Charge exchange of low-energy mesic hydrogen in helium and lithium

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We calculate the rates of formation of μ-mesic molecules by hydrogen and helium (or lithium) isotopes, the conversion electron having Hartree-Fock wave functions. The calculation results indicate that the rates of molecular charge exchange of the mesic hydrogen isotopes with helium nuclei is somewhat lower than in earlier preliminary calculations, and lead to better agreement with the experimental data.

1. INTRODUCTION

An important role in the study of muon absorption by a free proton and of the muon-catalysis reaction is played by capture of a muon from mesic hydrogen by nuclei of other elements contained in the hydrogen targets. It is known that direct muon capture from mesic hydrogen isotopes by a helium or a lithium nucleus is strongly suppressed,[1-3] so that molecular charge exchange of mesic hydrogen, which is decisive in case of interception by a helium nucleus, becomes important.

The mesic-molecule formation rate, which determines the rate of molecular charge exchange and is due to conversion of the target-atom electrons, was calculated approximately[4,8] with the residue electrostatic field acting on the conversion electron replaced by the field of the effective point charge. Molecular charge exchange of mesic hydrogen in helium was calculated[9] with allowance for the residue-ion atomic form factor, which hardly changed the results obtained[4] with an effective charge $Z_0 = 1.69$. A shortcoming of these approaches is that the exchange interaction was neglected when the multielectron system was considered.

We calculate here the rates of mesic-molecule formation in the Hartree-Fock approximation for atomic wave functions. The wave function of the conversion electron in the final state of the continuous spectrum was obtained both in the frozen-core model and with allowance for its static restructuring.

The calculation results are compared with the previously obtained approximate experimental data on charge exchange of mesic hydrogen in helium.

2. MESIC-MOLECULE FORMATION

A nonresonant method of mesic-molecule formation is conversion of the target atom in a reaction that takes for helium and lithium atoms the form

$$p\mu + \begin{matrix} \mathrm{He} \longrightarrow [(p\mu\,\mathrm{He}^{++})\,e]^{+} + e, & (1) \\ \mathrm{Li} \longrightarrow [(p\mu\,\mathrm{Li}^{+++})\,2e]^{+} + e, & (2) \end{matrix}$$

where p stands for the nucleus of any hydrogen isotope, and reaction (2) is possible only as a result of conversion of a lithium valence electron.[5]

The equation for the rate mesic-molecule formation in reactions (1) and (2) has the following common form[6,7]:

$$\lambda_m=\beta(16\pi^2/3)N_0 a_e{}^3\xi^5 q^{-1}|I(q)|^2|\langle d\rangle|^2\tau_e{}^{-1}\ \mathrm{s}^{-1}, \tag{3}$$

where $N_0 = 4.25\cdot 10^{22}$ cm^{-3} is the density of the liquid hydrogen, a_e is the Bohr radius of the hydrogen atom, $\xi = m_e/m^*$, m_e is the electron mass, m^* is the reduced mesic-hydrogen mass, $(m^*)^{-1} = m_\mu^{-1} + M_p^{-1}$, m_μ is the muon mass, M_p is the mass of the hydrogen-isotope nucleus, and $\tau_e = \hbar^3/(m_e e^4)$ is the atomic unit of time.

The conversion-electron momentum is

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

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

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

$M_{\mathrm{He(Li)}}$ is the mass of the helium (lithium) isotope nucleus (we neglect here the electron mass), $\beta = 1$ ($\frac{1}{2}$) for helium (lithium), since conversion in helium, in contrast to lithium, is due to two electrons.

The quantities $\langle d\rangle$ are calculated in units $\hbar = e = m^* = 1$. They are determined by the overlap integral of the wave function corresponding to the initial (continuous spectrum) and final (mesic molecule) states of the nuclei and of the muon, and were determined for helium and lithium in Refs. 4 and 5, respectively. The radial wave functions $x^{(i,f)}(R)$ (R is the distance between the nuclei) that enter in $\langle d\rangle$ satisfy the equation

$$\left[\frac{d^2}{dR^2}+2M(\varepsilon-W)-\frac{J(J+1)}{R^2}\right]\chi(R)=0 \tag{5}$$

with boundary conditions

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

The effective potential W is determined by the corresponding terms of the two-center problem,[10] by the adiabatic correction,[11] and by the interaction of the mesic atom with the electrons of the target-atom shell.[12] The effective single-channel approximation of the adiabatic representation of the three-body problem[13] (called the simple approach[14]), to

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which (5) and (6) correspond, leads to a correct asymptotic form of the initial state.

Equation (5) with boundary conditions (6) is solved numerically. At the same time, the screening potential V contained in W is determined by a perturbation theory in which the small parameter is the ratio $(m_e/m_\mu)^{1/2}$ (Ref. 12).

In first-order perturbation theory, the screening potential obtained with Hartree-Fock wave functions is given by[12]

$$V^{(1)}=-m^{*}\varkappa_\mu\xi^2(Za_\mu/2R)\sum_i\gamma_i\lambda_i^2\exp(-\lambda_iR/a_e), \qquad (7)$$

where $\varkappa_\mu=(M_p-m_\mu)/(M_p+m_\mu)$, a_μ is the Bohr radius of the mesic hydrogen, and the parameters γ_i and λ_i are given in Ref. 15.

