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TEMPERATURE DEPENDENCE OF THE FORMATION RATES OF HYDROGEN-HELIUM MESIC MOLECULES IN COLLISIONS OF SLOW HYDROGEN ATOMS WITH HELIUM

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The rates of the molecular muon transfer from the ground state muonic hydrogen to helium isotopes are calculated in an improved adiabatic approximation. The results obtained by us at various temperatures are compared with the available experimental data.

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Muon transfer from the ground state of the muonic hydrogen to nuclei with $Z > 1$ is one of the important problems of mesic-atom physics for more than 30 years. The transfer to helium is of special interest, since it is connected with the problem of muon-catalyzed fusion in the deuterium-tritium mixture. Helium nuclei are unavoidably accumulated in the mixture due to the nuclear fusion reactions and tritium decay. Muon transfer in collisions of muonic hydrogen atoms with helium stops the cycle of the catalysis, so the transfer rate is an important characteristic of the muon catalyzed fusion.

The rate of the direct muon transfer to helium is rather small ($\sim 10^6$ s^{-1}) [1,2], because the crossing point of the lowest terms of the system ($2p\sigma$ and $1s\sigma$), which corresponds to the initial and final states of the reaction, turns out to be deep under the barrier at energies ~ 1 eV.

Another possible mechanism for muon transfer with the formation of the intermediate molecular state via the conversion of the atomic electron was proposed in [3]. The resulting molecular ion is in an excited state (in the muon motion) and undergoes deexcitation to the lower term $1s\sigma$ in a time $\sim 10^{-12}$ s. As a result, the muon turns out to be bound on a helium nucleus, forming a muonic helium atom in the ground state $(\mathrm{He}^{++}\mu)_{1s}$.

Since the rate of formation of the muonic molecule ($\sim 10^8$ s^{-1}) is much smaller than that of its decay ($\sim 10^{12}$ s^{-1}), the muon transfer rate nearly coincides with the formation rate. The latter was calculated in a number of papers [3–6] in various approximations.

In this paper we focus special attention on the construction of the effective potential in accordance with the prescription given in [7] («simple-approach approximation»). We calculated the muon transfer rates at low energy collisions of hydrogen isotopes with helium isotopes and compared them with the new experimental data.

The rate of the formation of the muonic molecule[1)] is determined by a dipole transition with the conversion of the atomic electron and is given by a formula [6]:

$$d\lambda = \frac{16\pi^2}{3} N_0\, a_e^3\, \xi^5 q^{-1} I^2(q) \langle d\rangle^2 \nu_e\,, \qquad (1)$$

where $\nu_e = m_e e^4/\hbar^3 = 4.134 \cdot 10^{16}$ s^{-1} is an atomic frequency unit, $a_e = \hbar^2/m_e e^2 = 0.529 \cdot 10^{-8}$ cm is a Bohr radius of the hydrogen atom, $\xi = m_e/m$ (here m_e is the electron mass and m is the reduced mass of mesic hydrogen; $m^{-1} = m_\mu^{-1} + M_1^{-1}$, where m_μ is the muon mass, and M_1 is the mass of the nucleus of the hydrogen isotope), and $N_0 = 4.25 \cdot 10^{22}$ cm^{-3} is a liquid-hydrogen density. The value $q^{-1}I^2(q)$ is calculated in atomic units and determines the rate of the electron transition from the bound $1s$-state of the helium atom to the continuum. The value $\langle d\rangle^2$ is calculated in mesic atom units (see below) and determines the rate of the dipole transition of the system of three bodies from the continuum to the bound state on the term $2p\sigma$.

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[1)] For brevity we shall call a molecular ion $(\mathrm{H}\mu\mathrm{He})^{++}$, $\mathrm{H} \equiv p, d$ or t, mesic molecule.

The momentum q and the energy ε_e of the conversion electron are given by

$$q = \sqrt{2m_e\varepsilon_e}, \quad \varepsilon_e = \varepsilon + |\varepsilon_{Jv}| - I_e \,, \tag{2}$$

where ε is the collision energy, ε_{Jv} is the energy of the mesic molecule in the rotational-vibrational state (J, v) (here J is the rotational and v the vibrational quantum numbers), and I_e is the binding energy of the $1s$-electron in the helium atom.

