The influence of spectator nuclear motion on the nonresonant formation of muonic hydrogen molecules

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Abstract

A new approach has been developed in order to estimate the influence of the nuclear motion of the hydrogenic molecules on the nonresonant formation of the muonic hydrogen molecules. The rates of such nonresonant reactions, in collisions of the muonic hydrogen atoms with the symmetric and asymmetric hydrogenic molecules, have been calculated for a wide range of kinetic energies up to 100 eV. It has been shown that the internal nuclear motion significantly affects the nonresonant formation processes at specified low collision energies. The energy-dependent formation rates are indispensable in the interpretation of the already-measured data and for the upcoming and planned experiments in low-energy muon physics.

Keywords: muonic atoms, muonic hydrogenic molecules, nonresonant formation

1. Introduction

The formation of muonic molecules is a crucial link in the chain of physical processes caused by the negative muons $\mu^-$ in hydrogen-isotope mixtures (see reviews [1–3] and references therein). The interpretation and analysis of the data obtained in various experiments with low-energy muons requires a knowledge of the energy-dependent formation rates of various muonic hydrogen molecules; for example, in the studies of muon-catalyzed $pt$ and $tt$ fusion [4, 5], in the PSI measurements [6–8] of the basic weak muon capture on the hydrogen-isotope nuclei, as well as in the planned determination of the Zemach radius of protons by the FAMU collaboration [9] at RAL and by the CREMA collaboration [10, 11] at PSI. Also, the rates of nonresonant formation of different muonic molecules in H/D targets have been employed for the present investigation of nuclear structure with radioactive muonic atoms by the muX collaboration at PSI [12].

The muonic molecule, being the three-body system (ion, in reality), consists of the two hydrogen-isotope nuclei and the muon. Such $\mu$-molecular systems are formed in collisions of the muonic $a\mu$-atoms ($a = p, d, t$) with the hydrogen-isotope (hydrogenic) molecules $BX (B, X = H, D, or T)$. The quantum states of the muonic molecules formed are defined by the different rotational ($J$) and vibrational ($\nu$) quantum numbers (see table I). The loosely bound ($J = 1, \nu = 1$) states of the $dd\mu$ and $dt\mu$ molecules refer to the formation, as a rule, by the resonance mechanism [16] in the reaction of the following type

$$t\mu + D_2 \rightarrow [(dt\mu)_1 e e]^{+}_{K_\nu},$$

where the released energy of about $|\epsilon_1|$ is transferred to the excitation of the rotational-vibrational states ($K\nu$) of the molecular complex $[(dt\mu)_1 e e]$. The rates $\lambda_{dd\mu}$ and $\lambda_{dt\mu}$ of such resonance reactions depend on the target temperature $T$.  

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Table 1. The binding energies \( \epsilon_{J\nu} \) (in eV) of the muonic molecules \( ab\mu \) in the states \( (J\nu) \). The table is compiled from the data of [13], whereas the binding energies of the state \( (J = 1, \nu = 1) \) are taken from [14] (see also [15]).

| State \((J\nu)\) | \(pp\mu\) | \(pd\mu\) | \(pt\mu\) | \(dd\mu\) | \(dt\mu\) | \(tt\mu\) |
|------------------|--------|--------|--------|--------|--------|--------|
| (11)             | —      | —      | —      | —      | 1.965  | 0.631  | 45.206 |
| (30)             | —      | —      | —      | —      | —      | 48.838 |
| (01)             | —      | —      | —      | —      | 35.844 | 34.834 | 83.771 |
| (20)             | —      | —      | —      | —      | 86.494 | 102.649| 172.702|
| (10)             | 107.266| 97.498 | 99.126 | 226.682| 232.471| 289.142|
| (00)             | 253.152| 221.549| 213.840| 325.074| 319.140| 362.910|

For the room temperature \( T = 300 \) K, these rates are in the order of \( 10^8 \) s\(^{-1}\) [2] and \( 10^6 \) s\(^{-1}\) [3, 17], respectively.

In any other state \((J\nu)\), the muonic molecular ions \( ab\mu \) are formed via the nonresonant process [1, 18, 19]

\[
a\mu + BX \rightarrow [(ab\mu)_0, xe]^+ + e^-, \tag{2}
\]

with conversion of the released energy into the electron ionization of the BX molecule. The rates of transitions (2) to all \((J\nu)\)-states of \( ab\mu \) have been calculated [20] for kinetic energies \( \leq 50 \) eV, except that for the \((J = 1, \nu = 1)\) states of the molecules \( dd\mu \) and \( dt\mu \). Later on, the nonresonant formation in such a loosely bound state was also considered for collision energies higher than the electron ionization potential of the BX molecule [21]. It was shown that the corresponding rates of reactions (2) could be significant. The rates of such nonresonant formation reach magnitudes of up to \( 10^7 \) s\(^{-1}\), depending on the energy of the \( ab\mu \) collision with a BX molecule.

A comparison of the measured [3, 22, 23] and calculated [20, 21] rates of nonresonant transitions in reactions (2) demonstrated a very good agreement for different muonic molecules, although some differences between the theory and experiments were observed in the case of low-temperature H/D targets. In order to improve the calculating scheme [20], in which the distance between the center of mass (CM) of molecule \( ab\mu \) and the spectator nucleus \( x \) of the molecule BX was kept constant, the internal motion of both the nuclei \( b \) and \( x \) within the BX molecule was taken into account in the present work.

In section 2, a transformation of the nonresonant formation rates calculated in CM of the \( ab\mu + b \) system [20] to the laboratory system \( ab\mu + BX \) was carried out taking into account the internal motion of nuclei \( b \) and \( x \) within the molecule BC. To describe quantitatively the internal nuclear motion within the hydrogenic molecules, a harmonic model of the molecular vibrations is used in section 3. The results and discussion are included in section 4.

2. Transformation of the nonresonant formation rates between the center of mass and laboratory systems

The rates \( \lambda \) of the nonresonant formation of \( ab\mu \) molecules were calculated in [20] assuming that the nucleus \( x \) in the molecule BX is a distant spectator, which is located at a fixed position \( \mathbf{R}_0 \) with respect to the nucleus \( b \) (see figure 1). These rates, which were calculated in the center of mass of the \( ab\mu + b \) system (nuclear CMS), are functions of collision energy \( \epsilon \) in this system: \( \lambda = \lambda(\epsilon) \). A dependence of \( \epsilon \) on the momentum \( \mathbf{k} \) of relative motion of the \( ab\mu \) atom and the nucleus \( b \) is expressed as follows

\[
\epsilon = \frac{\mathbf{k}^2}{2\mu}, \quad \mathbf{k} = \frac{d\mathbf{r}_b}{dt}, \tag{3}
\]

where the reduced mass \( \mu \) of the \( ab\mu + b \) system is given by the relations

\[
\mu^{-1} = \mu_{\text{ab}}^{-1} + \mu_b^{-1}, \quad M_{ab} = M_a + M_b, \tag{4}
\]

in which \( M_b \) is the muon mass and the masses of nuclei \( a \) and \( b \) are denoted by \( M_a \) and \( M_b \), respectively.

