## De-excitation rates of $\mu$ -mesic molecules of hydrogen isotopes

S. I. Vinitskiĭ, L. I. Ponomarev, and M. P. Faïfman

Joint Institute for Nuclear Research (Submitted 29 August 1981) Zh. Eksp. Teor. Fiz. **82**, 985–990 (April 1982)

The rates of dipole E1 transitions of the mesic molecules  $pd\mu pt\mu$ , and  $dt\mu$  to the ground state with conversion on an electron of a molecular complex, one of whose nuclei is the produced  $\mu$ -mesic molecule, are calculated. The adiabatic representation in the three-body problem is used in the calculation.

PACS numbers: 36.10.Dr

## 1. INTRODUCTION

It is known<sup>1,2</sup> that fusion of mesic-molecule nuclei and  $\mu^-$ -meson capture by the protons of the nuclei take place in  $\mu$ -mesic molecules. The rates of these processes depend substantially on the quantum state of the mesic molecules.<sup>3,4</sup>

The mesic molecules  $pp\mu$ ,  $pd\mu$ ,  $pt\mu$ , and  $tt\mu$  are produced in reactions of the type<sup>1,5,6</sup>

$$d\mu + H_2 \rightarrow [(pd\mu)pe]^+ + e \tag{1}$$

with conversion on the electrons of the molecular complex  $[(pd\mu)p2e]$ , while the molecules  $dd\mu$  and  $dt\mu$  are produced in the resonance reactions<sup>7,8</sup>

$$d\mu + D_2 \rightarrow [(dd\mu)d2e]^{\bullet}, \quad t\mu + D_2 \rightarrow [(dt\mu)d2e]^{\bullet}$$
 (2)

with excitation of the vibrational levels of the complexes  $[(dd\mu)d2e]$  and  $[(dt\mu)d2e]$ . The mesic molecules  $pp\mu$ ,  $pd\mu$ , and  $pt\mu$  are produced predominantly in states with total orbital momentum J=1 and vibrational quantum number v=0, while the mesic molecules  $dd\mu$ ,  $dt\mu$ , and  $tt\mu$  are produced in states with J=1 and v=1.

For mesic molecules with like nuclei  $(pp\mu, dd\mu, tt\mu)$ the rate of the (J=1) - (J=0) transition into the ground state within the lifetime of the  $\mu^-$  meson is extremely small (for example,  $\lambda \sim 10^4$  sec<sup>-1</sup> in the case of the  $pp\mu$ mesic molecule<sup>9</sup>), since this transition is accompanied by a change of the total spin of the nuclei of the molecules, and is due to relativistic effects.

The mesic molecules  $pd\mu$ ,  $pt\mu$ , and  $dt\mu$  go over into the ground state via E1 transitions with conversion on an electron<sup>1)</sup> of molecular complexes of type I:  $[(pd\mu)pe]^*, [(pt\mu)pe]^*$  and  $[(dt\mu)de]^*)$ , or II:  $[(pd\mu)p2e]$ ,  $[(pt\mu)p2e]$  and  $[(dt\mu)d2e]$ , depending on the relation between the rates  $\lambda_A$  of the Auger transitions and the rate  $\lambda_{ex}$  of the charge exchange reaction of the type

$$[(pd\mu)pe]^{+}+H_{2} \xrightarrow{\text{res}} [(pd\mu)p2e] +H_{2}^{+}, \qquad (3)$$

as a result of which the initially produced ion  $[(pd\mu)pe]^*$  captures an electron.

Only one transition  $(J=1, v=0) \rightarrow (J=0, v=0)$ , is possible in the mesic molecules  $pd\mu$  and  $pt\mu$ , since they exist only in these two states<sup>10</sup> (see Table I). The mesic molecules  $dt\mu$  exist in five states<sup>10</sup> (see Fig. 1). Their de-excitation from the state (J=1, v=1) into the

ground state (J=0, v=0) proceeds mainly via cascade E1 transitions.

