Charge exchange of excited mesic hydrogen with helium nuclei

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The rates of direct and molecular charge exchange between excited mesic atoms of hydrogen isotopes and helium nuclei are calculated. It is shown that direct charge exchange is decisive for the capture of muons form mesic-hydrogen states with principal quantum numbers 2 and 3. The calculation results are compared with available experimental data on mesoprotium charge exchange with ^{4}He nuclei.

1. INTRODUCTION

The behavior of mesic hydrogen in hydrogen-isotope mixtures is of considerable interest for both weak-interaction physics[1] and mesic-atom physics.[2] Of particular interest at present is muon-catalyzed fusion, which is most effective in a *d–t* mixture.[3] Since hydrogen mixtures can contain impurities, it is very important to study muon transfer from mesic hydrogen to other nuclei.[1,2,4] In connection with muon catalysis, an important role is played by charge exchange of hydrogen-isotope mesic atoms with helium nuclei that accumulate in a hydrogen mixture via nuclear fusion and via tritium decay.[3,5–7]

Muon transfer from hydrogen-isotope mesic atoms in the ground state to helium nuclei has been investigated theoretically[8–13] as well as experimentally.[14–18] Account must be taken, however, of the charge exchange of excited mesic hydrogen with helium nuclei in the course of de-excitation stager of the mesic-atom[7,13,19,20] In connection with muon catalysis, allowance for this process (just as for charge exchange of mesic hydrogen in the ground state with helium nuclei) should decrease the number of catalysis cycles per muon. Calculated rates of charge exchange of hydrogen-isotope mesic atoms in the metastable $2S$ state with helium nuclei, obtained for a molecular charge-exchange mechanism via formation of a quasistationary molecular state, are given in Refs. 21 and 22.

We consider here direct charge exchange of hydrogen-isotope mesic atoms in the metastable $2S$ state with helium nuclei, and also direct and molecular transfer of a muon to helium from mesic hydrogen with principal quantum number $n = 3$.

2. MOLECULAR CHARGE EXCHANGE

It is known that the molecular mechanism dominates in the charge exchange of ground-state mesic hydrogen with helium nuclei.[10–13] Molecular charge exchange is possible also for excited mesic hydrogen with helium if the molecular term that describes the initial state of the system contains an attractive region. Such a region, as follows from Fig. 1 of Ref. 21, exists at a distance $R \sim 20\,a_\mu$ (a_μ is the Bohr radius of mesic hydrogen) for charge exchange of mesic hydrogen in a metastable $2S$ state with helium nuclei in a $5g\sigma$ term describing the initial state. As for the $8k\sigma$ term that corresponds asymptotically to a mesic-hydrogen excited state with $n = 3$ and to a helium nucleus (see Fig. 1), the attractive region is characterized by an energy minimum at $R \sim 50a_\mu$. A mesic molecule can be formed in two ways: by Auger conversion of the helium atom electron (1) and by a resonance process with formation of a final complex similar to an excited helium atom (2)[13,21,22]:

$$(H\mu)_{n'}^{*} + \mathrm{He} \rightarrow \begin{cases} [((H\mu)_{n'}^{*}\,\mathrm{He}^{2+})e]^{+} + e, & (1) \\ [((H\mu)_{n'}^{*}\,\mathrm{He}^{2+})2e]_{n''}^{**}. & (2) \end{cases}$$