For the analysis of the experimental data, it is often more convenient to use the formation rates as functions of kinetic energy \( E \) of the \( ab\mu \) atoms in the laboratory frame (LAB). Such rates in LAB were estimated in [21, 24] using the rates \( \lambda(\epsilon) \), which were calculated in the nuclear CMS, and the transformation of the following form [25, 26]:

\[
\lambda(E, T) = \int_0^\infty \lambda(\epsilon_Q) G(p, \epsilon_Q) d\epsilon_Q, \tag{5}
\]

with the following ‘distribution function’:

\[
G(p, \epsilon_Q) = \frac{M_{\text{ms}}}{2\pi T} \frac{M_{ab}}{\mu_p} \left\{ \exp \left[ -\frac{M_{\text{ms}}}{2T} \frac{Q - p}{\mu_p} \right]^2 \right\} = \exp \left[ -\frac{M_{\text{ms}}}{2T} \frac{Q + p}{M_{ab}} \right]. \tag{6}
\]
This function was derived assuming the Maxwellian distribution of kinetic energies of the thermalized hydrogenic molecules. The total mass $M_t$ and the reduced mass $\mu_e$ of the $a\mu + BX$ system (henceforth called the molecular system) are given by the relations

$$M_t = M_{a\mu} + M_{BX}, \quad \mu_e^{-1} = M_{a\mu}^{-1} + M_{BX}^{-1},$$

$$M_{BX} = M_b + M_a,$$  \hspace{1cm} (7)

where $M_a$ denotes the mass of nucleus $a$. In equations (5)–(6), the momentum $p$ of the $a\mu$ atom in LAB and the momentum $Q$ of the relative motion of the $a\mu$ atom and molecule $BX$ are related to the corresponding kinetic energies $E$ and $\varepsilon_Q$ by the following expressions:

$$E = p^2/(2M_{a\mu})$$ \hspace{1cm} (8)

and

$$\varepsilon_Q = Q^2/(2\mu_e), \quad Q = \mu_e d\mathbf{r}_m/dt.$$ \hspace{1cm} (9)

The employment of equations (5)–(6) for calculating the formation rates [25, 26] was based on the assumption that the target molecules $BX$ are point-like objects. Therefore, the dependencies

$$\varepsilon_Q = (\mu_e/\mu)\varepsilon, \quad Q = (\mu_e/\mu)k$$ \hspace{1cm} (10)

between the relative energies $\varepsilon_Q$ and $\varepsilon$, as well as between the corresponding momenta $Q$ and $k$, are inferred from equations (3) and (9) using the approximation $\mathbf{r}_m \approx \mathbf{r}_b$.

The simplified procedure of the formation-rate transformation between the nuclear (or molecular) CMS and LAB, which is briefly described above, denotes in fact that the internal motion of the nuclei in a target molecule $BX$ is neglected and that the correct masses $M_{BX}$ and $\mu_e$ of the system $a\mu + BX$, which are defined in (7), are substituted into equations (5)–(8) instead of the masses $M_b$ and $\mu$ of the system $a\mu + b$ (from equation (4)).

Since the hydrogenic molecules are very light, the kinetic energy $\varepsilon_q$

$$\varepsilon_q = q^2/2\mu_{BX}, \quad q = \mu_{BX} d\mathbf{r}_0/dt, \quad \mu_{BX}^{-1} = M_b^{-1} + M_x^{-1},$$ \hspace{1cm} (11)

which corresponds to the relative momentum $q$, is quite large. Even in the ground state of a molecule $BX$, this energy is in the order of its vibrational quantum $\hbar \omega \approx 0.3$–0.5 eV [27] due to the zero-point vibrations. Therefore, the above-mentioned simple scheme of $\lambda(\varepsilon)$ transformation between CMS and LAB is not valid in general. In order to improve this scheme, it is vital to consider the $a\mu$ atom collision with a real $BX$ molecule of finite dimensions, instead of a point-like molecule $BX$ that is located at the position of a free nucleus $b$.

The following relations between different vectors of the $a\mu + BX$ system are inferred from figure 1:

$$\mathbf{R}_0 = \mathbf{R}_a - \mathbf{R}_b = \mathbf{r}_a - \mathbf{r}_b,$$

$$\mathbf{R}_m = \frac{M_b \mathbf{R}_b + M_a \mathbf{R}_a}{M_{BX}}, \quad \mathbf{r}_m = \frac{M_a \mathbf{r}_a + M_b \mathbf{r}_b}{M_{BX}},$$

$$\mathbf{R}_b = \frac{M_b \mathbf{R}_b}{M_{BX}}, \quad \mathbf{r}_b = \mathbf{r}_m - \frac{M_b}{M_{BX}} \mathbf{R}_b,$$

$$\mathbf{R}_x = \mathbf{R}_m + \frac{M_b}{M_{BX}} \mathbf{r}_b, \quad \mathbf{r}_x = \mathbf{r}_m + \frac{M_b}{M_{BX}} \mathbf{R}_b$$ \hspace{1cm} (12)

in which vectors $\mathbf{R}_b$, $\mathbf{R}_x$, and $\mathbf{R}_m$ denote the positions of nuclei $b$ and $x$ and their center of mass in LAB, respectively. Vectors $\mathbf{r}_b$, $\mathbf{r}_x$, and $\mathbf{r}_m$ correspond to the same positions with respect to $a\mu$. Vector $\mathbf{r}_n$ can be expressed as

$$\mathbf{r}_n = \mathbf{R}_m - \mathbf{R}_{a\mu},$$ \hspace{1cm} (13)

where $\mathbf{R}_{a\mu}$ denotes the $a\mu$ position in LAB. This equation enables us to represent $\mathbf{r}_n$ from equations (12) as follows:

$$\mathbf{r}_b = \mathbf{R}_m - \mathbf{R}_{a\mu} - \frac{M_b}{M_{BX}} \mathbf{R}_b.$$ \hspace{1cm} (14)

The momentum $p$ of the muonic atom and the momentum $p_m$ of the molecule in LAB are related to their positions

$$p = M_{a\mu} \frac{d\mathbf{R}_{a\mu}}{dt}, \quad p_m = M_{BX} \frac{d\mathbf{R}_m}{dt}.$$ \hspace{1cm} (15)

