

Variational calculations of the energy levels of μ -mesic molecules of hydrogen isotopes

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A variational calculation has been carried out of the level energies $\epsilon_{J\nu}$ of nine vibrational-rotational states ($J\nu$) of the mesic molecules of hydrogen isotopes with angular momentum $J = 1$. About 1000 basis functions were used in the calculation, which ensured that the binding energies could be determined to within 0.001 eV. For weakly-bound states ($J = 1, \nu = 1$) of the mesic molecules $dd\mu$ and $dt\mu$, which are of particular interest in muon catalysis, it was found that $\epsilon_{11}(dd\mu) = -1.9749 \pm 0.0002$ eV and $\epsilon_{11}(dt\mu) = -0.663 \pm 0.002$ eV.

1. INTRODUCTION

The binding energies of twenty-two vibrational-rotational states of the mesic molecules of hydrogen isotopes were reported in Ref. 1. They were calculated to within 0.1 eV in the adiabatic representation of the three-body problem.² There is particular interest in the energy levels of the mesic molecules $dd\mu$ and $dt\mu$ in the $J = 1, \nu = 1$ state because they determine the resonance mechanism of formation of these mesic molecules³ and are important in calculations of the rate of nuclear fusion reactions.⁴ These weakly-bound states must be calculated to within 0.001 eV if they are to be used in reliable calculations of the rates and kinetics of processes involving muon catalysis, and in the accurate interpretation of recent experiments.⁵ A call was made in Ref. 1 for an independent confirmation of the calculations reported in that paper by methods other than the adiabatic approach, and for higher precision.

This program has been implemented along two lines. The first approach involves increasing the precision of algorithms within the framework of the adiabatic method, and was presented in a recent paper.⁶ We note that it was not until quite recently that new variational calculations^{7–10} of the energy levels of mesic molecules became available. They were found to agree to within the stated precision with calculations performed by the adiabatic method, but claimed higher precision.

In order to improve the results reported in Ref. 1, and to compare them with those reported in Refs. 6–10, we have implemented a variational scheme for the solution of the three-body Schrodinger equation in spheroidal coordinates,^{2,11} for which a solution had previously been obtained within the framework of the adiabatic method. As already noted in Ref. 12, these coordinates reflect most completely the symmetry and dynamics of three-particle interactions in mesic molecules. They have the further advantage that the variational calculations mentioned above^{7–10} use perimetric coordinates, and it is interesting to compare the properties of these independent computational schemes.

The first success in the calculation of the rotational levels of mesic molecules by the variational method using spheroidal coordinates was reported in Ref. 13. In our scheme, we use a system of trial functions similar to that

employed in Ref. 13, but with an extended set of nonlinear parameters and significantly better trial functions, so that the wave function can be described correctly both in the interaction and the asymptotic regions.

The implementation of this variational scheme together with the variational-difference method¹⁴ is the second line of approach, which involves the development of independent methods of calculating the energy levels of μ -mesic molecules of the hydrogen isotopes. In this paper, we report variational calculations of the energy levels of mesic molecules of hydrogen isotopes in the $J = 1$ state, using about 1000 basis functions. This enabled us to reach a precision of about 0.001 eV, which meets the current requirements of theory and experiment.

2. SCHROEDINGER EQUATION FOR THE $J=0$ AND $J=1$ ROTATIONAL STATES OF MESIC MOLECULES, AND CHOICE OF VARIATIONAL WAVE FUNCTIONS

A mesic molecule is usually understood to be a molecular ion consisting of the nuclei of the hydrogen isotopes p, d , or t and a negatively charged muon.¹⁵ The Hamiltonian for the three particle system is¹ ($e = \hbar = m_e = 1$)

$$H = - (2M_0)^{-1} \{ (\nabla_{\mathbf{R}} + \kappa \nabla_{\mathbf{r}} / 2)^2 - [(1 + \kappa) / 2]^2 \Delta_r \} + \hbar_a + R^{-1} \quad (1)$$

where \mathbf{R} is the position vector of nucleus a relative to nucleus b , \mathbf{r} is the position vector of the muon relative to the midpoint of the segment R , $M_0 = M_a M_b / (M_a + M_b)$ is the reduced mass of the nuclei ($M_a \geq M_b$), $\kappa = (M_b - M_a) / (M_a + M_b)$, $\frac{1}{2}\kappa R$ is the distance between the midpoint of the segment R and the center of mass of the nuclei,