Here $H \equiv p$, d, or t; n' is the principal quantum number of the final excited complex (2). The rate of the nonresonant reaction (1), referred to the liquid-hydrogen density $N_0 = 4.25 \times 10^{22}\ \mathrm{cm}^{-3}$, is given by[23]

$$\lambda_m^{nres} = \frac{16\pi^2}{3} N_0 a_e^3 \xi^5 \tau_e^{-1} \sum_v |I(q_v)|^2 |\langle d_v \rangle|^2 q_v^{-1} c^{-1}, \quad (3)$$

where a_e is the Bohr radius of the hydrogen atom, $\xi = m_e/m^*$, m_e is the electron mass, m^* the reduced mass of mesic hydrogen: $(m^*)^{-1} = m_\mu^{-1} + M_{\mathrm{H}}^{-1}$, m_μ is the muon mass, M_{H} the mass of the hydrogen-isotope nucleus, and $\tau_e = \hbar^3/(m_e e^4)$ the atomic unit of time. The momentum of the conversion electron is

$$q_v = [2m_e(|\varepsilon_{Jv}| + \varepsilon - |\varepsilon_I|)]^{1/2}, \quad (4)$$

where $\varepsilon = k^2/2M$ is the collision energy, ε_{Jv} is the binding energy of a mesic molecule in a state with total orbital momentum J of the three particles and with a vibrational quantum number v, $|\varepsilon_I| = 24.58$ eV is the helium-atom ionization potential, M is the reduced mass of the mesic atom and the target atom:

$$M^{-1} = (M_{\mathrm{H}} + m_\mu)^{-1} + M_{\mathrm{He}}^{-1},$$

and M_{He} is the mass of the helium-isotope nucleus.

The quantity $I(q_v)$ given in Eq. (3) in atomic units, has been determined in Ref. 12, where Hartree–Fock wave functions in the frozen-core model were used.

The quantities $\langle d_v \rangle$, calculated in units $\hbar = m^* = e = 1$, are determined by the overlap integral of the wave functions corresponding to the initial (continuous spectrum) and final (mesic-molecule) states of the nuclei and of the muon. We use for $\langle d_v \rangle$ an expression similar to that in Ref. 10, except that the wave functions of the $2p\sigma$ term are replaced by those of the $8k$ term that corresponds asymptotically to the $(H\mu)_{n=3}^{*} + \mathrm{He}^{2+}$ state.

The radial wave functions $\chi^{(i,f)}(R)$ contained in $\langle d_v \rangle$ satisfy the equation

$$[d^2/dR^2 + 2M(\varepsilon - V) - J(J+1)/R^2]\chi(R) = 0 \quad (5)$$

with boundary conditions

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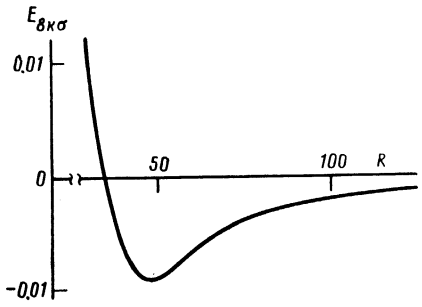

FIG. 1. The $8k\sigma$ term corresponding asymptotically to the $(p\mu)^*_{n=3}$ + He system.

$$\chi^{(i,\,f)}(0)=0,$$
$$\chi^{(i)}(R)\propto \sin(kR-\pi J/2+\delta_J) \quad \text{as} \quad R\to\infty, \tag{6}$$
$$\chi^{(f)}(R)\propto \exp[-(2M|\varepsilon_{Jv}|)^{1/2}R] \quad \text{as} \quad R\to\infty.$$

The effective potential is

$$V=E_{8k\sigma}+d_n(\varepsilon(R)-Z/R^2), \tag{7}$$

where $E_{8k\sigma}$ is the potential of the $8k\sigma$ term (see Fig. 1), $d_n = 3n\Delta/2$ is the dipole moment of the excited mesic hydrogen, Z is the charge of the target nucleus ($Z = 2$ for helium), $\Delta = n_1 - n_2$, and n_1 and n_2 are the mesic-atom parabolic quantum numbers. For the $8k\sigma$ term we have here $n = 3$ and $\Delta = -2$; $n_1 = 0$, $n_2 = 2$. The asymptote of the $8k\sigma$ term $E_{8k\sigma}\propto d_nZ/R^2 = -18/R^2$ corresponds as $R\to\infty$ to the linear Stark effect for the $(H\mu)^*_{n=3}$ mesic atom in the field of a helium nucleus, and $\varepsilon(R)$ is the field strength of an atom at an internuclear distance R (assuming the mesic atom to be pointlike on the atomic scale).