Using (14) and definitions (3), (11) and (15), the momentum $k$ can be written down as

$$k = \frac{1}{M} \left( \frac{M_{a\mu} M_b}{M_{BX}} p_m - M_{a\mu} q - M_b p \right).$$ \hspace{1cm} (16)

As a result, the corresponding collision energy $\varepsilon$ is expressed as a function of the momenta $p$, $p_m$ and $q$

$$\varepsilon = \varepsilon(p, q, p_m) = \frac{1}{2 \mu M^2} (M_b p + M_{a\mu} q - \frac{M_{a\mu} M_b}{M_{BX}} p_m)^2.$$ \hspace{1cm} (17)

Averaging the formation rate $\lambda(\varepsilon)$ over the distribution $W(q)$ of momentum $q$ and over the distribution $F(p_m, T)$ of the translational momentum $p_m$ of the molecule, in a given target at temperature $T$, results in

$$\lambda(E, T) \equiv \lambda(p(E), T) = \int \lambda(\varepsilon(p, q, p_m)) W(q) 	imes F(p_m, T) \, dq \, dp_m.$$ \hspace{1cm} (18)

Function $\lambda(E, T)$ is interpreted as the formation rate in the LAB frame, which takes into account the internal motion of nuclei within molecule $BX$. The probability $W(q)$ can be expressed in the standard form [27]

$$W(q) = \frac{1}{(2\pi)^3} \left| \int \phi(R_0) \exp(-i \mathbf{q} \cdot \mathbf{R}_0) \, d^3 R_0 \right|^2,$$ \hspace{1cm} (19)

where $\phi(R_0)$ is the nuclear wave function of the molecule in its center of mass system.
Collision energy $\varepsilon$ can also be expressed as a function of the momenta $Q$ and $q$. Using $\mathbf{r}_m$ from (12), together with definitions (3), (9) and (11), leads to the relation

$$k = \mu(Q/\mu_t - q/M_b),$$  

which results in

$$\varepsilon = \varepsilon(Q, q) = \frac{\mu}{2}(Q/\mu_t - q/M_b)^2.$$  

(20)

Averaging the rate $\lambda(\varepsilon(Q, q))$ over the distribution of momentum $q$ gives the following function:

$$\Lambda(\varepsilon_0) = \int \Lambda(\varepsilon(Q, q))W(q)d^3q,$$  

(22)

which depends on collision energy $\varepsilon_0$ and thus can be interpreted as the ‘formation rate’ in the molecular CMS. It is convenient to introduce a distribution function

$$g(\varepsilon_0, \varepsilon) \equiv \int W(q)\delta(\varepsilon - \varepsilon)\,d^3q,$$  

(23)

which enables us to treat (22) as averaging over collision energies $\varepsilon$ in nuclear CMS

$$\Lambda(\varepsilon_0) = \int_0^\infty \Lambda(\varepsilon)g(\varepsilon_0, \varepsilon)\,d\varepsilon.$$  

(24)

A relation between the formation rate $\Lambda(E, T)$ in LAB and the rate $\Lambda(\varepsilon_0)$ in molecular CMS can be derived using the following equations:

$$Q(p, P_m) = \mu_s(P_m/M_{bx} - p/M_{bx}),$$

$$\varepsilon_0(p, P_m) = \mu_s(P_m/M_{bx} - p/M_{bx})^2/2,$$  

(25)

which are inferred from the vector dependence $r_m = R_m - \mathbf{R}_{ax}$ ($\mathbf{R}_{ax}$ denotes the position of $\mu_0$ in LAB) and the definitions of momenta $Q$, $P$ and $p$ and energy $\varepsilon_0$. On substitution of (22) into (18) with the help of (25) one obtains

$$\Lambda(E, T) \equiv \lambda(p(E), T) = \int \Lambda(\varepsilon_0(p, P_m))$$

$$\times F(P_m, T)d^3P_m.$$  

(26)

After introducing the following distribution function

$$G(\varepsilon_0, \varepsilon) \equiv \int F(P_m, T)\delta(\varepsilon(Q(p, P_m) - \varepsilon_0))\,d^3P_m,$$  

(27)

the rate (26) is expressed as averaging over collision energies in the molecular CMS

$$\Lambda(E, T) \equiv \lambda(p(E), T) = \int_0^\infty \Lambda(\varepsilon_0)G(\varepsilon, \varepsilon_0)d\varepsilon.$$  

(28)

Let us note that this equation has a form similar to that of (5).

In the above reasoning, we have not assumed any specific form of momentum distribution $F(P_m, T)$. In the case of Maxwellian distribution

$$F(P_m, T) = (2\pi M_{bx}T)^{-3/2}\exp(-P_m^2/2M_{bx}T),$$  

(29)

function (27) can be strictly calculated. As a result, for a real hydrogenic molecule, we recover the distribution (6). When $p \rightarrow 0$, this distribution tends to the following limit:

$$G(0, \varepsilon_0) = 2\sqrt{\frac{1}{\pi T^{3}}}\left(\frac{M_{bx}}{\mu_t}\right)^{5/2}\sqrt{\varepsilon_0}\exp\left(-\frac{M_{bx} \varepsilon_0}{\mu_t T}\right),$$  

(30)

The Gaussian form (29) of distribution of the molecular momenta $P_m$ is valid not only for perfect hydrogenic gases. This distribution also applies to dense gases [28] as well as to liquid hydrogens, which are Boltzmann quantum fluids (see, e.g., [29]). However, at densities comparable to that of liquid hydrogen, the mean translational energy of hydrogenic molecules is significantly larger than $3k_B T/2$ ($k_B$ is Boltzmann’s constant) [30]. As a result, the Maxwellian distribution (29) can be applied provided that temperature $T$ is replaced by an effective temperature $T_{eff} > T$. The density of the hydrogenic target at a given temperature and pressure and, in particular, validity of the perfect-gas model can be determined using the extensive data from the handbook [31].