The contribution of the corrections to the screening potential is taken into account in second-order perturbation theory in accordance with the results of Ref. 12.

In Eq. (5), the initial state corresponds to the collision energy in low-energy s-scattering ($J=0$), so that mesic molecules with binding energy $\varepsilon_b\equiv\varepsilon_{10}$ are produced in the dipole transition to the final state.

The quantity $I(q)$ given in (3) in atomic units is a matrix element of the quantity $1/\rho^2$ calculated with the radial wave functions of the conversion electron in the initial and final states

$$I(q)=\int_0^\infty d\rho\,R_{ns}(\rho)R_{q1}(\rho), \qquad (8)$$

where ρ is the electron coordinate measured from the mass center of the mesic molecule, R_{q1} is the radial wave function of the continuum electron having a momentum q in the p-state, and R_{ns} is the radial wave function of the bound electron in a state with quantum number n. The wave functions are normalized in accordance with the conditions

$$\int R_{ns}^2\rho^2\,d\rho=1, \qquad \int R_{q1}R_{q'1}\rho^2\,d\rho=\delta(q-q').$$

In the calculations of $I(q)$ we used the Hartree-Fock wave functions of the initial and final states obtained using the algorithm given in Refs. 16 and 17. The wave function of the initial ns state was chosen from the set of single-particle wave functions of the atom ground state determined by solving a self-consistent system of Hartree-Fock equations. The wave function R_{q1} of the continuous spectrum was calculated in the models of frozen and thawed cores (i.e., with allowance for static restructuring). Both models give close results for the lithium atoms [the values of $I(q)$ differ by not more than 0.5%]. The restructuring of the final state is more appreciable in the helium atom [the difference in the values of $I(q)$ reaches 5%]. This is natural, since the absence of 1s electrons from the helium atom influences more strongly than the absence of the 2s electron in the lithium atom the self-consistent field in which the escaping electron moves.

It should be noted that with increasing q, which increases with increasing $\varepsilon_{J\upsilon}$ [see (4)] and accordingly M (Ref. 9), restructuring of the core within the emission time of the conversion electron is less probable, so that the calculation carried out in the frozen-core model are more plausible.

3. RESULTS

Table I lists the rates of the charge exchange of hydrogen mesic atoms with helium nuclei, obtained in the frozen-core model. These rates, averaged over the Maxwellian distribution of the mesic-atom velocities, are given in Table II. The values of λ_m calculated in a model with a restructurable core can be obtained by decreasing the corresponding values in Tables I and II by approximately 10%. Table III gives the binding energies of hydrogen-lithium mesic molecules, obtained in the simple approach. They turn out to be 0.3–0.6 eV deeper than those calculated in the single-channel approximation.[5] The energy-level shift due to allowance for screening does not exceed several meV.

Tables IV and V give respectively the rates, unaveraged and averaged over the Maxwellian distribution, of the charge exchange of mesic hydrogen with lithium nuclei.[2)] It can be seen that molecular charge exchange of mesic deuterium with lithium nuclei is strongly suppressed, so that direct charge exchange should be regarded as decisive in these cases.[5]

Table VI gives the experimental results on charge exchange of mesic protium[18] and mesic deuterium[19] in helium, compared with our calculated data. Results obtained in the frozen- as well as unfrozen-core models are listed. They are compared in the table with analogous results from Ref. 9, which differ only in the method used to calculate $I(q)$ (no account of the exchange interaction was taken in Ref. 9). It can be seen that the data of Ref. 9 agree less with experiment than our data.

Figure 1 shows the results, taken from Table I, on charge exchange of mesic tritium with ^{3}He nuclei, compared

TABLE I. Rates λ_m (10^8 s^{-1}) of formation of hydrogen-helium mesic molecules, calculated in the simple approach with allowance for screening.

ε, eV	$p\mu^3$He	$p\mu^4$He	$d\mu^3$He	$d\mu^4$He	$t\mu^3$He	$t\mu^4$He
0.004	0.64	0.43	2,14	7.93	26.7	1.81
0.02	0.56	0.37	1.55	3.44	8.35	1,45
0.04	0.52	0.34	1.29	2.25	4.95	1,24
0.06	0.49	0.32	1,15	1.73	3.62	1.09
0.1	0.46	0.30	0.97	1.22	2.42	0,90
1.0	0.30	0.17	0.33	0.22	0.39	0,21

TABLE II. Rates $\bar{\lambda}_m$ (10^{-8} s^{-1}) of formation of hydrogen-helium mesic molecules, averaged over a Maxwellian distribution of the mesic-atom velocities.