In first-order perturbation theory, $\varepsilon(R)$ obtained using Hartree–Fock wave functions is of the form[24]

$$\varepsilon(R)=\frac{Z}{R^2}\sum_i\gamma_i\left(1+\lambda_i\frac{R}{a_e}\right)\exp\left(-\frac{\lambda_iR}{a_e}\right), \tag{8}$$

where the parameters γ_i and λ_i are given for $Z = 2$ in Ref. 25.

It follows from Fig. 1 that the effective interaction is characterized by rather large distances, so that the choice of a potential in the form (7) is justified. We solve Eq. (5) with boundary conditions (6) numerically. Tables I and II list the binding energies, which we calculated with and without allowance for screening, of the quasimolecules formed by helium nuclei and excited mesic hydrogen in the $n = 3$ state.

Assuming a Maxwellian mesic-atom energy distribution with temperature T, we average the rates λ_m^{nres} calculated from Eq. (3) for the reaction (1) with the function $\gamma(\varepsilon, \varepsilon_T)$ given, for example in Ref. 21 ($\varepsilon_T = 3/2k_0T$ and k_0 is the Boltzmann constant). Tables III and IV contain the averaged charge-exchange rates calculated without and with allowance for screening. It can be seen that allowance for screening is most significant in scattering of mesoprotium in state $n = 3$ by ^{3}He nuclei. The lesser role of screening in scattering of mesic hydrogen in the $2S$ state by helium nuclei is due in part to the smaller effective-interaction range.

Resonant charge exchange is possible under the condition

$$\varepsilon_T=\varepsilon_r\equiv|\varepsilon_{1v}+\varepsilon_{n'p}-\varepsilon_I|, \tag{9}$$

where $\varepsilon_{n'p}$ is the binding energy of an electron in the excited p-state of the final complex (2), with principal quantum number n'. The energy levels of the mesic molecules for which the resonance condition (9) is met are underlined in Table I. The rate of resonant formation of a mesic molecule in reaction (2) is given by[26]

$$\lambda_m^{res}=\tfrac{8}{3}\pi^2N_0a_e^3\xi^5I^2(q_v)\,|\langle d_v\rangle|^2\gamma(\varepsilon_r,\varepsilon_T)\tau_e^{-1}c^{-1}, \tag{10}$$

where ε_r is defined in (9). The rate of resonant formation of mesic molecules reaches a maximum at energies $\varepsilon_T\approx\varepsilon_r$ (actually at lower energy, in view of the factor $1/k$ in $\langle d_v\rangle$).

The value of $I(q_v)$ (in atomic units) was determined in Ref. 21.

Resonant formation of mesic molecules is accompanied by excitation of He-atom levels with principal quantum numbers $n' = 2$, 3, and 4 (see Table I). The binding energies of these levels, calculated with the program described in Ref. 27, are $\varepsilon_{2p} = -3.499$ eV, $\varepsilon_{3p} = -1.543$ eV, and $\varepsilon_{4p} = -0.864$ eV. The corresponding overlap integrals are equal to 0.239, 0.137, and 0.0902.

The rates of resonant formation of mesic molecules, calculated without allowance for screening, are shown in Fig. 2. It can be seen that at room temperature the most substantial is charge exchange of mesodeuterium with ^{3}He atoms.

Comparing the rates of resonant formation of mesic molecules for various isotope mixtures (Fig. 2), we see that $\lambda_m^{res}(d\mu^3\text{He})$ is smaller than $\lambda_m^{res}(p\mu\ \text{He})$ since $n' = 3$ for the case $(d\mu)^*_{n=3} + {}^3$He, as against $n' = 2$ for $(p\mu)^*_{n=3}$ + He. This decrease is even more noticeable for the system $(d\mu)^*_{n=3} + {}^4$He, where $n' = 4$. The rates of resonant formation of mesic molecules for the system $(t\mu)^*_{n=3}$ + He are smaller than for $(p\mu)^*_{n=3}$ + He because in the former case the mesic-molecule level that enters into resonance is the one with $v = 3$, which oscillates faster than the level with $v = 2$ for $(p\mu)^*_{n=3}$ + He.