3. Internal nuclear motion within a hydrogenic molecule

Equation (21) can be expressed (see definitions (9) and (11)) in terms of kinetic energies $\varepsilon_0$ and $\varepsilon_p$, which correspond to the momenta $Q$ and $q$, respectively:

$$\varepsilon = \frac{\mu}{\mu_t} + \beta_p^2\frac{\varepsilon_q}{\mu_{bx}} - 2\beta_p \sqrt{\frac{\varepsilon_q}{\mu_t} \mu_{bx} \varepsilon},$$

$$\varepsilon = \cos \vartheta, \quad \beta_p = M_e/M_{bx},$$  

(31)

where the angle between vectors $Q$ and $q$ is denoted by $\vartheta$. When $\varepsilon_0 \gg \varepsilon_p$, equation (31) takes a simple asymptotic form (10): $\varepsilon = (\mu/\mu_t)\varepsilon_0$. When $\varepsilon_0 \ll \varepsilon_p$ kinetic energy $\varepsilon$ is mainly determined by the internal molecular energy $\varepsilon_p$. In particular, at $\varepsilon_0 \rightarrow 0$, the characteristic energy $\varepsilon$ tends to a constant value, which is given by the second term of (31). The width of the $\varepsilon$ spectrum is ruled by the term $\sqrt{\varepsilon_0^2/\varepsilon_q}$ and thus rises with increasing $\varepsilon_0$. On the other hand, as (31) indicates, a fixed kinetic energy $\varepsilon_0$ (9) in CM of the molecular $\mu_0 + BX$ system corresponds to a wide spectrum of energies $\varepsilon$ in the nuclear CMS. As a result, the formation rate $\Lambda(\varepsilon_0)$ in the molecular CMS, which is given in (24), has been obtained on averging the input formation rates $\lambda(\varepsilon)$ over such a spectrum. This leads to an additional smearing of these rates (apart from the thermal motion of the molecules), if they significantly change within the spectrum of energies $\varepsilon$. This problem has already been considered in the case of $\alpha\mu$ scattering from hydrogenic molecules [32], where it has been shown there that the above-mentioned smearing effect is of importance for many low-energy scattering cross sections $\alpha\mu + BX$.

In order to obtain the distribution $g(\varepsilon_0, \varepsilon)$ as a function of collision energies $\varepsilon$ in the nuclear CMS for a fixed collision energy $\varepsilon_0$ in the molecular CMS (see (31)), we follow the calculating scheme from [32]. It is assumed here that the orientation of the molecule with respect to the vector $\mathbf{r}_m$ is random. In a general case, the wave function $\Phi_\mu(\mathbf{R}_d)$ of molecule $BC$ in the quantum state $n$ can be written as follows:

$$\Phi_\mu(\mathbf{R}_d) = \frac{\mu_s(\mathbf{R}_d)}{R_0}Y_{K_{\mu\nu}}(\mathbf{R}_d), \quad \mathbf{R}_d \equiv \frac{\mathbf{R}_d}{R_0}$$  

(32)

where $n \equiv (\nu, K, M_k)$, the vibrational quantum number is denoted by $\nu$, the rotational quantum number is specified by the quantum
numbers $K$ and $M_k$, and $Y_{K0}$ stands for the corresponding spherical harmonics. The radial wave function $u_r$ in the harmonic approximation takes the form

$$u_r(R_0) = N_r H_n(\alpha \rho_0) \exp \left(-\frac{1}{2} \alpha^2 \rho_0^2 \right),$$

$$N_r = \sqrt{\frac{\alpha}{2^{n+1} \sqrt{\pi}}} \quad \alpha = \sqrt{\mu_{\text{ex}} \omega_0}, \quad \rho_0 = R_0 - \bar{R}_0,$$

where $H_n$ denotes the $n$th Hermite polynomial and $\rho_0$ is the displacement of $R_0$ from a mean distance $\bar{R}_0$ between the nuclei $b$ and $x$ in $BX$. The rotational $E_R$ and vibrational $E_v$ energy levels are given as

$$E_R = B_{\text{tot}} K(K + 1), \quad E_v = (\nu + \frac{1}{2}) \omega_0,$$

where the rotational $B_{\text{rot}}$ and vibrational $\omega_0$ constants depend on the type of hydrogen isotopes $b$ and $x$.

At temperatures usually applied in experiments, the molecules are in the ground vibrational state $\nu = 0$. Thus, the distribution function (23) for this state $(\nu = 0)$ is $\langle \nu = 0, K, M_K \rangle$ takes the form

$$g(\varepsilon_Q, \overline{z}) = \frac{1}{2\pi} \int \left| f_{0k}(q) \right|^2 \delta(\varepsilon - \overline{z}) \, dq,$$

where

$$f_{0k}(q) = \frac{2\alpha}{\sqrt{\pi}} J_0(q; K), \quad \bar{q} = q/\rho_0,$$

$$J_0(q; K) = \int_0^{\infty} j_k(qR_0) \exp \left(-\frac{1}{2} \alpha^2 R_0^2 \right) \, dR_0,$$

and $j_k(qR_0)$ denotes the $k$th spherical Bessel function. The main contribution to the integral (38) comes from the vicinity of $\rho_0 \approx 0$ ($R_0 \approx \bar{R}_0$). Thus, we obtain a good approximation of $J_0$, if the lower integration limit is extended to $-\infty$. Then, we can use the asymptotic form of the function $j_k(x)$ for $x \gg K(K + 1)$ [33]

$$j_k(x) \approx \frac{1}{x} \cos \left[x - \frac{1}{2} K(K + 1) \pi \right],$$

which is the exact form for $K = 0$ at any $x$. As a result, we obtain the following approximation:

$$\bar{J}_0(q; K) \approx \sqrt{\frac{\pi}{2}} R_0 \alpha \frac{\rho_0}{\rho_0} \exp \left[-\frac{q^2}{2\alpha^2} \right].$$

In the case of $K > 0$ and $qR_0 \ll K(K + 1)$, the integral $\bar{J}_0$ should be estimated numerically.

Further evaluation of (36) for $g(\varepsilon_Q, \overline{z}) = \bar{g}_K(\varepsilon_Q, \overline{z})$ is performed using the additional averaging over the projections $M_K$ with a uniform weight $(2K + 1)^{-1}$ for a fixed $K$

$$\bar{g}_K(\varepsilon_Q, \overline{z}) = \frac{1}{2K + 1} \sum_{M_k} \int f_{0k}(q) \left| Y_{K0}(\bar{q}) \right|^2 \times \delta(\varepsilon - \overline{z}) \, dq,$$

Since for any solid angle $\omega$ the identity

$$\frac{1}{2K + 1} \sum_{M_k} \left| Y_{K0}(\omega) \right|^2 = \frac{1}{4\pi},$$

is valid, for a random-oriented molecule averaging over $M_K$ in (41) results in

$$\bar{g}_K(\varepsilon_Q, \overline{z}) = \frac{1}{4\pi} \int f_{0k}(q) \delta(\varepsilon - \overline{z}) \, q^2 \, dq \, d\Omega,$$

where the solid angle $\Omega(\vartheta, \phi)$ determines the orientation of vector $\bar{q}$ with respect to a fixed vector $\Omega$: $d\Omega = \sin \vartheta \, d\vartheta \, d\phi = -dz \, d\phi$. On integration over $\varphi$ in (43) we obtain

$$\bar{g}_K(\varepsilon_Q, \overline{z}) = \frac{1}{2} \int_0^\infty f_{0k}(q) \mathcal{T}(\varepsilon_q) \, q^2 \, dq,$$

where, by virtue of (31), the integral $\mathcal{T}(\varepsilon_q)$ is defined as

$$\mathcal{T}(\varepsilon_q) = \int_{-1}^1 \delta \left( \frac{\mu}{\mu_1} \varepsilon_q + \frac{\beta_b^2}{\mu_b} \varepsilon_q - \overline{z} \right) \frac{2\beta_b}{\mu_b} \frac{\mu}{\mu_1} \varepsilon_q = \overline{z},$$

