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RESONANT FORMATION
OF dd_{μ} MESIC MOLECULES

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1. INTRODUCTION

The phenomenon of the mesic molecule resonant formation has been established experimentally for the first time in the works of V.P.Dzhelepov with the collaborators.¹⁾ In contrast to the $dd\mu$ molecule non-resonant formation, when the binding energy of the formed mesic molecule is transferred by the conversion electron:



the very essence of the resonant mechanism of $dd\mu$ molecule formation suggested by E.A.Vesman in 1967²⁾ is the following. Mesic atom $d\mu$ with the kinetic energy ϵ_p when approaching one of the nuclei of D_2 molecule forms with it mesic molecule $dd\mu$ (to be more precise, the mesic molecular ion $(dd\mu)^+$) in a loosely bound rotational-vibrational state ($J = v = 1$), which becomes a "heavy nucleus" of mesic molecular complex $[(dd\mu)dee]$:

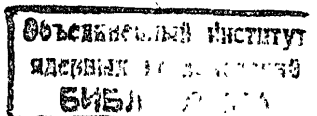


The released binding energy $|\epsilon_{JV}| = |\epsilon_{11}|$ of $dd\mu$ mesic molecule is transmitted to the excitation of vibrational-rotational states (νK) of mesic molecular complex $[(dd\mu)dee]_{\nu K}$ (see Fig. 1).

If $|\epsilon_{11}| \approx 2$ eV, the rate of reaction (2) at deuterium temperatures $T \gtrsim 100$ K is $\lambda_{dd\mu} \sim 10^6$ s⁻¹, that exceeds the rate of non-resonant process (1) in tens times. The existence of a loosely bound state ($J = v = 1$)³⁾ was firmly established in theoretical works in the period 1973 - 1983. It made possible to carry out the first well-grounded calculation of the $dd\mu$ molecule formation rate $\lambda_{dd\mu}(T)$ as a function of medium temperature T ⁴⁾. But on the whole this calculation was of illustrative character because the value of ϵ_{11} was known at that time with an accuracy of ~ 0.1 eV only and was determined just from the comparison of theoretical curve $\lambda_{dd\mu}(T)$ with experiment⁵⁾ at $T = 300$ K. Besides, the calculation⁴⁾ did not take into account the spin structure of $d\mu$ atom and $dd\mu$ molecule energy levels and the energy levels rotational structure of D_2 molecules and $[(dd\mu)dee]$ complexes. Some peculiarities of the kinetics of the mesic molecular processes in deuterium, namely, the deintegration ("back decay") and stabilization of the mesic molecular complexes $[(dd\mu)dee]$, fusion and cascade transitions in $dd\mu$ mesic molecule, the process of $d\mu$ atom spin-flip in collisions, etc., were not induced into consideration, as well.

All the effects listed above are taken into account in the present paper.* The energy of the ($J = v = 1$) state of $dd\mu$ mesic molecule has

* The first attempt to include the hyperfine structure of energy levels of $(d\mu)_F$ and $(dd\mu)_S$ was presented in paper⁶⁾.



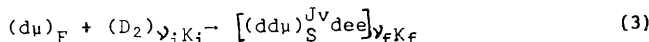
been calculated in recent years with a high accuracy (10^{-3} eV)^{7,8} the rates of fusion λ_f^{Jv} and de-excitation λ_{dex}^{Jv} to the state ($J = 1, v = 0$) have been also found for $dd\mu$ mesic molecule. Besides, in papers¹¹⁻¹³ the new refined expression has been obtained for the rate $\lambda_{dd\mu}^{(T)}$ (see also^{14,15}). Basing on the results of the listed papers, we present here the theoretical calculation of rates $\lambda_{dd\mu}^{(T)}$ for reactions



where $A = D, H, T$; $a = d, p, t$. This calculation does not involve any free parameters and additional hypotheses. The calculated dependence $\lambda_{dd\mu}^{(T)}$ fits well all the available experimental data on reaction (2) which is taken in the following as an example to demonstrate our method of the resonant rate calculations.

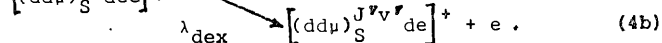
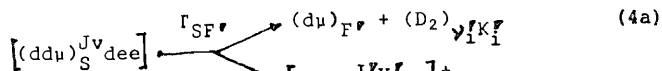
2. SCHEME OF THE CALCULATION OF RATES $\lambda_{dd\mu}^{(T)}$

In collisions of mesic atoms $(d\mu)_F$ in spin state F with molecule $(D_2)\psi_{iK_i}$ in vibrational-rotational state (ψ_{iK_i}) the excited mesic molecular complexes $[(dd\mu)dee]_{\psi_{fK_f}}$ are formed in vibrational-rotational state (ψ_{fK_f}) :

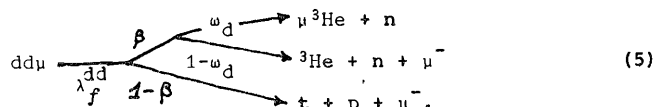


with rate λ_{FK_i, SK_f} where S is the total spin of $dd\mu$ mesic molecule.

The formed complexes either decay with rate Γ_{SF} into initial fragments (in the general case $F' \neq F, \psi_{i'} \neq \psi_i$ and $K_{i'} \neq K_i$), or are stabilized with rate λ_{dex} due to de-excitation of $dd\mu$ molecule:



The nuclear fusion reactions with the rates λ_f also prevent the complexes desintegration (4a):



The reaction channels probabilities are equal $\beta = 0.58$ and $1-\beta = 0.42$, respectively,^{16,17} the muon sticking probability in the first channel being $\omega_d = 0.122$ ^{17,18}, λ_f^{dd} is the rate of nuclear reaction.

The rate of reaction (3) equals^{11,13}*

$$\Lambda_{FK_i, SK_f} = \lambda_{FK_i, SK_f} \varphi$$

$$\lambda_{FK_i, SK_f} = 2\pi N_0 W_{FS} \int d^3p f(\epsilon_p, T) |V_{fi}|^2 \delta(E_i - E_f), \quad (6)$$

where $N_0 = 4.25 \cdot 10^{22} \text{ cm}^{-3}$ is the liquid hydrogen density, $\varphi = N/N_0$ is the deuterium density, \vec{p} is the momentum of relative motion of $d\mu$ atom and D_2 molecule, $f(\epsilon_p, T) = 2(\epsilon_p/\pi)^{1/2} T^{-3/2} \exp\{-\epsilon_p/T\}$ is the Maxwellian distribution over the relative collision energy ϵ_p at given temperature T , V_{fi} is the coordinate matrix element of the transition from the initial state i to the final state f :

$$|V_{fi}|^2 = 1/(2K_i+1) \sum_{M_{K_i}, M_{K_f}, M_J} |\langle \Psi^{(f)} | \hat{V} | \Psi^{(i)} \rangle|^2, \quad (7)$$

M_{K_i}, M_{K_f} and M_J are third projections of angular momenta K_i, K_f and J . Overlapping between the spin functions of initial (F) and final (S) states is given by the factor¹¹

$$W_{FS} = 2(2S+1) \begin{Bmatrix} 1/2 & 1 & F \\ 1 & S & 1 \end{Bmatrix}^2, \quad (8)$$

where $\begin{Bmatrix} S_\mu & S_d & F \\ S_d & S & I \end{Bmatrix}$ is the Wigner 6j-symbol, $I = 1$ is the total spin of

deuterium nuclei in $dd\mu$ molecule (identity of nuclei in $dd\mu$ molecule being taken into account).