We calculate in this paper the rates  $\lambda_A^{(1)}$  and  $\lambda_A^{(2)}$  of the Auger transitions in the mesic molecules  $pd\mu$ ,  $pt\mu$ , and  $dt\mu$ , which are the "nuclei" of the molecular complexes of type I and II, respectively.

## 2. DE-EXCITATION VIA E1 TRANSITION

The probability of the transition of a mesic molecule from an initial (i) state into a final (f) state with emission of an Auger electron in the momentum interval between q and q + dq is<sup>6</sup>

$$dW_{fi} = \frac{2\pi}{\hbar} |T_{fi}|^2 \delta(E_f - E_i) d\mathbf{q}.$$
(4)

Here  $E_i$  and  $E_j$  are the total energies of the initial and and final states of the complex (I or II),

$$E_i = \varepsilon_{Jv}^{(f)} + \varepsilon_I,$$
  
$$E_j = \varepsilon_{Jv}^{(f)} + q^2/2m_e,$$

 $\varepsilon_{Jv}^{(i)}$  and  $\varepsilon_{Jv}^{(f)}$  are the energies of the quasimolecule in the initial and final states with total angular momenta  $J^{(i,f)}$  and vibrational quantum numbers  $v^{(i,f)}, \varepsilon_I$  is the binding energy of the electron in the ground state of the complex, **q** is the momentum of the conversion electron, and  $m_e$  is the electron mass.

The matrix element of the transition is

$$T_{R}|^{s} = \frac{1}{2J^{(i)} + 1} \sum_{m_{J}^{(i)}} \sum_{m_{J}^{(j)}} \left| \int d\mathbf{R} \, d\mathbf{r}_{\mu} d\rho \, \Psi^{(l)*}(\mathbf{r}_{\mu}, \mathbf{R}) \, \psi^{(l)*}(\rho) \, \hat{H}_{int} \right| \\ \times \psi^{(i)}(\rho) \, \Psi^{(i)}(\mathbf{r}_{\mu}, \mathbf{R}) \Big|^{2}, \tag{5}$$

where  $\psi^{(i)}(\rho)$  and  $\psi^{(f)}(\rho)$  are the wave functions of the conversion electron in the initial and final states,  $\rho$  is the electron coordinate measured from the mass center of the mesic molecule,  $\Psi^{(i)}(\mathbf{r}_{\mu}, \mathbf{R})$  and  $\Psi^{(f)}(\mathbf{r}_{\mu}, \mathbf{R})$  are the wave functions of the mesic molecule, R is the radius vector joining the nuclei of the mesic molecule, and  $r_{\mu}$  is the  $\mu$ -meson coordinate measured from the

TABLE I. Rates of dipole Auger transition in the mesic molecules  $pd\mu$  and  $pt\mu$ .

Molecule	$-\varepsilon_{10}^{(i)}, eV$	$-\varepsilon_{00}^{(f)}$ , eV	{d}	$\lambda_A^{(1)}, 10^{11}  \mathrm{sec}^{-1}$	$\lambda_A^{(2)}, 10^{11} \text{ sec}^{-1}$
pdµ	97.4	221.5	0.28	1.2	2.7
ptµ	99.0	214.0	0.38	2.2	5.1

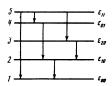


FIG. 1. Cascade E1 transitions between the states (Jv) of the mesic molecule  $dt\mu$  with energies:  $\varepsilon_{11} = -0.64$ ,  $\varepsilon_{01} = -34.9$ ,  $\varepsilon_{20} = -102.5$ ,  $\varepsilon_{10} = -232.4$ ,  $\varepsilon_{00} = -319.2$  eV.

center of the segment R. Expression (5) is averaged over the projections  $m_J^{(i)}$  of the orbital momentum  $J^{(i)}$ in the initial state and summed over the projections  $m_J^{(f)}$  in the final state.