The delta function imposes the following condition on $\varepsilon_q$:

$$\varepsilon_q = \varepsilon_0 \equiv \cos \vartheta, \quad \varepsilon_0 = \frac{1}{2\beta_b} \frac{\mu}{\mu_1} \varepsilon_q + \frac{\beta_b^2}{\mu_b} \varepsilon_q - \overline{z},$$

for all $\varepsilon_0$ such that $|\varepsilon_0| \leq 1$. The result of integration over $\varepsilon_q$ can be written down as

$$\mathcal{T}(\varepsilon_q) = \frac{1}{2\beta_b} \frac{\mu}{\mu_1} \varepsilon_q + \frac{\beta_b^2}{\mu_b} \varepsilon_q - \overline{z},$$

where $\Theta$ is the Heaviside step function and

$$\varepsilon_q, \overline{z} = \frac{1}{\beta_b^2} \beta_b \mu_1 \varepsilon_q + \frac{\beta_b^2}{\mu_b} \varepsilon_q \overline{z},$$

Substituting (47) into (44) and changing the integration variable $q$ to variable $\varepsilon_q$, which is defined in (11), leads to the following relation

$$\bar{g}_K(\varepsilon_Q, \overline{z}) = \frac{1}{4\beta_b} \frac{\mu}{\mu_1} \varepsilon_q \overline{z} \int_{\varepsilon_0}^{\varepsilon_q} f_{0k}(\varepsilon_q) \, d\varepsilon_q,$$

where

$$f_{0k}(\varepsilon_q) \equiv \sqrt{2\mu_b} f_{0k}(q(\varepsilon_q)).$$

On employing a convenient variable

$$\omega = 2\varepsilon_q/\omega_0$$

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and equations (11), (33) and (50), the distribution (49) takes the final form
\[
g_k(\varepsilon_Q, \bar{\varepsilon}) = \frac{4\alpha^2R_0^2}{\beta_b2\pi^3} \frac{\mu_{bs}}{\mu} \sqrt{\frac{\mu_{bs}}{\mu}} \frac{1}{\sqrt{\omega_0^2Q}} \\
\times \int_{\omega_1}^{\omega_2} J_k(\alpha\sqrt{\omega}; K) d\omega, \quad \omega_{1,2} \equiv \frac{2\varepsilon_Q\omega_0}{\omega_0},
\]
for a fixed collision energy \(\varepsilon_Q\) in the molecular CMS.

Let us consider the limit \(\varepsilon_Q \to 0\). Then, according to (31), the corresponding distribution of \(\bar{\varepsilon}\) is solely determined by the distribution of internal kinetic energy \(\varepsilon_q\) of the molecule BX:
\[
\bar{\varepsilon} \sim \varepsilon_q \gg \varepsilon_Q.
\]
In this approximation
\[
\omega_{1,2} \approx \bar{\omega} = \frac{2\mu_{bs}}{\beta_b^2} \frac{\bar{\varepsilon}}{\mu_0},
\]
\[
d\omega \to \Delta\omega = \omega_2 - \omega_1 = \frac{8\mu_{bs}}{\beta_b^2} \frac{\bar{\varepsilon}}{\mu_0} \sqrt{\frac{\varepsilon_Q}{\omega_0}},
\]
so that
\[
g_k(\varepsilon_Q, \bar{\varepsilon}) = \frac{2\alpha^2R_0^2}{\beta_b^2\pi^3} \frac{\mu_{bs}}{\mu} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\mu_{bs}}{\mu}} \frac{1}{\sqrt{\omega_0^2Q}} \\
\times \int_{\omega_1}^{\omega_2} J_k(\alpha\sqrt{\omega}; K) d\omega,
\]
when \(\varepsilon_Q \to 0\). In this limit, if the approximation (40) is valid, equations (52) and (55) take the following asymptotic forms:
\[
g_k(\varepsilon_Q, \bar{\varepsilon}) = \frac{4\alpha^2R_0^2}{\beta_b2\pi^3} \frac{\mu_{bs}}{\mu} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\mu_{bs}}{\mu}} \frac{1}{\sqrt{\omega_0^2Q}} \\
\times \int_{\omega_1}^{\omega_2} J_k(\alpha\sqrt{\omega}; K) d\omega,
\]
and
\[
g_k(\varepsilon_Q, \bar{\varepsilon}) = \frac{4\alpha^2R_0^2}{\beta_b2\pi^3} \frac{\mu_{bs}}{\mu} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\mu_{bs}}{\mu}} \frac{1}{\sqrt{\omega_0^2Q}} \\
\times \int_{\omega_1}^{\omega_2} J_k(\alpha\sqrt{\omega}; K) \exp(-\omega) d\omega,
\]
respectively.

In the limit \(\varepsilon_Q \to \infty\), the argument of the \(\delta\) function in (45) tends to \(\bar{\varepsilon} - \mu \varepsilon_Q/\mu_0\), which means that
\[
\bar{\varepsilon} \to (\mu/\mu_0)\varepsilon_Q, \quad \text{when} \quad \varepsilon_Q \to \infty.
\]
Let us note once more that it is invalid to use the above asymptotic relation, which is equivalent to (10), when the condition \(\varepsilon_Q \gg \varepsilon_q \sim \omega_Q/4\) is not fulfilled.

### 4. Results and discussion

The distribution density (52), which was calculated using a numerical integration in the case of the \(p\mu + H_2\) system, is shown in figure 2 \(^4\) as a function of kinetic energy \(\varepsilon\) in the nuclear CMS for several values of \(\varepsilon_Q\) (in the molecular CMS).

\(^4\) For simplicity of notation, the integration variable \(\bar{\varepsilon}\) in the presented plots of the functions (52) and (55) is displayed without the ‘tilde’ sign.

