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FORMATION OF HYDROGEN MESIC MOLECULES

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An effective mechanism is described for the formation of hydrogen mesic molecules. It consists of dipole transitions from S-wave repulsive states to the $K = 1$ rotational level with energy transfer to a conversion electron. The calculations give $1.5 \times 10^6\ \text{sec}^{-1}$ for the probability of formation of a mesic molecule $(pp)^+_\mu$ in liquid hydrogen. The process under consideration is relevant to the meson catalysis of the $p + d$ nuclear reaction as well as to the $\mu^- + p \rightarrow n + \nu$ process in liquid hydrogen.

THE formation of μ-mesic hydrogen molecules is of interest in the theory of μ-mesonic catalysis[1] of nuclear reactions for two reasons. First, the yield of the nuclear reaction depends on the probability of formation of mesic molecules since the mesic molecules are the initial stage for the nuclear reaction. Second, formation of the mesic molecule $(pp)^+_\mu$ (as well as the decay of the μ-meson) depletes the supply of μ mesons available for catalysing the nuclear reactions; this explains the dependence of the reaction yield on the concentration of deuterium. The formation of $(pp)^+_\mu$ is also of interest in the study of the elementary interaction $(pn\mu\nu)$, which is one of the more important problems in the theory of weak interactions. It has been shown[2] that the probability of formation of mesic molecules can be considerably increased by the resonance phenomena if the transition is from an initial state (in which the meson function is Σ_g and the nuclei are in a relative S state) to an excited vibrational level of the mesic molecule with $K = 0$ (a 0-0 transition). However, even in this case the probability of formation of mesic molecules during the μ-meson lifetime is not more than 30 to 40%.*

A rather effective mechanism, as was already noted,[4] for the formation of mesic molecules from various nuclei is provided by electric dipole transitions to the rotational $K = 1$ level accompanied by electron conversion.

The dipole moment of the mesic ion relative to its center of mass (this is necessary since the total charge is different from zero) is

$$\mathbf{d} = -\frac{e}{2}\left\{\frac{M_2 - M_1}{M_2 + M_1}\mathbf{R} + (\mathbf{r}_1 + \mathbf{r}_2)\right\}, \tag{1}$$

where $\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$, $\mathbf{r}_1 = \mathbf{r} - \mathbf{R}_1$, $\mathbf{r}_2 = \mathbf{r} - \mathbf{R}_2$; $\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{r}$ are the coordinates of the nuclei and the μ meson, M_2 and M_1 are the nuclear masses.

The computation of the probability of formation of mesic molecules with transfer of the binding energy to the electron of the hydrogen atom is analogous to the computation of the probability of internal conversion in nuclear transitions since the dimension of a mesic molecule is small compared to atomic dimensions. Taking the exact hydrogenic Coulomb functions for the electron wave function in the initial and final states (neglecting the fact that the mesic atom combines with a proton, which in turn is bound in a normal H_2 molecule) and integrating over the electron coordinates and the direction of electron emission, we obtain for the probability of formation of the mesic molecule

$$W = \frac{16}{3}(Na_e^3)\left(\frac{m_e}{m_\mu}\right)^5 \eta\zeta^2 \frac{e}{a_e\hbar} \sum_{M_K} \left| \int \Psi^{(f)*}_{\text{mol}} \mathbf{d} \Psi^{(i)}_{\text{mol}} (d\mathbf{R})(d\mathbf{r}) \right|^2, \tag{2}$$

where

$$\eta = \frac{e^2}{\hbar v_e}, \quad \zeta = \left[\frac{2\pi\eta}{(1 - e^{-2\pi\eta})(1 + \eta^2)}\right]^{1/2} \exp\{-2\eta \cot^{-1} \eta\},$$

$N = 4.2 \times 10^{22}$ is the number of nuclei in cm^3, a_e the Bohr radius, and v_e the electron velocity. The integral in (2) is written in mesic atom units ($e = 1$,

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*We note that in reference 3 the probability for formation of mesic molecules in 0 – 0 transitions is overestimated by three orders of magnitude in comparison with reference 2. In calculating the Coulomb interaction (D.6) Jackson[3] stopped at the first term, independent of the mesic molecule coordinates, which would give a transition probability of exactly zero if the orthogonality of the initial and final state wave functions were taken into account. The calculation (D.6) in higher orders would give, as it should for a 0 – 0 transition, $\Sigma e_i r_i^2$.

