugarman, (McGraw-Hill Book Company, Inc., New York, 1951), Paper 52, National Nuclear Energy Series, Plutonium Project Record, Vol. 9, Div. IV.

² L. E. Glendenin, Technical Report No. 35, Laboratory for Nuclear Science and Engineering, Massachusetts Institute of Technology, 1949 (unpublished).

³ A. C. Pappas, Technical Report No. 63, Laboratory for Nuclear Science, Massachusetts Institute of Technology, 1953 (unpublished).