Since the characteristic kinetic energy \(\omega_{bs}\) in the molecular ground state is determined by the zero-point vibrations: \(\omega_{bs} \sim \sqrt{E_{n=0}} = \omega_0/4\), the magnitude of \(\omega_{bs}\) for the \(H_2\) molecule is in the order of 0.1 eV. Therefore, the curve plotted in figure 2 for \(\varepsilon_Q = 0.001\) eV practically represents the limit (55). It is evident that the averaging over the distribution density \(g \equiv g_k\) in equation (24) is important when the rate \(\lambda(\varepsilon)\) significantly changes within the characteristic width of \(g_k\), which occurs in the case of \(pp\mu\) formation presented in this figure.

A dependence of \(g_k\) on the rotational quantum numbers \(K\) is shown in figures 3 and 4 for \(\varepsilon_Q = 0.001\) and 1 eV, respectively.

At \(\varepsilon_Q < 0.001\) eV, the distribution of \(\varepsilon\) is practically determined by the rotational-vibrational state of the \(H_2\) molecule. However, this distribution substantially changes for subsequent rotational numbers. The distribution maximum decreases with rising \(K\). At \(\varepsilon_Q > 1\) eV, the location of maximum of \(g_k\) is proportional to \(\varepsilon_Q\), according to the asymptotic relation (58). The rotational-vibrational motion of the molecule causes a significant broadening of this maximum, which is wider at
higher $\varepsilon_0$. The distribution $g_K$ is flatter for greater $K$. The presented changes of $g_K$ for various $K$ can lead to an appreciable dependence of the formation rates (24) and (26) on the initial rotational distribution of the target molecules.

In order to demonstrate effects of the internal nuclear motion in the target molecules, the molecular formation rate $\Lambda(\varepsilon_0, \varepsilon)$, which was calculated using equation (24), and the input nuclear formation rate $\lambda(\varepsilon)$ are plotted below for some interesting cases. For the sake of comparison, the pairs of corresponding rates $\Lambda(\varepsilon_0, \varepsilon)$ and $\lambda(\varepsilon)$ are shown together with the help of asymptotic relation (58) between kinetic energies $\varepsilon_0$ and $\varepsilon$. The internal-motion effect in $\mu p\mu$ formation for the transition $J = 0 \rightarrow J = 0$, $\nu = 0$ is shown in figure 5. The apparent difference between the rates below about 0.2 eV is due to a significant variation in the input rate $\lambda(\varepsilon)$ within a relatively narrow interval $5 \text{ meV} \lesssim \varepsilon \lesssim 0.2 \text{ eV}$, which is comparable with the characteristic width of the distribution $g_K$. This effect disappears at higher energies. The nuclear-motion smearing of the formation rate for the $\mu p\mu$ formation in the transition $J = 1 \rightarrow J = 0$ is shown in figure 6. Here, this effect is due to the small magnitude of $\lambda(\varepsilon)$ for the $\mu p\mu + p$ scattering at $\varepsilon \rightarrow 0$ in the initial $J = 1$ state. In general, such a behavior is typical for the nonresonant formation at the muonic atom scattering in the higher partial ($J > 0$) wave state.

A dependence of the formation rate $\Lambda$ on the initial rotational state of the target molecule is shown in figure 7, for the $\mu p\mu$ formation in the transition $J = 0 \rightarrow J = 0$. The appreciable differences of $\Lambda$ for various $K$ lead to different values of the average formation rate $\lambda(E, T)$ in the LAB frame, depending on the rotational population for a specified target and temperature. For example, strong nuclear motion and rotational effects occur at relatively high energies (target temperatures) for the transition $J = 2 \rightarrow J = 2$ in the nonresonant $\mu p\mu$ formation within the $T_2$ molecule (see figure 8). This is due to the existence of the $\mu p\mu$ quasi-stationary state, which appears as a narrow peak in the elastic $\mu p + t$ cross section at the scattering energy $\sim 3 \text{ eV}$ and $J = 2$ [34, 35].

Figure 9 refers to the nonresonant formation of the $d\mu t\mu$ molecule (2) in the loosely bound state $J = \nu = 1$ (see details in [21]). For the thermalized $d\mu$ atoms, the nonresonant process (2) is unfeasible. However, such a reaction is effective in the case of nonthermalized $d\mu$ atoms with collision energies exceeding the ionization threshold of the $D_2$ molecule. The rate $\Lambda(\varepsilon_0, \varepsilon)$ plotted in this figure was estimated by averaging the corresponding input rate $\lambda(\varepsilon)$ for $d\mu t\mu$ formation in the $J = \nu = 1$ state [21], with the use of (24) and (52). A
smearing of the rate $\Lambda$ due to the internal nuclear motion is quite strong near the threshold. However, this effect cannot significantly affect the kinetics of $dd$-fusion, since the threshold is located at energy much higher than the thermal energies of typical $D_2$ targets. Thus, a fraction of the nonthermalized $d\mu$ atoms with such high energies ($\sim 15$ eV) is small. The analogous around-threshold smearing effect is shown in figure 10 for nonresonant formation of the $d\mu$ molecule in the loosely bound state $J = \upsilon = 1$. This muonic molecule is created in the collision of $\mu$ with the $D_2$ molecule. In this case, the threshold energy of 16 eV is somewhat greater than that for the $dd\mu$ molecule.

The molecular rates $\Lambda(E)$ of nonresonant $dd\mu$ formation in the state $J = 0$, in the case of $d\mu$ collision with the molecules $D_2$ and HD, are presented in figure 11 as functions of LAB kinetic energy $E$. These rates were calculated using (28) and (6). The corresponding nuclear rate $\lambda(E)$ is plotted for a comparison. A strong smearing of $\Lambda(E)$ appears at low collision energies ($E \lesssim 0.1$ eV), where the input rate $\lambda(\varepsilon)$ rises rapidly in the interval of energies $\varepsilon \ll \omega_0$. As a result, the molecular rates are much greater than the corresponding nuclear rate for thermalized $d\mu$ atoms. Also, an appreciable isotopic effect can be observed in figure 11 at low energies. This effect is due to the different distributions $g(\varepsilon_{Q', \varepsilon})$ of the deuteron kinetic energy in the molecules $D_2$ and HD. Since most kinetic energy in the HD molecule is carried by the lighter proton, it follows that the mean kinetic energy of the deuteron in HD is smaller than that in the $D_2$ molecule. Let us note that the nonresonant $dd\mu$ formation rate in the state ($J = 1, \upsilon = 0$) is very flat at low collision energies. As a result, there is no appreciable differences between the rates $\lambda(E)$ and $\Lambda(E)$ in this case.