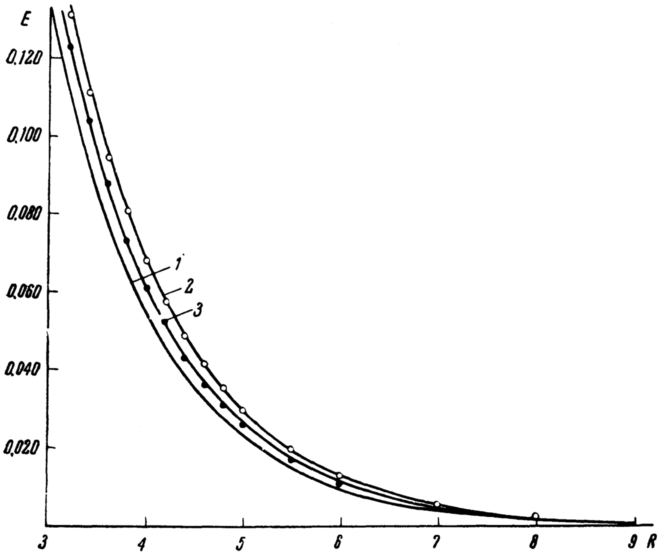

FIG. 1. The potential $E_u(R)$ in the repulsive Σ_u state (from reference 5) – curve 1. The effective potential in the Σ_u state including the corrections (computed in reference 6) due to nuclear motion, for protons – curve 2, for deuterons – curve 3. Values of the approximating exponential: ○ – $V_u = 1.850\ e^{1.826R}$ (for protons), ● – $V_u = 2.017\ e^{-0.873R}$ (for deuterons). (E and R in mesic atom units).

$\hbar = 1$, $m_\mu = 1$) assuming that $\Psi^{(i)}_{\mathrm{mol}}$ is normalized to unit probability density in the incident wave. The summation in (2) is over all possible final states of the mesic molecule.

The first term in the expression (1) for the dipole moment (it is nonzero for different nuclei only, e.g., for the $(pd)^+_\mu$ mesic molecule) takes part only in transitions in which the parity of the meson function is unchanged ($\Sigma_g \to \Sigma_g$). The second term, whose role in conversion has not been considered previously,* is relevant for different [$(pd)^+_\mu$, $(dt)^+_\mu$, $(pt)^+_\mu$] as well as for identical nuclei [$(pp)^+_\mu$, $(dd)^+_\mu$, $(tt)^+_\mu$] and gives rise to transitions of the type $\Sigma_u \to \Sigma_g$.

An approximate analytic expression may be given for $\Psi^{(i)}_{\mathrm{mol}}$ and $\Psi^{(f)}_{\mathrm{mol}}$ in the case of identical nuclei.

The initial state wave function, corresponding to a dissociated mesic molecule, is of the form

$$\Psi'^{(i)}_{\mathrm{mol}} = \frac{f(R)}{R} \Sigma_u(R, r_1, r_2). \qquad (3)$$

The relative motion of the nuclei is described by an S wave, since formation of mesic molecules takes place only after mesic atoms have been slowed down to thermal velocities. The function f(R) is determined from the Schrödinger equation with a known repulsive potential $E_u(R)$. The numerical values of $E_u(R)$,[5] including corrections ΔE_u which take into account the motion of the nuclei accurate to terms of order $\sim m_\mu/M$,[6] may be approximated by an exponential in the region R of interest in this problem (see Fig. 1):

$$V_u = E_u(R) + \Delta E_u(R) \simeq B \exp(-\beta R). \qquad (4)$$

The Schrödinger equation with the potential (4) may be transformed into the Bessel equation by a change of variable. The function f(R) (including normalization) for the energy of relative motion tending to zero is of the form

$$f(R) = \frac{2}{\beta} K_0\left(\frac{2\sqrt{MB}}{\beta} e^{-\beta R/2}\right) \qquad (5)$$

[$K_0(z)$ is the Bessel function of the third kind, M is the mass of one of the nuclei]. f(R) falls off rapidly for small R, and for $R \geq 8$ it goes over into the wave function corresponding to free motion.