T, K	ε, eV	$p\mu{}^3$He	$p\mu{}^4$He	$d\mu{}^3$He	$d\mu{}^4$He	$t\mu{}^3$He	$t\mu{}^4$He
30.9	0.004	0.64	0.43	2.17	8.74	32.9	1.83
154.7	0.02	0.57	0.38	1.68	4.60	13.5	1.52
309.5	0.04	0.53	0.35	1.43	3.22	8.56	1.32
464.2	0.06	0.51	0.34	1.29	2.56	6.45	1.19
773.7	0.1	0.48	0.31	1.11	1.89	4.47	1.02
7737	1.0	0.33	0.19	0.45	0.40	0.78	0.33

TABLE III. Binding energies ε_{10} of hydrogen-lithium mesic molecules (eV), calculated in the simple approach.

$p\mu{}^6$Li	$p\mu{}^7$Li	$d\mu{}^6$Li	$d\mu{}^7$Li	$t\mu{}^6$Li	$t\mu{}^7$Li
7.40	8.20	13.5	14.7	16.9	18.3

TABLE IV. Rates λ_m (10^6 s^{-1}) of formation of hydrogen-lithium mesic molecules, calculated in the simple approach with allowance for screening.

ε, eV	$p\mu{}^6$Li	$p\mu{}^7$Li	$d\mu{}^6$Li	$d\mu{}^7$Li	$t\mu{}^6$Li	$t\mu{}^7$Li
0.004	2.76	1.26	0.060	0.00136	0.57	0.47
0.02	2.33	1.05	0.028	0.00065	0.19	0.26
0.04	2.03	0.91	0.018	0.00052	0.12	0.17
0.06	1.84	0.82	0.014	0.00049	0.085	0.13
0.1	1.60	0.71	0.0098	0.00050	0.058	0.089
1.0	0.46	0.19	$3\cdot10^{-6}$	0.00223	0.018	0.022

TABLE V. Rates $\bar{\lambda}_m$ (10^6 s^{-1}) of formation of hydrogen-lithium mesic molecules averaged over Maxwellian distribution of the mesic-atom velocities.

T, K	ε, eV	$p\mu{}^6$Li	$p\mu{}^7$Li	$d\mu{}^6$Li	$d\mu{}^7$Li	$t\mu{}^6$Li	$t\mu{}^7$Li
30.9	0.004	2.76	1.26	0.063	0.00149	0.65	0.48
154.7	0.02	2.40	1.09	0.036	0.00085	0.29	0.31
309.5	0.04	2.15	0.97	0.025	0.00067	0.19	0.23
464.2	0.06	1.98	0.89	0.020	0.00062	0.15	0.18
773.7	0.1	1.76	0.78	0.015	0.00060	0.10	0.14
7737	1.0	0.68	0.29	0.0024	0.00222	0.026	0.034

TABLE VI. Comparison of the values of $\bar{\lambda}_m$ (10^8 s^{-1}), calculated at room temperatures in different atomic models and averaged over the maximum Maxwellian distribution of the mesic-atom velocities.

Charge-exchange reaction	Kravtsov *et al.*[9]	Present work		Experiment
		thawed core	frozen core	
$p\mu + {}^4$He	0.52	0.32	0.35	0.36±0.10 [18]
$d\mu + {}^3$He	2.01	1.30	1.43	1.27±0.11 [19]
$d\mu + {}^4$He	4.22	2.96	3.22	3.68±0.18 [19]
$t\mu + {}^3$He *	6.59	4.47	4.95	4.7±0.7 [20]

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*The calculated data for this reaction are not averaged over the Maxwellian distribution of the mesic atoms.

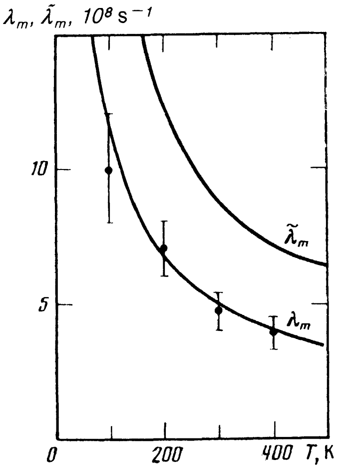

FIG. 1. Temperature dependences of the charge-exchange rates λ_m and $\tilde{\lambda}_m$ in the reaction $t\mu + {}^3\mathrm{He} \rightarrow t\mu{}^3\mathrm{He} \rightarrow {}^3\mathrm{He}\mu + t$. The theoretical curves were calculated in the "simple approach" with allowance for screening. The electrons were described by Hartree-Fock wave functions. The frozen-core model was used for the outgoing electron. The experimental results were taken from Ref. 20.

with the temperature dependence, measured in Ref. 20, of the charge-exchange rate in this reaction. The good agreement between theory and experiment, in contrast to the results of using the data of Table II indicates that, in all probability, charge exchange is more likely than thermalization of mesic atoms under the conditions of this experiment, carried out at high pressure ($\sim$700 atm).

4. CONCLUSION

The agreement of experiment with our results on charge exchange of mesic atoms of hydrogen and helium isotopes is evidence of the need for correctly taking into account the atomic shell in the calculation of bound states of mesic molecules. At the same time, it confirms the applicability of the effective single-channel approximation (the "simple approach") rather than the single-channel approximation which underestimates the results of analogous calculations.

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2) Data on the rate of this charge exchange are important for a discussion of the feasibility of using LiH targets in lieu of hydrogen ones.

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