TABLE I. Binding energies (eV) of mesic molecules with $J = 1$, formed by excited mesic hydrogen with $n = 3$ ($8k\sigma$ term) and helium nuclei. The levels responsible for resonant charge exchange are underlined.

n'	2	2	3	4	2	2
v	$(p\mu)^*+{}^3$He	$(p\mu)^*+{}^4$He	$(d\mu)^*+{}^3$He	$(d\mu)^*+{}^4$He	$(t\mu)^*+{}^3$He	$(t\mu)^*+{}^4$He
0	−39,0	−39.2	−42,4	−42,7	−43,7	−44,1
1	−26,5	−27,1	−30,9	−31,7	−32,9	−33.9
2	<u>−18.0</u>	<u>−18,6</u>	<u>−22,4</u>	−23,4	−24,6	−25,8
3	−12,2	−12,8	−16,2	−17.2	<u>−18.3</u>	<u>−19,6</u>

TABLE II. The same as in Table I, but with allowance for screening.

v	$(p\mu)^*+{}^3He$	$(p\mu)^*+{}^4He$	$(d\mu)^*+{}^3He$	$(d\mu)^*+{}^4He$	$(t\mu)^*+{}^3He$	$(t\mu)^*+{}^4He$
0	−34,1	−34,3	−37,8	−38,1	−39,3	−39,7
1	−21,5	−22,1	−26,3	−27,1	−28,4	−29,3
2	−12,9	−13,5	−17,6	−18,6	−19.9	−21,2
3	−7,1	−7.7	−11,4	−12,4	−13,6	−14,9

TABLE III. Rates of nonresonant molecular charge exchange ($10^8\ s^{-1}$) without allowance for screening. $8k\sigma$ term.

T, K	$(p\mu)^*+{}^3He$	$(p\mu)^*+{}^4He$	$(d\mu)^*+{}^3He$	$(d\mu)^*+{}^4He$	$(t\mu)^*+{}^3He$	$(t\mu)^*+{}^4He$
20	5,78	3,84	1,69	1,32	0,99	0,90
50	4,19	2,81	1,23	0,96	0,72	0,61
100	3,09	2,11	0,92	0,72	0,54	0,44
400	1,58	1,10	0,48	0,38	0,28	0,23
800	1,12	0,78	0,34	0,27	0,20	0,16
1000	1,01	0,69	0,30	0,24	0,18	0,15

TABLE IV. The same as in Table III with allowance for screening.

T, K	$(p\mu)^*+{}^3He$	$(p\mu)^*+{}^4He$	$(d\mu)^*+{}^3He$	$(d\mu)^*+{}^4He$	$(t\mu)^*+{}^3He$	$(t\mu)^*+{}^4He$
20	0.55	1,17	2,26	0,93	1,09	0,77
50	0,39	0,87	1,70	0,69	0,76	0,53
100	0,30	0,65	1,26	0,53	0,56	0,39
400	0,17	0,33	0,63	0,29	0,29	0,20
800	0,12	0,23	0,44	0,21	0,21	0,14
1000	0.11	0,21	0,39	0,19	0,19	0,13

TABLE V. Rates of direct charge exchange ($10^{11}\ s^{-1}$) of excited mesic hydrogen with $n = 2$ and 3 with helium nuclei for a thermal energy $\varepsilon = 0.04$ eV. Screening is disregarded.

