RESONANT MESOMOLECULE FORMATION

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Resonant formation of mesomolecules in the mixture of hydrogen isotopes plays a key role in muon catalyzed fusion [1]. In the standard theory the rate of this process is calculated in the first order of perturbation theory, and perturbation potential \( \hat{V} \) is calculated only in dipole approximation [4, 5]. The finite width of the resonance [6] and the anharmonism of the potential [7] contribute essentially to the result. In the formation of the mesomolecule the most important perturbation is the shift of the deuteron ion in respect to the centre of mass [4, 5]:

\[
\hat{V}(\hat{\rho}, \hat{R}) = U(|\hat{\rho} - \beta_2 \hat{R}|) - U(\rho) .
\]  

(1)

Here \( U(\rho) \) is the \( 1^1\Sigma_g \) term of the \( DX \) mesomolecule \((X = H, D, T)\); \( \hat{\rho} \) is the distance between \( d^+ \) and \( X^+ \) ions, \( \hat{R} \) is the distance between mesoatom and \( d^+ \) inside the mesomolecule, parameter \( \beta_2 \) (which depends on mass ratios) is \( \beta_2 \approx 0.5–0.6 \). The potential \( U(\rho) \) is calculated in Born-Oppenheimer approximation (infinite mass of nuclei) and corrections to the finite nuclei mass are known to be small [5].

Dipole interaction is only the first term of the multipole expansion for potential of Eq. (1). Meanwhile, the expansion parameter appears to be not a small number. Indeed, this parameter is equal to the ratio of \( \beta_2 R \) to vibrational amplitude \( a = (M\Omega)^{-1/2} \) which is \( \beta_2 R(M\Omega)^{1/2} \approx 0.2–0.35 \). For this reason the next (quadrupole) term of the multipole expansion changes formation rate significantly.

In Ref. [5] we developed a method which does not make use of the multipole expansion — the potential of Eq. (1) is taken into account exactly. We do not need the wave function of the mesomolecule, it is enough to know only its asymptotics. This is due to the fact that in the loosely bound mesomolecules \( dy\mu \) \((v = J = 1; y = d, t)\) the mesoatom \((y\mu)_1\) is located in the average at large distances from the deuteron and hence one can neglect their interaction. Only exact binding energy \( \tilde{E}_{11} \) and constant \( C_{dy\mu} \) which enters the asymptotics of the wave function [4] are required for the calculation of formation rate. At the moment the binding energy \( \tilde{E}_{11} \) is known with accuracy of the order of 1 meV. The most accurate values of the constant \( C_{dy\mu} \) are obtained in Ref. [14].

On the basis of the method developed in [5] we elaborated the computer code designed for the calculation of mesomolecule formation rates [14]. The subroutine MATEL of the code solves the Schrödinger equation with potential \( U(\rho) \) for \( DX \)-molecules and mesomolecular complexes (MMC). It determines the energy levels with different vibrational \((v)\) and rotational \((K)\) quantum numbers and also calculates their wave functions. On the next stage the code calculates the matrix elements \( \langle \nu_i, K_i, F | \hat{V} | \nu_f, K_f, S \rangle \) where \( F \) is the spin of the original mesoatom and \( S \) is the spin of the mesomolecule. We need to know something like 200 matrix elements and their dependence on the energy. The code calculates also the position of all resonances below and above the threshold. Next subroutine (SPEED) sums up all Breit-Wigner resonance contributions to the probability of mesomolecular complex formation \( \lambda_{F \rightarrow S}^{F \rightarrow S} \) and translates them from the centre-of-mass frame to the lab. one:

\[
\lambda_{F \rightarrow S}^{F \rightarrow S}(E_L, T) = \int dE_c \frac{\lambda_{F \rightarrow S}^{F \rightarrow S}(E_c) F(E_c \rightarrow E_L, T)}{E_c}.
\]  

(2)

Here the function \( F(E_c \rightarrow E_L, T) \), which takes into account the motion of gas molecules, leads to the Doppler broadening of resonances with the width \( \Delta_{DD} = (4E_{QL} T/A)^{1/2} \). In the spirit of the Bohr theory of compound nuclei, we consider the decay of mesomolecular complex as being independent of the channel by which it was formed. Therefore in order to obtain the rate of formation we have to multiply \( \lambda_{F \rightarrow S}^{F \rightarrow S}(E_L, T) \) by the ratio \( \Gamma_f/\Gamma_t \) where \( \Gamma_t \) is the total and \( \Gamma_f \) is the partial reaction width \((\Gamma_f \rightarrow F \rightarrow F^* \rightarrow \text{back decay}, \text{and so on})\). One has to average the values of \( \lambda_{F}^{F}(E_L, T) \) over the spectrum of mesoatoms \( f(E_L) \).