Coordinate wave functions and transition operator are

$$\Psi^{(i)} = \Psi_{d\mu}(\vec{r}_1) \Psi_{D_2}^{\psi_{iK_i}}(\vec{\rho}_1) e^{i\vec{p}\vec{\rho}_2}$$

$$\Psi^{(f)} = \Psi_{dd\mu}^{Jv}(\vec{r}, \vec{R}) \Psi_{MD}^{\psi_{fK_f}}(\vec{\rho}) \quad (9)$$

$$\hat{V} = \vec{\rho} \cdot \vec{d} / \rho \cdot \partial W(\rho) / \partial \rho,$$

\vec{r}_1 and $\vec{\rho}_1$ are intrinsic coordinates of $d\mu$ atom and D_2 molecule, $\vec{\rho}_2$ is their relative coordinate, \vec{r} and \vec{R} are Jacobi coordinates of $dd\mu$ molecule, $\vec{\rho}$ is an internuclear coordinate of mesic molecular complex $MD = [(dd\mu)dee]$, \vec{d} is the $dd\mu$ molecule dipole moment. (The choice of expressions (6)-(9) is justified in papers¹¹⁻¹⁵.)

* Another expression for (6) with $\delta(E_i - E_f)$ substituted by the Breit-Wigner factor is suggested in paper¹⁹. For the discussion of this question see^{13,20}.

** The cross-section $\sigma_{el} \approx 2 \cdot 10^{-19} \text{ cm}^2$ ³⁴ of the elastic scattering $d\mu + d$ is large enough for the Maxwell distribution establishing in times $\sim 3 \cdot 10^{-8} \varphi^{-1} \text{ s}$. See paper⁴⁵, where the kinetics in $D_2 + T_2$ mixture at small φ is considered.

The initial (E_i) and final (E_f) energies for reaction (3) equal, respectively,

$$\begin{aligned} E_i &= E_F(d\mu) + E_{\nu_i K_i}(D_2) + \epsilon_p \\ E_f &= \epsilon_S(dd\mu) + E_{\nu_f K_f}(MD) \\ E_F(d\mu) &= E_{1s}(d\mu) + \Delta E_F \\ \epsilon_S(dd\mu) &= \epsilon_{J\nu}(dd\mu) + \Delta \epsilon_S, \end{aligned} \quad (10)$$

where $E_{1s}(d\mu)$ and ΔE_F are the nonrelativistic energy and relativistic hyperfine splitting of $d\mu$ atom $1s$ state, corresponding to the total spin F , $\epsilon_{J\nu}(dd\mu)$ and ϵ_S are the corresponding quantities for ($J\nu$) state of $dd\mu$ mesic molecule with the total spin $S^{21,22}$. The resonance condition $E_f = E_i$ can be presented as $\epsilon_p = \epsilon_{if}$, where

$$\epsilon_{if} = \epsilon_{i1} + \Delta \epsilon_{FS} + \Delta E_{\nu_i K_i, \nu_f K_f} = \epsilon_0 + \Delta \epsilon_{FS} + \Delta E_{if} \quad (11)$$

$\epsilon_0 = \epsilon_{i1} + \Delta E_{\nu}$ is the resonance defect, $\Delta E_{\nu} = \Delta E_{\nu_i 0, \nu_f 0} = E_{\nu_f 0}(MD) - E_{\nu_i 0}(D_2)$; $\epsilon_{i1} = E_{11}(dd\mu) - E_{1s}(d\mu)$ the nonrelativistic energy $\epsilon_{J\nu}$ of the state ($J = \nu = 1$), $\Delta \epsilon_{FS} = \Delta \epsilon_S - \Delta E_F$ is the spin splitting of ϵ_{i1} ,

$$\Delta E_{\nu_i K_i, \nu_f K_f} = E_{\nu_f K_f}(MD) - E_{\nu_i K_i}(D_2) = \Delta E_{\nu} + \Delta E_{if}$$

$$\Delta E_{if} = \left\{ E_{\nu_f K_f}(MD) - E_{\nu_f 0}(MD) \right\} - \left\{ E_{\nu_i K_i}(D_2) - E_{\nu_i 0}(D_2) \right\} = \epsilon_f - \epsilon_i$$

Energies $E_{\nu_i K_i}(D_2)$ and $E_{\nu_f K_f}(MD)$ of rotational-vibrational states of D_2 molecule and complexes MD have been calculated with an accuracy of $\sim 10^{-4}$ eV in paper²³.

The general scheme of the $dd\mu$ -resonant formation is presented in Fig. 1. This process is possible if the sum $\epsilon_p + |\epsilon_{i1}|$ of the $d\mu$ atom kinetic energy ϵ_p and $dd\mu$ molecule binding energy $|\epsilon_{i1}|$ is equal to the transition energy ΔE_{ν} from the ground state $\nu_i = 0$ of D_2 molecule to the excited vibrational state $\nu_f = 7$ of the complex $[(dd\mu)dee]$.

The scheme of splitting of energy levels of initial and final states is shown in Figs. 2 and 3. In our calculations were used the quantities $\epsilon_{i1} = -1.964$ eV, $\Delta \epsilon_{FS}$ and ΔE_{if} , which can be found in papers^{8,21-25}.

* The used value of $\epsilon_{i1} = \epsilon_{i1}^{nrel} + \Delta \epsilon_{i1}^{rel} + \Delta \epsilon_{i1}^{dim}$ is a sum of the non-relativistic energy for point-like nuclei $\epsilon_{i1}^{nrel} = -1.9750$ eV⁸, relativistic corrections $\Delta \epsilon_{i1}^{rel} = 0.0097$ eV²² and corrections to the finite size of $dd\mu$ mesic molecule in the mesic molecular complex $\Delta \epsilon_{i1}^{dim} = 0.0010$ eV^{24,25} therefore $\epsilon_{i1} = -1.9643$ eV with the possible error

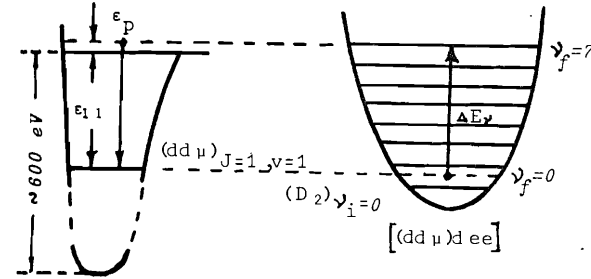


Fig. 1. Scheme of the resonance formation of $dd\mu$ mesic molecules: the reaction is allowed if the resonance condition $\epsilon_p + |\epsilon_{i1}| = \Delta E_{\nu}$ is fulfilled.

For reaction (1) $\nu_i = 0$, $\nu_f = 7$, the resonance defect is $\epsilon_0 = 0.0337$ eV, and values of $\Delta \epsilon_{FS}$ equal:

$$\begin{aligned} \Delta \epsilon_{1/2 \ 1/2} &= 0.0163 \text{ eV} & \Delta \epsilon_{1/2 \ 3/2} &= 0.0403 \text{ eV} \\ \Delta \epsilon_{3/2 \ 1/2} &= -0.0322 \text{ eV} & \Delta \epsilon_{3/2 \ 3/2} &= -0.0082 \text{ eV}. \end{aligned} \quad (12)$$

The rate λ_{FS} of the $(dd\mu)_S$ mesic molecule formation from the initial states of mesic atoms $(d\mu)_F$, averaged over the rotational states of $(D_2)_{K_i}$ molecule and summed over the final states of complex $(MD)_{K_f}$ equals

$$\lambda_{FS} = \sum_{K_i, K_f} \omega(K_i) \lambda_{FK_i, SK_f} \Theta(\epsilon_{if}), \quad (13a)$$

where

$$\Theta(x) = \begin{cases} 1 & \text{at } x > 0 \\ 0 & \text{at } x < 0 \end{cases}$$

$$\omega(K_i) = \xi(K_i) Z_i^{-1} (2K_i + 1) \exp \{ -\epsilon_i / T \}, \quad (13b)$$

$\epsilon_i = E_{\nu_i K_i}(D_2) - E_{\nu_i 0}(D_2)$ is the rotational energy of molecule D_2 , $\omega(K_i)$ is the Boltzmann distribution of molecules D_2 over rotational degrees of freedom, Z_i is the statistical sum over rotational