$$\hbar_a = - (2m_a)^{-1} \Delta_r - r_a^{-1} - r_b^{-1} \quad (2)$$

is the Hamiltonian of the muon in the field of fixed nuclear charges, r_a and r_b are the distances between the muon and the two nuclei, and $m_a = m_\mu M_a / (m_\mu + M_a)$ is the reduced mass of the muon in the mesic atoms ($a\mu$), where $a \equiv p, d, \text{ or } t$. The Hamiltonian shows explicitly the dependence on the reduced mass of the muon because we are interested not in the total energy E of the mesic molecule, but in its binding energy $-\epsilon_{J\nu} = (E + \frac{1}{2}m_a)2R_y$. This energy differs from the energy $E_{a\mu} = -m_a R_y$ of the ground state of the mesic atoms ($a\mu$) of mass $M_a \geq M_b$. The following

constants are used in our calculations: $Ry = 13.6058041$ eV, $M_p = 1836.151527$, $M_d = 3670.481$, $M_t = 5436.918$, $m_\mu = 206.769$.

The Hamiltonian (1) was obtained in Ref. 16 in the representation of the total orbital angular momentum J in a rotating spheroidal coordinate system $\{\mathbf{R}, \mathbf{r}\} = \{R\theta\Phi, \xi\eta\varphi\}$, and is given in an explicit form in Refs. 2 and 11.¹⁾ In the latter papers, the three-particle Schrodinger equation was obtained in the spheroidal coordinate system for a $(J+1)$ -component wave function $\{F_m^{J\lambda}(\xi\eta R)\}_{m=0, J}$ in the region $\Omega = \{1 \leq \xi < \infty, -1 \leq \eta \leq 1, 0 < R < \infty\}$, where $m = 0, 1, \dots, J$ are the eigenvalues of the projection of J onto R that label the components of the wave function for fixed J and total parity $\lambda = \sigma_{yz} (-1)^J = \pm 1$, which determines the sign of the rotational state.²⁾ This equation can be used to calculate any rotational-vibrational state (Jv) of mesic molecules. For $J=0$, $\lambda=1$, and $J=+1$, $\lambda=-1$, it takes the form ($e = \hbar = m_a = 1$)

$$J=0: (H_{00}^{0+} - E)F_0^{0+} = 0, \quad (3)$$

$$H_{00}^{0+} = -\frac{1}{2M} \frac{1}{R^2} \frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} + \frac{1}{MR^2} \frac{1}{\xi^2 - \eta^2} \left[(\xi - \kappa\eta) (\xi^2 - 1) \left(\frac{\partial}{\partial \xi} + R \frac{\partial^2}{\partial \xi \partial R} \right) + (\eta - \kappa\xi) (1 - \eta^2) \left(\frac{\partial}{\partial \eta} + R \frac{\partial^2}{\partial \eta \partial R} \right) - \frac{1}{2} \left\{ 1 + \frac{1}{4M} [\xi^2 + \eta^2 - 2 - 2\kappa(\xi\eta + 1)] \right\} \frac{4}{R^2} \frac{1}{\xi^2 - \eta^2} \left[\frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} \right] - \frac{4}{R} \frac{\xi}{\xi^2 - \eta^2} + \frac{1}{R} \right]$$

$$\int d\xi d\eta dR \tau (F_0^{0+})^2 = 1, \quad \tau = 1/8 R^5 (\xi^2 - \eta^2),$$

$$J=1: \begin{pmatrix} H_{00}^{1-} - E & H_{10}^{1-} \\ H_{10}^{1-} & H_{11}^{1-} - E \end{pmatrix} \begin{pmatrix} F_0^{1-} \\ F_1^{1-} \end{pmatrix} = 0, \quad (4)$$

$$H_{00}^{1-} = H_{00}^{0+} + \frac{1}{MR^2},$$

$$H_{11}^{1-} = H_{00}^{0+} + \frac{2}{R^2} \frac{\{1 + (4M)^{-1} [\xi^2 + \eta^2 - 2 - 2\kappa(\xi\eta + 1)]\}}{(\xi^2 - 1)(1 - \eta^2)},$$

$$H_{01}^{1-} = -H_{10}^{1-} - \frac{1}{MR^2} \frac{\xi\eta - \kappa}{[(\xi^2 - 1)(1 - \eta^2)]^{1/2}},$$