The perturbation operator  $\hat{H}_{int}$  takes in the dipole approximation the form

$$\hat{H}_{int} = -e d\rho / \rho^3, \tag{6}$$

where the dipole moment  $d = d(r_{\mu}, R)$  of the mesic molecule is<sup>6</sup>

$$\mathbf{d} = -e \left[ \frac{\varkappa}{2} \left( 1 - \frac{M_{\mu}}{M_{tot}} \right) \mathbf{R} + \left( 1 + \frac{M_{\mu}}{M_{tot}} \right) \mathbf{r}_{\mu} \right],$$
  
$$\mathbf{x} = (M_{b} - M_{a}) / (M_{b} + M_{a}), \quad M_{tot} = M_{a} + M_{b} + M_{\mu}.$$
 (7)

Here  $M_{\mu}$  is the mass of the  $\mu$  meson,  $M_a > M_b$  are the masses of the mesic-molecule nuclei, and  $M_{tot}$  is the total mesic-molecule mass.

The wave functions of the electron in the initial and final states (in atomic units  $e = \hbar = m_e = 1$ ) were chosen respectively in the form<sup>5,6</sup>

$$\psi^{(i)}(\rho) = \left[\frac{Z_{0}^{3}}{2\pi (1+\Delta)^{-}}\right]^{\nu_{0}} \left[\exp\left(-Z_{0}\rho\right) + \exp\left(-Z_{0}|\rho-\mathbf{R}_{p}|\right)\right], \quad (8a)$$

$$\psi^{(I)}(\rho) = \frac{3i}{4\pi q} e^{-i\sigma_{1}}R_{q_{1}}(\rho)\cos\theta_{q_{0}},$$

$$R_{q_{1}}(\rho) = \frac{2}{3}q^{2} \left[\frac{\eta(1+\eta^{3})}{(1-e^{-2\pi\eta})}\right]^{\nu_{0}}\rho F(2+i\eta, 4; 2iq\rho),$$

$$R_{q_{1}}(\rho) \stackrel{+}{\to} \sqrt{\frac{2}{\pi}}\frac{1}{\rho}\sin\left(q\rho+\eta\ln 2q\rho-\frac{\pi}{2}+\sigma_{1}\right), \quad \eta = \frac{Z^{*}}{q}.$$
(8b)

Here  $Z_0$  and  $Z^*$  are the effective charges in whose field the electron moves in the initial and final states of the complex,  $R_{\rho}$  is the radius vector between the mass center of the mesic molecule and the other nucleus of the complex;  $\theta_{a\rho}$  is the angle between the vectors q and  $\rho$ , and  $\sigma_1 = \arg \Gamma(2 - i\eta)$  is the Coulomb phase shift in the state with angular momentum l = 1.

We use in this paper the following values of the parameters<sup>11</sup> that characterize the molecular complexes of type I (analogous to the molecular ion  $H_2^*$ ) and II (analogous to the  $H_2$  molecule):

for the complexes I

$$Z_0=1.25; R_p=2.00, \Delta=0.468; Z^*=2;$$
 (9a)

for the complexes II

$$Z_0 = 1.19; \quad R_p = 1.40; \quad \Delta = 0.677; \quad Z^* = 1.$$
 (9b)

The wave functions of the mesic molecules are cal-

culated in the adiabatic representation of the threebody  $problem^{12}$ :

$$\Psi^{(i,f)}(\mathbf{r}_{\mu},\mathbf{R}) = \sum_{m=0}^{j^{(i,f)}} \sum_{j} F_{jm}^{j^{(i,f)}}(\mathbf{r};R,\Theta,\Phi) \frac{1}{R} \chi^{(i,f)}_{jm}(R), \qquad (10)$$

$$F_{jm}{}^{J}(\mathbf{r}; R, \Theta, \Phi) = [2(1+\delta_{0m})]^{-l_{j}} \{\varphi_{jm}(\mathbf{r}; R) \mathcal{D}_{mm_{j}}{}^{J}(\Phi, \Theta, 0) + \varphi_{j,-m}(\mathbf{r}; R) \mathcal{D}_{-mm_{j}}{}^{J}(\Phi, \Theta, 0) \},$$