The integral $I(q)$ is the matrix element of the variable $1/\rho^2$ (ρ is the distance between the electron and the center of mass of the system) calculated with the electron wave functions:

$$I(q) = \int\limits_0^\infty d\rho R_{q1}(\rho) R_{1s}(\rho) \,, \tag{3}$$

where $R_{1s}(\rho)$ is the radial ground-state wave function of the electron in the helium atom, and $R_{q1}(\rho)$ is the radial wave function of the p-wave electron ($l = 1$) in the continuum.

The functions $R(\rho)$ are normalized by the conditions

$$\begin{aligned} &\int\limits_0^\infty R_{1s}^2(\rho)\rho^2 d\rho = 1, \\ &\int\limits_0^\infty R_{q'1}(\rho) R_{q1}(\rho)\rho^2 d\rho = \delta(q'-q). \end{aligned} \tag{4}$$

The Hartree—Fock wave functions were used as $R(\rho)$. The wave function of the emitted electron was calculated in the frozen core model (in the model with the core reconstruction the results for $I^2(q)$ are about 10% smaller [6]). The values of the integral $I(q)$ for several energies ε_e are given in Table 1.

The dipole matrix element calculated with the wave functions of the system of three bodies has the form [5]

$$\langle d \rangle = a I_1 + b\, I_2 \,, \tag{5}$$

$$\begin{aligned} &a = \frac{M_2 - M_1}{M_t} - \frac{1}{2}, \quad b = 1 + \frac{2m_\mu}{M_t}, \\ &M_t = M_1 + M_2 + M_\mu, \end{aligned} \tag{6}$$

$$\begin{aligned} I_1 &= \frac{1}{k}\int\limits_0^\infty \chi_f(R)\,\chi_i(R)\,R\,dR\,, \\ I_2 &= \frac{1}{k}\int\limits_0^\infty \chi_f(R)\,\chi_i(R)\,dR \int \phi^2_{2p\sigma}(R,\mathbf{r})\,\frac{\mathbf{R}\cdot\mathbf{r}}{R}\,d\mathbf{r}\,. \end{aligned} \tag{7}$$

M_2 is the mass of the helium isotope, $\phi_{2p\sigma}(R,\mathbf{r})$ is the wave function of the muon in the state $2p\sigma$ in the field of the two Coulomb centers, R is the internuclear distance, and $\mathbf{r}$ is the muon coordinate calculated from the middle of the internuclear distance. The radial wave functions $\chi_i(R)$ and $\chi_f(R)$ describe the relative motion of the nuclei in the initial and final states, respectively. In the one-channel approximation they are obtained from the Schrödinger equation

$$\left[\frac{d^2}{dR^2} + 2M(\varepsilon - W) - \frac{J(J+1)}{R^2}\right]\chi(R) = 0\,. \tag{8}$$

Here J is the total orbital angular momentum of the system of three particles, M is the reduced mass of the nuclei, $\varepsilon = k^2/2M$ is the collision energy, and k is the asymptotic momentum of the relative nuclear motion in the effective potential W [the same momentum enters formulas (7)]. All the quantities in Eq. (8) are used in the mesic atom units $e = \hbar = m = 1$, where $m = M_1 m_\mu/(M_1 + m_\mu)$. In these units

$$m_\mu = 1 + \lambda_1, \quad \lambda_1 = m_\mu/M_1\,. \tag{9}$$

The effective potential W consists of the term E, the adiabatic corrections, and the energy of the Coulomb repulsion of the nuclei [8]:

$$W = E + \frac{2}{R} + \frac{1}{2M}[H^+ - H^* + \kappa(H^- - 2H^*)], \tag{10}$$

$$M = \frac{M_2 M_1}{M_2 + M_1}\,, \qquad \kappa = \frac{M_2 - M_1}{M_2 + M_1}\,. \tag{11}$$

Table 1.