$$H_{10}^{1-} = \frac{1}{MR^2} \frac{[(\xi^2 - 1)(1 - \eta^2)]^{1/2}}{\xi^2 - \eta^2} \left[(\eta - \kappa\xi) \frac{\partial}{\partial \xi} - (\xi - \kappa\eta) \frac{\partial}{\partial \eta} \right],$$

$$\int d\xi d\eta dR \tau [(F_0^{1-})^2 + (F_1^{1-})^2] = 1,$$

where³⁾ $M = M_0/M_a$ is the reduced mass of the nuclei and the superscripts (\pm) represent the rotational states $\lambda = \pm 1$. The binding energy is given by $-\epsilon_{Jv} = (E + 1/2m_a)2Ry$.

Three-dimensional boundary value problems such as (3)–(4) can be solved in various ways, including the method in which a reduction is made to the Kantorovich ordinary differential equations¹⁷ or to the Bubnov-Galerkin and Rayleigh-Ritz algebraic equations. Many variational procedures can be reduced in this way and can be used even in the case of nonlinear parameters, since these parameters are usually op-

timized independently of the linear parameters. The first line of approach was used in Ref. 1, in which $F(\xi\eta R)$ was expanded in terms of a complete set of solutions for the two-body problem (2). In our calculations, we employed a variational procedure based on the minimax principle, using several sets of nonlinear parameters chosen on the basis of our previous experience with the adiabatic basis. Thus, in constructing the basis functions, we took into account the properties of the π -components, the (g, u) symmetry⁴ and certain known asymptotic properties of the solutions.² The expansions for the variational σ - and π -functions with $J=1$ have the following form:

$$F_0^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(0s)} R^{i-1} \xi^{j-1} \eta^{k-1} e^{-\alpha_s R} e^{-\beta_s R \xi}, \quad (5a)$$

$$i, j, k = 1, 2, \dots; i > j,$$

$$F_1^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(1s)} (\xi^2 - 1)^{1/2} (1 - \eta^2)^{1/2} R^{i-1} \xi^{j-1} \eta^{k-1} e^{-\gamma_s R} e^{-\nu_s R \xi}, \quad (5b)$$

$$i, j, k = 1, 2, \dots; i > j + 1.$$

For mesic molecules with identical nuclei ($\kappa = 0$), the presence of the additional (g, u) symmetry leads to a restriction on the possible combinations of quantum numbers $(-1)^{J+I} = p$ for given total nuclear spin I , to a reduction in the size of the region Ω in the variable η : $\{0 \leq \eta \leq 1$, and, correspondingly, to a less dense set of basis functions for the σ - and π -functions:

$$F_{0g}^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(0s)} R^{i-1} \xi^{j-1} \eta^{2k-2} e^{-\alpha_s R} e^{-\beta_s R \xi}, \quad (6a)$$

$$i, j, k = 1, 2, \dots; i > j,$$

$$F_{1g}^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(1s)} (\xi^2 - 1)^{1/2} (1 - \eta^2)^{1/2} R^{i-1} \xi^{j-1} \eta^{2k-1} e^{-\gamma_s R} e^{-\nu_s R \xi}, \quad (6b)$$

$$i, j, k = 1, 2, \dots; i > j + 1.$$

The basis functions with the first set of nonlinear parameters $\{\alpha, \beta, \gamma, \nu\}$ were used to approximate the asymptotic behavior of the variational functions for $R \rightarrow 0$, whereas the second set $\{\alpha, \beta, \gamma, \nu\}$ was used for $R \rightarrow \infty$.

The dynamics of the $J=1, v=1$ weakly-bound state of the mesic molecule $d\mu$ was correctly taken into account by taking the variational σ -function as the sum of the g - and u -components $F_0^{1-} = F_{0g}^{1-} + F_{0u}^{1-}$, where

$$F_{0g}^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(0sg)} R^{i-1} \xi^{j-1} \eta^{2k-2} e^{-\alpha_{sg} R} e^{-\beta_{sg} R \xi}, \quad (7a)$$

$$F_{0u}^{1-} = \sum_{s=1}^2 \sum_{ijk} a_{ijk}^{(0su)} R^{i-1} \xi^{j-1} \eta^{2k-1} e^{-\alpha_{su} R} e^{-\beta_{su} R \xi}, \quad (7b)$$

$$i, j, k = 1, 2, \dots; i > j.$$

This representation is justified, on the one hand, by the small value $\kappa(2M)^{-1} \approx 0.01$ and, consequently, the approximate conservation of (g, u) symmetry, while, on the other hand, it ensures that the correct dissociation limit is obtained for the $d\mu$ mesic molecule decaying into the mesic atom μ and the

TABLE I. Calculated binding energies of mesic molecules with angular momentum $J = 1$.

