

Ground state of positronium hydride

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The ground bound state in the positronium hydride molecule (HPs) is determined from extensive variational four-body calculations with the James-Coolidge four-body variational expansion in the relative coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$, and r_{34} . For the positronium hydride with the infinitely heavy nucleus (${}^\infty$ HPs) the total energy found, $E = -0.789\,136\,9$ a.u., is one of the lowest variational values published to date. A number of bound-state properties have been calculated also, including the δ -function expectation values, two-body cusps, and the two-photon annihilation rate. [S1050-2947(97)00708-7]

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In the present study we consider the bound-state spectrum in the positronium hydride (HPs). The four-body HPs systems consist of two electrons e^- , one positron e^+ , and one positive heavy particle p^+ (the proton for short). Actually, the bound-state spectrum of HPs contains only one bound state. The boundness of this state is well known from the paper by Ore [1]. Later, the ground state in the HPs hydride was studied very intensively in a number of theoretical works [2–4]. The structure of bound-state spectra in the HPs hydride and all references before 1981 can be found in [5]. It was shown in that work that positronium hydride and a few related systems may play a remarkable role in some astrophysical theories. Recently, bound positronium hydride has been created and observed in the laboratory [6]. Our previous work [7] contains the most extensive variational results for some properties of such hydrides (with the different proton masses).

In this paper we report variational results (energies and some other properties) for the ground bound state of the HPs hydride. In order to determine the energy of this state we use variational expansions in the four-body relative coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$, and r_{34} , where $r_{ij} = |\vec{r}_i - \vec{r}_j|$. Our present goal was to obtain a better or comparable value for the ground-state energy in the HPs hydride than the result found in [7]. In [7] we used the variational ansatz [Kolesnikov-Tarasov (KT) expansion] from [8],

$$\Psi = \mathcal{A} \sum_{i=1}^N C_i \exp(-\alpha_{12}^i r_{12}^2 - \alpha_{13}^i r_{13}^2 - \alpha_{23}^i r_{23}^2 - \alpha_{14}^i r_{14}^2 - \alpha_{24}^i r_{24}^2 - \alpha_{34}^i r_{34}^2), \quad (1)$$

where the α_{kl}^i are the nonlinear parameters, the C_i are the linear (or variational) parameters, and \mathcal{A} is the appropriate symmetrizer (or antisymmetrizer), i.e., a projection operator which produces the final wave function with the correct permutation symmetry. In the HPs system there are two identical particles (electrons). They are designated as particles 1 and 2, while 3 stands for the positron and 4 means the proton [9]. Therefore \mathcal{A} takes a very simple form: $\mathcal{A} = 1 + \hat{P}_{12}$, where \hat{P}_{12} is the permutation operator. Note that the KT expansion has an incorrect asymptotic behavior in each of the decay channels for an arbitrary Coulomb four-body system, and therefore it cannot be regarded as an accurate variational expansion for such systems.

Nevertheless, as it follows from the results of [7], the KT expansion produces variational results for the HPs hydride which are energetically better (and even significantly better) than the values found earlier by other methods [2–4]. This was completely unexpected, since the methods used in [2–4] have a partially correct asymptotic behavior, i.e., the appropriate wave functions have the correct asymptotics in some decay channels. Presently, we consider the variational ansatz for the four-body wave function due originally to James and Coolidge (JC) [10]. As it is applied to ${}^\infty$ HPs the expansion takes the form (below we shall call this the JC expansion, for short [11,12])

$$\Psi = \mathcal{A} \left[\left(\sum_{i=1}^N C_i p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}) \right) \times \exp(-\alpha r_{14} - \beta r_{24} - \gamma r_{34}) \right], \quad (2)$$

