ANNIHILATION OF SLOW POSITRONS IN HYDRIDES OF ALKALI METALS. II.

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The self-consistent field method was used to calculate five excited states of positronium hydride. The average lifetime 1.27×10^{-9} sec calculated for these levels is in satisfactory agreement with the experimental value of the long-lived component $\tau_2 = (1.52 \pm 0.8) \times 10^{-9}$ sec. Curves are presented of the angular correlation of the gamma quanta, corresponding to two-photon annihilation from these levels.

IT was shown in a paper by Gol'danskiĭ and the authors [1] that the system e^+H^- (positronium hydride) has a series of bound levels. The ground state $1s^2(1s)$ and the first two excited states $1s^2(2s)$ and $1s^2(2p)$ were calculated by the self-consistent field method. The results of the calculations explained the complicated character of the spectrum of the positron lifetimes in the hydrides of alkali metals. It was found that two-photon annihilation from the first two excited levels gives a positron lifetime $\tau = 2.84 \times 10^{-10}$ sec, which was in good agreement with the experimental value of the short-lived component in lithium hydride $\tau_1 = (2.1 \pm 0.3) \times 10^{-10}$ sec.[2] A hypothesis was advanced that the long-lived component is due to annihilation from higher excited levels. The results of calculations for the next five excited levels, performed in the present work, have confirmed this assumption. Indeed, the calculated mean value of the lifetime for these levels (with account of their populations is 1.27×10^{-9} sec and agrees satisfactorily with the experimental value of the long-lived component $\tau_2 = (1.52 \pm 0.8) \times 10^{-9}$ sec.[2]

Let us present the main results of the calculation. Single-positron wave functions for 3s, 3p, 3d, 4s, and 4p states of the positron in the e^+H^- bound system, obtained from the Hartree-Fock equations with full self consistency[1)], are shown in Fig. 1. The corresponding eigenvalues of the energies $\mu_{nl,nl}$ (for the positron) and $\lambda_{10,10}$ (for the electrons), in atomic units, are listed in Table I. The same table lists the values of the binding energy of the positron with the negative hydrogen ion as compared with the binding energies of the positron with the Cl^- ion, calculated by Simons [4] by the Hartree method.

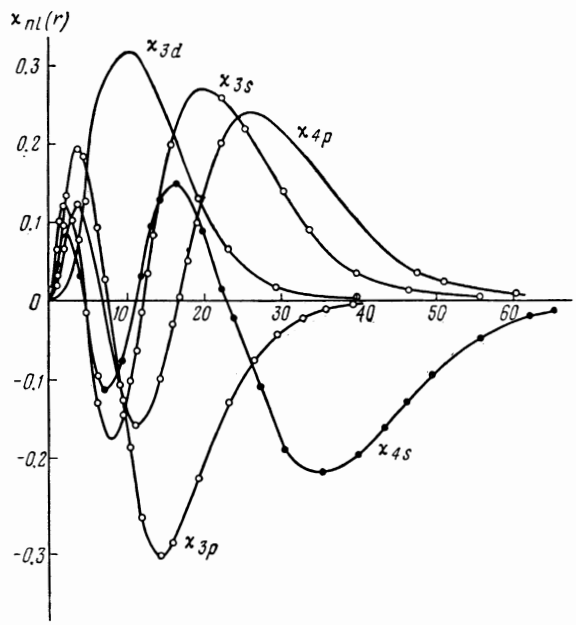

FIG. 1. Single-positron wave functions of the system for the states $1s^2(3d)$, $1s^2(3p)$, $1s^2(3s)$, $1s^2(4p)$, and $1s^2(4s)$.

As can be seen from Table I, the excited energy levels for the systems e^+H^- and e^+Cl^- differ by not more than 13% (3d level), and in

Table I

State of positron	$-\lambda_{10,10}$	$-\mu_{nl,nl}$	Binding energy (in eV)	
			e+H−	e+Cl−
1*s*	0.2987	0.1910	4.57	3.82
2*p*	0.2144	0.1033	2.72	2.68
2*s*	0.1592	0.0705	1.53	1.60
3*d*	0.1542	0.0543	1.29	1.49
3*p*	0.1365	0.0486	1.15	1.27
3*s*	0.1160	0.0376	0.91	0.91
4*p*	0.1027	0.0282	0.69	0.745
4*s*	0.0929	0.0231	0.58	0.59

[1)] A detailed description of the calculation procedure is given in[1,3].