Significant differences between the rates $\lambda(E)$ and $\Lambda(E)$ at the lowest energies are of special importance when the conditions of steady-state kinetics are reached, e.g., as in the case of experiments reported in [3]. Under such conditions, the kinetics is described in terms of the thermally averaged rates of various $\mu$CF processes for a fixed target temperature. In calculations it is assumed that the distributions of LAB kinetic energies of the molecules and muonic atoms in a gaseous target have the Maxwellian shape. The rotational levels of the target molecules obey the Boltzmann distribution. The thermally averaged total nonresonant rates $\lambda(T)$ and
\( \Lambda(T) \) are plotted in figure 12 as functions of the target temperature, for the D\(_2\) and HD gases. Also, the contribution from the state \( J = 1 \) to the total rate is shown, which is practically identical for both the nuclear and molecular rates. The experimental data points at \( T = 50, 150, \) and \( 300 \) K were determined in [3] using the steady-state kinetics for a pure HD target. The calculated rates \( \Lambda(T) \) and \( \Lambda(\nu) \) do not well describe the data. Nevertheless, the molecular rate \( \Lambda(T) \) for the HD target, which takes into account the deuteron motion within the molecule HD, is closer to the data than the nuclear rate \( \nu(T) \). From figure 12 one can conclude that the theoretical rate \( \Lambda(T) \), which takes into account an appreciable isotopic effect, is closer to the experimental data (compare the rates for D\(_2\) and HD).

The contributions to the total rate \( \Lambda(\mu) \) from the nonresonant \( dd\mu \) formation in the rotational states \( J = 0 \) and 2 are shown in figure 13 as functions of LAB energy. For the sake of clarity, a higher-energy contribution from the state \( J = \nu = 1 \) of \( dd\mu \), which is plotted in figure 10, is not included here. A negligible contribution from the state \( J = 1, \nu = 0 \) of \( dd\mu \) is not visible in this plot. The presented rates have been calculated assuming the 300 K Boltzmann distribution of the rotational levels of the target D\(_2\) molecules.

Our calculations of the thermally averaged molecular rates \( \Lambda(T) \) for the gaseous 30 K and 300 K hydrogenic targets are summarized in tables 2 and 3.

In the case of symmetric molecules H\(_3\), D\(_2\), and T\(_2\), the transitions between the even and odd rotational states are very slow unless a catalyst is used [31]. Since low-temperature hydrogenic targets are usually obtained by fast cooling of gaseous hydrogens from the room temperature, both the rotational levels \( K = 0 \) and \( K = 1 \) are populated in resulting cold targets. A relative distribution of these states is statistical: 2:1 for D\(_2\) and 1:3 for H\(_2\) and T\(_2\). This is due to the different values of the nuclear spin: 1 for deuterium and 1/2 for protium and tritium. After a long time or after using a catalyst, the rotational distributions eventually take the Boltzmann form. Different experiments with cold hydrogenic targets are performed for the statistical or Boltzmann rotational distribution. Sometimes the \( K = 0 \) targets are employed. Therefore, in table 2 for the symmetric molecules, the 30 K results are separately presented for the states \( K = 0, K = 1 \) and for the statistical mixture of these states (label ‘Statistical’). The rates for the 30 K Boltzmann distribution can be estimated by summing the rates for \( K = 0 \) and \( K = 1 \) with the appropriate Boltzmann factors. Let us note that a significant difference of the average \( dd\mu \) formation rate in the states \( K = 0 \) and \( K = 1 \) of D\(_2\) is due to a strong increase in the dominant nuclear formation rate \( J = 1 \rightarrow J = 0 \) in the interval 0–0.1 eV and to a greater internal kinetic energy of D\(_2\) in the state \( K = 1 \).

Contributions from different rotational states \( J \) of the created muonic molecules to the total nonresonant formation rate \( \Lambda(T) \) are shown in table 3 for 30 and 300 K.

Here the Boltzmann distribution of the rotational levels of the target molecules is assumed for the sake of better comparing the rates for the both temperatures. One can see that the molecular rates \( \Lambda(T) \) of nonresonant \( dd\mu \) formation (in HD and D\(_2\)) and \( dd\mu \) formation (in D\(_2\) and DT) display a significant isotope effect, in particular at the lower temperature.

In table 4, the available experimental formation rates \( \lambda(T) \), which are averaged over kinetic energies of the impinging muonic atoms, are compared with the theoretical results. The values of theoretical rates from [1, 18] and [19, 20] are quoted at collision energy approaching zero and at \( \varepsilon = 0.04 \) eV, respectively. The value of \( \lambda_{ppp} \) from the work [18] has been corrected due to the updated value of the density of nuclei in liquid hydrogen \( N_0 = 4.25 \times 10^{22} \) cm\(^{-3}\), which is used in the present work, and in accordance with the remark of review [1], where it is pointed out that the corrected value should be two times less. The label ‘Present work’ denotes the average rate for the 22 K or 300 K Maxwell distribution of muonic atom energies. As can be seen from this table, for the majority of muonic molecules, the calculated rates are in good agreement with the experimental data. Only the value of \( ppp \) formation rate, which is topical due to the forthcoming experiments [9, 10], is a special case because
Table 2. The calculated averaged nonresonant formation rates of muonic molecules $[10^6 \text{ s}^{-1}]$ for different populations of the rotational numbers $K$ of the target hydrogenic molecules.

| Muonic molecule | Target molecule | Temperature $T = 30 \text{ K}$ | Temperature $T = 300 \text{ K}$ |
|-----------------|-----------------|-------------------------------|---------------------------------|
|                 | $K = 0$         | $K = 1$          | Statistical          | Boltzmann          |
| $pp\mu$         | H$_2$           | 1.806            | 1.805              | 1.805              | 1.799             |
| $pd\mu$         | H$_2$           | 5.626            | 5.618              | 5.620              | 5.582             |
| $pt\mu$         | H$_2$           | 6.375            | 6.363              | 6.366              | 6.317             |
| $dd\mu$         | D$_2$           | 0.078            | 0.082 9            | 0.080 1            | 0.139             |
| $dt\mu$         | D$_2$           | 4.083            | 4.433              | 4.200              | 7.249             |
| $tt\mu$         | T$_2$           | 2.685            | 2.681              | 2.682              | 2.639             |

Table 3. The calculated averaged nonresonant formation rates $[10^6 \text{ s}^{-1}]$ for different rotational numbers $J$ of the muonic-molecule states $J\nu$. The Boltzmann distribution of rotational states of the target molecules is assumed for both temperatures.