where $p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}) = r_{23}^{n_{1,i}} r_{13}^{n_{2,i}} r_{12}^{n_{3,i}} r_{14}^{m_{1,i}} r_{24}^{m_{2,i}} r_{34}^{m_{3,i}}$, and all $n_{k,i}$ and $m_{l,i}$ are non-negative integer numbers. The α, β , and γ are the only three nonlinear parameters. They do not depend on the number of basis functions used, and in our present calculations with the JC expansion the values $\alpha = 0.65, \beta = 1.00$, and $\gamma = 0.59$ have been chosen for these parameters. The functions $p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34})$ are homogeneous polynomial functions of all relative coordinates: $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$, and r_{34} . All other notation is exactly the same as in Eq. (1) [9]. Note that in contrast with all previous studies (with the JC ansatz) there is no assumption that some of the $[n_{1,i}, n_{2,i}, n_{3,i}, m_{1,i}, m_{2,i}, m_{3,i}]$ equal zero (or each other, etc.) *a priori*. Likewise, our goal is to use all possible complete families of basis functions. Such a family of basis functions is represented by the single non-negative integer number ω : $\omega_{g(i)} = n_{1,i} + n_{2,i} + n_{3,i} + m_{1,i} + m_{2,i} + m_{3,i}$, where $i = 1, 2, \dots, N$ and $\omega_{g(i)}$ is a non-negative integer and equals 0, 1, 2, 3, 4, 5, 6 in this study. The physical meaning of $\omega_{g(i)}$ is obvious: it is the total power of the homogeneous polynomial function $p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34})$, i.e., ω can be determined as an eigenvalue for the following operator:

$$\left(\sum_{k \neq l} r_{kl} \frac{\partial}{\partial r_{kl}} \right) p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}) = \omega p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}). \quad (3)$$

TABLE I. The expectation values in atomic units ($m_e=1, \hbar=1, e=1$) of some properties for the ground bound S state ($L=0$) of the positronium hydride ${}^{\infty}\text{HPs}$ as a function of the total number of basis functions N .^a

