

Catalysis of nuclear reactions in hydrogen in a strong magnetic field

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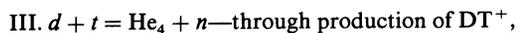
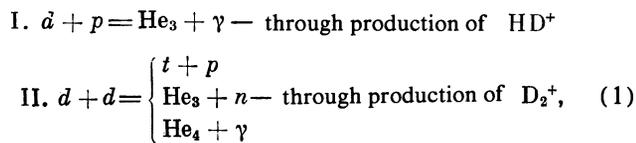
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In the strong magnetic field $B = 10^{12}$ – 10^{13} G typical of the surface of a neutron star, the thickness of the barrier separating the nuclei in molecules decreases, and its transmission increases substantially. This circumstance is a cause of the acceleration of nuclear reactions. The catalysis is determined mainly by the properties of the molecules and the value of the magnetic field. In this article we carry out calculations of the probabilities of nuclear reactions in a strong magnetic field occurring in the molecular ions HD^+ , D_2^+ , and DT^+ . It is shown that on change of the field strength from 10^{12} to 10^{13} G the nuclear-reaction probabilities increase by ten orders of magnitude. The influence of the vibrational-rotational state from which tunneling occurs into the nuclear potential well on the reaction probabilities is taken into account.

1. INTRODUCTION

As is shown by calculations of the structure of hydrogen and helium atoms¹ and of the molecular ion of hydrogen,²⁻⁴ all placed in a strong magnetic field $B = 10^{12}$ – 10^{13} G typical of the surface of a neutron star, the ionization and dissociation energies in such magnetic fields increase substantially, reaching tens and hundreds of electron volts. The same thing can take place in a neutral hydrogen molecule H_2 and other molecules. In addition, the internuclear distances in molecules decrease significantly in the direction of the magnetic field. The decrease of the thicknesses of the potential barriers separating the nuclei in molecules leads to an increase of the coefficient of tunneling through the barrier. In particular, in a previous article⁵ we showed that on change of the magnetic field strength from 10^{11} to 10^{13} G the internuclear distance in H_2^+ decreases from 0.33 to 0.086 Å. Here the transmission coefficient rises by sixteen orders of magnitude. In this way the magnetic field facilitates the penetration of nuclei into the nuclear potential well and consequently can catalyze a nuclear reaction. This effect is analogous to the muon catalysis of nuclear reactions (see for example Ref. 6). The magnitude of the effect considered is determined mainly by the properties of the molecules (i.e., the characteristics of the potential barriers) and by the magnetic field strength. The temperature of the gas affects the reaction probability only in the sense that it determines the populations of the vibrational-rotational levels, while the barrier penetrability depends on which of these levels the molecule or molecular ion occupies.

The purpose of the present work consists of estimating the probabilities of the following nuclear reactions



which can occur in a hydrogenous medium in a strong magnetic field.

2. NUCLEAR REACTION PROBABILITIES

In calculation of the probabilities of the nuclear reactions under discussion in a strong magnetic field we shall follow the same procedure that was used in calculations of similar quantities for muon catalysis.⁶ The probability of a nuclear reaction can be defined as

$$P_i(n, B) = C_i \xi_i(n, B), \quad i = \text{I, II, III.} \quad (2)$$

In this formula n is the set of quantum numbers characterizing the nuclear motions in the molecular ion. The factor C_i is the rate constant of the nuclear reaction between nuclei which are within a nuclear potential well. The second factor $\xi_i(n, B)$ is the square of the modulus of the wave function $\Psi_n^{(i)}$ that describes the motion of the nuclei in the molecular ion and is defined at the boundary of the nuclear potential well. In other words, the quantity ξ_i is the probability that the nuclei are at such a distance from each other that their interaction is determined not by Coulomb forces, but by nuclear forces. In cylindrical coordinates, which will be used everywhere below (the z axis if directed along the magnetic field), this factor is given by the formula

$$\xi_i(n, B) = \int_0^{2\pi} |\Psi_n^{(i)}(\rho = \rho_n, \varphi, z = z_n)|^2 d\varphi, \quad (3)$$

in which ρ_n and z_n are the dimensions of the potential well of the nucleus (which is formed as the result of the reaction) in the transverse and longitudinal directions relative to the magnetic field direction. It must be mentioned at once that the magnetic fields discussed have practically no effect on the nature of the nuclear potential well, which as is customary is assumed everywhere below to be spherically symmetric. We shall assume also that the radial dependence of the interaction potential at distances of the order of nuclear distances has a rectangular form, and the dimensions of the well are

$$\rho_n = z_n \approx 1.2 \cdot 10^{-13} A^{1/2},$$

where A is the mass number of the nucleus. Integration over the azimuthal angle in Eq. (3) permits one to take into ac-

count the axial symmetry of the system in the presence of a magnetic field.

