

## Electronic configuration in the ground state of atomic lawrencium\*

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Self-consistent relativistic Dirac-Hartree-Fock calculations have been made of some low-lying electronic energies for the atoms of all elements in ground-state  $ds^2$  electron configurations. The results indicate that, contrary to some previous estimates, the ground electronic state of atomic Lr could be in either the  $5f^{14}6d7s^2$  or the  $5f^{14}7p7s^2$  electron configuration. The separation between the lowest energy level of the  $5f^{14}6d7s^2$  configuration and the lowest energy level of the  $5f^{14}7p7s^2$  configuration is estimated to be  $(0 \pm 3) \times 10^3 \text{ cm}^{-1}$  for atomic Lr.

Conflicting claims have appeared on whether the ground state of atomic Lr is in the  $5f^{14}6d7s^2$  electron configuration, as might be expected from the simple systematics of the Periodic Table, or in the  $5f^{14}7p7s^2$  electron configuration, as predicted from relativistic calculations. Brewer<sup>1</sup> smoothly extrapolated the difference  $\Delta_{pd}(q)$  between the lowest energy level of the  $5f^q7p7s^2$  configuration and the lowest energy level of the  $5f^q6d7s^2$  configuration as a function of  $q$ , or atomic number  $Z = 89 + q$ . His extrapolation proceeded from where these data are known for the atoms of the elements in the left half of the actinide series to where they are not known for the atoms of the elements in the right half. He estimated that the lowest energy level of the  $5f^{14}7p7s^2$  configuration of Lr is the ground level, and that the lowest energy level of the  $5f^{14}6d7s^2$  configuration is  $(8 \pm 2) \times 10^3 \text{ cm}^{-1}$  above this ground level. Mann<sup>2</sup> estimated the same energy separation to be  $(4 \pm 2) \times 10^3 \text{ cm}^{-1}$  on the basis of a self-consistent relativistic Dirac-Hartree-Fock calculation,<sup>3-5</sup> and this appeared to substantiate Brewer's extrapolation. Subsequently, on the basis of a generalized systematics in the relative energies of the lowest energy levels of the  $f^q ps^2$ ,  $f^q ds^2$ , and  $f^{q+1} s^2$  configurations for the atoms of the lanthanide and actinide series, Vander Sluis and Nugent<sup>6</sup> estimated the lowest energy level of the  $5f^{14}7p7s^2$  configuration of Lr to be above the lowest energy level of the  $5f^{14}6d7s^2$  configuration by  $(2.3 \pm 3) \times 10^3 \text{ cm}^{-1}$ . This latter result suggested that the ground state of atomic Lr may, after all, be in the  $5f^{14}6d7s^2$  configuration; however, a  $5f^{14}7p7s^2$  ground state was not precluded because of the  $\pm 3 \times 10^3 \text{ cm}^{-1}$  uncertainty.

The purpose of the present article is twofold. First we report the results of a study of the accu-

racy of self-consistent relativistic Dirac-Hartree-Fock calculations of  $\Delta_{pd}(Z)$  for all elements with atoms in  $x ds^2$  ground-state electron configurations, where  $x$  represents  $Z - 3$  electrons in closed shells. Second, we extrapolate the first results to obtain  $\Delta_{pd}(103)$  for Lr, and we show that with the present uncertainty of  $\pm 1 \times 10^3 \text{ cm}^{-1}$  in the value of  $\Delta_{pd}(89)$  for Ac, the self-consistent relativistic Dirac-Hartree-Fock method cannot resolve with certainty whether the ground state of atomic Lr is in the  $5f^{14}6d7s^2$  or in the  $5f^{14}7p7s^2$  configuration.

The elements with atoms known to be in  $x ds^2$  electronic ground-state configurations are presented in the order of atomic number in the first column of Table I. In the second column are measured values of  $\Delta_{pd}(Z)$ , and in the third column are values of  $\Delta_{pd}(Z)$  as calculated via the self-consistent relativistic Dirac-Hartree-Fock method with neglect of configuration interaction. In the fourth column are  $\delta_{pd}(Z)$ , the difference between the respective measured and calculated values of  $\Delta_{pd}(Z)$ .