Mesic molecule	Variant #1						Variant #2						Variant #3						Variant #4						Variant #5											
	σ			π			σ			π			σ			π			σ			π			σ			π								
	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η	N_R	N_ξ	N_η						
$pd\mu, ddt\mu, \nu=0$	6	4	4	4	2	2	7	4	6	4	2	3	7	5	6	4	3	3	—						—											
	6	3	4	4	2	2	6	4	4	4	2	2	7	4	6	4	2	2	—						—											
Total: 200						Total: 304						Total: 438																								
$dt\mu, \nu=1$	6	3	4	3	2	2	6	4	4	4	2	2	7	4	5	4	2	2	7	5	5	4	3	3	7	6	6	5	3	3	7	6	6	5	3	3
	6	3	6	3	2	3	7	4	6	4	2	3	7	5	7	4	3	4	7	6	8	5	3	4	8	6	9	6	3	4	8	6	9	6	3	5
Total: 210						Total: 304						Total: 449						Total: 607						Total: 819												
$dd\mu, \nu=1$	6	4	4	4	2	2	7	4	5	4	2	2	7	5	5	4	3	3	7	6	6	5	3	3	8	7	7	6	4	4	8	7	10	7	4	6
	7	4	6	4	2	3	7	5	7	4	3	4	7	6	8	5	3	4	8	6	9	6	3	5	9	7	10	7	4	6						
Total: 304						Total: 449						Total: 607						Total: 819						Total: 1286												
$pd\mu, dt\mu, \nu=0$	6	3	7	3	2	4	7	4	9	4	2	6	7	5	10	4	3	7	—						—											
	6	3	7	3	2	4	6	4	7	4	2	4	6	4	9	4	2	6	—						—											
Total: 300						Total: 500						Total: 698																								
$dt\mu, \nu=1$	6	3	4	3	2	4	6	4	4	4	2	2	7	4	5	4	3	4	7	5	5	4	3	5	7	6	6	5	3	3	7	6	6	5	3	3
	6	3	5	3	2	4	7	4	6	4	2	3	7	5	7	5	3	7	8	6	7	5	3	7	9	6	8	6	3	5	9	6	8	6	3	5
Total: 330						Total: 568						Total: 844						Total: 982						Total: 1495												

nucleus d . We note that the correct origin was used for E_{μ} in the Hamiltonian (1) and, as shown in Ref. 2, is asymptotically reproduced in (3) and (4).

To improve the convergence of the expansions (5)–(7), we have thinned out the series of basis functions. This is possible because the sequences used in (5)–(7) are not the minimum sequences as defined in Ref. 18. A numerical experiment was used to choose certain sequences of basis functions in (5)–(7) in order to achieve the most successful approximation to the required solution. The following sets of basis functions were used in our calculations for the σ - and π -functions, respectively:

$$J = 1, \kappa \neq 0$$

$$j = 1, 2, 3, \dots; i = j + s_i, s_i = 1, 2, 3, 5, 7, 9, \dots;$$

$$\kappa = 1, 2, 3, 4, 5, 6, 9, 10, 13, 14, \dots \quad (5c)$$

$$j = 1, 2, 3, \dots; i = j + s_i + 1, s_i = 1, 2, 4, 6, \dots;$$

$$k = 1, 2, 3, 4, 7, 8, 11, 12, \dots, \quad (5d)$$

$$J = 1, \kappa = 0$$

$$j = 1, 2, 3, 4, 6, 8, 10, \dots; i = j + s_i, s_i = 1, 2, 3, 5, 7, 9, 11, \dots;$$

$$k = 1, 2, 3, 5, 7, 9, \dots \quad (6c)$$

$$j = 1, 2, 3, 5, 7, \dots; i = j + s_i + 1, s_i = 1, 2, 4, 6, 8, \dots;$$

$$k = 1, 2, 4, 8, \dots \quad (6d)$$

The corresponding versions are shown in Table I, where N_R , N_ξ , and N_η represent, respectively, the number of basis functions in the coordinates R , ξ , and η , chosen in accordance with (5) and (6).

