

Annihilation of Positrons in LiH†

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(Received November 23, 1960)

The angular correlation of photons from positron annihilation in LiH and NaH has been measured. The data yield a wave-function product density distribution much wider than the outer-shell electron density around the negative ion. This result is in contrast with the observations for other alkali halides for which these two distributions are much alike.

A NEW effect has been observed in the annihilation of positrons in crystals. Previous work¹⁻⁴ in a variety of alkali halide crystals has shown that, for fluorides and chlorides at least, the electron-positron wave-function products which give fits to the observed momentum distribution of the annihilation gamma rays resemble the Hartree-Fock free-ion wave functions of the outer shell of electrons of the negative ion. For these alkali halides both the wave-function products and the free-ion electron wave functions yield density distributions in agreement with the density distributions obtained by x-ray measurement.⁵⁻⁷ The situation is different, however, for positron annihilation in LiH. For this crystal the electron-positron wave-function product is much wider at the half-maximum position and at the same time falls much faster toward zero at about one atomic spacing than does the electron wave function obtained from the measured x-ray data⁸ or from the calculated free-ion wave functions.⁹

The experimental results follow. Figure 1 shows the angular correlation of photons from positrons annihilating in polycrystalline LiH and NaH. The two curves are hardly distinguishable. These data were obtained using the parallel slit geometry previously discussed.¹⁰ The slopes of chords of these data are plotted on Fig. 2 where we also show that an analytic function happens to provide a good one-parameter fit to the data. Follow-

ing the usual analysis,^{11,12} we have taken the observed distribution in momentum space, $\rho(p)$, to be proportional to the sum over all electrons of the squares of

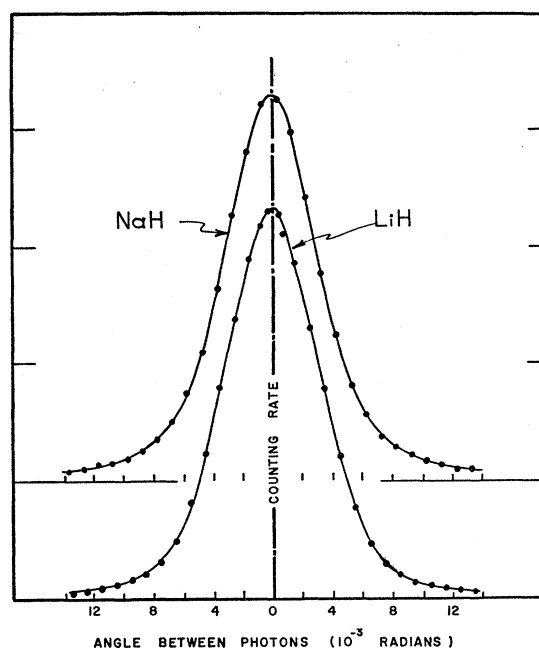


FIG. 1. Angular correlation of the two-photon annihilation radiation from positrons annihilating in LiH and NaH. The instrumental resolution function has a width of less than 1 milliradian.

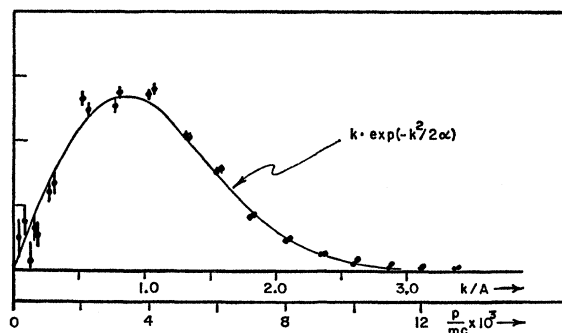


FIG. 2. Slope of angular correlation data and fit of analytic function.

† This research has been supported by the National Research Council of Canada and by Atomic Energy of Canada Limited.

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¹ W. E. Millett and R. Castillo-Bahena, *Phys. Rev.* **108**, 257 (1957).

² N. K. Pope and A. T. Stewart, *Bull. Am. Phys. Soc.* **4**, 217 (1959). But see reference 3.

³ A. T. Stewart and N. K. Pope, *Phys. Rev.* **120**, 2033 (1960).

⁴ N. K. Pope, *Bull. Am. Phys. Soc.* **5**, 262 (1960).

⁵ H. Witte and E. Wölfel, *Z. physik Chem.* **3**, 296 (1955).

⁶ J. Krug, H. Witte, and E. Wölfel, *Z. physik Chem.* **4**, 36 (1955).

⁷ H. Witte and E. Wölfel, *Revs. Modern Phys.* **30**, 51 (1958).