$\delta \epsilon_{i1} = \pm 0.0010$ eV which is comparable with the fine structure splitting (0.0006 eV) in $dd\mu$ molecule²². (See Fig. 2)

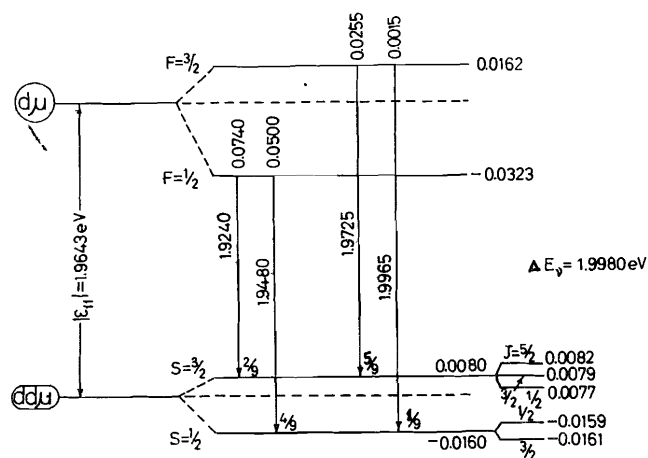


Fig. 2. Scheme of hyperfine and fine splitting of energy levels of atoms $(d\mu)_F$ and mesic molecules $(dd\mu)_{S}^{J\bar{V}}$: $\bar{F} = \bar{S}_\mu + S_d$ is a total spin of $d\mu$ atom, $\bar{S} = \bar{F} + \bar{S}_d = \bar{S}_\mu + \bar{I}$ and $\bar{J} = \bar{S} + \bar{J}$ are total spin and total angular momentum of $dd\mu$ molecule, respectively, $\Delta E_\nu = E_{\nu,0} - E_{\nu,F} = 1.9980 \text{ eV}$, $\epsilon_0 = \Delta E_\nu - |\epsilon_{11}| = 0.0337 \text{ eV}$. Transition energies are given at vertical arrows showing transitions $(F \rightarrow S)$, their resonance energies $\epsilon_0 + \Delta\epsilon_{FS}$ are given at the beginning, while corresponding weights W_{FS} at the end of the arrows.

states of D_2 molecule at given temperature T ,

$$\xi(K_i) = \begin{cases} 2/3 & \text{for even } K_i \\ 1/3 & \text{for odd } K_i \end{cases} \quad (13c)$$

(for the case of equilibrium population of ortho- and para-states of D_2 molecule).

Resonance process (2) is possible only if $\epsilon_{if} > 0$. At temperatures $T \lesssim 10^3 \text{ K}$ rotational states $K_i < 10$ are excited, i.e., in resonance condition (11) ~ 100 various values of ΔE_{if} are possible, corresponding to various combinations (K_i, K_f) and 209 terms in sum (13), limited only by a condition $\epsilon_{if} > 0$. In reality, at given temperature T an essential contribution to sum (13) comes only from 2 - 3 terms, for which $\epsilon_{if} \sim T$.

The rate Γ_{SF} of complex back decay (4a) equals*

$$\Gamma_{SF} = \sum_{K_i, K_f} \Gamma_{SK_f, F'K_i} \omega(K_f) \xi(K_i') \quad (14)$$

* Rates of the rotational relaxation ($\sim 10^{13} \varphi \text{ s}^{-1}$ 26) of the formed complexes noticeably exceed rates λ_f, λ_{dex} and Γ_{SF} , hence, during the

$$\omega(K_f) = Z_f^{-1} (2K_f + 1) \exp \{-\epsilon_f/T\} \quad (14)$$

$$Z_f = \sum_{K_f} (2K_f + 1) \exp \{-\epsilon_f/T\}$$

where $\Gamma_{SK_f, F'K_i}$ is defined by the expression^{13,26,27)}

$$\Gamma_{SK_f, F'K_i} = 2/\pi (2\nu_2^3 \epsilon_{if})^{1/2} W_{FS} (2F+1)(2S+1)(2K_i+1)(2K_f+1) |V_{fi}|^2 \theta(\epsilon_{if}) \quad (15)$$

with $\mu_2^{-1} = m_{d\mu}^{-1} + m_{D_2}^{-1}$ being the inverse reduced mass of system $d\mu + D_2$, and the spin overlapping factor W_{FS} being defined with (9).

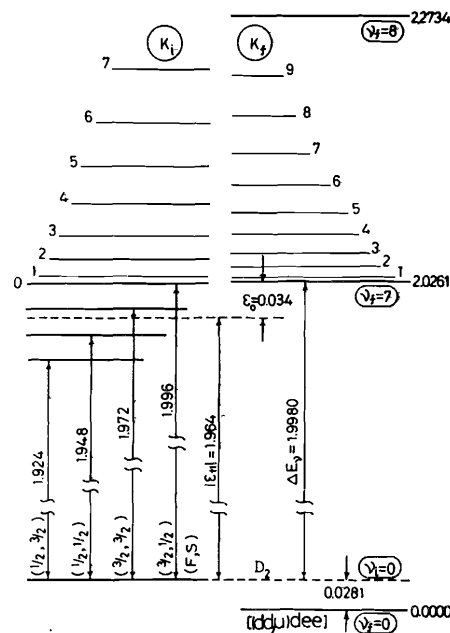


Fig. 3. Scheme of resonance transitions in reaction (3) with taken into account the rotational level splitting of molecule $(D_2)_{\nu_i, K_i}$ and complex $[(dd\mu)dee]_{\nu_f, K_f}$. On the left are shown values $\epsilon_{11} + \Delta\epsilon_{FS} + \epsilon_i$, on the right $\Delta E_\nu + \epsilon_f$, the energies being reckoned from the energy of the molecule $(D_2)_{\nu_i=0, K_i=0}$ ground state.

lifetime of complex $[(dd\mu)dee]$ the Boltzmann distribution over rotational states K_f is established.

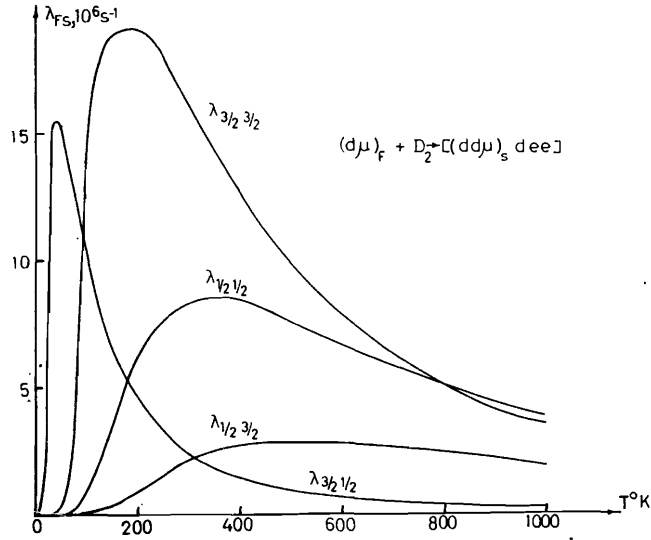


Fig. 4. Temperature dependence of partial rates λ_{FS} corresponding to the scheme of transitions in Fig. 2. The sharp maximum of rate $\lambda_{3/2 1/2}$ at $T \approx 46$ K corresponds to resonance energy $\epsilon_{if} = 5.9$ meV of dipole transition ($F = 3/2, K_f = 0$) \rightarrow ($S = 1/2, K_f = 1$).