3. METHOD OF CALCULATION

The well-known minimax principle¹⁸ is implemented in our computational scheme. Thus, the approximate values of the energy levels corresponding to a particular ν in the n -dimensional space described by a finite set of n basis functions $\{\varphi_j\}, j = 1, \dots, n$ are given by

$$E_\nu^{(n)} = \min_{\chi_\nu^{(n)}(\omega)} \max_{\Psi^{(n)}} \left\{ \frac{(\Psi^{(n)}, H\Psi^{(n)})}{(\Psi^{(n)}, \Psi^{(n)})} \right\}, \quad \nu = 0, 1, \dots, \quad (8)$$

where $\Psi^{(n)}$ is an arbitrary linear combination of basis functions, which can also depend on the choice of nonlinear parameters ω , and $\chi_\nu^{(n)}(\omega)$ is the $(\nu + 1)$ -dimensional subspace on the set of basis functions. It is well-known,¹⁹ for a fixed set of nonlinear parameters ω , that $E_\nu \leq E_\nu^{(n)}(\omega)$, and this bound continues to hold as additional minimization of $E_\nu^{(n)}(\omega)$ with respect to the set ω is carried out.

Our computational scheme is implemented as follows. With a given set ω , we first calculate $E_\nu^{(n)}(\omega)$ in accordance with (8). The determination of the coefficients in (5)–(7), for which (8) is satisfied, then reduces to the solution of the algebraic eigenvalue problem:

$$\mathbf{A}(\omega)\mathbf{X} = \lambda\mathbf{B}(\omega)\mathbf{X}, \quad (9)$$

where

$$\mathbf{A}(\omega) = \{a_{ij}\} = \{(\varphi_i(\omega), H\varphi_j(\omega))\},$$

$$\mathbf{B}(\omega) = \{b_{ij}\} = \{(\varphi_i(\omega), \varphi_j(\omega))\}.$$

The basis functions are normalized to unity.

The eigenvalue problem (9) was solved in two ways. In the first method, the problem was reduced to the standard form.²⁰ The following regularization procedure was em-

TABLE II. Nonlinear parameters used in calculations ($J = 1$)

v	Mesic molecule	α_1	β_1	γ_1	ν_1	α_2	β_2	γ_2	ν_2
0	$pp\mu$	3.2	1.45	3.2	1.4	1.3	1.1	1.3	1.1
0	$dd\mu$	4.0	1.45	3.6	1.4	1.6	1.1	1.5	1.1
0	$tt\mu$	4.8	1.45	4.4	1.4	3.8	1.1	3.4	1.1
1	$dd\mu$	3.5	1.375	3.5	1.4	0.001	1.0	0.01	1.1
1	$tt\mu$	4.6	1.375	3.9	1.4	1.4	1.15	1.4	1.1
0	$pd\mu$	3.6	1.45	3.7	1.4	1.4	1.1	1.5	1.1
0	$pt\mu$	3.7	1.45	3.7	1.4	1.4	1.1	1.4	1.1
0	$dt\mu$	4.3	1.45	4.1	1.4	2.2	1.1	2.1	1.1
1	$g\text{-четн.}$	4.6	1.35	4.0	1.4	0.01	1.15	0.1	1.2
	$d\mu$								
	$u\text{-нечетн.}$	2.4	0.85	4.0	1.4	0.001	0.85	0.1	1.2

Footnote. The state $J = 1, v = 1$ has even and odd components for the σ -function of the mesic molecule $d\mu$. The values of all the parameters are multiplied by the coefficient $q = 2m_\sigma/m_0$, $m_0^{-1} = (M_a + M_b)^{-1} + M_c^{-1}$.

ployed. If, for a given set d_{ij} , the condition

$$\left\| \varphi_i - \sum_{j < i} d_{ij} \varphi_j \right\| < \varepsilon,$$

was satisfied, where ε is the regularization parameter, the columns and rows containing these elements of the matrices A and B were deleted and (9) was solved for the lower dimensionality. This procedure was incorporated in an algorithm for the expansion of the matrix B in accordance with the Choleski scheme, which enabled us to obtain a stable algorithm that was no less effective than the standard procedure used in Ref. 20.