The mesic molecule final state wave function, corresponding to the rotational K = 1 level, has the form

$$\Psi'^{(f)}_{\mathrm{mol}} = \frac{g(R)}{R} Y_{1, M_K}(\theta, \varphi) \Sigma_g(R, r_1, r_2). \qquad (6)$$

The numerical values of the attractive potential $E_g(R)$ (taken from reference 5) together with the corrections ΔE_g (calculated in reference 6) and the centrifugal potential are well approximated near the minimum R_e by the Morse function (Fig. 2)

$$V_g = E_g(R) + \Delta E_g(R) + \frac{2}{MR^2} \simeq D \times [e^{-2\alpha(R-R_e)} - 2e^{-\alpha(R-R_e)}]. \qquad (7)$$

The solution of the Schrödinger equation for the potential (7) gives, in the case of the mesic molecule $(pp)^+_\mu$, only one K = 1 level with an energy $E \simeq -109$ ev. The corresponding wave function is

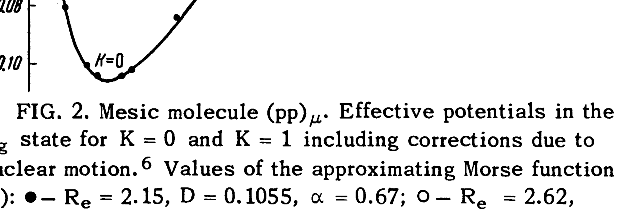

FIG. 2. Mesic molecule $(pp)_\mu$. Effective potentials in the Σ_g state for K = 0 and K = 1 including corrections due to nuclear motion.[6] Values of the approximating Morse function (7): ● – $R_e = 2.15$, $D = 0.1055$, $\alpha = 0.67$; ○ – $R_e = 2.62$, $D = 0.065$, $\alpha = 0.69$, (E and R in mesic atom units).

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*It has been mentioned in radiative transitions.[2]

of the form

$$g(R) = [\alpha/\Gamma(2s)]^{1/2} e^{-\xi/2} \xi^s, \tag{8}$$

where

$$\xi = \frac{2\sqrt{MD}}{\alpha} e^{-\alpha(R-R_e)}; \quad s = \frac{\sqrt{-ME}}{\alpha}.$$

The deviations of the interaction potential from the Morse function (7) at large and small R do not substantially affect the magnitude of the energy level since in these regions of R the wave function is exponentially small.[*] The influence of these deviations on the form of the wave function at large R is also insignificant since for $R \gtrsim 5$, $e^{-\xi/2}$ is already $\simeq 1$, and the wave function corresponds to free motion: $g(R) \sim \exp\{-R\sqrt{-ME}\}$.

Since f(R) falls off rapidly for small R only the region $R > 4$ is important in the integral (2). The following approximation is good enough for such R[†]

$$\Sigma_{g,u} = [2\pi(1 \pm S)]^{-1/2} (e^{-r_1} \pm e^{-r_2}), \tag{9}$$

where

$$S = \frac{1}{\pi} \int e^{-r_1} e^{-r_2} d\tau = \left(1 + R + \frac{R^2}{3}\right) e^{-R}.$$

Integration in (2) over the μ-meson coordinates then gives for the dipole moment matrix element

$$\langle \mathbf{d} \rangle_{gu} = -(1 - S^2)^{-1/2} \mathbf{R}/2 \simeq -\mathbf{R}/2.$$

The integration in (2) over the angles of the mesic molecule and the summation over the orbital angular-momentum projections M_K is simple to carry out. The remaining integral over the radial functions is computed easily with the help of (3), (5), (6), and (8).[‡] By multiplying (2) by $\frac{3}{4}$, which represents the probability that the spin wave function of the protons is in the state Σ_u, $K = 0$ ("ortho-mesic-hydrogen"), we finally obtain for the probability of formation of mesic molecules $(pp)^+_\mu$

$$W \approx 1.5 \cdot 10^6 \text{ sec}^{-1}$$

(i.e., three times the probability for the decay $\mu \rightarrow e + \nu + \tilde{\nu}$). Consequently the formation of $(pp)^+_\mu$ must be considered in the discussion of the dependence of the rate of the nuclear reaction $p + d \rightarrow He^3$ on the concentration of deuterium. The qualitative agreement with experiment obtained in reference 4 is, however, not upset since the cross section for μ-meson capture by deuterons[7] turns out to be larger than was assumed in reference 4.[*] The probability of formation of a deuterium mesic atom in natural hydrogen and in hydrogen containing 0.3% deuterium was found experimentally[1] to be 24 and 80% respectively (the calculation gives 44 and 94%). Apparently the probability of formation of $(pp)^+_\mu$ is even greater, or (and) the probability of the exchange $p_\mu + d \rightarrow d_\mu + p$ is less than our calculations indicate.