The details of calculations of λ_{FS} and Γ_{SF} are given in papers¹¹⁻¹³, the dependence of these rates on temperature T is presented in Figs. 4 and 5. The observed rate of $dd\mu$ molecule formation $\lambda_{dd\mu}$ is expressed through λ_{FS} and Γ_{SF} , the rates of fusion λ_{μ}^{JV} (5) and Auger transitions λ_{dex}^{JV} (4), the rate λ_{nr} of nonresonance formation of $dd\mu$ molecules in reaction (1) and rates λ_{FF} , of $d\mu$ atom spin-flip in collisions with deuterium nuclei. To find adequate expressions for $\lambda_{dd\mu}$, one should consider the kinetics of muon catalysis processes in deuterium.

3. KINETICS OF MUON CATALYSIS PROCESSES IN DEUTERIUM

During the time $t_0 \sim 10^{-12} \varphi^{-1}$ s²⁹) muons with energy ~ 10 keV in deuterium form mesic atoms $d\mu$ in highly excited states $n \geq 14$ ³⁰). During $t_a \sim 10^{-11} \varphi^{-1}$ s they go down to the ground 1s-state of $d\mu$ atom³¹) and statistically populate sublevels $F = 1/2$ and $F = 3/2$ of its hyper-

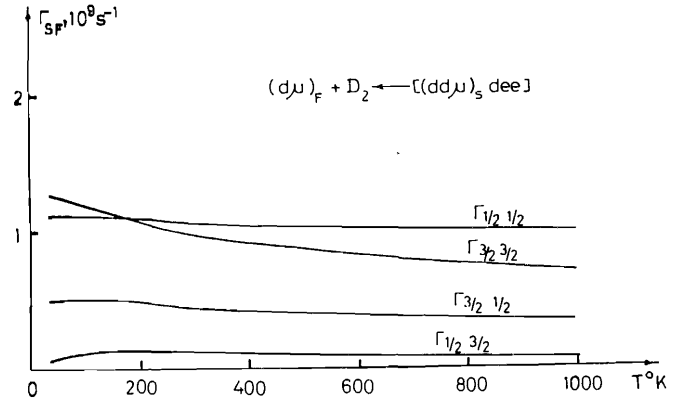
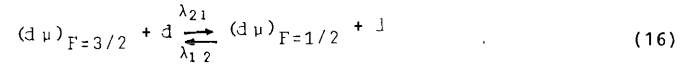


Fig. 5. Temperature dependence of complex back decay rates in reaction (4a).

Approximate equalities are valid $\sum_F \Gamma_{3/2 F} \approx \sum_F \Gamma_{1/2 F} \approx \text{const}$.

fine structure³²) (which subsequently will be denoted by indices 1 and 2, respectively) with weights $h_1 = 1/3$ and $h_2 = 2/3$. After this process (3) and (17) of $dd\mu$ molecule formation take place as well as spin-flip processes^{33,34}:



the ratios of direct and inverse processes (16) being connected by the detailed balance relation

$$\lambda_{12} = \gamma \cdot \lambda_{21}, \quad \gamma = 2 \exp(-\Delta E/T) \\ \Delta E = \Delta E_{d\mu}^{hfs} = 0.0485 \text{ eV}. \quad (17)$$

The general case of muon catalysis kinetics in hydrogen isotope mixtures is rather complicated and is considered in papers^{35,36}). The scheme of processes in pure deuterium is depicted in Fig. 6, and the system of equations describing the kinetics of these processes has the form

$$\begin{aligned} \frac{dN_F}{dt} &= -(\lambda_0 + \lambda_{nr} + \lambda_F + \lambda_{FF}) N_F + \lambda_{FF'} N_{F'} + \sum_{\alpha} \left\{ \Gamma_{\alpha F} + F(1-\omega) \lambda_{\alpha F}^{(\alpha)} \right\} N_{\alpha}, \\ &\quad F' \neq F \\ \frac{dN_{\alpha}}{dt} &= -(\lambda_0 + \lambda_{\alpha F}^{(\alpha)} + \Gamma_{\alpha} + \sum_{\alpha'} \lambda_{\alpha \alpha'}) N_{\alpha} + \sum_{\alpha' \neq \alpha} \lambda_{\alpha' \alpha} N_{\alpha'} + \sum_F \lambda_{F \alpha} N_F \\ \frac{dN_n}{dt} &= \beta \sum_{\alpha} \lambda_{\alpha n}^{(\alpha)} N_{\alpha} \end{aligned} \quad (18)$$

$$\lambda_F = \sum_S \lambda_{FS}, \quad \Gamma_S = \sum_F \Gamma_{SF}, \quad \Gamma_{\alpha F} = 0, \quad \lambda_{nr} = \sum_{\alpha \neq S} \lambda_{F \alpha}$$

at $\alpha \neq S$

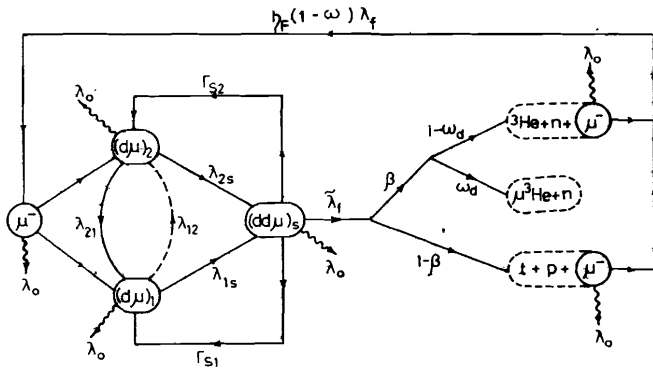


Fig. 6. Kinetics of μ -catalysis processes in deuterium. Rates λ_{FS} , Γ_{SF} , λ_{FF} , and λ_f are defined with formulas (13a), (14), (24) and (22) at $\varphi = 1$.

with initial conditions

$$N_F(0) = \eta_F, \quad N_\alpha(0) = N_n(0) = 0. \quad (19)$$

Here the notation is introduced: N_F is the number of mesic atoms $(d\mu)_F$, N_α is the number of $(dd\mu)_\alpha$ mesic molecules in state $\alpha = \{S, J\nu\}$ (for the resonance state ($J = \nu = 1$) we put in the following $\alpha = S$), N_n is the number of neutrons emitted in reaction (5), $\omega = \omega_d$ is the total muon sticking probability in reaction (5), $\lambda_0 = 0.455 \cdot 10^6 \text{ s}^{-1}$ is the muon decay rate, $\lambda_f^{(\alpha)}$ is the nuclear fusion rate for the state $(dd\mu)_\alpha$, λ_{nr} is the rate of the nonresonance $dd\mu$ molecule formation in reaction (1) in various states $\alpha = (S, J\nu)$ (except the state ($J = \nu = 1$)), for which $\Gamma_{\alpha F} = 0$, $\lambda_{\alpha\alpha}$ are the rates of Auger transitions (4b), λ_{FF} is the rate of spin-flip reactions (16). All the rates λ_F , λ_{FF} , $\lambda_{F\alpha}$ and λ_{nr} are normalized to the liquid hydrogen density $N_0 = 4.25 \cdot 10^{22} \text{ cm}^{-3}$. In the calculations below we use the following values of rates:

$$\begin{aligned} \lambda_{FF} &= 4.7 \cdot 10^7 \text{ s}^{-1} \quad (34) & \lambda_{nr} &= 0.4 \cdot 10^5 \text{ s}^{-1} \quad (4, 28) \\ \lambda_F^{(S)} &= 0.43 \cdot 10^9 \text{ s}^{-1} \quad (9) & \lambda_f^{(\alpha)} &= 1.5 \cdot 10^9 \text{ s}^{-1} \quad (9) \\ \lambda_{S\alpha} &= 0.08 \cdot 10^9 \text{ s}^{-1} \quad (10) & \omega &= 0.071 \quad (17, 18). \end{aligned} \quad (20)$$

Rates $\lambda_{FS(T)} \approx 10^6 + 10^7 \text{ s}^{-1}$ and $\Gamma_{SF} \approx 10^8 + 10^9 \text{ s}^{-1}$ are calculated in the present paper (see Figs. 4 and 5).