where  $\mathscr{D}_{mmJ}^{J}(\Phi, \Theta, 0)$  are the normalized Wigner  $\mathscr{D}$  functions,  $\varphi_{jm}(\mathbf{r}; R)$  is the complete set of solutions of the problem of two Coulomb centers,<sup>13</sup>  $\mathbf{r}$  are the coordinates of the meson in a rotating coordinate frame whose Z axis is directed along the vector  $\mathbf{R}$ . The connection between the components of the vector  $\mathbf{r}_{\mu} = (x_{\mu}, y_{\mu}, z_{\mu})$  in the laboratory frame with the components of the vector  $\mathbf{r} = (x, y, z)$  is given by the relations<sup>12</sup>

$$\begin{pmatrix} x_{\mu} \\ y_{\mu} \\ z_{\mu} \end{pmatrix} = \begin{pmatrix} \cos \Theta \cos \Phi & -\sin \Phi & \sin \Theta \cos \Phi \\ \cos \Theta \sin \Phi & \cos \Phi & \sin \Theta \sin \Phi \\ -\sin \Theta & 0 & \cos \Theta \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$
(11)

The symbol  $\Sigma_j$  in Eqs. (10) means summation over the discrete spectrum and integration over the continuous spectrum of the two-center problem,<sup>12</sup> and  $j = [n_1 n_2 p]$  is the parabolic-quantum-number set corresponding to even (p = g) and odd (p = u) solutions of the two-center problem.<sup>13</sup>

The wave functions  $\varphi_{jm}(\mathbf{r};R)$  are orthonormalized by the condition

$$d\mathbf{r}\varphi_{jm}(\mathbf{r};R)\varphi_{j'm'}^{*}(\mathbf{r};R) = \delta_{jj'}\delta_{mm'}.$$
(12)

The functions  $\chi_{jm}^{(i,f)}(R) \equiv \chi_{jm}^{(Jv)^{i,f}}(R)$  represent the relative motion of the nuclei of the quasimolecule in the initial (i) and final (f) states with respective energies  $\varepsilon_{Jv}^{(i)}$  and  $\varepsilon_{Jv}^{(f)}$ , and satisfy the orthogonality relation<sup>10</sup>

$$\sum_{m=0}^{7} \sum_{j} \int dR \chi_{jm}^{sv}(R) \chi_{jm}^{sv'}(R) = \delta_{vv'}.$$
 (13)

Separating the dimensional factors for all the quantities in the expression for  $T_{fi}$  in<sup>2)</sup> (5), and integrating over the coordinates  $\rho$ , r, and R and the momenta q of the electron in the final state, we obtain for the rates  $\lambda_A^{(1,2)}(E1) \equiv W_{fi}$  of the E1 transition in the mesic molecule the expression

$$\lambda_{A}^{(1,2)}(E1) = \beta \frac{4\pi}{3} \left(\frac{m_{\bullet}}{m_{\bullet}}\right)^{2} \frac{Z_{\bullet}^{3}}{1+\Delta} \frac{1}{q} |I(q)|^{2} |\langle d \rangle|^{2} \frac{m_{\bullet}e^{4}}{\hbar^{3}} c^{-1}.$$
(14)

Here  $\beta = 1$  for transitions in complexes of type I,  $\beta = 2$  for complexes of type II, and  $m_a^{-1} = M_\mu^{-1} + M_a^{-1}$ , where  $M_a$  is the mass of the heavier nucleus of the mesic molecule,

$$I(q) = \int_{0}^{\infty} d\rho R_{q_{1}}(\rho) \exp(-Z_{0}\rho) + \frac{1}{2} \int_{0}^{\infty} d\rho R_{q_{1}}(\rho) \int_{-1}^{1} d\cos\theta_{\rho R_{p}} \exp(-Z_{0}|\rho - R_{p}|),$$
  
$$|\langle d \rangle|^{2} = \frac{1}{2J^{(i)} + 1} \sum_{m_{j}^{(i)}} \sum_{m_{j}^{(i)}} \left| \int d\mathbf{R} \, d\mathbf{r}_{\mu} \Psi^{(\prime)}(\mathbf{r}_{\mu}, \mathbf{R}) \, d(\mathbf{r}_{\mu}, \mathbf{R}) \, \Psi^{(i)}(\mathbf{r}_{\mu}, \mathbf{R}) \right|^{2}.$$
(15)