⁸ W. Cochran, *Revs. Modern Phys.* **30**, 47 (1958).

⁹ The charge density plotted is obtained from $\int f(r_1, r_2, r_{12}) d^3r_2$, where $f = [1 + \beta r_{12} + \gamma(r_1 - r_2)^2] \exp[-\alpha(r_1 + r_2)]$ is the three-parameter wave function for the H^- ion obtained by H. A. Bethe [*Z. physik* **57**, 815 (1929)]. See also H. A. Bethe and E. E. Salpeter's article in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. XXXV, p. 241.

¹⁰ A. T. Stewart, *Can. J. Phys.* **35**, 168 (1957).

¹¹ S. DeBenedetti, C. E. Cowan, W. R. Konneker, and H. Primakoff, *Phys. Rev.* **77**, 205 (1950).

¹² R. A. Ferrell, *Revs. Modern Phys.* **28**, 308 (1956).

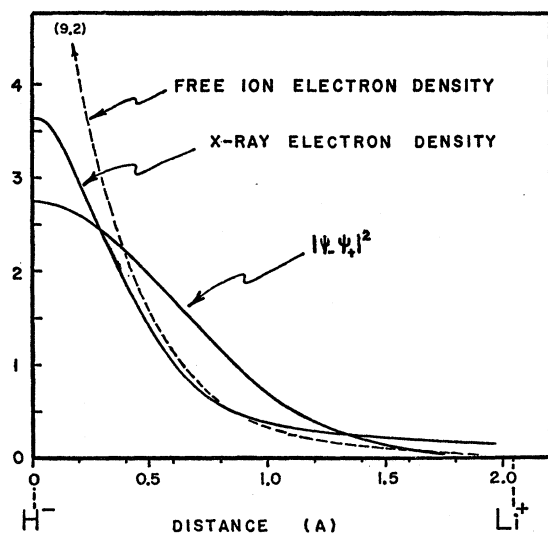


FIG. 3. Comparison of electron density distribution obtained from x-ray diffraction and from free-ion calculations with "wave-function product" squared obtained from this experiment.

moduli of the Fourier transforms of the wave-function products, $\psi_j\psi_+$;

$$\rho(\mathbf{p}) = \sum_j |\chi_j(\mathbf{p})|^2 = \text{const} \sum_j \left| \int e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_j \psi_+ d\tau \right|^2.$$

For the case of LiH it is expected that the positrons annihilate chiefly with the electrons of the H^- ion so that the above sum has one term only. The slope of the angular correlation data, which can easily be shown to be proportional to $p\rho(p)$, is seen (Fig. 2) to fit the function $p \exp(-k^2/2\alpha)$ for $\alpha = 0.70/\text{\AA}^2$. ($k = p/\hbar$.) From this we obtain by Fourier transform $|\psi_j\psi_+|^2 = \exp(-2\alpha r^2)$, the wave-function product density. This is compared in Fig. 3 with the electron density obtained by Cochran⁸ from x-ray scattering and with the calculated free-ion electron density.⁹ The three curves are normalized to give approximately the same number of electrons around the H^- ion.

The considerable difference between charge density and wave-function product density for positrons annihilating in LiH is in contrast with their similarity for positrons annihilating in, for example, NaF. This contrast is somewhat strange for, as we show below, one might expect any difference to be in the other direction. Consider the behavior of the positron wave function and of the wave function of the outer closed shell of electrons around the negative ions in LiH and NaF. The charge density is known to peak at about 0.5 Å from both H^- and F^- although the distribution in H^- has a much longer tail than in F^- . [This is to be expected when one considers the binding energies of the last electron in H^- (0.7 eV) and in F^- (4.1 eV).] The positron wave function starts at zero at the ion positions and increases with radius at a rate which is much greater in the field of H^+ than in the field of F^{+7} . Therefore, one would expect that the peak of the wave-function product distribution would be displaced outward past the charge density maximum, more in the fluoride results than in the hydride. The opposite is observed.

A detailed cellular calculation of the positron wave function in LiH and in NaF could, of course, disprove these simple qualitative conclusions. On the other hand, it is interesting to speculate that these data may require the use of electron wave functions perturbed by the positron or even correlations between the positron and the electrons. Both of these effects would be stronger in H^- than in F^- and would be in the right direction, i.e., they would reduce the momentum of the center of mass and make the wave function product appear more spread out than the charge distribution. In any case, this experiment has furnished a criterion, the wave-function product in single-particle terminology, for the testing of calculations of positron annihilation in a simple ionic crystal.

ACKNOWLEDGMENTS

We are indebted to Mr. J. M. Robson and Dr. N. K. Pope for consultation and assistance.