The rate constants of the reaction I–III under discussion are given in Ref. 6 and are respectively

$$C_I = 1.3 \cdot 10^{-22} \text{ cm}^3/\text{sec}, C_{II} = 2.0 \cdot 10^{-16} \text{ cm}^3/\text{sec},$$

$$C_{III} = 2.0 \cdot 10^{-14} \text{ cm}^3/\text{sec}. \quad (4)$$

Note that the reaction $d + d = \text{He}_4 + \gamma$ is highly improbable as the result of the smallness of the electromagnetic interaction, and also for reasons of isotopic invariance. The rate constant C_{II} is the combined value for the two remaining channels of reaction II.

Therefore in calculation of the probabilities P_i it is necessary to calculate the values of $|\Psi_n^{(i)}(\rho_n, \varphi, z_n)|^2$ as a function of the magnetic field for the molecular ions HD^+ , D_2^+ , and DT^+ .

The further discussion is based on the results of Refs 4 and 7. In the first of these articles we calculated the potential energy surface of the molecular ion H_2^+ in a strong magnetic field, and in the second we discussed in detail the structure of the vibrational-rotational spectrum and the wave functions which describe the vibrational-rotational motion of the nuclei of this ion. For estimates we shall use the adiabatic approximation, i.e., we shall assume that the potential surface for the ions HD^+ , D_2^+ , and DT^+ is the same as for H_2^+ . Then all of the results which apply to the structure of the spectrum and the wave function describing the motion of the nuclei can be obtained from the data for H_2^+ by a simple recalculation taking into account the differences in the reduced nuclear masses of the molecular ion considered. In the formulas used below, the index i which relates the molecular parameters to a specific isotope replacement configuration HD^+ , D_2^+ , or DT^+ has been omitted for simplicity of notation, which should not lead to any confusion in the formulas.

The potential surface of the H_2^+ ion in a strong magnetic field is axially symmetric. Numerical calculations of this surface for various values of field strength⁴ have shown that in the region of the molecular potential well it can be approximately described by the function⁷

$$U(\rho, z) = V(\rho) + W(z), \quad (5)$$

where

$$V(\rho) = A\rho^2, \quad (6)$$

$$W(z) = -E_a + D_e [\text{sh}^4(\alpha_p z_e) / \text{sh}^2(\alpha_p z) - \text{ch}^4(\alpha_p z_e) / \text{ch}^2(\alpha_p z)]. \quad (7)$$

In these formulas E_a is the energy of the hydrogen atom in the ground state (the energy of the tightly bound ground state in a strong magnetic field); D_e is the H_2^+ dissociation energy; α_p , z_e , and A are approximation parameters determined from the condition of best matching of Eq. (5) with the calculated potential surface (Table I). In Ref. 7 we showed that the vibrational-rotational spectrum of H_2^+ in a strong magnetic field consists of several systems of bands of vibrational levels, each of which corresponds to a definite rotational state. The vibrational levels (vibrations of the nuclei along the internuclear axis) are characterized by a quantum number v . The rotational states (precession of the internuclear axis around the direction of the magnetic field) are characterized by a quantum number N (the Landau level number) and by the projection Λ of the angular momentum on the direction of the magnetic field. The expression for the energy of a vibrational-rotational level (without taking into account the interaction of the nuclear spins with the magnetic field) can be represented approximately in the form⁷

$$\epsilon_{N\Lambda v} = -E_a - D_e + \hbar\omega_B \alpha_B^{1/2} [N + (1 + |\Lambda|)/2 - \Lambda/2\alpha_B^{1/2}] + \hbar\omega_e (v + 1/2) [1 - x_e (v + 1/2)]. \quad (8)$$

Here we have used the following notation:

$$\omega_B = eB/\mu c, \quad \alpha_B = 1 + 8A/\mu\omega_B^2, \quad (9)$$

$$\hbar\omega_e = 2\hbar^2\alpha_p^2/\mu x_e,$$

$$x_e = \{ [1/4 + (2\mu D_e/\hbar^2\alpha_p^2) \text{ch}^4(\alpha_p z_e)]^{1/2} - [1/4 + (2\mu D_e/\hbar^2\alpha_p^2) \text{sh}^4(\alpha_p z_e)]^{1/2} \}^{-1}, \quad (10)$$

and μ is the reduced mass of the nuclei.