	$N=462$	$N=588$	$N=589$	$N=783$	$N=924$	KT [15]
$\langle r_{12} \rangle$	3.551109	3.550723	3.551163	3.555187	3.554741	3.573452
$\langle r_{13} \rangle$	3.469798	3.469411	3.469624	3.471350	3.471097	3.479507
$\langle r_{14} \rangle$	2.298693	2.298455	2.298681	2.300959	2.300684	2.310887
$\langle r_{34} \rangle$	3.638839	3.638248	3.638657	3.642593	3.642103	3.660417
$\langle r_{12}^2 \rangle$	15.56987	15.56819	15.57341	15.61738	15.61330	15.85396
$\langle r_{13}^2 \rangle$	15.44102	15.43839	15.44111	15.46176	15.45925	15.57139
$\langle r_{14}^2 \rangle$	7.658638	7.657744	7.660105	7.682908	7.680700	7.802988
$\langle r_{34}^2 \rangle$	15.96190	15.95924	15.96389	16.00648	16.00208	16.23445
π_{12}	0.484445	0.484722	0.484696	0.485402	0.485389	0.491471
π_{13}	0.531536	0.531330	0.531660	0.532076	0.532056	0.534931
π_{14}	0.670376	0.670250	0.670595	0.671667	0.671614	0.679102
π_{34}	0.453295	0.453728	0.453594	0.454261	0.454254	0.460052
$\langle r_{12}^3 \rangle$	81.0942	81.1006	81.1545	81.5679	81.5341	84.2409
$\langle r_{13}^3 \rangle$	82.7032	82.6934	82.7228	82.9268	82.9053	84.1828
$\langle r_{14}^3 \rangle$	33.5537	33.5577	33.5796	33.7794	33.7629	35.0711
$\langle r_{34}^3 \rangle$	81.8475	81.8559	81.9007	82.2974	82.2609	84.8012
$\langle r_{12}^4 \rangle$	488.597	488.880	489.436	493.288	492.984	523.417
$\langle r_{13}^4 \rangle$	513.720	513.755	514.068	516.037	515.842	530.169
$\langle r_{14}^4 \rangle$	180.767	180.909	181.117	182.864	182.726	196.829
$\langle r_{34}^4 \rangle$	480.078	480.428	480.853	484.548	484.210	511.689
$\langle r_{12}^{-1} \rangle$	0.3717022	0.3717575	0.3717336	0.3714797	0.3715203	0.3705098
$\langle r_{13}^{-1} \rangle$	0.4187259	0.4188448	0.4183785	0.4188055	0.4188283	0.4185147
$\langle r_{14}^{-1} \rangle$	0.7305630	0.7306299	0.7306103	0.7304066	0.7304515	0.7297236
$\langle r_{34}^{-1} \rangle$	0.3485038	0.3485687	0.3485463	0.3483100	0.3483512	0.3475001
$\langle -\frac{1}{2}\nabla_1^2 \rangle$	0.3262654	0.3263277	0.3263251	0.3263045	0.3263244	0.3261727
$\langle -\frac{1}{2}\nabla_3^2 \rangle$	0.1367618	0.1368619	0.1368590	0.1368908	0.1369023	0.1368539
$\langle \delta_{12} \rangle$	0.449379×10^{-2}	0.445403×10^{-2}	0.445375×10^{-2}	0.448405×10^{-2}	0.442663×10^{-2}	0.449550×10^{-2}
$\langle \delta_{13} \rangle$	0.241086×10^{-1}	0.243188×10^{-1}	0.243229×10^{-1}	0.243544×10^{-1}	0.244158×10^{-1}	0.241519×10^{-1}
$\langle \delta_{14} \rangle$	0.177488	0.177495	0.177493	0.177439	0.177484	0.174616
$\langle \delta_{34} \rangle$	0.160766×10^{-2}	0.161920×10^{-2}	0.162000×10^{-2}	0.161731×10^{-2}	0.162165×10^{-2}	0.168874×10^{-2}
ν_{12} ^b	0.4587343	0.4715450	0.4713573	0.4708562	0.4793652	0.0
ν_{13}	-0.4804015	-0.4902103	-0.4904605	-0.4907653	-0.4945145	0.0
ν_{14}	-1.0009363	-1.0002769	-1.0003399	-0.9996877	-1.0004014	0.0
ν_{34}	1.0353583	1.0239807	1.0209628	1.0241008	1.0196266	0.0
$\langle \delta_{123} \rangle$	0.37631×10^{-3}	0.38059×10^{-3}	0.38027×10^{-3}	0.37413×10^{-3}	0.37941×10^{-3}	0.37515×10^{-3}
$\langle \delta_{134} \rangle$	0.86090×10^{-3}	0.86746×10^{-3}	0.86768×10^{-3}	0.85689×10^{-3}	0.85815×10^{-3}	0.90685×10^{-3}
$\langle \delta_{124} \rangle$	0.77587×10^{-2}	0.77224×10^{-2}	0.77219×10^{-2}	0.77261×10^{-2}	0.76892×10^{-2}	0.71512×10^{-2}
$\langle \delta_{1234} \rangle$	0.19827×10^{-3}	0.20269×10^{-3}	0.20273×10^{-3}	0.19668×10^{-3}	0.20163×10^{-3}	0.17332×10^{-3}
$\langle T \rangle$	0.7892925	0.7895173	0.7895092	0.7894997	0.7895511	0.7891964
$\langle \frac{1}{2}V \rangle$	-0.7891859	-0.7893116	-0.7893085	-0.7893172	-0.7893440	-0.7891891
E	-0.7890730	-0.7891060	-0.7891077	-0.7891348	-0.7891369	-0.7891818
χ	0.1350×10^{-3}	0.2605×10^{-3}	0.2543×10^{-3}	0.2311×10^{-3}	0.2623×10^{-3}	0.9235×10^{-5}

^aThe particles 1 and 2 designate the electrons, 3 stands for the positron, and 4 means the infinitely heavy proton ${}^{\infty}\text{H}^+$. Such notation differs from our previous choice used in [7] (for more details see [9]).