The values of  $\delta_{pd}(Z)$  from Table I are plotted as a function of  $Z$  in the figure where it is shown that  $\delta_{pd}(Z)$  is essentially zero, within  $\pm 1 \times 10^3 \text{ cm}^{-1}$ , up to and including La. After La,  $\delta_{pd}(Z)$  increases approximately linearly to Ac. Our extrapolation to Lr is  $\delta_{pd}(103) = (3.6 \pm 3) \times 10^3 \text{ cm}^{-1}$ , as represented by the dashed line (b) in Fig. 1 and as listed in the table. We make this extrapolation by setting  $\delta_{pd}(103) \approx \delta_{pd}(89)$ , the same as for the preceding element Ac, and by expanding the error limit to  $\pm 3 \times 10^3 \text{ cm}^{-1}$  as represented by dashed lines (a) and (c). We can see from the other  $\delta_{pd}(Z)$  results in the table that this approximation—setting  $\delta_{pd}(Z) \approx \delta_{pd}(Z')$ , where  $Z'$  is the next atomic number below  $Z$  in the table—would

TABLE I. Measured and calculated  $\Delta_{pd}(Z)$  energies for the atoms of all elements in  $nds^2$  electronic ground-state configurations.

$M(Z)$	$\Delta_{pd}(Z)$		$\delta_{pd}(Z)$
	Meas. ( $10^3 \text{ cm}^{-1}$ )	Calc.	
Sc(21)	24.223 <sup>a</sup>	23.678	0.545
Y(39)	10.529 20 <sup>b</sup>	11.463	-0.934
La(57)	15.220 <sup>c</sup>	16.296	-1.076
Lu(71)	4.14 <sup>c</sup>	3.142	1.00
Ac(89)	$9.5 \pm 1$ <sup>c</sup>	6.129	$3.4 \pm 1$
Lr(103)	$(0 \pm 3)$ <sup>d</sup>	-3.632	$(3.6 \pm 3)$

<sup>a</sup>This is a measured value for  $\Delta_{pd}(21)$  as determined by Racah from a spectral analysis of ScI after analytic elimination of the unusually strong interactions between the nearly degenerate  $spd$  and  $s^2p$  electron configurations. [Cf. G. Racah, *Phys. Rev.* **62**, 523 (1942); and C. Roth, *J. Res. Natl. Bur. Stand.* **73**, 497 (1969).]

<sup>b</sup>C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. Circ. No. 467, (U. S. GPO, Washington, D. C., 1952), p. 196.

<sup>c</sup>References 1 and 6.

<sup>d</sup>This is our best estimated value of  $\Delta_{pd}(103)$  for Lr. It is obtained from the sum of the adjacent calculated value of  $-3.632 \times 10^3 \text{ cm}^{-1}$  and the value  $3.6 \pm 3 \times 10^3 \text{ cm}^{-1}$  extrapolated for  $\delta_{pd}(103)$  from Fig. 1.

lead to errors in  $\delta_{pd}(Z)$  of no more than  $\pm 3 \times 10^3 \text{ cm}^{-1}$ . The expanded error limit here also accounts for the  $\pm 1 \times 10^3 \text{ cm}^{-1}$  uncertainty in the value of  $\Delta_{pd}(89)$  for Ac, and it accounts for the following two contingencies: The first, dashed line (a), accounts for the possibility that relativistic effects which progressively lower the energy of the  $ps^2$  configuration relative to the  $ds^2$  configuration with increasing  $Z$ , may, in fact, be less than calculated from the theory. The second, dashed line (c), accounts for the possibility that  $\delta_{pd}(103)$  for Lr may be approximately equal to  $\delta_{pd}(71)$  for Lu, the electronic, chemical, and periodic analog of Lr in the lanthanide series.

Next we compare the results from our present extrapolation with previous results for Lr. If we take the estimate  $\Delta_{pd}(103) = (2.3 \pm 3) \times 10^3 \text{ cm}^{-1}$  of Vander Sluis and Nugent as the measured value for Lr, we obtain the point VN in Fig. 1. Similarly, if we take the estimate  $\Delta_{pd}(103) = -(8 \pm 2) \times 10^3 \text{ cm}^{-1}$  of Brewer as the measured value for Lr, we obtain the point B in the figure. We see that the present extrapolation is in reasonable agreement with the point VN, and that the point B is well outside of all the reasonable trends.