The wave function describing the vibrational-rotational state of a molecular ion in the zero approximation of perturbation theory is

$$\Psi_{N\Lambda v}(\rho, \varphi, z) = (2\pi)^{-1/2} e^{-i\Lambda\varphi} \chi_{N\Lambda}(\rho) \eta_v(z). \quad (11)$$

In this formula $\chi_{N\Lambda}(\rho)$ and $\eta_v(z)$ are the wave functions of the transverse motion (i.e., rotational motion) and the vibrational motion of the nuclei. The wave function of the transverse motion is given by the expression⁸

$$\chi_{N\Lambda}(\rho) = G_{N\Lambda} e^{-x/2} x^{|\Lambda|/2} {}_1F_1(-N, 1 + |\Lambda|, x), \quad (12)$$

where

$$x = \frac{\alpha_B^{1/2}}{2} \left(\frac{\rho}{a_B} \right)^2, \quad a_B = \left(\frac{\hbar}{\mu\omega_B} \right)^{1/2},$$

$$G_{N\Lambda} = \frac{\alpha_B^{1/4}}{a_B} \frac{1}{|\Lambda|!} \left[\frac{(N + |\Lambda|)!}{N!} \right]^{1/2}. \quad (13)$$

TABLE I. Values of parameters approximating the potential surface of H_2^+ .

B, G	10^{12}	$3 \cdot 10^{12}$	$5 \cdot 10^{12}$	10^{13}
D_e, eV	64.7	107.2	137.6	195.5
E_a, eV	145.3	204.2	234.4	279.1
$\alpha_p, \text{\AA}^{-1}$	2.6	3.3	3.7	4.5
$z_e, \text{\AA}$	0.172	0.122	0.106	0.086
$A, \text{eV} \cdot \text{\AA}^{-2}$	1.14(4)	6.15(4)	1.22(5)	4.69(5)

Note. $a(n)$ denotes $a \cdot 10^n$.

In what follows we shall be interested in the values of the function $\chi_{N\Lambda}(\rho)$ and the complete wave function for values $\rho = \rho_n$ [see Eq. (3)]. It can be seen from Eq. (12) that the function $\chi_{N\Lambda}(\rho)$ for small ρ ($\rho \ll 1$) is determined only by the power dependence $\rho^{|\Lambda|}$. Consequently for $\Lambda \neq 0$ the function $\chi_{N\Lambda}(\rho_n)$ will have a much smaller value than for $\Lambda = 0$. Therefore rotational states with $\Lambda \neq 0$ do not present significant interest in the framework of the problem posed and will not be discussed in what follows. For state with $\Lambda = 0$ instead of the value $\rho = \rho_n$ we shall use the value $\rho = 0$, which will not lead to an appreciable error. The wave function of the vibrational motion in the region of the molecular potential well can be obtained as the exact solution of the Schrödinger equation with the potential (7).⁷ However for the purposes of the present work it is necessary to know the behavior of the wave function of the longitudinal motion not only in the region of this well, but also in the entire sub-barrier region, where the approximation (7) is already not sufficiently good. Therefore in solution of the problem we shall use the quasiclassical expression for the wave function of the longitudinal motion in the sub-barrier region:

$$\eta_v(z) = \left[\frac{\mu \omega_v}{2\pi p(z)} \right]^{1/2} \exp \left\{ -\frac{1}{\hbar} \int_z^{z_v} p(z) dz \right\}, \quad (14)$$

where the momentum of the particle is given by the expression

$$p(z) = [2\mu(W(z) - \varepsilon_{N\Lambda v})]^{1/2}. \quad (15)$$

The quantity ω_v is the characteristic cyclic frequency of periodic vibrations of nuclei along the internuclear axis:

$$\omega_v \approx \omega_e - x_e(v + 1/2), \quad (16)$$

and z_v is the coordinate of the classical turning point for the vibrational-rotational state $N\Lambda v$ in the molecular potential well. It is determined as the smaller of the roots of the equation

$$W(z_v) = \varepsilon_{N\Lambda v}. \quad (17)$$

Here we have used $W(z)$ as given by Eq. (7). The solution of Eq. (17) has the form

$$z_v = (2\alpha_p)^{-1} \ln \left[\frac{(1 + \delta_{N\Lambda v})}{(1 - \delta_{N\Lambda v})} \right], \quad (18)$$

where we use the following notation:

$$\delta_{N\Lambda v} = \{A + B - C - [(A + B - C)^2 - 4AB]^{1/2}\} / 2B, \quad (19)$$

$$\xi_e = \text{th}^2(\alpha_p z_e),$$

$$A = \frac{D_e}{|\varepsilon_{N\Lambda v}|} \frac{\xi_e^2}{(1 - \xi_e)^2}, \quad B = \frac{D_e}{|\varepsilon_{N\Lambda v}|} \frac{1}{(1 - \xi_e)^2},$$

$$C = 1 - \frac{E_a}{|\varepsilon_{N\Lambda v}|}.$$

The barrier transmission coefficient in the sub-barrier region with coordinate z is given by the formula

$$D_{N\Lambda v}(z) = \exp \left\{ -\frac{2}{\hbar} (2\mu |\varepsilon_{N\Lambda v}|)^{1/2} \int_z^{z_v} \left(\frac{W(z)}{|\varepsilon_{N\Lambda v}|} + 1 \right)^{1/2} dz \right\}. \quad (20)$$