For the mesoatom spin \( F = 0 \) we calculated the rates of resonant formation and fusion in reactions \((t\mu)^0 + D_2 \) and \((t\mu)^0 + DH \) at moderate gas density, when one can neglect rescattering of the MMC on the gas molecules [12]. In this case the decay of the MMC occurs from the state where it was formed. At small \( T \) the fusion rate is determined by underthreshold resonance with the energy \( E_r = -14 \) meV:

\[
\lambda_f^0(T) = B \frac{\Gamma_f}{E_f^2} \left| \langle 0, 0, 0 | \hat{V} | 2, 1, 1 \rangle \right|^2,
\]  

(3)

that corresponds to the transition \( \nu = 0 \rightarrow 2, K = 0 \rightarrow 1 \). Here \( B = N_0 a_0 (\hbar c)^2/m_\mu = 0.7085 \cdot 10^{16} \text{eV}/\text{a.u.} \), \( \Gamma_f = 0.65 \) meV and \( |\langle 0, 0 | \hat{V} | 2, 1 \rangle|^2 = 0.60 \cdot 10^{-8} \) a.u. [13]. According to Eq. (3), the rate \( \lambda_f^0 \) does not depend on the temperature \( T \). Account for other resonances leads to small variations of \( \lambda_f^0 \) with temperature (see Fig. 1). This should be compared with the strong
temperature dependence for the rate of $dd\mu$ formation (Fig. 2). Let us notice that, if one takes account of resonances above the threshold only (dashed line in Fig. 1), then the rate of formation restores its strong temperature dependence. Also let us point out that dipole approximation overestimates the matrix element of Eq. (1) more than 3 times [7, 12].

We plot on the Fig. 1 the single known experimental point. For the first time without any fitting parameter we reach the agreement with data on the level of 15% [13]. The disagreement of previous models with data we reach the agreement with data on the level of 15% [13]. The disagreement of previous models with data we reach the agreement with data on the level of 15% [13]. The disagreement of previous models with data we reach the agreement with data on the level of 15% [13]. The disagreement of previous models with data we reach the agreement with data on the level of 15% [13].

The other limiting case when the collision width is much larger than all other widths takes place for the resonant formation of $dd\mu$-mesomolecules in $D_2$-gas [14]. After formation of the mesomolecular complex in the state with rotational quantum number $K_f$ it can be changed due to collisions to some new $K'_f$. It is enough time to reach the equilibrium Boltzmann distribution in rotational quantum numbers $K'_f$. For this reason the back decay of the mesomolecular complex takes place independently of the value $K_f$ with which it was formed. Rates of the $dd\mu$ formation with subsequent fusion for two values of the mesomolecule spin $F = 1/2, 3/2$ are presented on Fig. 2 [15]. They are considerably less than for $dt\mu$ case. This fact is a consequence of the sharp decrease of transition matrix elements with the energy of the bound state ($\bar{\varepsilon} = -0.632$ eV for $dt\mu$ and $\bar{\varepsilon} = -1.966$ eV for $dd\mu$).

The rate $\lambda^{3/2}_f(T)$ depends weakly on $T$ owing to the strong Doppler broadening of the $K = 0 \rightarrow 1$ resonance with small positive resonance energy $E^r_L = 4.2$ meV. On the contrary, the rate $\lambda^{1/2}_f(T) \approx 15$ (which is mainly due to the far resonances with positive energy ) depends on the temperature rather strongly.

At Fig. 2 we plot also recent experimental data of Ref. [16] which were obtained for the non-equilibrium mixture of ortho- and para-deuterium in the ratio of 2 to 1 (independent of $T$). In such a non-equilibrium gas due to the extra inelastic acceleration of mesoatoms on para-deuteroniums (which are excited by 7.4 meV), the mesoatom spectrum $f(E_L)$ below $\approx 70$ K should decrease with $E_L$ considerably faster than the equilibrium Maxwell spectrum $f_M(E_L)$. Meanwhile in our paper [15] the fusion rate of Eq. (2) was averaged over $f_M(E_L)$ spectrum. For this reason it makes sense to compare the results of Ref. [15] with data only at temperatures $T > 70$ K. The calculation (taking into account non-resonant formation of $dd\mu$ [15]) based on purely theoretical values of all quantities, reproduces the data on the level of 10%. The accuracy of our calculations is limited mainly by insufficient accuracy of the estimation of fusion width $\Gamma_f = 460(70) \mu$ sec$^{-1}$ [16]. If one uses $\Gamma_f$ as a single fitting parameter it is
Table 1:

| Source        | $|C_{matr}|^2$ | $\Gamma_f, \mu\text{sec}^{-1}$ |
|---------------|-------------|-----------------------------|
| IAE, 1993     | 0.62(13)    | 337(40)                     |
| IAE, 2001     | 0.56(3)     | 407(20)                     |
| PNPI, 1998    | 1           | 400(46)                     |
| PNPI, 2001    | 1           | 397(40)                     |

possible to achieve an excellent relative accuracy of 3% for $\lambda_f^{3/2}(T)$ and 4% for $\lambda_f^{1/2}(T)$. The best fit corresponds to $\Gamma_f = 397(40) \mu\text{sec}^{-1}$. This value lies within the errors of theoretical estimate.

Let us compare our results with calculations of Refs. [16, 19]. These calculations coincide with the data only if one introduces an additional fitting parameter $|C_{matr}|^2 = 0.56$ which is used as factor to multiply all transition matrix elements squared. In other words, this approach overestimates $\lambda_f^T$ by a factor of 1.8 (see Table 1). In our calculations this fitting parameter is absent. The discrepancy between the data and our calculations in the region of $T < 70 K$ (up to 14% at $T = 28.3 K$) can be, in our opinion, attributed to the distortion of the spectrum $f(E_L)$ due to the mesatom acceleration in non-equilibrium medium. This new effect awaits for calculation.

Thus the theory of the mesomolecule resonant formation [2]–[4] by Vesman mechanism developed in Refs. [2]–[4] and improved significantly in Refs. [7, 11, 12] describes now the data with sufficient accuracy (see Figs. 1,2).

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