ε_e, eV	q	$I(q)$	$q^{-1}I^2(q)$
4	0.542	0.491	0.445
8	0.767	0.607	0.481
12	0.939	0.712	0.540
16	1.084	0.805	0.598
20	1.212	0.887	0.649
24	1.328	0.964	0.700
28	1.435	1.030	0.739
32	1.534	1.089	0.774
36	1.627	1.144	0.805
40	1.715	1.196	0.834
44	1.798	1.248	0.866
48	1.878	1.300	0.899
52	1.955	1.352	0.934
56	2.029	1.403	0.971
60	2.100	1.455	1.008

For $R \to \infty$ we have $E_{2p\sigma} \to -1/2$, $H^{+}_{2p\sigma} \to 1/4$, $H^{*}_{2p\sigma} \to 1/4$, $H^{-}_{2p\sigma} \to 1/2$, so

$$W_{2p\sigma} \to -\frac{1}{2} = E_{1s}(H\mu). \tag{12}$$

The asymptotic value of $W_{2p\sigma}$ coincides with the energy of the $H\mu$-atom in the ground state (which corresponds to the initial conditions of the collision). However, the reduced mass M in Eq. (11) (and hence the asymptotic momentum k), which enters Eq. (8) differs from the true reduced mass of the system $H\mu + He$, which is

$$\tilde{M} = \frac{M_2\,(M_1 + m_\mu)}{M_2 + M_1 + m_\mu} = M\,\frac{1+\lambda_1}{1+\lambda}\,, \qquad \lambda = \frac{m_\mu}{M_2 + M_1}\,. \tag{13}$$

If one makes the replacement $M \to \tilde{M}$ in Eq. (8), the calculated energy levels of the mesic molecule ε_{Jv} [9] turn out to be in better agreement with accurate calculations[2)] [10–12] than those obtained earlier [3] with the mass M. Even better agreement can be obtained if one replaces κ in Eq. (10) by $\tilde{\kappa}$, which gives the correct asymptotic value of the effective potential in the $1s\sigma$ channel. We are solving a one-level problem; however, the $1s\sigma$ channel is the second open channel in the problem of slow collisions of mesic hydrogen with helium, and its influence can be taken into account indirectly[3)] by the replacement $\kappa \to \tilde{\kappa}$. In order to obtain $\tilde{\kappa}$ let us write the asymptotics of the potentials in the $1s\sigma$ channel: for $R \to \infty$ $E_{1s\sigma} \to -2$, $H^{+}_{1s\sigma} \to 1$, $H^{*}_{1s\sigma} \to 1$, $H^{-}_{1s\sigma} \to -2$,

$$W_{1s\sigma} \to -2 + \frac{1}{2\tilde{M}}\,[1 - 1 + \tilde{\kappa}\,(-2-2)] = = -2\left(1 + \frac{\tilde{\kappa}}{\tilde{M}}\right)\,. \tag{14}$$

Actual asymptotic value of the potential in the $1s\sigma$ channel should coincide with the ground-state energy of the $He\mu$-atom:

$$E_{1s\sigma}(He\mu) = -2m', \quad m' = \frac{m_\mu M_2}{M_2+\mu} = \frac{1+\lambda_1}{1+\lambda_2}, \qquad \lambda_2 = \frac{m_\mu}{M_2}. \tag{15}$$

Let us choose such $\tilde{\kappa}$ that $W_{1s\sigma} \to E_{1s\sigma}(He\mu)$. Then

$$\tilde{\kappa} = \kappa\,\frac{(1+\lambda_1)^2}{(1+\lambda)(1+\lambda_2)}\,. \tag{16}$$