^bThe ‘‘exact’’ cusp values are $\nu_{12}=0.5, \nu_{13}=-0.5, \nu_{14}=-1.0$, and $\nu_{34}=1.0$, respectively.

In other words, ω is the so-called representation (or subspace) index in a more general infinite-dimensional polynomial space $\{P_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34})\}$. The total number of basis functions $N(B_\omega)$ in these subspaces or families B_ω are, respectively, 1, 6, 21, 56, 126, 252, 462 for $\omega = 0, 1, 2, 3, 4, 5, 6$, respectively. If it is mentioned below that all basis functions from the families with $\omega \leq \Omega$ (Ω is the so-called Pekeris number) are used in a calculation, then this means that the total number of basis functions is equal to $N(\Omega) = N(B_0) + N(B_1) + \dots + N(B_\Omega)$. For the total number of basis functions one easily finds $N(\Omega) = 1, 7, 28, 84, 210, 462, 924$ for $\Omega = 0, 1, 2, 3, 4, 5, 6$, respectively.

In our present calculations we used $N = 462, 588, 589, 783$, and 924 basis wave functions, respectively. The first value corresponds to the basis set which includes all complete families B_ω with $\omega \leq 5$. The basis set with $N = 588$ basis functions contains all complete families with $\omega \leq 5$ plus those from the $\omega = 6$ family for which the inequality $\max_i(n_{1i}, n_{2i}, n_{3i}, m_{1i}, m_{2i}, m_{3i}) \geq 4$ is obeyed. This means that this basis set includes the $(0, 2, 0, 4, 0, 0)$ basis function, but not the $(0, 2, 0, 2, 0, 2)$ basis function. The basis set with 589 basis functions consists of these 588 functions from the previous basis set plus the first $(3, 3, 0, 0, 0, 0)$ function from the subfamily with $\omega = 6$ for which $\max_i(n_{1i}, n_{2i}, n_{3i}, m_{1i}, m_{2i}, m_{3i}) = 3$. As it follows from Table I such an elementary $N \rightarrow N + 1$ increment may produce quite large changes in some properties, while the other properties remain almost unchanged. Analogously, the basis set with the $N = 783$ basis functions contains the basis functions from complete families with $\omega \leq 5$ plus those from the $\omega = 6$ family, for which $\max_i(n_{1i}, n_{2i}, n_{3i}, m_{1i}, m_{2i}, m_{3i}) \geq 3$. Unfortunately, the set of all 924 basis functions with $\omega \leq 6$ is nearly linear dependent and could not be taken into account (see also below). The basis set with 924 basis functions which we used in our present study includes the previous set with 783 basis functions plus all those basis functions from the family $\omega = 7$ for which $\max_i(n_{1i}, n_{2i}, n_{3i}, m_{1i}, m_{2i}, m_{3i}) \geq 4$. To compute the needed four-body integrals we applied our method developed in [13] (see also the Appendix).

The numerical results for some of the properties (i.e., expectation values) of the ground bound state in the ${}^\infty\text{HPs}$ hydride are presented in Table I, where the convergence for each of the properties is shown as a function of the total number of basis functions N . Since we use incomplete families of basis functions, such a convergence may have a quite nonsmooth form. For an arbitrary self-adjoint operator \hat{X} its expectation value is determined as follows: $\langle X \rangle = \langle \Psi | \hat{X} | \Psi \rangle / \langle \Psi | \Psi \rangle$, where $|\Psi\rangle$ is the respective wave function. The physical meaning of almost all of these expectation values seems to be quite clear, and we make only a few remarks. In Table I $\langle T \rangle$ and $\langle V \rangle$ are the expectation values for the kinetic and potential energies, respectively. The parameter E designates the total energy: $E = \langle T \rangle + \langle V \rangle$, while the deviation of the so-called virial parameter $\chi = |1 + \langle V \rangle / 2\langle T \rangle|$ from zero is an indicator of the quality of the wave function used. The π_{ij} are the Pearson correlation coefficients, $\pi_{ij} = \sqrt{\langle r_{ij}^2 \rangle - \langle r_{ij} \rangle^2} / \langle r_{ij} \rangle$, that express the uncertainty in the expected value of the coordinate r_{ij} , i.e., $\langle r_{ij} \rangle$, or the length of the ‘‘bond’’ between particles i and j .