Taking into account inequalities $\{\Gamma_{SF}, \lambda_f^{(\alpha)}\} \gg \{\lambda_{FS}, \lambda_0\}$ it follows from equations (18) that at $t \gg (\lambda_f^{(\alpha)} + \Gamma_\alpha)^{-1} \sim 0.5 \cdot 10^{-9} \text{ s}$ the quasistationary regime is achieved, i.e. the following relations are fulfilled

$$dN_\alpha/dt \approx 0, \quad N_\alpha \approx \sum_F \lambda_{F\alpha} / (\lambda_f^{(\alpha)} + \Gamma_\alpha) N_F \ll 1 \quad (21)$$

$$\begin{aligned} N_S &\approx \varphi \sum_F \lambda_{FS} / (\lambda_f^{(S)} + \Gamma_S) N_F \\ \lambda_\alpha^{(\alpha)} N_\alpha &= \sum_F (\lambda_F + \lambda_{nr}) \varphi N_F - \sum_S \Gamma_S N_S \\ \tilde{\lambda}_F &= \lambda_f^{(S)} + \sum_\alpha \lambda_{S\alpha}. \end{aligned} \quad (21)$$

In this case the system of equations (18) is reduced to more simple one within the accuracy $\{\lambda_{FS}, \lambda_0\} / \{\Gamma_{SF}, \lambda_f^{(\alpha)}\} \sim 10^{-2}$:

$$\begin{aligned} dN_F/dt &= -(\lambda_0 + \lambda_F \varphi + \lambda_{FF} \varphi) N_F + \tilde{\lambda}_F \varphi N_F + \eta_F (1-\omega) \tilde{\lambda}_F N_{dd\mu} \\ dN_n/dt &= \beta \tilde{\lambda}_F N_{dd\mu}, \\ N_{dd\mu} &= \sum_\alpha N_\alpha = \tilde{\lambda}_F^{-1} \varphi \sum_F \lambda_{F\alpha} N_F \end{aligned} \quad (22)$$

to which corresponds the scheme of the processes presented in Fig. 7. The effective rates in this scheme are given by:

$$\begin{aligned} \tilde{\lambda}_F &= \lambda_{nr} + \sum_S \lambda_{FS} \tilde{\lambda}_F / (\tilde{\lambda}_F + \Gamma_S) \\ \tilde{\lambda}_{FF} &= \lambda_{FF} + \sum_S \lambda_{FS} \Gamma_{SF} / (\tilde{\lambda}_F + \Gamma_S) \end{aligned} \quad (23)$$

and $\bar{\lambda}_F \approx \lambda_f^{(S)}$ within accuracy $\sim \lambda_{nr} / \tilde{\lambda}_F$.

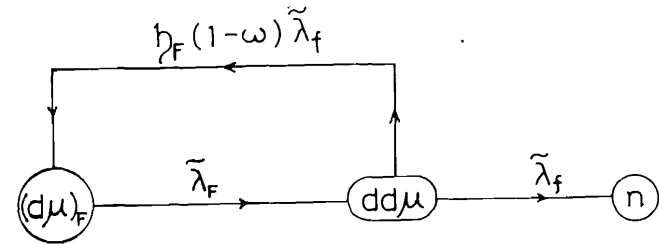


Fig. 7. The principal scheme of μ -catalysis processes in deuterium, valid at $t \gg (\tilde{\lambda}_F + \Gamma_S)^{-1} \approx 0.5 \cdot 10^{-9} \text{ s}$.

It is seen from (23) that the rates λ_{FS} of the $dd\mu$ molecule resonance formation is about three times as small at the value of the rates (20) than that calculated by formulas (13) which do not take into account the back decay of mesic molecular complexes (4a). (The importance of this process was first pointed out in papers^{26,27}, see³⁷, as well).

For the same reason the effective rate λ_{FF} of spin-flip process differs from the rate λ_{FF} of reaction (16), as the process (4a) changes the populations of the spin states $(d\mu)_F$ and that is equivalent to the additional depolarization ($F = 3/2$) \rightarrow ($F = 1/2$). The second term

for $\tilde{\lambda}_{FF}$, in (23) describes this process. The more detailed discussion of this effect is performed in³⁸⁾.

At $t \gg (\lambda_{21}\varphi)^{-1}$ the dynamical equilibrium of the spin-flip processes (16) gives as a result the quasistationary populations P_F of the spin states $(d\mu)_F$. In this case the time distributions $N_F(t)$ become universal:

$$\begin{aligned} N_F(t) &= P_F N_{d\mu}(t) \\ \sum_F P_F &= \sum_F \tilde{h}_F = 1. \end{aligned} \quad (24)$$

Taking into account these relations we obtain from (22):

$$\begin{aligned} dN_{d\mu}/dt &= -\lambda_c N_{d\mu} \\ dN_n/dt &= \beta \lambda_{dd\mu} \varphi N_{d\mu} = \beta \lambda_{dd\mu} \varphi e^{-\lambda_c t} \\ \lambda_c &= \lambda_0 + \omega \lambda_{dd\mu} \varphi, \quad \lambda_{dd\mu} = \sum_F P_F \tilde{\lambda}_F, \end{aligned} \quad (25a)$$

where the populations P_F are equal to

$$\begin{aligned} P_1 &= (1 + \tilde{\gamma})^{-1}, \quad P_2 = 1 - P_1, \\ \tilde{\gamma} &= (\tilde{\lambda}_{12} + \tilde{h}_2 \tilde{\lambda}_1) / (\tilde{\lambda}_{21} + \tilde{h}_1 \tilde{\lambda}_2). \end{aligned} \quad (25b)$$

Neglecting the terms of order $\sim \omega^2$ it is possible to represent the solution of the system (22) in the analytical form:

$$\begin{aligned} N_F(t) &= P_F e^{-\lambda_c t} + Q_F e^{-\Lambda t} \\ Q_F &= \tilde{h}_F - P_F \\ \Lambda &= \lambda_0 + (\tilde{\lambda}_{21} + \tilde{\lambda}_{12} + \tilde{h}_1 \tilde{\lambda}_2 + \tilde{h}_2 \tilde{\lambda}_1) \varphi. \end{aligned} \quad (26)$$

Taking into account relations (22)-(25) we finally obtain:

$$dN_n/dt = \beta \varphi \{ \lambda_{dd\mu} e^{-\lambda_c t} + (\tilde{h}_2 - P_2)(\tilde{\lambda}_2 - \tilde{\lambda}_1) e^{-\Lambda t} \}. \quad (27)$$

The multiplicity of muon catalysis χ_c (the number of neutrons per one muon) is equal to

$$\chi_c = \beta \varphi \{ \lambda_{dd\mu} \lambda_c^{-1} + (\tilde{h}_2 - P_2)(\tilde{\lambda}_2 - \tilde{\lambda}_1) \Lambda^{-1} \}. \quad (28)$$

At low deuterium temperatures $10 \lesssim T \lesssim 100$ K, when the inequalities are valid:

$$\begin{aligned} \lambda_{3/2} \gg \lambda_{1/2}, \quad \lambda_{21} \gg \{ \lambda_{12}, \lambda_1, \lambda_2 \}, \quad \tilde{\lambda}_1 \approx \lambda_{nr}, \\ P_1 \approx 1, \quad P_2 \approx \tilde{\gamma} \approx 2/3 \lambda_{nr} / \lambda_{21} \sim 10^{-2}, \quad \lambda_{dd\mu} \approx 1.05 \lambda_{nr} \end{aligned}$$

the time distribution of neutron is simplified:

$$dN_n/dt \approx \beta \varphi e^{-\lambda_0 t} \{ \tilde{\lambda}_1 \exp\{-\omega \tilde{\lambda}_1 \varphi t\} + 2/3 \tilde{\lambda}_2 \exp\{-\tilde{\lambda}_{21} \varphi t\} \}. \quad (29)$$

Just this distribution was used at SIN experiment⁴²⁾ for the measurement of the ratio $\tilde{\lambda}_{3/2} / \tilde{\lambda}_{1/2}$.