The probability of formation of the mesic molecule $(pd)^+_\mu$ will be substantially larger than the probability of formation of $(pp)^+_\mu$ due to transitions Σ_g, $K = 0 \rightarrow \Sigma_g$, $K = 1$, caused by the first term in the expression (1) for the dipole moment. Furthermore, the resonance[2] may play a significant role if the mesic molecule $(pd)^+_\mu$ has a vibrational level close to the energy of the $p + d_\mu$ system infinitely separated; it could lead to an increase in the amplitude of the wave function near the nuclei. (The resonance plays no role in the repulsive Σ_u state.)

It has been shown[8] that, given a quantity of deuterium sufficient for all mesons to form d_μ atoms, the number of nuclear reactions would be 0.36 ± 0.06 per meson. The measured rate equals $0.36 = W_1W_2/(W_1 + W)(W_2 + W)$ where W_2 is the probability of formation of the molecule, W_1 the probability of a nuclear reaction in the molecule and W the probability of the decay of a μ-meson per second. On the other hand, the time dependence of the nuclear reaction measured in reference 8 was given by the difference of two exponentials $[\exp(-\lambda_2 t) - \exp(-\lambda_1 t)]$ where $\lambda_1 = W_1 + W$, $\lambda_2 = W_2 + W$. The experiment gives $0.19 \times 10^6 < \lambda_1 < 0.88 \times 10^6$; $0.55 \times 10^6 < \lambda_2 < 2 \times 10^7$. Only $W_2 > 1.4 \times 10^6$ and $0.24 \times 10^6 < W_1 < 0.43 \times 10^6$ are consistent with the observed reaction probability, which is in agreement with our calculations and other experiments. (The second solution $W_1 > 1.4 \times 10^6$ and $0.24 \times 10^6 < W_2 < 0.43 \times 10^6$ is unreasonable.)

The formation of mesic molecules changes the conclusions drawn in reference 9 on total polarization of neutrons formed in the process $\mu + p \rightarrow n + \nu$, since in liquid hydrogen this process proceeds to a large extent from the mesic molecule state. In the mesic molecule $(pp)^+_\mu$ the $K = 1$

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[*] The level shift caused by these deviations may be calculated numerically using perturbation theory: $\Delta E = \int g^2(R)(V_g - V_{Morse})\,dR$.

[†] We recall that mesic atom units are being used.

[‡] We note that the integrand $f(R)\,Rg(R)$ has, in the case of $(pp)^+\mu$, a maximum at $R \approx 8.5$; a comparatively good result is thus obtained by replacing f(R) and g(R) by their asymptotic expressions for large R, and the integration can then be carried out analytically.

[*] In the final result in reference 7 there is a misprint; the actual capture cross section is $\sigma \approx 6\pi a_\mu^2 k_0/k_1$.

state is possible only for a parallel spin orientation $I = 1$ for the two protons ("ortho-mesic-hydrogen"). Owing to fast transitions to the lowest hyperfine-structure state[9] the initial state of the mesic atom is $F = 0$ and the mesic molecules $(pp)^+_\mu$ are formed in the $K = 1$ state with a total spin $J = 1/2$, so that the μ-meson spin is antiparallel to both protons. Although the transition probability from the metastable "ortho-mesic-hydrogen" state into "para-mesic-hydrogen" is small, already in the state with parallel spin protons $I = 1$ and antiparallel μ-meson spin $(J = 1/2)$ we get the product $\mathbf{i}_1 \cdot \mathbf{s} + \mathbf{i}_2 \cdot \mathbf{s} = -1$ ($\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{s}$ are the protons and μ-meson spins respectively), while in the mesic atom we get $\mathbf{i}_1 \cdot \mathbf{s} = -3/4$ for $F = 0$ and $\mathbf{i}_1 \cdot \mathbf{s} = 1/4$ for $F = 1$. Thus the mesic molecule in the ortho-state with spin $J = 1/2$ is equivalent to a mixture of atoms consisting of 75% $(F = 0)$ and 25% $(F = 1)$. In spite of this, owing to the interaction between the rotation of the molecule and the spins, the $K = 1$, $J = 1/2$ state is partially transformed into the $K = 1$, $J = 3/2$ state (corresponding to a pure $F = 1$ state). The process $\mu^- + p \rightarrow n + \nu$ in the $F = 0$ state without admixtures of $F = 1$ can be observed at hydrogen densities 20 or more times smaller than the density of liquid hydrogen.* At that the transition probability in $F = 0$ state remains sufficiently large (10^9 sec^{-1}) and the probability of formation of mesic molecules during the meson lifetime will be 15% or less. The influence of the relative proton — μ-meson spin orientation on the process $\mu + p \rightarrow n + \nu$ will be discussed in a subsequent note.

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*Gaseous hydrogen of that density has a pressure of 40 atmos at room temperature.

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