| Temperature [K] | State | Muonic molecule (target molecule) |
|-----------------|-------|-----------------------------------|
|                 |       | $pp\mu$ (H$_2$) $dd\mu$ (HD) $dd\mu$ (D$_2$) $dt\mu$ (D$_2$) $dt\mu$ (DT) $tt\mu$ (T$_2$) |
| 30              | 0     | 0.008 0.056 8 0.065 3 3.655 3.893 0.003 |
|                 | 1     | 1.798 0.011 9 0.011 9 0.000 0.000 2.680 |
|                 | 2     | —     0.001 5 0.001 9 0.454 0.484 0.000 |
|                 | Total | 1.806 0.070 2 0.079 1 4.109 4.377 2.683 |
| 300             | 0     | 0.007 0.117 0 0.123 4 6.444 6.550 0.003 |
|                 | 1     | 1.792 0.011 8 0.011 8 0.000 0.000 2.636 |
|                 | 2     | —     0.003 8 0.004 1 0.805 0.819 0.000 |
|                 | Total | 1.799 0.132 6 0.139 3 7.249 7.369 2.639 |

Table 4. Experimental and calculated rates $[10^6 \text{ s}^{-1}]$ of nonresonant formation of the muonic hydrogen molecules in different hydrogenic targets. The asterisk superscript denotes the assumed value, when the experimental temperature is not explicitly given in the corresponding reference.

| Muonic molecule | Rate $[10^6 \text{ s}^{-1}]$ | Conditions | Paper | Rate | Authors | Paper |
|-----------------|------------------------------|------------|-------|-------|---------|-------|
| $pp\mu$         | 0.6$_{+0.5}^{-0.3}$         | Gas, 300 K* | [36]  | 2.6   | Zel’dovich and Gershtein | [1]  |
|                 | 1.89 ± 0.20                 | Liquid, 22 K* | [37]  | 3.9   | Cohen et al | [18]  |
|                 | 2.55 ± 0.18                 | Liquid, 22 K* | [38]  | 2.20  | Ponomarev and Faifman | [19]  |
|                 | 2.74 ± 0.25                 | Gas, 300 K*  | [39]  | 1.80  | Faifman | [20]  |
|                 | 2.34 ± 0.17                 | Gas, 300 K*  | [40]  | 1.81  | Present work, 22 K |       |
|                 | 3.21 ± 0.24                 | Solid, 3 K   | [41]  | 1.80  | Present work, 300 K |       |
|                 | 2.01 ± 0.09                 | Gas, 300 K   | [22]  | 1.3   | Zel’dovich and Gershtein | [1]  |
| $pd\mu$         | 5.8 ± 0.3                   | Liquid, 22 K* | [37]  | 3.0   | Cohen et al | [18]  |
|                 | 6.82 ± 0.25                 | Liquid, 22 K* | [38]  | 5.91  | Ponomarev and Faifman | [19]  |
|                 | 5.53 ± 0.16                 | Gas, 300 K*  | [40]  | 5.63  | Faifman | [20]  |
|                 | 5.9 ± 0.9                   | Liquid, 22 K* | [42]  | 5.63  | Present work, 22 K |       |
|                 | 5.6 ± 0.2                   | Liquid, 22 K* | [43]  | 5.58  | Present work, 300 K |       |
| $pt\mu$         | 7.5 ± 1.3                   | Liquid, 23 K* | [44]  | 0.4   | Zel’dovich and Gershtein | [1]  |
|                 | 6.49                        | Present work, 22 K | [19]  | 6.38  | Faifman | [20]  |
|                 | 6.38                        | Present work, 22 K | [19]  | 6.32  | Present work, 300 K |       |
| $tt\mu$         | 1.8 ± 0.6                   | Liquid, 23 K | [45]  | 0.65  | Zel’dovich and Gershtein | [1]  |
|                 | 2.3 ± 0.6                   | Solid, 16 K  | [46]  | 2.96  | Ponomarev and Faifman | [19]  |
|                 | 2.84 ± 0.32                 | Liquid, 22 K | [47]  | 2.64  | Faifman | [20]  |
|                 |                             | Present work, 22 K |       | 2.64  | Present work, 300 K |       |
of the disagreements between the theory and experiments. Moreover, the experimental data measured in different gaseous, liquid and solid hydrogen targets differ among themselves and are not sufficiently consistent. Therefore it is rather complicated to draw a conclusion about the degree of agreement between the experimental and the theoretical values of the $pp\mu$ formation rates.

5. Conclusions

The nonresonant formation of the muonic hydrogen molecules has been considered taking into account the internal nuclear motion in the target hydrogenic molecules. The rates of such processes have been calculated for collision energies $\lesssim 100$ eV in nuclear CMS. The corresponding rates in the LAB system have been obtained for gaseous hydrogenic targets at fixed temperatures, for collision energies $\gtrsim 200$ eV. A knowledge of the high-energy formation rates is needed since the initial energies of the ground-state muonic atoms can reach many hundreds of electron volts, after the atomic muon capture and subsequent cascade. Also, in gaseous $H_2$ mixtures with small amounts (a fraction of 1%) of deuterium or tritium, the $d\mu$ or $t\mu$ atoms with energies of a few tens of eV are always present due to muon transfer from $p\mu$ to deuteron or triton. As a result, the mean free path of the created $dp$ and $tp$ atoms is much larger than that of $p\mu$ atoms. This phenomenon is employed by the muX collaboration for the effective formation of muonic atoms of high-$Z$ elements and a precise determination of their nuclear charge radii [12]. Let us note that energetic $dp$ or $tp$ always present in experiments performed in natural-hydrogen targets.

In general, the internal nuclear motion leads to a significant smearing of the energy-dependent formation rate $\lambda(\varepsilon)$ of the reaction $(2)$ in the $a\mu + BX$ system. This occurs when the corresponding input rate $\lambda(\varepsilon)$, which was calculated in the $a\mu + b$ system [20], strongly changes within the energy interval comparable with the magnitude of vibrational quantum of the target molecule $BX$ ($\sim 0.1$ eV). In particular, this effect is essential in the case of nonresonant $d\mu$ and $t\mu$ formation at $\varepsilon \lesssim 0.1$ eV, which significantly affects the steady-state kinetics of $\mu$CF processes. Also, the internal nuclear motion results in appreciable isotopic effects, which can be seen in the case of $dd\mu$ nonresonant formation in $D_2$ and HD gas.

It follows from table 4 that, for the presented experimental conditions, the internal nuclear motion in the target hydrogenic molecules does not appreciably affect the thermally averaged total formation rates. This is due to the practically constant dominant contribution to the total rates from different $J\nu$ states of the created muonic molecules, at collision energies $\lesssim 0.1$ eV. Therefore, the nuclear-motion effects can be confirmed only in experiments, in which it is important to take into account the presence of higher-energy muonic atoms or different $J\nu$ states.

The calculated energy-dependence formation rates are required for accurate simulations of the muonic atomic and molecular processes in the hydrogenic mixtures, data analysis and interpretation of different experiments in low-energy muon physics (e.g., the investigations of the collaborations FAMU, CREMA and muX).

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