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Muon transfer in excited muonic hydrogen

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The cross sections and rates of muon transfer between excited states of muonic hydrogen are presented as functions of collision energy for different isotope combinations. Electron screening of the field of the target nucleus is taken into account. The ground-state population, q_{1s} , of muonic hydrogen is obtained for different collision energies, target densities, and relative hydrogen isotope concentrations, considering cascade processes for the principal quantum numbers $n \leq 12$. The obtained results for q_{1s} are significantly smaller than the recent experimental data for D-T and H-D mixtures (tenfold and twice, respectively) and indicate that some new effects must be considered to improve the agreement.

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I. INTRODUCTION

The isotopic exchange reactions in the excited states of muonic atoms,

$$(d\mu)_n + t \to (t\mu)_n + d , \qquad (1)$$

$$(p\mu)_n + d \to (d\mu)_n + p , \qquad (2)$$

$$(p\mu)_n + t \to (t\mu)_n + p , \qquad (3)$$

play an important role in the kinetics of the processes occurring in hydrogen isotope mixtures and have been studied in a number of papers [1,2,8,11,18-20]. In particular, they have to be taken into account in investigations of weak muon capture by protons [1] and muon-catalyzed fusion [2].

At collision energies smaller than the isotopic energy difference, the muon transfer reactions (1)-(3) are irreversible and can be considered as quasiresonance processes with a resonance defect $\Delta U_n = (\mu_2 - \mu_1)/2n^2 \sim 0.01/n^2$ (in muonic atom energy units) μ_1 and μ_2 being reduced masses of the initial and final muonic atoms, respectively.

The ground-state population of muonic atoms in mixtures of hydrogen isotopes is determined by muon transfer, which competes with deexcitation processes, i.e., radiative or Coulomb deexcitation, dissociation of the target molecules, and external Auger processes on target atoms (or molecules). The latter process has been considered by Leon and Bethe [3] and by Bukhvostov and Popov [4] in the Born and eikonal approximation, respectively. Deexcitation via target molecule dissociation was investigated in Ref. [3] and radiative deexcitation in Ref. [5]. The detailed considerations for Coulomb deexcitation were presented in Refs. [3,6-12].

In Refs. [8,13–16] it has been assumed that for n > 5



FIG. 1. Scheme of the muonic atom cascade.

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the rates of deexcitation and thermalization of muonic hydrogen are much greater than the corresponding rates of muon transfer. Therefore, the initial conditions corresponded there to populations $q_5=1$, $q_{n<5}=0$, and muonic atoms were considered to be fully thermalized. However, according to the experimental data of Refs. [21,22], the residual energy of muonic hydrogen can be larger than thermal energy $\varepsilon_T=0.04$ eV. Consequently, in Refs. [11,17,18,19] the ground-state population of muonic hydrogen, q_{1s} , was calculated for collision energies $\varepsilon > 0.04$ eV. Moreover, the results of Ref. [20] demonstrate that the states $5 < n \le 7$ also significantly influence the value of q_{1s} .

In this paper we present the rates for reactions (1)-(3) as a function of collision energy for $2 \le n \le 10$. We also calculate the q_{1s} parameter for muonic atom cascade presented in Fig. 1, including states up to n = 12.

II. MUON TRANSFER

The effective potential of interaction of the muonic hydrogen atom in an excited state with a hydrogen nucleus is asymptotically determined by

$$U(R) \approx \frac{3}{2} [n(n_1 - n_2)/R^2]$$
,

(in units of $m_{\mu} = \hbar = e = 1$, m_{μ} being the reduced mass of muonic atom), where R is internuclear distance and (n, n_1, n_2) are parabolic quantum numbers. The validity condition for the WKB approximation $d\lambda/dR \ll 1$ is fulfilled here, since for $n_1 \neq n_2$,

$$d\lambda/dR \approx (3Mn|n_1-n_2|)^{-1/2} \ll 1$$

which is the case for transfer processes in excited states [13]. M is the reduced mass of the colliding atoms. The cross section can be then written as

$$\sigma = \pi \int_0^{\rho_{\max}^2} P \, d\rho^2 \,, \tag{4}$$

where ρ is the classical impact parameter (ρ_{max} is the maximum impact parameter determined by the potential barrier) and *P* is the reaction probability.