4. RESULTS AND DISCUSSION

It is clear from the previous consideration that the calculated values $\lambda_{dd\mu}(T)$ in the framework of accepted calculation scheme

depend on two parameters only: the binding energy $|\epsilon_{11}|$ of the state $(1 \cdot v \cdot 1)$ and the effective nuclear fusion rate $\tilde{\lambda}_F$ in the $dd\mu$ molecule.

In Fig. 0 there are presented theoretical values of $|\epsilon_{11}| \pm \delta\epsilon_1$ and $\tilde{\lambda}_F \pm \delta\tilde{\lambda}_F$, as well as the range of their allowed values, following from experiments¹⁷⁾ and⁴²⁾. The lower range corresponds to pairs of $|\epsilon_{11}|$ and $\tilde{\lambda}_F$ for which the values $\lambda_{dd\mu}$ calculated by (23) - (26) fall on the boundaries of the interval of measured value¹⁷⁾

$$\lambda_{dd\mu}(T = 298 \text{ K}) = (2.76 \pm 0.08) \cdot 10^6 \text{ s}^{-1}$$

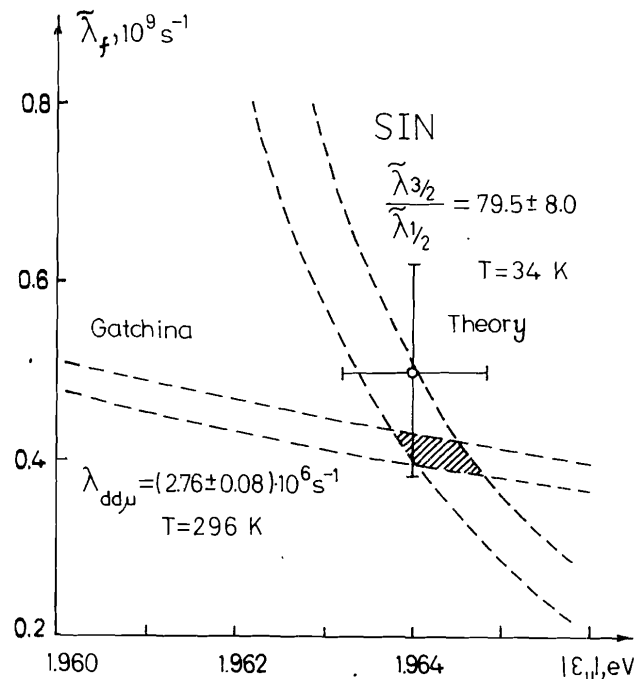


Fig. 0. The range of allowed values of $|\epsilon_{11}| \pm \delta\epsilon_1$ and $\tilde{\lambda}_F \pm \delta\tilde{\lambda}_F$ following from experiments¹⁷⁾ and⁴²⁾ (shaded). The cross represents the theoretical values of $|\epsilon_{11}|$ and $\tilde{\lambda}_F$ with their possible uncertainties.

The upper range corresponds to the measured ratio⁴²⁾

$$\tilde{\lambda}_{3/2} / \tilde{\lambda}_{1/2} (T = 34 \text{ K}) = 79.5 \pm 8.0$$

of the rates of the $dd\mu$ molecule formation from states $F = 3/2$ and $F = 1/2$ of $(d\mu)_F$ mesic atom. It is easily seen that the shadowed area of $|\epsilon_{11}|$ and $\tilde{\lambda}_F$ values compatible with results of both experiments¹⁷⁾

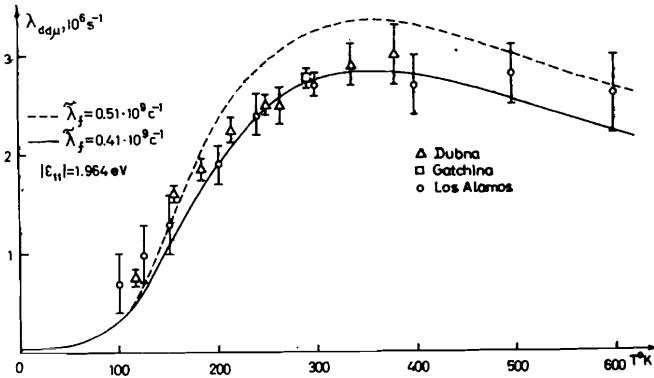


Fig. 9. The dependence of reaction (1) rate $\lambda_{dd\mu}(T)$ on temperature T . Experimental points: Δ - Dubna⁵⁾, \square - Gatchina¹⁷⁾, \circ - Los Alamos⁴²⁾ (Dubna data are renormalized to the value $\lambda_{dd\mu}(T = 298 \text{ K})$ measured at Gatchina). A solid line presents the calculation at $\epsilon_{11} = -1.964 \text{ eV}$, $\tilde{\lambda}_f = 0.41 \cdot 10^9 \text{ s}^{-1}$, a dashed line was calculated at $\epsilon_{11} = -1.964 \text{ eV}$, $\tilde{\lambda}_f = 0.51 \cdot 10^9 \text{ s}^{-1}$.

and⁴²⁾ is within theoretical uncertainties of $|\epsilon_{11}|$ and $\tilde{\lambda}_f$:

$$|\epsilon_{11}| = 1.964 \pm 0.001 \text{ eV}, \quad \tilde{\lambda}_f = (0.51 \pm 0.10) 10^9 \text{ s}^{-1}. \quad (30a)$$

The solid line in Fig. 9 presents $\lambda_{dd\mu}(T)$ calculated at

$$|\epsilon_{11}| = 1.964 \text{ eV} \text{ and } \tilde{\lambda}_f = 0.41 \cdot 10^9 \text{ s}^{-1} \quad (30b)$$

taken from the shadowed area in Fig. 8. It can be easily seen that these values of ϵ_{11} and λ_f provide a good fit of all the experiments^{5,17,39)} (Data from paper⁵⁾ are multiplied by the normalization factor $B = 3.6$, which equals the ratio of rates $\lambda_{dd\mu}$ from¹⁷⁾ and⁵⁾ at $T = 298 \text{ K}$). The supplementary analysis in respect to criterion χ^2 confirms that the best fit of theory and experiment is achieved at these very values (30b).

The dashed line in Fig. 9 represents the calculated rates $\lambda_{dd\mu}(T)$ at the theoretical values (30a) of ϵ_{11} and $\tilde{\lambda}_f$. It is seen that the deviations of dashed line from solid one do not exceed $\sim 20\%$. Since the accuracy of calculation scheme¹³⁾ is estimated by $\sim 1\%$, they are mainly caused by the uncertainties in the nuclear rate $\tilde{\lambda}_f$, which today is known with the accuracy $\sim 20 \div 30\%$ ⁹⁾.

The presented calculation of $\lambda_{dd\mu}(T)$ is carried out for the equilibrium mixture of ortho- and para-states of D_2 molecules, corresponding to values of $\xi(K_i)$ (13c). The curves for the cases of pure ortho- and para-states of D_2 differ from each other not more than by 5% (Fig. 10, see also paper⁴³⁾, specially devoted to this question).

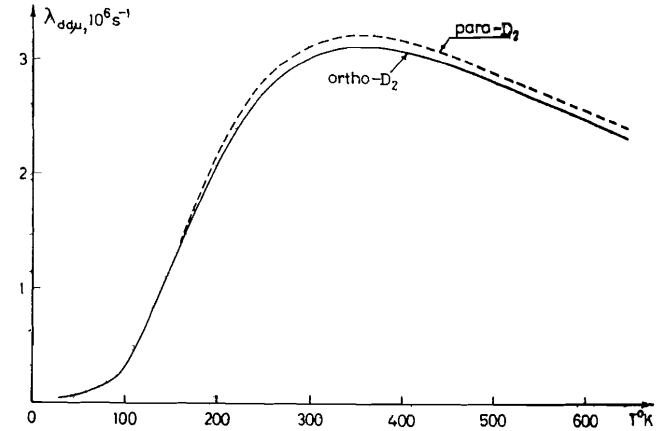


Fig. 10. The comparison of the $\lambda_{dd\mu}$ molecules formation rates in pure ortho and para deuterium.