Table II

State of positron	K	ω_A, 10^{10} sec.$^{-1}$	$A_{n'n}$, 10^8 sec.$^{-1}$	ω_{cap} 10^8 sec.$^{-1}$	State of position	K	ω_A, 10^{10} sec.$^{-1}$	$A_{n'n}$, 10^8 sec.$^{-1}$	ω_{cap}, 10^8 sec.$^{-1}$
1s	0.91	1.25	0.565 ($2p \to 1s$)	0.24	3p	0.89	0.115	0.0074 ($3s \to 3p$)	170
2p	0.88	0.43	0.057 ($3p \to 1s$)	49.6	3s	0.89	0.092		30.2
2s	0.88	0.24	0.067 ($2s \to 2p$)	3.3	4p 4s	0.89	0.0039		370 131
3d	0.88	0.070	0.018 ($3p \to 2s$)	3.3	$1s^2$ (E_0, 1) $1s^2$ (E_0, 0)		0.000033 0.0066		

Remark. Here $E_0 = 0.025$ eV is the energy of the thermalized positron.

many cases (2p, 3s, 4s) they practically coincide. The latter indicates that for the system e^+H^- one can employ the interpolation formula proposed by Simons [4] for e^+Cl^-, namely

$$E \sim -1/2(n+\alpha)^2$$

($\alpha = 1$ for $l = 0$; $\alpha = 0$ for $l \geq 1$), which makes it possible to estimate the energy of the highly excited levels. The appreciable difference in the values of the energy for the ground state ($\sim 20\%$) can be attributed to the fact that the electron structure of the negative ion is especially important in this state. In particular, in the ground state there is an especially strong deforming action of the positron on the electron shell of the H^- ion. In the calculation for positronium chloride,[4] the deformation of the Cl^- by the positron was not taken into consideration.

The self-consistent field wave functions obtained were used to calculate the probabilities of the interaction between thermalized positrons and negative hydrogen ions and the angular correlation curves for annihilation radiation of two-photon annihilation. In Table II are listed the probabilities of the annihilation ω_A and radiative $A_{n'n}$ transitions of bound positronium, and the probabilities ω_{cap} of radiative capture and of the annihilation of thermalized positrons (the last two lines of Table II). The calculation was based on formulas (5)—(8) of [1]. In the second column of Table II are given also the values of the superposition integrals K [see formula (7) of [1]]. We see from the data of Table II that the annihilation of thermalized positrons in collisions with the electrons of the ion H^- can be neglected as compared with the radiative captures and subsequent annihilation from the bound states. Comparison of the obtained values of the annihilation rates of the bound positrons and the probabilities of radiative transitions for the same levels shows that in practice only annihilation is effected at all the levels in question.

Figure 2 shows curves of angular correlation of the annihilation gamma quanta in two-photon annihilation of bound positrons in different states and of free thermalized positrons with electrons of the K shell of the H^- ion. Calculation of the relative probability $P(k_z)$, which depends on the z component of the summary vector **k** of the radiated photons, was carried out by formulas (9) and (10) from [1]. For comparison, Fig. 2 shows the experimental curve obtained by Stewart and March.[5] The calculated angular-correlation curves for the ground state and for several excited states duplicate the shape of the experimental curve, thus arguing in favor of the proposed mechanism of annihilation of thermalized positrons.

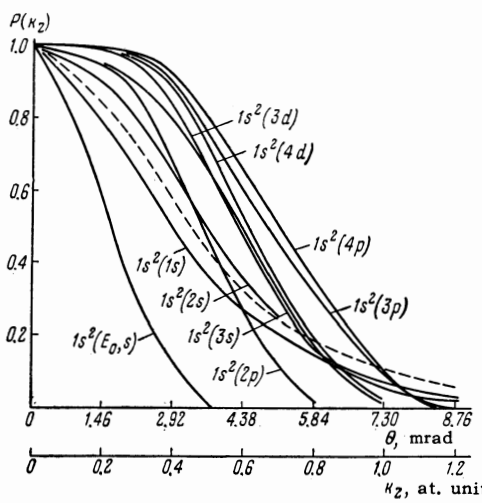

FIG. 2. Plots of the angular correlation of gamma quanta in two-photon annihilation: the solid curves were calculated for the annihilations of (1s), (2s), (3s), (2p), (3p), (4p), (3d), and (4d) positrons and free thermalized positrons (E_0, 0); the dashed curve is experimental for LiH.[2]

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[1] Gol'danskiĭ, Ivanova, and Prokop'ev, JETP 47, 659 (1964), Soviet Phys. JETP 20, 440 (1965).

[2] Bisi, Fiorentini and Zappa, Phys. Rev. 133, 1023 (1963).

[3] Gol'danskiĭ, Ivanova, and Prokop'ev, Collection: Yadernaya khimiya (Nuclear Chemistry), Nauka, 1965.

[4] L. Simons, Phys. Rev. 90, 165 (1953).

[5] A. Stewart and R. March, Phys. Rev. 122, 75 (1961).

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