To compute the two-particle δ -function expectation values, we used the definition $\hat{X} = \delta(\vec{r}_i - \vec{r}_j)$, where $i \neq j = 1, 2, 3, 4$. The three- and four-particle δ functions have been determined in an analogous manner, i.e., $\delta_{ijk} = \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_i - \vec{r}_k)$ and $\delta_{ijkl} = \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_i - \vec{r}_k) \delta(\vec{r}_i - \vec{r}_l)$, where $i \neq j = 1, 2, 3, 4$. The two-body cusp values are determined in the traditional way, i.e., the cusp between the particles i and j takes the form $\nu_{ij} = \langle \Psi | \delta(\vec{r}_i - \vec{r}_j) \partial / \partial r_{ij} | \Psi \rangle / \langle \Psi | \delta(\vec{r}_i - \vec{r}_j) | \Psi \rangle$ where $i \neq j = 1, 2, 3, 4$. In an arbitrary Coulomb system the exact ν_{ij} values equal $q_i q_j m_i m_j / (m_i + m_j)$, where q_i and q_j are the charges and m_i and m_j are the masses of particles i and j , respectively [14]. Note also that with the KT-variational expansion all appropriate cusp values equal zero identically [7]. Obviously, this is not true for the exact wave function. The results for the KT-variational expansion can also be found in Table I (in the right-hand column) [9]. The nonlinear parameters (α_{ij}) in the present KT wave function have been optimized a little bit better than in our earlier work [7]. Now, by applying the expectation value for the electron-positron δ function ($\langle \delta_{13} \rangle = \langle \delta_{+-} \rangle$) from Table I ($N = 924$) we can compute the two-photon annihilation rate for the ${}^\infty\text{HPs}$ hydride [4,7]: $\Gamma_{2\gamma} = 2\pi\alpha^4 c a_0^{-1} \langle \delta_{+-} \rangle \approx 100.617 480 9 \times 10^9 \langle \delta_{+-} \rangle \approx 2.4567 \times 10^9 \text{ sec}^{-1}$. The appropriate many-photon annihilation rates $\Gamma_{n\gamma}$, where $n \geq 3$ as well as $\Gamma_{1\gamma}$ and $\Gamma_{0\gamma}$ can be computed by using the formulas from [7]. Here, we do not wish to repeat all such calculations in detail.

In general, the agreement between our results from [7] and those given in Table I for most of the properties can be recognized as very good (even for the many-particle δ functions). The variational energies in Table I are slightly higher than those obtained in the KT expansion [7,15]. Likewise, the virial parameters χ are comparable with the respective values obtained in [7]. However, in comparison with the KT expansion [7] the JC-variational expansion has at least the two following advantages: (1) it can be used to compute the nontrivial two-body cusp values ν_{ij} for Coulomb systems, and (2) the expectation values for some of the properties, e.g., the outer moments $\langle r_{ij}^k \rangle$, where $k \geq 2$, are certainly more accurate than the appropriate values determined from the KT method. The inner moment $\langle r_{ij}^{-1} \rangle$ is slightly smaller for the KT expansion than for the JC expansion. In contrast, the outer moments $\langle r_{ij}^k \rangle$, where $k \geq 1$, are slightly larger for the KT expansion than for the JC expansion. The deviation increases with k . This means that the KT expansion describes HPs as slightly more diffuse than does the JC expansion [16].