The values of  $|\langle d \rangle|^2$  for the transitions  $(J^{(i)}=1) \rightarrow (J^{(f)}=0)$  and  $(J^{(i)}=1) \rightarrow (J^{(f)}=2)$  are respectively

$$(2J^{(i)}+1)|\langle d \rangle|^{2} = \left[\frac{\varkappa}{2}\left(1-\frac{M_{\mu}}{M_{tot}}\right)\int_{0}^{\infty} dR \cdot RD_{00}^{(0)} + \left(1+\frac{M_{\mu}}{M_{tot}}\right)\int_{0}^{\infty} dR (D_{00}^{(1)}-\sqrt{2}D_{01}^{(1)})\right]^{2}, \qquad (16a)$$

$$(2J^{(i)}+1) |\langle d \rangle|^{2} = 2 \left[ \frac{\varkappa}{2} \left( 1 - \frac{M_{\mu}}{M_{tot}} \right) \int_{0}^{1} dR \cdot R \left( D_{00}^{(i)} + \frac{\gamma 3}{2} D_{11}^{(i)} \right) + \left( 1 + \frac{M_{\mu}}{M_{tot}} \right) \int_{0}^{1} dR \left( D_{00}^{(i)} + \frac{\gamma 3}{2} D_{11}^{(i)} + \frac{1}{\sqrt{2}} D_{01}^{(i)} + \sqrt{\frac{3}{2}} (D_{10}^{(i)} + D_{21}^{(i)}) \right) \right]^{2}.$$

$$(16b)$$

We have introduced here the notation

$$D_{mm}^{(0)} = D_{mm}^{(0)}(R) = \sum_{j} \chi_{jm}^{(f)}(R) \chi_{jm}^{(i)}(R), \quad m = 0, 1,$$

$$D_{m'm}^{(i)} = D_{m'm}^{(i)}(R) = \sum_{j,j'} \langle j'm' | r_k | jm \rangle \chi_{j'm'}^{(f)}(R) \chi_{jm}^{(i)}(R), \quad m = 0, 1, 2,$$
(17)

where  $\langle j'm' | r_k | jm \rangle$  are the dipole moments of a  $\mu^-$  meson moving in the field of two fixed Coulomb centers<sup>14</sup>:

$$\langle j'm' | r_{k} | jm \rangle = \int d\mathbf{r} \phi_{j'm'}^{*}(\mathbf{r}; R) r_{k} \phi_{jm}(\mathbf{r}; R),$$

$$r_{k} = z, \quad m' = m, \quad k = 0,$$

$$r_{k} = \frac{1}{\sqrt{2}} (x \pm iy), \quad m' = m \mp 1, \quad k = \pm 1.$$
(18)

For the transitions  $(J^{(f)}=0) \rightarrow (J^{(f)}=1)$  and  $(J^{(f)}=2) \rightarrow (J^{(f)}=1)$  it is necessary to make in (16a, b) the interchange  $D_{mm}^{(1)} \rightarrow D_{mm'}^{(1)}$ .

If the mesic-molecule de-excitation rates exceed the rate of the charge-exchange reaction (3), i.e., if  $\lambda_A(E1) > \lambda_{ex}$ , the de-excitation of the molecules takes place in complexes of type I [ $\beta = 1$  in Eq. (14)], while at  $\lambda_A(E1) < \lambda_{ex}$  the complex of type I manages to capture an electron and the E1 transition in the mesic molecule is effected in the complex of type II ( $\beta = 2$ ).

## 3. DISCUSSION OF RESULTS

Table I lists the rates of the E1 transitions in the mesic molecules  $pd\mu$  and  $pt\mu$  from the state (J=1, v=0) with energy  $\varepsilon_{J}^{(i)}$  into the state (J=0, v=0) with energy  $\varepsilon_{J}^{(i)}$ , and the values of  $|\langle d \rangle|$  defined by Eqs. (16)-(18) in the system of units  $(e=\hbar=m_a=1)$ . The rates  $\lambda_A^{(1)}$  and  $\lambda_A^{(2)}$  correspond to E1 transitions with conversion on electrons of the molecular complexes of type I and II. We note that the transition rate calculated by us in the mesic molecule  $pd\mu$  differs considerably from the value  $0.25 \times 10^{11} \text{ sec}^{-1}$  obtained in Ref. 5. Since the details of the numerical calculation are not given in that reference, we were unable to determine the cause of the discrepancy.