So the wave functions $\chi_{i,f}(R)$ are solutions of the equation

$$\left[\frac{d^2}{dR^2} + 2\tilde{M}\,(\varepsilon - \tilde{W}_{2p\sigma}) - \frac{J_{i,f}(J_{i,f}+1)}{R^2}\right] \times \chi_{i,f}(R) = 0\,, \tag{17}$$

where

$$\tilde{W}_{2p\sigma} = E_{2p\sigma} + \frac{2}{R} + + \frac{1}{2\tilde{M}}[H^{+}_{2p\sigma} - H^{*}_{2p\sigma} + \tilde{\kappa}(H^{-}_{2p\sigma} - 2H^{*}_{2p\sigma})] \tag{18}$$

with the boundary conditions

$$\chi_i(0) = \chi_f(0) = 0,$$

$$\chi_i(R)_{R\to\infty} = \sin(kR - J\pi/2 + \delta_J), \quad k = \sqrt{2\tilde{M}\varepsilon}, \qquad \chi_f(R)_{R\to\infty} = \exp[-(2\tilde{M}|\varepsilon_{Jv}|)^{1/2}R]. \tag{19}$$

The energy of the rovibrational state (J, v) of the molecular ion $(\mathrm{H}\mu\mathrm{He})^{++}$ is obtained together with the wave function $\chi_f(R)$ when solving the Schrödinger equation. For slow collisions it is enough to consider $J_i = 0$ for initial and $J_f = 1$ for final states (the molecule is formed via the dipole transition). There exist only three bound states in the $2p\sigma$-channel, which have $v = 0$ and $J = 0, 1, 2$. The level energies ε_{00} and ε_{10} obtained in the present paper are given in Table 2 together with the results of other papers.

As can seen from the table, the level energies calculated in the present paper are very close to the high accuracy calculations with large number of basis functions [10–12]. For this reason, when calculating the rates of the formation of mesic molecules, we use Eq. (17), where $\tilde{M}$ and $\tilde{\kappa}$ are defined by Eqs. (13) and (16).

When calculating the wave function of the initial state $\chi_i(R)$, the electron screening was taken into account by an additional term in the potential of Eq. (17). The influence of the electron shell of the helium atom on the final (bound) state of the molecule is negligible because of the short length of the corresponding wave function (see Refs. [4–6] for more details).

Table 3 shows the rates of the molecule formation λ (10^8 s^{-1}) averaged over the Maxwell energy distribution. The electron screening is taken into account.

Recently new experimental data on λ have been obtained. In the experiment the total muon transfer rate from the ground-state muonic hydrogen to helium is measured:

$$\lambda_{p\mathrm{He}} = \lambda_{p\mu\mathrm{He}} + \lambda^{dir}_{p\mathrm{He}}\,, \tag{20}$$

[2)] These calculations make use of about 300 to 3000 basis functions.

[3)] A similar procedure for solving the two-channel problem was proposed earlier in [7] («simple approach», or «improved two-channel approximation»).

Table 2. The binding energies (eV) of the hydrogen-helium muonic molecules

Energy	Reference	$p\mu^3$He	$p\mu^4$He	$d\mu^3$He	$d\mu^4$He	$t\mu^3$He	$t\mu^4$He
$-\varepsilon_{00}$	[3][a]	67.2	73.9	69.5	77.6	71.6	80.5
	[9][b]	69.0	75.4	70.6	78.7	72.3	81.3
	This paper[c]	73.2	80.8	71.0	79.4	72.3	81.4
	[10]			70.7			
	[13]	67.7	74.4	70.0	78.0	71.9	80.8
	[14]	72.8	80.6	69.4	77.5		
$-\varepsilon_{10}$	[3][a]	34.9	41.6	46.5	55.9	52.4	62.9
	[9][b]	38.1	45.4	48.2	57.6	53.4	63.9
	This paper[c]	41.5	50.0	48.5	58.3	53.4	64.0
	[10]		50.0	47.9	57.8		
	[11]			48.4	58.2		
	[12]			48.4	58.2		
	[13]	33.8	41.2	46.8	56.1	52.7	63.1
	[14]	38.8	47.4	46.3	55.7		

[a] One-channel approximation with M and κ.
[b] One-channel approximation with $\tilde{M}$ and κ.
[c] One-channel approximation with $\tilde{M}$ and $\tilde{\kappa}$.