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APPENDIX

Let us discuss briefly (all details can be found in [13]) the problem related with the calculations of the basic four-body integral $\mathcal{I} = \mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$ [17]:

$$\mathcal{I} = \int \int \int r_{14}^{K+2} r_{24}^{L+2} r_{34}^{M+2} r_{12}^{n_3} r_{13}^{n_2} r_{23}^{n_1} \times \exp(-\alpha r_{14} - \beta r_{24} - \gamma r_{34}) dr_{14} dr_{24} dr_{34}, \quad (\text{A1})$$

where K, L, M, n_1, n_2, n_3 are integer numbers, while α, β, γ are three real (positive) numbers. Actually, by applying the well known, routine procedure (see, e.g., [18,19]) this integral is expressed as a finite or, sometimes, an infinite sum of the auxiliary functions $A_1(k, a), A_2(k, \ell, a, b)$, and $A_3(k, \ell, m, a, b, c)$. Now, the central problem is to find very effective, fast, and numerically stable formulas in order to compute these auxiliary functions:

$$A_1(k, a) = A(k, a) = \int_0^{+\infty} x^k \exp(-ax) dx = \frac{k!}{a^{k+1}},$$

$$A_2(k, \ell, a, b) = \int_0^{+\infty} x^k \exp(-ax) dx \int_x^{+\infty} y^\ell \exp(-by) dy,$$

$$A_3(k, \ell, m, a, b, c) = \int_0^{+\infty} x^k \exp(-ax) dx \int_x^{+\infty} y^\ell \times \exp(-by) dy \int_y^{+\infty} z^m \exp(-cz) dz,$$

where all values k, ℓ, m are integers (k is always non-negative, while ℓ and m can be positive or negative) and a, b, c are real positive numbers. The case when all k, ℓ, m are positive is reduced to finite term expressions [13], while for the negative values of some of these parameters, prob-

ably, the best computational formula for the $A_2(k, \ell, a, b)$ (when $\ell < 0$) takes the form [13]

$$A_2(k, \ell, a, b) = \frac{A(k + \ell + 1, a + b)}{k + 1} \times {}_2F_1\left(1, k + \ell + 2; k + 2; \frac{a}{a + b}\right),$$

where ${}_2F_1(\alpha, \beta; \gamma; z)$ is the Gaussian hypergeometric function, i.e., ${}_2F_1(\alpha, \beta; \gamma; z) = 1 + \sum_{n=1}^{\infty} [(\alpha)_n (\beta)_n / (\gamma)_n n!] z^n$, and $(\alpha)_0 = 1, (\alpha)_1 = \alpha, \dots, (\alpha)_n = \alpha(\alpha + 1) \cdots (\alpha + n - 1) = \Gamma(\alpha + n) / \Gamma(\alpha)$, where $\Gamma(x)$ is the usual gamma-function (n is always a positive integer). In terms of this notation $(1)_n = n!$. The presented formal series for ${}_2F_1(\alpha, \beta; \gamma; z)$ is absolutely convergent only for $|z| < 1$. The analogous formula for the A_3 auxiliary function ($m < 0$) is [13]

$$A_3(k, \ell, m, \alpha, \beta, \gamma) = A(k + \ell + m + 2, \alpha + \beta + \gamma) \times \sum_{n=0}^{\infty} \frac{(k + \ell + m + 3)_n}{(k + 1)_{n+1}} \left(\frac{\alpha}{\alpha + \beta + \gamma}\right)^n \times D_{k+\ell+n+3}^m\left(\frac{\alpha + \beta}{\alpha + \beta + \gamma}\right), \quad (\text{A2})$$

where all notations are the same as before and the coefficients $D_K^m(y) = {}_2F_1(1, K + m; K; y) / (K - 1)$, where $K \geq 2, K + m \geq 0$ and $0 \leq y < 1$ always. Note that the last formula can be reduced to the form found in [19].