The second method includes the regularization of the matrix B : $\tilde{B} = B + \varepsilon E$, where E is a unit matrix and ε is the regularization parameter. The solution of (9) with the regularized matrix \tilde{B} was performed by inverse iteration. The

initial approximation to the eigenvalues were taken from Ref. 1, and the approximations converged with the required precision after three or four iterations. The efficient Bunch algorithm was used in each iteration to solve the set of algebraic equations. The matrices were stored in symmetric form, which meant that we could work with matrices of dimensionality 1000 in computer memory.

The computational error of the inverse iteration method was monitored in the course of the solution of the regularized problem (9) (with matrices of dimensionality up to 500) by comparison with a solution of (9) of known precision, obtained by the standard reduction method. This error was less than 10^{-5} eV when the regularization parameter was equal to 10^{-12} . For large dimensionalities ($m > 500$), the estimated error in the solution of (9) was obtained by comparing calculations made by the inverse iteration method with different values of the regularization parameter

TABLE III. Binding energies $-\varepsilon_{Jv}$ (in eV) of the mesic molecules of hydrogen with angular momentum $J = 1$.

Reference	$pp\mu$ $v=0$	$dd\mu$ $v=0$	$tt\mu$ $v=0$	$dd\mu$ $v=1$	$tt\mu$ $v=1$	$pd\mu$ $v=0$	$pt\mu$ $v=0$	$dt\mu$ $v=0$	$dt\mu$ $v=1$
[1]	106.96 (264)	226.61 (264)	289.15 (264)	1.956 ** (844)	45.24 (264)	97.40 (264)	99.01 (264)	232.44 (844)	0.656 ** (844)
[7]	107.266 (286)	226.662 (286)	289.12 (286)	1.862 (364)	45.096 (286)	97.493 (440)	99.119 (440)	232.436 * (300)	0.623 * (500)
Extrapolation	107.266	226.680	289.12	1.87	45.187	97.493	99.119	-	-
[8]	107.26563 (250)	226.68157 (250)	289.13931 (250)	1.97110 *** (350)	45.19359 (250)	97.42990 (250)	99.10104 (250)	232.42049 (250)	0.60719 *** (400)
Extrapolation	107.267	226.683	289.146	1.972±0.001 ***	45.22	97.66	99.13	232.48	0.6554± ±0.0150 ***
Present work	107.26364 (200)	226.68106 (200)	289.14142 (200)	1.96933 (304)	45.20093 (210)	97.49232 (300)	99.12044 (300)	232.47020 (300)	0.60304 (330)
	107.26533 (304)	226.68160 (304)	289.14191 (304)	1.97274 (449)	45.20451 (304)	97.49624 (500)	99.12471 (500)	232.47142 (500)	0.64772 (568)
	107.26568 (438)	226.68164 (438)	289.14195 (438)	1.97368 (607)	45.20524 (449)	97.49774 (698)	99.12608 (698)	232.47155 (698)	0.65228 (844)
	-	-	-	1.97431 (849)	45.20552 (607)	-	-	-	0.65371 (982)
	-	-	-	1.97465 (1286)	-	-	-	-	0.65889 (1495)
Extrapolation	107.2659	226.6817	289.1420	1.9749±0.0002	45.2058	97.4990	99.1271	232.4717	0.663±0.002

*Results from Ref. 9; **results from Ref. 6; ***results from Ref. 10b.

($\varepsilon = 10^{-11}$ and 10^{-12}). The error was then less than 10^{-4} eV.

The calculations were performed for a number of sets of nonlinear parameters. This was used to find the optimum values of these parameters and the minimum values of $E_{Jv}^{(n)}(\omega)$. The optimum values of the nonlinear parameters for mesic molecules with $J = 1$ are listed in Table II.

4. RESULTS

Table III lists the calculated binding energies $-\varepsilon_{Jv}$ of the mesic molecules of hydrogen isotopes for the ground ($v = 0$) and excited ($v = 1$) vibrational states with orbital angular momentum $J = 1$. The table also lists the best results of adiabatic^{1,6} and variational⁷⁻¹⁰ calculations. The number in parentheses under each value of $-\varepsilon_{Jv}^{(n)}$ is the number n of basis functions used in the calculation.

Our results were obtained for a sequence of five increasing sets of basis functions with $n = n_1 < n_2 < \dots < n_s$, $3 \leq s \leq 5$, which enabled us to follow their convergence. Table I lists the necessary information on the sets of basis functions (5)–(7) for each state (Jv).