Because reactions (1)-(3) are quasiresonant processes, *P* can be calculated using the fully solvable Rozen-Zener-Demkov model [23(a)]. The molecular terms of the two-center problem with Coulomb repulsion U_i (i = 1,2 for the initial and final states of the transfer process, respectively) are considered in this model as branches of the complex potential U(R) in a complex *R* plane [23(b),23(c)]. The difference between $U_1(R)$ and $U_2(R)$ in the neighborhood of the branch points of U(R)can be expressed as [23(c)]

$$\Delta U(R) = \sqrt{d^2 + w^2(R)}$$

where $w(R) \sim \exp(-\alpha R)$ represents exchange interaction and $d = \Delta U(\infty)$ is resonance defect. Muon transfer occurs when $\Delta U(R)=0$. It is satisfied for an infinite *P* series of complex, equidistant branch points $R_j = R_P + i\pi(j-1/2)\alpha^{-1}, J = 1, 2, ...,$ which determine the transition probability.¹ For single passing of the transition region (ReR either increasing or decreasing),

$$P_1 = \frac{1}{2}(1 - \tanh \delta) = \sum_{j=1}^{\infty} (-1)^{j+1} \exp(-2j\delta) , \quad (5)$$

where δ is the Massey parameter

$$\delta = \left| \operatorname{Im} \int_{C} p_{i} dR \right| . \tag{6}$$

Contour C in integral (6) encloses the branch point R_1 , which is the closest one to the real axis ReR; and

$$p_i = \sqrt{2M \left[\varepsilon - U_i(R) - \varepsilon \rho^2 / R^2\right]}$$
(7)

is the relative radial momentum of colliding atoms for the initial (i=1) and final (i=2) state of reactions (1)-(3), respectively, with ε being collision energy at infinite R. The total transition probability (the transition region is passed twice) is

$$P = 2P_1(1 - P_1) = (2\cosh^2\delta)^{-1} .$$
(8)

In the calculations of U_i , electron screening of the field of the target nucleus was taken into account according to Ref. [24], which asymptotically $(R \rightarrow \infty)$ is given by

$$U_{i}(R) = -\mu_{i}/2n^{2} + \{(\frac{3}{2})n(n_{1}-n_{2})-(n^{2}/2R)[6(n_{1}-n_{2})^{2}-n^{2}+1]\}E(R) -\lambda^{3}\exp(-2\beta)(n^{2}/2)[9(n_{1}-n_{2})^{2}+n^{2}-m^{2}+3],$$
(9)

where $\lambda = a_{\mu}/a_e$, $\beta = R/a_e$ (a_{μ} and a_e are Bohr radii of the muonic and electronic hydrogen atom, respectively), and E(R) is the atomic electric field

$$E(R) = (1/R^2)(1+2\beta+2\beta^2)\exp(-2\beta), \qquad (10)$$

sensed by the muonic atom. In the calculation of transfer cross sections and rates the molecular degrees of freedom of hydrogen molecules colliding with muonic atoms were neglected. In order to obtain the transfer cross sections we have calculated the molecular terms and their branch points for $n \leq 10$.

III. RESULTS AND DISCUSSION

The rates for reactions (1)-(3), obtained with electron screening taken into account, are shown in Figs.

¹It should be noted that for nonresonant reactions, e.g., Coulomb deexcitation or muon transfer to helium, only one branch point of the potential is practically important, so the reaction probability is $P_1 = \exp(-2\delta)$ [23(d)].



FIG. 2. (a)–(c) Muon transfer rates calculated with electron screening taken into account for reactions (1)–(3), respectively, for different principal quantum numbers n indicated on curves.

2(a)-2(c), respectively.² Figure 3 shows the corresponding rates for reaction (1), calculated without electron screening. Comparison of Figs. 2(a) and 3 shows a significant influence of electron screening on the transfer processes [the cross sections and rates obtained with electron screening are much smaller due to the decrease of ρ_{max} in Eq. (4)].

The rates of radiative deexcitation were obtained using the formulas of Ref. [5], and the rates of Auger deexcitation and target molecule dissociation were calculated for muonic hydrogen using the data of Ref. [3]. In muonic hydrogen the Auger transitions $n \rightarrow n - 1$ for *n* between 8-12 are energetically forbidden; hence, in order to con-

²Transfer rates are normalized to liquid-hydrogen density (LHD), $N_0 = 4.25 \times 10^{22}$ cm⁻³, i.e., $\lambda_n = \sigma_n V N_0$, where V is relative velocity of the colliding atoms at infinite R.



FIG. 3. Muon transfer rates for reaction (1) without electron screening.