Table 3. The rates of the molecule formation λ (10^8 s^{-1}) averaged over the Maxwellian energy distribution. The electron screening is taken into account

T, K	$p\mu^3$He	$p\mu^4$He	$d\mu^3$He	$d\mu^4$He	$t\mu^3$He	$t\mu^4$He
15	0.52	0.33	2.40	12.7	51.2	1.89
20	0.52	0.33	2.34	11.8	45.5	1.86
25	0.51	0.32	2.28	11.0	41.1	1.84
30	0.51	0.32	2.24	10.4	37.6	1.82
35	0.51	0.32	2.20	9.8	34.7	1.79
40	0.50	0.31	2.16	9.3	32.3	1.77
50	0.50	0.31	2.09	8.5	28.6	1.74
100	0.47	0.29	1.85	6.2	18.8	1.60
150	0.46	0.28	1.70	5.1	14.4	1.51
200	0.45	0.27	1.60	4.4	11.9	1.43
250	0.44	0.27	1.52	3.8	10.2	1.37
300	0.43	0.26	1.45	3.5	9.0	1.31
350	0.42	0.25	1.39	3.2	8.1	1.27
400	0.42	0.25	1.34	2.9	7.3	1.22
450	0.41	0.25	1.30	2.7	6.7	1.19
500	0.40	0.24	1.26	2.6	6.2	1.15

Table 4. Muon transfer rates (10^8 s^{-1}) for various isotopes and temperatures

	Experiment		Theory
$\lambda(p^3\mathrm{He}, 30\ \mathrm{K})$	0.46 ± 0.15	[15]	0.57
$\lambda(p^4\mathrm{He}, 30\ \mathrm{K})$	0.42 ± 0.07	[15]	0.38
$\lambda(p^4\mathrm{He}, 300\ \mathrm{K})$	0.36 ± 0.10	[16]	0.32
$\lambda(p^4\mathrm{He}, 300\ \mathrm{K})$	0.44 ± 0.20	[17, 9]	0.32
$\lambda(p^4\mathrm{He}, 300\ \mathrm{K})$	0.5 ± 0.1	[18, 19]	0.32
$\lambda(d^3\mathrm{He}, 30\ \mathrm{K})$	1.86 ± 0.08	[20]	2.25
$\lambda(d^3\mathrm{He}, 40\ \mathrm{K})$	2.25 ± 0.15	[21]	2.17
$\lambda(d^3\mathrm{He}, 300\ \mathrm{K})$	1.24 ± 0.05	[22]	1.46
$\lambda(d^4\mathrm{He}, 30\ \mathrm{K})$	10.50 ± 0.21	[20]	10.4
$\lambda(d^4\mathrm{He}, 300\ \mathrm{K})$	3.68 ± 0.18	[23]	3.48
$\lambda(t^3\mathrm{He}, 15\ \mathrm{K})$	46 ± 4	[24]	51

where $\lambda_{p\mathrm{He}}^{dir}$ is the rate of the direct muon transfer without the molecule formation. This rate was calculated in [1] for the systems $p\mu + {}^{3,4}$He and $d\mu + {}^{3,4}$He. For collision energies $\varepsilon \leq 0.1$ eV the rate of the direct muon transfer does not depend on energy and amounts to

$$\lambda_{p\mathrm{He}}^{dir} \approx 0.06 \cdot 10^8\ \mathrm{s}^{-1} \quad \text{and} \quad \lambda_{d\mathrm{He}}^{dir} \approx 10^6\ \mathrm{s}^{-1}. \qquad (21)$$

As was mentioned, the rate of the molecular transfer coincides with the rate of the molecule formation (see Table 3). So when comparing experimental rates with theoretical ones (Table 4), the latter were enlarged according to Eqs. (20) and (21).

As a matter of fact, the genuine muon transfer to the helium nucleus occurs when the molecular ion decays into hydrogen and muonic helium. Such a decay may be radiative (or via the electron conversion), as well as via predissociation. The latter channel was not considered in the first papers on the molecular charge exchange. This led to large discrepancies when comparing the calculations with the experiments, in which the probability of the transfer was obtained by the measurement of the X-ray yield. These discrepancies were removed when the predissociation channel was pointed out [13, 9] and taken into account.

Comparing the experimental and theoretical values for muon transfer from ground-state muonic hydrogen to helium, one can see that they are in a reasonable agreement. This means that the main features of the process are understood correctly.

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