It follows from our calculations⁴⁾ that at $T = 34 \text{ K}$

$$\lambda_{dd\mu} \approx \tilde{\lambda}_{1/2} \approx \lambda_{nr} \approx 0.4 \cdot 10^5 \text{ s}^{-1} \quad (31)$$

that noticeably differs from experimental values $(0.76 \pm 0.15) \cdot 10^5 \text{ s}^{-1}$ ⁴⁰⁾ and $(1.03 \pm 0.04) \cdot 10^5 \text{ s}^{-1}$ ⁴¹⁾. A possible reason of such a discrepancy may be the method of data analysis: in particular, to the neutron time distribution (27) two exponentials should be included.

In such a situation it seems necessary to make a new measurement of $\lambda_{dd\mu}$ in the liquid deuterium because they allow one to calculate the absolute value of $\tilde{\lambda}_{3/2}$ from the measured ratio $\tilde{\lambda}_{3/2} / \tilde{\lambda}_{1/2}$. The rate $\lambda_{dd\mu}$, being extremely sensitive to the value of ϵ_{11} (see the Table and Fig. 9), the level energy ϵ_{11} can be found with a high accuracy ($\sim 10^{-4} \text{ eV}$). At low deuterium temperatures practically only one term contributes to sum (13) for partial rates λ_{FS} , namely, the one corresponding to the dipole transition ($F = 3/2, K_i = 0$) - ($S = 1/2, K_f = 1$) with resonance energy $\epsilon_{if} = 5.9 \text{ meV} = 69 \text{ K}$. In this case $\omega(K_i) \approx 1$ and dependence (6), (13) of $\lambda_{dd\mu}(T)$ at $T \lesssim 100 \text{ K}$ can be put in the analytical form:

$$\lambda_{1,1/2}(T) \approx \lambda_{3/2, 1/2}(T) \approx 4\sqrt{\pi} N_0 W_{3/2, 1/2} |V_{if}|^2 \sqrt{\epsilon_{if}} T^{-3/2} \exp\{-\epsilon_{if}/T\} = 2.5 \cdot 10^{10} \cdot T^{-3/2} \exp\{-69/T\} \text{ s}^{-1}, \quad (32)$$

where $W_{3/2, 1/2} = 1/9$, $|V_{if}|^2 = 4.63 \cdot 10^{-11} \text{ a.u.}$

Note that the shape of the curve for $\lambda_{dd\mu}(T)$ is very sensitive to the value of ϵ_{11} , hence accurate measurements of the temperature

dependence of the $dd\mu$ molecule resonance formation rate will allow experimental studies of relativistic effects in a three-body system⁴⁴⁾. The degree of sensitivity of $\lambda_{dd\mu}(T)$ to ϵ_{11} is demonstrated in Fig. 11: ϵ_{11} variation of 10 meV twice changes the value of $\lambda_{dd\mu}$ at $T \lesssim 100$ K.

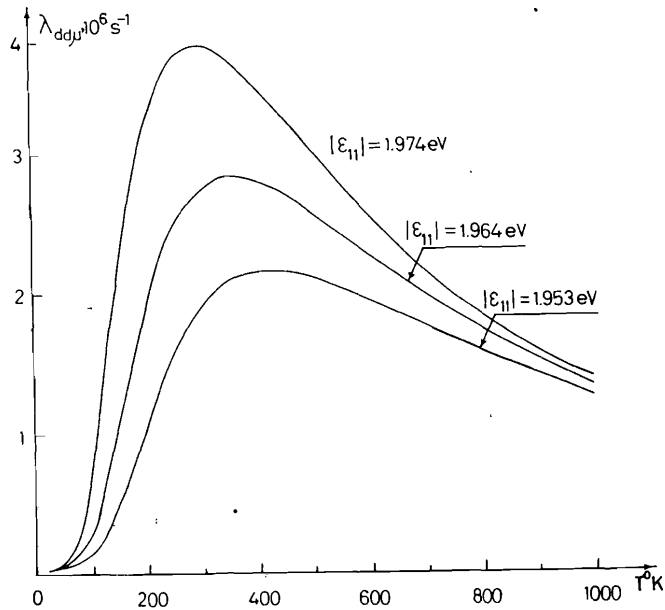


Fig. 11. The dependence of the shape of $\lambda_{dd\mu}(T)$ curve for reaction (1) on the value $|\epsilon_{11}|$ at $\tilde{\lambda}_F = 0.41 \cdot 10^9 \text{ s}^{-1}$.

In Fig. 12 there are presented spin-flip rates ($F = 3/2$) - ($F = 1/2$) (16) without (λ_{21}) and with ($\tilde{\lambda}_{21}$) formation and desintegration of $[(dd\mu)dee]$ complexes taken into account. It is seen that $\tilde{\lambda}_{21}$ exceeds λ_{21} by 20% at low temperatures. It is seen from the Table that λ_{21} ³⁴⁾ coincide with experiment⁴²⁾ better than $\tilde{\lambda}_{21}$. The reason for this disagreement is still unclear.

5. RESONANT FORMATION OF $dd\mu$ MOLECULES IN THE COLLISIONS $d\mu + DT$ AND $d\mu + DH$

The scheme of calculations¹³⁾ can be used directly for calculation of λ_F rates of $dd\mu$ molecules in reactions:

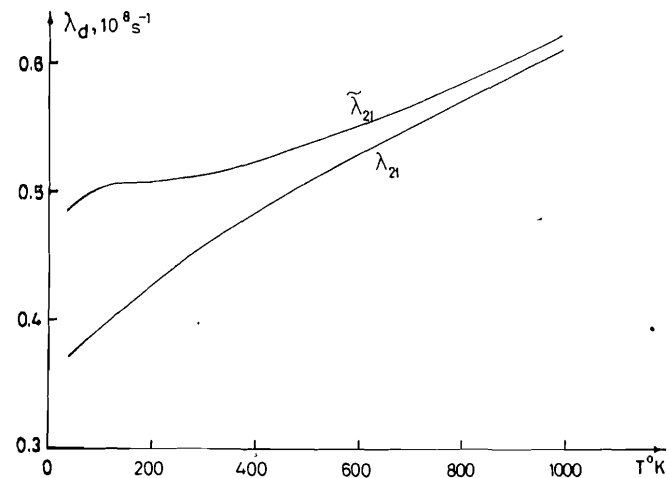
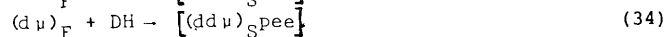


Fig. 12. Ratio λ_{FF} and $\tilde{\lambda}_{FF}$ (23) of spin flip in direct reaction (16) and with the back decay processes (4a) taken into account. The contribution from the latter process reaches $\sim 20\%$ at $T \sim 34$ K.

Table

References	$\tilde{\lambda}_{3/2} / \tilde{\lambda}_{1/2}$	$\tilde{\lambda}_{21}, 10^6 \text{ s}^{-1}$
Kimmel et al. ⁴³⁾	79.5 ± 8	37.4 ± 1.5
Present paper $\tilde{\lambda}_F = 0.41 \cdot 10^9 \text{ s}^{-1}$	73.3	48.6
$0.51 \cdot 10^9 \text{ s}^{-1}$	87.7	48.1

Resonance defects for these reactions equal, respectively:

for reaction (33) $\epsilon_0 = -0.1789 \text{ eV}$ ($\nu_F = 7$)

$\epsilon_0 = 0.0478 \text{ eV}$ ($\nu_F = 8$)

for reaction (34) $\epsilon_0 = -0.1078 \text{ eV}$ ($\nu_F = 5$)

$\epsilon_0 = 0.2151 \text{ eV}$ ($\nu_F = 6$).