n	$(p\mu)^*_n+{}^3He$	$(p\mu)^*_n+{}^4He$	$(d\mu)^*_n+{}^3He$	$(d\mu)^*_n+{}^4He$	$(t\mu)^*_n+{}^3He$	$(t\mu)^*_n+{}^4He$
2	7,1	6,3	2,8	2,2	1,6	1,2
3	78	75	55	51	46	40

TABLE VI. The same as Table V but with allowance for screening.

n	$(p\mu)^*_n+{}^3He$	$(p\mu)^*_n+{}^4He$	$(d\mu)^*_n+{}^3He$	$(d\mu)^*_n+{}^4He$	$(t\mu)^*_n+{}^3He$	$(t\mu)^*_n+{}^4He$
2	1,5	1,3	0,62	0,49	0,38	0,27
3	10,5	10,1	7,9	7,3	6,7	5,9

The resonant charge-exchange rate is inversely proportional to the resonance energy ε_r. Therefore the shift of the mesic-molecule level (and accordingly of ε_r) owing, say, to allowance for screening or to adiabatic corrections, can change this rate substantially. For example, if a level shift displaces the resonance energy of the system $(p\mu)^*_{n=3}$ + He into the room-temperature region, the resonant charge-exchange rate increases by a factor of 50, reaching $\sim 10^9$ s^{-1}. In our present calculation of the resonant charge exchange rates we disregard screening and adiabatic or other corrections, including, for example, coupling with other channels, since the given upper bound of the resonant molecular charge exchange is substantially lower than the rates of mesic-hydrogen de-excitation and direct charge exchange (as shown below).

Note that the mesic molecules formed in reactions (1) and (2) dissociate and transfer a muon to the helium atom

$$(H\mu)_n{}^*He \to (He\mu)_{n'}{}^{**} + H. \qquad (11)$$

Analysis of the term structure indicates the existence of a dipole transition to the $7i\sigma$ term in reaction (11). The rate of this transition is high,[7] so that the charge-exchange rate is determined by the quasimolecule-formation rate (see above). At the same time, the rate of de-excitation of the $(H\mu)^*_{n=3}$ state as high ($\sim 10^{11}$ s^{-1}).[28,29] It follows therefore from our results (see Tables III and IV) that molecular charge exchange of mesic hydrogen with helium nuclei cannot play a significant role in the kinetics of the excited molecules.

3. DIRECT CHARGE EXCHANGE

Direct charge exchange of ground-state hydrogen-isotope mesic atoms with helium nuclei is strongly suppressed by the absence of pseudocrossing of the molecular terms corresponding to the initial and final states of the reaction.[8] At the same time, as noted in Ref. 8, the rate of transfer of a muon from excited mesic hydogen can be high ($\sim 10^{11}$ s^{-1}) because of the large number of term crossings in this case. As regards transfer of a muon to helium, it is shown in Ref. 30 that direct charge exchange of mesic hydrogen in states with $n \leqslant 4$ is expected to be suppressed by the absence of term crossing. However, our calculations, based on an analysis[31,32] of nonadiabatic transitions in the complex R plane, show that the suppression predicted in Ref. 30 for the rates of the charge-exchange reaction does not take place at $n \geqslant 2$.

Using the analyticity of the terms in the complex R plane, we obtain quasicrossing of terms corresponding to the initial and final states of the reaction at a branch point R_c determined by the condition

$$\Delta E(R) = \text{const}\,(R-R_c)^{1/2} = 0. \qquad (12)$$

The inter-term transition probability connected with the branch point R_c is determined by the Massey parameter

$$\delta = \left| \operatorname{Im} \int_c p(R)\, dR \right|, \qquad (13)$$

where $p(R)$ is the relative radial momentum along the contour C with the point R_c bypassed at Re R = Re R_c;

$$p(R) = Mv(1 - E/\varepsilon - (\rho/R)^2)^{1/2}$$

(v is the collision velocity as $R \to \infty$ and ρ is the impact parameter). The transition cross section

$$\sigma = \pi \int_0^{\rho_{max}} P\, d\rho^2$$

is determined here by the probability[33]

$$P = 2e^{-2\delta}(1 - e^{-2\delta}). \qquad (14)$$

The transition rate referred to the liquid-hydrogen density N_0 is

$$\lambda = \sigma N_0 v. \qquad (15)$$

The total cross section σ was obtained, as in Ref. 34, with account taken of the statistical weight of the states corresponding to motion on the attracting term.