Let us now consider the extrapolation of the energies $\varepsilon_{Jv}^{(n)}$ to $n \rightarrow \infty$. We used the following extrapolation formula, which is commonly employed in variational calculations:

$$\varepsilon_{Jv} = \varepsilon_{Jv}^{(n)} + Cn^{-\alpha}. \quad (10)$$

Improved values of the energy ε_{Jv} and the parameters C , α can be found, by three suitably chosen calculations, from the available sequence with $n = n_1, \dots, n_s$, as was done, for example, in Refs. 7 and 10. The same problem can be solved by analyzing the entire series of calculations with $n = n_1, \dots, n_s$ by the method of least squares. We have used both methods and found that they yielded consistent values of ε_{Jv} . Analysis of the results listed in Table III and calculations based on the extrapolation formula (10) showed that the improved values of ε_{Jv} were subject to an uncertainty of less than 0.001 eV. The exception is the weakly-bound state ($J = 1, v = 1$) of the $dt\mu$ mesic molecule for which the improved energy was determined to within 0.002 eV.

All the calculations were performed on the ES-1061 computer, using double precision arithmetic. The most laborious calculation ($n = 1495$) was carried out with quadruple precision and required 12 hours of processor time. One variant with the lower figure of $n = 200$ took less than 2 min.

5. DISCUSSION OF RESULTS

Interest in variational calculations on mesic molecules practically ceased after 1976, but was rekindled by the work of Demkov and Filinskii.²¹ They considered mesic molecules with $J = 1$, and constructed three types of variational function in perimetric coordinates with nonstandard basis elements, namely, Laguerre polynomials, fractional powers, and exponentials. The expansion in terms of exponentials was extended in Refs. 8 and 10 to the $J \neq 0$ case. The intention of this work was to perform high-precision calculations, and this led to the use of a large number of basis functions. However, it is known that increasing the number of nonorthogonal basis functions leads to algebraic systems that are more difficult to handle, and improved precision cannot be achieved without regularizing procedures.²²

We also note that, when a large number of basis functions is used, the results of different variational calculations are not very sensitive to their form. This can be seen by comparing the different calculations listed in Table III for different sets of basis functions. The quality criterion adopted in variational calculations is the depth of the minimum of the variational function. Comparisons based on this criterion show that the basis functions expressed in terms of different coordinates still describe the three-particle wave functions with different precision, depending on the particle mass ratio. In the $dd\mu$ and $dt\mu$ mesic molecules, whose weakly-bound states are of particular interest, the reduced mass of the nuclei is large, and the basis functions employed in our calculations in terms of spheroidal coordinates are more optimal.

We note that the value found for $-\varepsilon_{Jv}$ in the case of the mesic molecule $dt\mu$ ($J = 1, v = 1$) agrees with the result obtained by the adiabatic approach in Ref. 6.

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¹The nuclei a and b are located at the respective foci $\{\xi = 1, \eta = -1\}$ and $\{\xi = 1, \eta = 1\}$ of the spheroidal coordinate system $\mathbf{r} = \{\xi, \eta, \varphi\}$, where $\xi = (r_a + r_b)/R$, $\eta = (r_a - r_b)/R$, and φ is the rotation angle about the major axis of the ellipse. The latter is oriented in the direction $\mathbf{R} = \{R\theta\Phi\}$, i.e., its orientation in the laboratory system of coordinates is given in spherical coordinates by the angles θ and Φ .

²Following molecular terminology, we will refer to the components with $m = 0, 1$ as σ and π components; $\sigma_{yz} = \pm 1$ is the eigenvalue of the reflection operator in the plane defined by the unit vectors \mathbf{e}_R and \mathbf{e}_Φ .

³The operator H_{10}^- can be represented more symmetrically as

$$H_{10}^- = \frac{1}{MR^2} \frac{1}{\xi^2 - \eta^2} \left\{ \frac{\partial}{\partial \xi} [(\xi^2 - 1)(1 - \eta^2)]^{1/2} (\eta - \kappa\xi) - \frac{\partial}{\partial \eta} [(\xi^2 - 1)(1 - \eta^2)]^{1/2} (\xi - \kappa\eta) \right\} - \frac{1}{MR^2} \frac{\xi\eta - \kappa}{[(\xi^2 - 1)(1 - \eta^2)]^{1/2}},$$

which, as was shown in Ref. 11, gives rise to a symmetric bilinear form in the Rayleigh-Ritz variational functional.