The temperature dependences of partial resonant rates $\lambda_F(T)$ for reactions (1) and (34) are given in Fig. 13 and 14.

It is necessary to keep in mind that presented rates give only the general outline of the resonance processes (33) and (34), but for the description of some important peculiarities of them it is necessary to perform the careful consideration of the μCF kinetics in the mixtures $D\mu + D_2$ and $D_2 + T_2$.

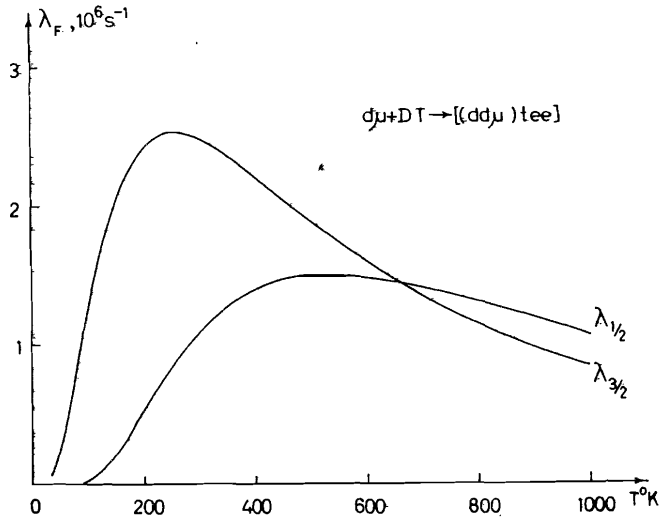
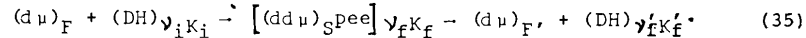


Fig. 13. Partial rates $\lambda_{dd\mu}(T)$ of complex $[(dd\mu)tee]$ formation in states $\gamma_f = 7$ and $\gamma_f = 8$ in reaction (33).

In particular, the deep minimum in the cross-section of elastic scattering $d\mu + p$ at $\epsilon \approx 1.6$ eV prevents from the fast thermalization of $d\mu$ atoms in the mixture $H_2 + D_2$. That in a turn will influence the processes of resonant formation of $dd\mu$ molecules in reaction (34) and leads to the spin-flip of $d\mu$ atoms in the chain of reactions



The detailed study of this depolarization mechanism of $d\mu$ atoms in $H_2 + D_2$ mixture may turn necessary for the consecutive description of the nuclear fusion in $pd\mu$ molecule studies experiments⁴⁶⁾, as well as for understanding of the well known but surprising results of the experiment⁴⁷⁾ devoted to the measurement of μ -capture rate by the deuterium nuclei in the $H_2 + D_2$ mixture.

6. CONCLUDING REMARKS

The presented calculations of the $dd\mu$ mesic molecule resonance formation rates crowns the program of studies outlined in paper³⁵⁾. The various characteristics of mesic molecules and mesic molecular complexes which are necessary for calculations, namely, nonrelativistic values of the $dd\mu$ molecule energy levels, their relativistic shifts including the vacuum polarization, nuclear recoil and nuclei form factors,

spin splitting and other relativistic effects, energy levels of mesic molecular complexes, the influence of a $dd\mu$ molecule finite size on the energy of the complexes rates of cascade transitions in $dd\mu$ molecule and of their nonresonance formation, etc., are also calculated without any free parameters. Only when calculating the fusion rate in $dd\mu$ mesic molecule the measured cross section of reaction $1(d, {}^3He)_n$ has been used. With this exception the presented calculations are the calculations *ab initio*.

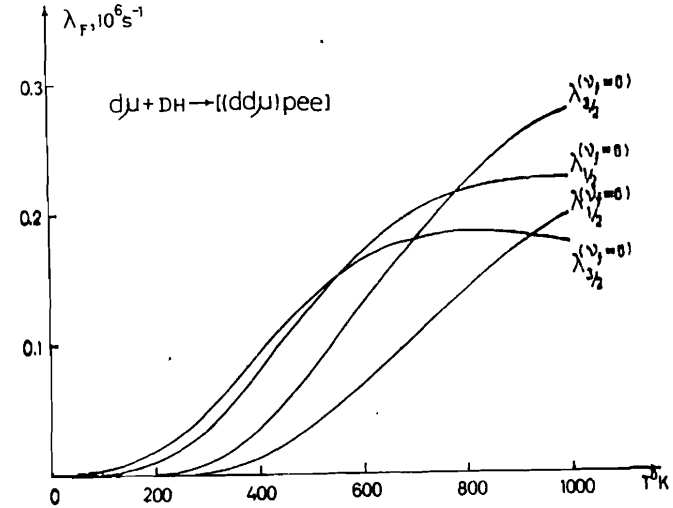


Fig. 14. Partial rates $\lambda_{dd\mu}(T)$ of complex $[(dd\mu)pee]$ formation in states $\gamma_f = 6$ and $\gamma_f = 8$ in reaction (34), total thermalization of $d\mu$ atoms being assumed.

The achieved agreement between theoretical and experimental values of $\lambda_{dd\mu}(T)$ evidences both the correctness of all the calculational scheme as a whole (the choice of wave functions, transition operator, method of averaging, etc.) and high accuracy of theoretical calculations of the $dd\mu$ molecules and $[(dd\mu)dee]$ complexes.

The performed investigation demonstrates a possibility and gives a theoretical basis for precise measurements of the binding energy of $dd\mu$ molecule ($J = 1, v = 1$) state with an accuracy of $10^{-3} - 10^{-4}$ eV, i.e. with a relative accuracy of $10^{-6} - 10^{-7}$ 44).

The analysis of experimental data in the framework of the developed calculation scheme (see Fig. 8) gives the following value for the binding energy of $dd\mu$ molecule bound state ($J = v = 1$):

$$|E_{11}| = 1.9643 \pm 0.0005 \text{ eV} \quad (36)$$

that is in a very good agreement with the theoretical value (30a). However, the presented analysis could be refined because in it the fine structure of $dd\mu$ mesic molecule energy levels (splitting ≈ 0.6 meV) having been not taken into account in the present analysis and the theoretical value λ_{nr} having been used. It is very desirable in this line to perform the new measurements of $\lambda_{dd\mu}$ in liquid deuterium.

The present calculation is a numerical realization of the theoretical scheme developed in papers¹¹⁻¹³ for the general case of resonance formation of $dd\mu$ and $dt\mu$ molecules. The achieved agreement between theory and experiment for the case of $dd\mu$ molecules allows one to use it with a confidence for a more complicated case of $dt\mu$ molecules. Corresponding calculations are being completed.

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Резонансное образование мезомолекул $dd\mu$

Вычислены скорости $\lambda_{dd\mu}(T)$ резонансного образования мезомолекул $dd\mu$ при столкновениях мезоатомов $d\mu$ с молекулами D_2 , HD и DT при температурах $10 \leq T \leq 1000$ K. Для реакции $d\mu + D_2 \rightarrow [(dd\mu)dee]$, вычисленные скорости $\lambda_{dd\mu}(T)$ хорошо согласуются с экспериментально измеренными на всем интервале изменения температуры дейтерия.

Работа выполнена в Лаборатории ядерных проблем ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1986

Faifman M.P. et al.

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Resonant Formation of $dd\mu$ Mesic Molecules

The rates $\lambda_{dd\mu}(T)$ of $dd\mu$ mesic molecule resonant formation in $d\mu$ mesic atom collision with molecules D_2 , HD and DT at temperatures $10 \leq T \leq 1000$ K are calculated. For reaction $d\mu + D_2 \rightarrow [(dd\mu)dee]$ the calculated rates $\lambda_{dd\mu}(T)$ are in good agreement with the experimentally measured ones for a wide range of deuterium temperature.

The investigation has been performed at the Laboratory of Nuclear Problems, JINR.

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