In the calculation of the charge-exchange rates, just as in the isotopic exchange reactions,[34] the value of P depended little on ρ in the effective integration region. The quantity ρ_{max} is defined here as the largest impact parameter for which the term crossing point R_c is located in the classically allowed region. For the values of n considered here it suffices to take screening into account only in the entry channel.

Allowance for screening in the semiclassical approach leads to the appearance at distances $R \sim a_e$ of a potential barrier that decreases ρ_{max}. In addition, transfer of a muon to the helium restructures the electron shell of the helium: one electron leaves the helium atom, and the other changes its state, since the compact complex $(He\mu)^+$ is similar to a nucleus with unit charge. The minimum energy needed for this restructuring is ~ 52 eV (the electron leaving the helium is trapped in this case in the ground state of the hydrogen atom). Charge exchange is therefore possible only if the difference between the binding energies of mesic helium and mesic hydrogen exceeds this value. Since the screening does not alter noticeably the terms in the region of their crossing, its contribution is ignored when R_c is calculated (Re $R_c \ll a_e$).

We consider now direct charge exchange of mesic atoms of hydrogen-isotopes in the metastable $2S$ state with helium nuclei

$$(H\mu)^*_{2S} + He \to (He\,\mu)_{n'}{}^{**} + H. \qquad (16)$$

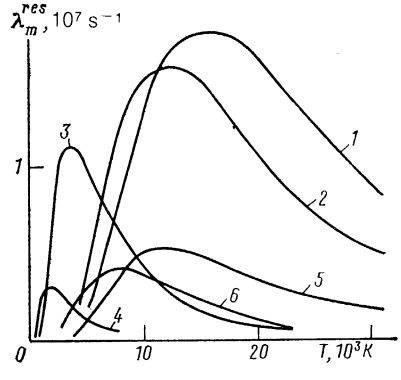

FIG. 2. Temperature dependence of the charge-exchange rates. Screening is disregarded: *1*—$p\mu$ + ^{3}He, *2*—$p\mu$ + ^{4}He, *3*—$d\mu$ + ^{3}He, *4*—$d\mu$ + ^{4}He, *5*—$t\mu$ + ^{3}He, *6*—$t\mu$ + ^{4}He.

We have calculated the branch points that correspond, for the energy-allowed $[5g\sigma-3d\sigma]$ and $[5g\sigma-4f\sigma]$ transitions, to the considered charge-exchange reaction (16).

For the charge exchange of mesic atoms of hydrogen isotopes in the state with $n = 3$

$$(H\mu)^{*}_{n=3} + He \rightarrow (He\,\mu)^{**}_{n} + H \qquad (17)$$

two transitions are energetically allowed: $[8k\sigma-7i\sigma]$ and $[7i\pi-6h\pi]$.

The calculated rates of charge exchange of excited hydrogen-isotope mesic atoms with helium nuclei are listed in Tables V and VI. Comparison with the experimental data on the scattering of mesoprotium and mesodeuterium by ^{4}He nuclei[7,14,20] attests to the importance of direct charge exchange of excited mesic hydrogen and of allowance for screening. It must be borne in mind at the same time that charge exchange of mesodeuterium and mesotritium with He, He^+ and He^{2+} can be observed in investigations of muon catalysis in a *d–t* mixture.

CONCLUSION

As shown by our analysis, direct charge exchange of excited hydrogen-isotope mesic atoms with helium nuclei is quite appreciable and should, in contrast with molecular charge exchange from these states, be taken into account in the analysis of the kinetics of mesic-atom processes in a hydrogen–helium mixture.

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