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TABLE I. Parameter q_{1s} for the D-T mixture as a function of tritium concentration c_t , and density ϕ in LHD units for collision energy $\varepsilon = 0.04$ eV.

c_t	0.01	0.05	φ (LHD) 0.1	0.5	1.0
0.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.0010	0.9787	0.9683	0.9620	0.9456	0.9398
0.0100	0.9152	0.8743	0.8488	0.7863	0.7663
0.0200	0.8753	0.8176	0.7814	0.6970	0.6721
0.0400	0.8078	0.7257	0.6754	0.5676	0.5388
0.0600	0.7482	0.6484	0.5896	0.4720	0.4429
0.0800	0.6942	0.5817	0.5180	0.3980	0.3701
0.1000	0.6451	0.5235	0.4574	0.3393	0.3131
0.2000	0.4552	0.3217	0.2611	0.1715	0.1545
0.3000	0.3296	0.2084	0.1608	0.0981	0.0872
0.4000	0.2439	0.1406	0.1045	0.0607	0.0535
0.5000	0.1838	0.0981	0.0709	0.0397	0.0348
0.6000	0.1408	0.0703	0.0497	0.0270	0.0236
0.7000	0.1094	0.0516	0.0358	0.0190	0.0166
0.8000	0.0861	0.0386	0.0264	0.0138	0.0119
0.9000	0.0685	0.0294	0.0198	0.0102	0.0088
1.0000	0.0551	0.0228	0.0151	0.0077	0.0066

sider levels n = 8-12, one has to take into account Auger transitions for $\Delta n > 1$. These transitions were consequently included also for lower levels (see Fig. 1). As for Coulomb deexcitation, we used our results of Ref. [12]. The rate of Stark-induced transition, $\lambda_{ind}(2s \rightarrow 2p \rightarrow 1s)$, and the rates of Stark mixing of the 2p and 2s states were obtained using the results of Refs. [14,17,25].

As is seen in Figs. 2(a)-2(c), the transfer rates λ_{10} and λ_9 are nearly equal for $\varepsilon \le 1$ eV; hence, to calculate q_{1s} in this energy region we put $\lambda_{12} = \lambda_{11} = \lambda_{10}$. The results

TABLE II. Parameter q_{1s} for the D-T mixture as a function of tritium concentration c_i , and density ϕ in LHD units for collision energy $\varepsilon = 1.0 \text{ eV}$.

			ϕ (LHD)		
c_t	0.01	0.05	0.1	0.5	1.0
0.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.0010	0.9964	0.9954	0.9947	0.9922	0.9907
0.0100	0.9650	0.9553	0.9482	0.9254	0.9120
0.0200	0.9315	0.9130	0.8996	0.8577	0.8336
0.0400	0.8688	0.8350	0.8111	0.7399	0.7006
0.0600	0.8111	0.7649	0.7330	0.6517	0.5932
0.0800	0.7581	0.7017	0.6639	0.5592	0.5055
0.1000	0.7092	0.6447	0.6025	0.4894	0.4334
0.2000	0.5156	0.4309	0.3813	0.2658	0.2162
0.3000	0.3827	0.2968	0.2511	0.1553	0.1185
0.4000	0.2892	0.2097	0.1708	0.0959	0.0696
0.5000	0.2220	0.1515	0.1194	0.0618	0.0431
0.6000	0.1728	0.1116	0.0855	0.0413	0.0279
0.7000	0.1361	0.0836	0.0625	0.0284	0.0187
0.8000	0.1084	0.0636	0.0465	0.0201	0.0129
0.9000	0.0872	0.0490	0.0351	0.0145	0.0091
1.0000	0.0708	0.0382	0.0269	0.0107	0.0066



FIG. 4. (a)-(c) Parameter q_{1s} for (a) $d\mu$ in the D-T mixture, (b) $p\mu$ in the H-D mixture, and (c) $p\mu$ in the H-T mixture as a function of the concentration of the heavier hydrogen isotope for collision energies $\varepsilon = 0.04$ eV (solid lines) and $\varepsilon = 1$ eV (dashed lines). Densities, ϕ in LHD units, are indicated at the curves.

were obtained by solving the system of kinetic equations with the initial conditions corresponding to $q_{12}=1$ and $q_{n<12}=0$. The dependence of q_{1s} on tritium concentration c_t , for different target densities and collision energies is shown for the D-T mixture in Tables I and II and Fig. 4(a). The analogous results for the H-D and H-T mixtures are presented in Figs. 4(b) and 4(c), respectively.