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- [1] A. Ore, Phys. Rev. **83**, 665 (1951).
 [2] C.F. Lebeda and D.M. Schrader, Phys. Rev. **178**, 24 (1969); P.B. Navin *et al.*, Phys. Rev. A **9**, 2248 (1974).
 [3] B.A. Page and P.A. Frazer, J. Phys. B **7**, L389 (1974).
 [4] Y.K. Ho, Phys. Rev. A **34**, 609 (1986).
 [5] R.J. Drachman, Can. J. Phys. **60**, 494 (1982); S.K. Houston and R.J. Drachman, Phys. Rev. A **7**, 819 (1973).
 [6] D.M. Schrader *et al.*, Phys. Rev. Lett. **69**, 57 (1992).
 [7] A.M. Frolov and V.H. Smith, Jr., Phys. Rev. A **55**, 2662 (1997).
 [8] N.N. Kolesnikov and V.I. Tarasov, Yad. Fiz. **35**, 609 (1982) [Sov. J. Nucl. Phys. **35**, 354 (1982)].
 [9] This notation differs completely from that used in our previous work [7]. In the James-Coolidge and related methods it is assumed that particle 4 has very large (even infinitely large) mass, while 1, 2, and 3 denote the so-called light particles. Such a choice is needed for all similar methods, which are based on calculations of the so-called basic four-body integral (see Appendix).
 [10] H.M. James and A.S. Coolidge, Phys. Rev. **49**, 688 (1936).
 [11] Both of our brief notations KT and JC expansions are not commonly used in the literature to designate the variational expansions Eqs. (1) and (2), respectively. We use these notations in the present study only for brevity, and to make a few comparisons between them. Note also that James and Coolidge proposed another variational method for the highly accurate molecular calculations in ellipsoidal coordinates [J. Chem. Phys. **1**, 825 (1933)]. However, in the present work the name JC expansion is used only for Eq. (2).
 [12] The variational expansion Eq. (2) can be considered as a generalization of the Hylleraas method to the four-body problem [1]. Obviously, Eq. (2) is only one of a few possible such generalizations (see, e.g., discussion in [13]).
 [13] A.M. Frolov and V.H. Smith, Jr., Int. J. Quantum Chem. **63**, 269 (1997).
 [14] R.T. Pack and W. Byers-Brown, J. Chem. Phys. **45**, 556 (1966).
 [15] Our previous work [7] contains the variational results for various HPs systems, i.e., ${}^{\infty}\text{H}$, TPs, DPs, ${}^1\text{HPs}$, and MuPs. For the present study we have reoptimized the wave function for ${}^{\infty}\text{HPs}$, and found the total energy $-0.789\,181\,8$ a.u. for the ${}^{\infty}\text{HPs}$ system (i.e., $-1.066\,192$ eV for its binding energy).
 [16] The appropriate JC results for other complete families of basis functions are $E(N=1, \omega=0) = -0.551\,631\,521$ a.u., $E(N=7, \omega \leq 1) = -0.744\,701\,881$ a.u., $E(N=28, \omega \leq 2) = -0.778\,527\,035$ a.u., $E(N=84, \omega \leq 3) = -0.786\,802\,75$ a.u., and $E(N=210, \omega \leq 4) = -0.788\,676\,668$ a.u.
 [17] This integral is often called the ‘‘basic’’ four-body integral, since if the expression for $\mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$ is known, then all matrix elements for the Hamiltonian, the overlap matrix, etc. can be found easily from this.
 [18] J.F. Perkins, J. Chem. Phys. **48**, 1985 (1968); Y.K. Ho and B.A.P. Page, J. Comput. Phys. **17**, 122 (1975).
 [19] G.W.F. Drake and Z.C. Yan, Phys. Rev. A **52**, 3681 (1995).