⁴The eigenvalues for the operator which inverts the muon coordinates $\mathbf{r} \rightarrow -\mathbf{r}$ are given by $p \equiv (g, u) = \pm 1$.

⁵S. I. Vinitiskii, V. S. Melezhik, L. I. Ponomarev, *et al.*, Zh. Eksp. Teor. Fiz. **79**, 698 (1980) [Sov. Phys. JETP **52**, 353 (1980)].

⁶S. I. Vinitiskii and L. I. Ponomarev, EChAYa **13**, 556 (1982).

⁷S. I. Vinitiskii, L. I. Ponomarev, I. V. Puzynin, *et al.*, Zh. Eksp. Teor. Fiz. **74**, 849 (1978) [Sov. Phys. JETP **47**, 444 (1978)].

⁸L. N. Bogdanova, V. E. Markushin, and V. S. Melezhik, Zh. Eksp. Teor. Fiz. **81**, 829 (1981) [Sov. Phys. JETP **54**, 42 (1981)].

⁹S. E. Jones, A. N. Anderson, A. J. Caffrey, *et al.*, Phys. Rev. Lett. **51**, 1757 (1983).

¹⁰A. D. Gocheva, B. B. Gusev, V. S. Melezhik, *et al.*, Phys. Lett. B **153**, 349 (1985).

¹¹A. K. Bhatia and R. J. Drachman, Phys. Rev. **30**, 2138 (1984).

¹²A. M. Frolov and V. D. Efros, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 449 (1984) [JETP Lett. **39**, 544 (1984)].

¹³C. Y. Hu, Phys. Rev. **32**, 1245 (1985).

¹⁴A. M. Frolov and V. D. Efros a) Yad. Fiz. **41**, 828 (1985) [Sov. J. Nucl. Phys. **41**, 528 (1985)]. b) J. Phys. B **18**, L265 (1985).

¹⁵M. Kaschiev and S. I. Vinitiskii, Preprint JINR, E4-85-467, Dubna, 1985.

¹⁶R. C. Whitten and J. S. Sims, Phys. Rev. A **9**, 1588 (1974).

- ¹³A. Halpern, *Phys. Rev. Lett.* **13**, 660 (1964).
- ¹⁴V. V. Gusev and M. S. Kaschiev, Preprint OIYaI, R11-85-758, Dubna, 1985.
- ¹⁵Ya. B. Zel'dovich and S. S. Gershtein, *Usp. Fiz. Nauk* **71**, 581 (1960) [*Sov. Phys. Uspekhi* **3**, 593 (1961)].
- ¹⁶S. I. Vinitskiĭ and L. I. Ponomarev, *Yad. Fiz.* **20**, 576 (1974) [*Sov. J. Nucl. Phys.* **20**, 310 (1975)].
- ¹⁷L. V. Kantorovich and V. I. Krylov, *Priblizhennyye metody vysshego analiza* Fizmatgiz, Moscow-Leningrad, 1962 (*Approximate Methods of Higher Analysis*, Wiley, New York, 1959).
- ¹⁸S. G. Mikhlin, *Chislennaya realizatsiya variatsionnykh metodov* (Numerical Implementation of Variational Methods), Nauka, Moscow, 1966.
- ¹⁹B. N. Parlett, *The Symmetric Eigenvalue Problem*, Prentice-Hall, 1980 [Russian translation, Mir, 1983].
- ²⁰J. H. Wilkinson and G. Reinsch, *Handbook for Automatic Computation. Linear Algebra* [Russian translation, Mashinostroenie, Moscow, 1976], Springer-Verlag, 1971, Vol. 2.
- ²¹Yu. N. Demkov and A. V. Filinskiĭ, in Abstracts of Papers read to the All-Union Conf. on the Theory of Atoms and Atomic Spectra, Academy of Sciences of the Belorussian SSR, Minsk, 1983; in Abstracts of a Conference on Quantum Chemistry, Dnepropetrovsk State University, 1983, p. 12.
- ²²A. N. Tikhonov and V. Ya. Arsenin, *Metody resheniya nekorrektnykh zadach* (Solutions of Ill-posed Problems), Nauka, Moscow, 1974.

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