Figures 5 and 6 illustrate, for the case of the D-T mixture, the influence of the maximum *n* taken into account in the calculations of q_{1s} . It is remarkable that inclusion of the level n = 8 leads to a sharp decrease of q_{1s} . The gap between the q_{1s} curves obtained for $n_{max} = 7$ and 8 is caused mainly by the absence of the Auger transition between levels 8 and 7 [4] (as opposed to pionic hydrogen where this transition is allowed [3]) and by the fact that the other deexcitations of n = 8 are comparable or slower than transfer to tritium. The curve obtained for $n_{max} = 9$ lies above the curve for $n_{max} = 8$ because the dominating Auger transition $9 \rightarrow 7$ bypasses n = 8 (the rates of molecular and Coulomb deexcitation of n = 9 are about 10 times slower than the Auger transition $9 \rightarrow 7$). A similar observation holds true for levels 11 and 12.

It follows from Figs. 5 and 6 that the dependence of q_{1s} on n_{max} becomes stronger with decreasing ϕ and increasing ε . It can be explained by a relatively strong *n* dependence of λ_n for large ε [see Fig. 2(a)] and a relatively slow deexcitation as compared with transfer for decreasing ϕ . The above observations remain valid also for other hydrogen isotopes.

The isotopic effect in the energy dependence of q_{1s} is illustrated in Fig. 7 for $\phi = 0.1$ and equal concentrations of the two components of the mixture. It is remarkable that the effect is strongest for the H-T mixture and q_{1s} increases by a factor of 2 between $\varepsilon = 0.1$ and 1.0 eV for all isotope combinations.

Figure 8 shows the comparison of our results for q_{1s}



FIG. 5. Parameter q_{1s} for $d\mu$ in the D-T mixture calculated for $\varepsilon = 0.04$ eV as a function of tritium concentration c_t for $\phi = 0.01$ LHD and for different n_{max} indicated at the curves. The ordering of the curves for other densities ($\phi = 0.1$ and 1.0 LHD) is the same as for $\phi = 0.01$ LHD.

with the present experimental data for the D-T [26] and H-D [27] mixtures. As is seen from Fig. 8(a) (the D-T case) the theoretical corridor for q_{1s} , bounded by the curves for $\phi = 0.1$ and 1.2 LHD calculated for $n_{max} = 12$ and $\varepsilon = 1$ eV, lies drastically lower than the experimental one (as is seen in Fig. 7, q_{1s} is maximal for $\varepsilon = 1$ eV), espe-



FIG. 6. Parameter q_{1s} for $d\mu$ in the D-T mixture as a function of tritium concentration c_t calculated for $\phi = 0.1$ LHD for different n_{\max} and ε .



FIG. 7. Isotopic effect in the energy dependence of q_{1s} calculated for $\phi = 0.1$ LHD and equal concentrations of mixture components.

cially for large c_t , where the experiment exceeds theory by a factor of 10.³ As is seen from Fig. 8(b), the discrepancy between theory for $n_{\text{max}} = 12$ and the experiment for the H-D mixture for $\phi = 1$ LHD is also large (the experimental value is about two times greater than the theoretical one).

It follows from Figs. 5 and 6 that increasing n_{max} (which automatically leads to inclusion of additional transfer channels) deteriorates further the agreement between theory and experiment. This could mean that the muon transfer rates are overestimated. On the other hand, the rates calculated for muon transfer from hydrogen to helium [18,19,30] are in good agreement with the experimental data [28,29]. Therefore, the reason for the discrepancy observed for hydrogen mixtures is possibly due to other effects which suppress muon transfer from highly excited states. A possible explanation can probably be given by inclusion of inverse muon transfer, i.e., muon transfer from a heavier to a lighter hydrogen isotope. The epithermal effects in D-T mixtures leave ample room for such transitions, particularly in the highly excited states. Calculations of inverse transfer rates are in progress.



FIG. 8. (a) Comparison of the experimental q_{1s} corridor obtained for ϕ in the range 0.1-1.2 LHD (solid line) for the D-T mixture [26] with the theoretical curves for $\phi=0.1$ and 1.2 LHD, calculated at $\varepsilon=1$ eV for $n_{\max}=12$ (dashed). (b) Comparison of the experimental point of q_{1s} for the H-D mixture for $\phi=1$ LHD [27] with theoretical results (dashed line) obtained at $\varepsilon=1$ eV for $n_{\max}=12$.

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³It should be noted, however, that the experimental corridor represents the error bars rather than the $\phi = 0.1$ and 1.2 LHD bounds. In fact, in Ref. [26] the ϕ dependence is found to be nearly negligible.

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