We obtain  $(0 \pm 3) \times 10^3 \text{ cm}^{-1}$  for our present estimate of  $\Delta_{pd}(103)$  for Lr, as listed in Table I from the sum of the adjacent calculated value  $-3.632 \times 10^3 \text{ cm}^{-1}$  and the extrapolated value  $\delta_{pd}(103)$

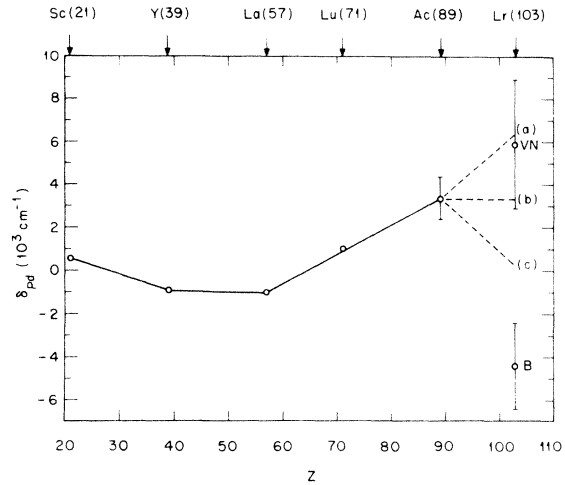


FIG. 1.  $\delta_{pd}(Z)$  vs atomic number  $Z$  for those elements with atoms in ground-state  $nds^2$  electron configurations. The dashed lines are extrapolations based on the preceding points. The point VN represents the difference between the extrapolated  $\Delta_{pd}(103)$  value of Vander Sluis and Nugent and the calculated  $\Delta_{pd}(103)$  value. The point B represents the difference between the extrapolated  $\Delta_{pd}(103)$  value of Brewer and the calculated  $\Delta_{pd}(103)$  value.

$= (3.6 \pm 3) \times 10^3 \text{ cm}^{-1}$ . So within the present  $\pm 3 \times 10^3 \text{ cm}^{-1}$  uncertainty, we cannot resolve whether the ground state of atomic Lr is in the  $5f^{14}6d7s^2$  or in the  $5f^{14}7p7s^2$  configuration.

We conclude with some general comments on the effects of configuration interaction. Most of the significant configurations move farther apart in energy with increasing atomic number progressing across the lanthanide or actinide series,<sup>1</sup> so the effects of configuration interaction are least for Lu and Lr. The  $ds^2$  and  $ps^2$  configurations are of opposite parity and hence do not interact in any case. All states that are of the proper symmetry to interact with the lowest energy level of the  $ds^2$  configuration lie in each case above this level, so one effect of configuration interaction is a slight lowering of the lowest energy level of the  $ds^2$  configuration. Similarly, all states that are of the proper symmetry to interact with the lowest energy level of the  $ps^2$  configuration lie in each case above that level, so another effect of configuration interaction is a slight lowering of the lowest energy level of the  $ps^2$  configuration. Since  $\Delta_{pd}(Z)$  represents the difference in energy between the lowest levels of these two configurations, most of the effects of configuration interaction are subtracted out, leaving only a small residual which is expected to be well within the other uncertainties in the present treatment.

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<sup>1</sup>L. Brewer, J. Opt. Soc. Am. 61, 1101 (1971).

<sup>2</sup>J. B. Mann, cited in G. T. Seaborg, J. L. Crandall, P. R. Fields, A. Ghiorso, O. L. Keller, and R. A. Penneman, Proceedings of the Fourth International Conference on the Peaceful Uses of Atomic Energy, Geneva, United Nations, A/Conf. 49, 841, 1972 (unpublished).

<sup>3</sup>J. B. Mann and J. T. Waber, J. Chem. Phys. 53, 2397 (1970).

<sup>4</sup>J. B. Mann and J. T. Waber, Atomic Data 5, No. 2, April, 1973.

<sup>5</sup>J. P. Desclaux, thesis (University of Paris, 1968) (unpublished).

<sup>6</sup>K. L. Vander Sluis and L. J. Nugent, Phys. Rev. A 6, 86 (1972).