Table II lists the rates  $\lambda_A^{(1)}$  and  $\lambda_A^{(2)}$  of the cascade E1 transitions in the mesic molecule  $dt\mu$ . This table does not contain the rates  $\lambda_A^{(1)}$  of the transitions from the state (J=1, v=1), since the mesic molecules  $dt\mu$  are produced in this state only in reactions of the type (1b), and transitions from this state are always accompanied by conversion on one of the two electrons of the complex  $[(dt\mu)d2e]$ . The numbering of the states together with the scheme of the cascade transitions is shown in Fig. 1.

We used in the calculations the wave functions  $\chi_{J_w}^{J_w}(R)$ and the energies  $\varepsilon_{J_w}$  of the mesic molecules, obtained

TABLE II. Rates of dipole Auger transitions in the mesic molecule  $dt\mu$ .

N→N′	(d)	$\lambda_A^{(1)}, 10^{11} \text{sec}^{-1}$	$\lambda_A^{(2)}$ , 10 <sup>11</sup> sec <sup>-1</sup>
$5 \rightarrow 4$ $5 \rightarrow 3$ $5 \rightarrow 1$ $4 \rightarrow 2$ $3 \rightarrow 2$ $2 \rightarrow 1$	0.52 0.27 0.03 0.24 0.16 0.11	- - 0.28 0.33 0.20	11.4 1.3 0.02 0.58 0.74 0.49

in Ref. 10, as well as the dipole moments (18) given in Ref. 14. In (17) we used the dipole moments  $\langle j'm' | r_k | \times jm \rangle$  which connect the first 26 states of the discrete spectrum of the two-center problem. As shown by the numerical calculations, the contribution of the higher states is ~10<sup>-2</sup>, so that to calculate  $|\langle d \rangle|$  with this accuracy it suffices to take into account only the contribution from the matrix element  $\langle 000g | r_0 | 000u \rangle$ .

The main error in the de-excitation rates calculated by us is due to insufficient knowledge of the conversionelectron wave functions in the initial and final states. The calculations show that variation of the value of  $Z^*$ in the range  $1 \le Z^* \le 2$  changes the de-excitation rate by 5-10% of the cited value.<sup>3)</sup>

The rates of de-excitation in the mesic molecules, calculated in this paper, are needed for the calculation of the kinetics muon catalysis in a mixture of hydrogen isotopes.

The accuracy attained in the present paper can be improved if necessary by using more accurate wave functions of the conversion electron, and also by including a larger number of terms in the expansion (10).

In conclusion, the authors thank V. S. Melezhik and L. N. Somov for help with the numerical calculations.

- <sup>1)</sup> The rates of the radiative transitions amount to  $\lambda_R \sim 10^5 10^6 \text{ sec}^{-1}$  and are small compared with the rates of Auger transitions in mesic molecules.<sup>1,4</sup>
- <sup>2)</sup> The quantity  $q^{-1}|I(q)|^2$  was calculated in atomic units, and  $|\langle d \rangle|_{*}^{2}$  in the units  $(e = \hbar = m_a = 1)$  of the problem. The dimensionalities of the wave functions (8a), (8b), and (10) are  $a_e^{-3/2}$ ,  $1 a_m^{-3/2}$ , respectively, where  $a_e = \hbar^2/m_e e^2$ ,  $a_m = \hbar^2/m_a e^2$ .
- <sup>3)</sup> The rates of the monopole E0 transitions in the mesic molecule  $dt\mu$ , calculated by the scheme given in Ref. 6, are small compared with E1 transitions and amount to  $\lambda_A(E0)$ ~10<sup>6</sup>-10<sup>8</sup> sec<sup>-1</sup>.
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Translated by J. G. Adashko