Consequently the square root of the wave function of the longitudinal motion at an arbitrary point z is

$$|\eta_v(z)|^2 = [\mu \omega_v / 2p(z)] D_{N\Lambda v}(z). \quad (21)$$

With inclusion of Eqs. (12) and (21) we obtain for the square of the modulus of the total wave function (for $\Lambda = 0$) at the boundary of the nuclear potential well

$$|\Psi_{N0v}(\rho_n, \varphi, z_n)|^2 = \frac{1}{2\pi} \frac{\alpha_B^{1/2}}{a_B^2} \frac{\mu \omega_v}{2p(z_n)} D_{N0v}(z_n). \quad (22)$$

Now the factor $\xi_i(N0v, B)$, which determines the reaction probability can be represented in the form

$$\xi_i(N0v, B) = \frac{\alpha_B^{1/2}}{a_B^2} \frac{\mu \omega_v}{2p(z_n)} D_{N0v}(z_n). \quad (23)$$

We recall that for simplification in writing the right-hand sides of Eqs. (22) and (23), as in the previous formulas for the energies and wave functions, the index i which relates the molecular parameters to a definite molecular ion has been omitted.

For the final calculation of the quantity ξ_i it is necessary to calculate $p(z_n)$ and $D_{N0v}(z_n)$. As was mentioned above, here we have assumed that the nuclear potential well is rectangular. At distances $z > z_n$ the dependence of the potential on distance initially has a Coulomb nature, and then drops more steeply. The quantity $p(z_n)$ can easily be calculated on the basis of Eq. (15) if instead of $W(z)$ we substitute the Coulomb potential energy $W(z)$ calculated for the point

For calculation of the integral entering into the transmission coefficient (20), it is necessary to know the behavior of the function $W(z)$ in the sub-barrier region. Numerical calculations of this function showed that for any values of the magnetic field strength from the interval considered in the present work $B = 10^{12} - 10^{13}$ G, in the region $z \leq z_k \approx 0.0001$ Å the function $W(z)$ is quite well described by a Coulomb dependence. In the region $z_p \leq z \leq z_v$, where z_p is some characteristic distance which depends on the magnetic field strength, the dependence is given by Eq. (7). The values of z_p are approximately 0.07, 0.05, 0.04, and 0.03 Å for the respective magnetic field strengths $B = 10^{12}$, $3 \cdot 10^{12}$, $5 \cdot 10^{12}$, and 10^{13} G. For the intermediate region of the longitudinal coordinate, $z_k \leq z \leq z_p$, the values of the function $W(z)$ are given in Table II. This set of data permits calculation of the integral in Eq. (20) and the coefficients ξ_i in accordance with Eq. (23).

3. DISCUSSION OF THE RESULTS OF THE CALCULATION

The results of calculations of the probabilities of the nuclear reactions (1) as functions of the magnetic field strength are given in Figs. 1-3 for reactions I-III respectively. The quantum number $\Lambda = 0$ has been omitted in the notation $P_i(N\Lambda v, B)$. In addition, in these figures we have not given the probabilities of reactions from $(2, v)$ levels, since they do not differ substantially from the results which were obtained for $(0, v)$ or $(1, v)$ levels and have been omitted in order to avoid encumbering the figures. In the figures we can see that certain curves [for example, (1,1) and (1,0) in Fig.

TABLE II. Values of the function $W(z)$ in the region $z_k \ll z \ll z_p$ (in eV).

$z, \text{\AA}$	B, G			
	10^{12}	$3 \cdot 10^{12}$	$5 \cdot 10^{12}$	10^{13}
0.0002	7.089 (4)	7.071 (4)	7.067 (4)	7.046 (4)
0.0003	4.713 (4)	4.695 (4)	4.685 (4)	4.671 (4)
0.0004	3.525 (4)	3.508 (4)	3.498 (4)	3.483 (4)
0.0005	2.812 (4)	2.795 (4)	2.785 (4)	2.770 (4)
0.0006	2.337 (4)	2.320 (4)	2.310 (4)	2.295 (4)
0.0007	1.998 (4)	1.980 (4)	1.971 (4)	1.956 (4)
0.0008	1.743 (4)	1.726 (4)	1.716 (4)	1.720 (4)
0.0009	1.545 (4)	1.528 (4)	1.518 (4)	1.504 (4)
0.001	1.387 (4)	1.370 (4)	1.360 (4)	1.345 (4)
0.002	6.742 (3)	6.570 (3)	6.474 (3)	6.327 (3)
0.003	4.368 (3)	4.197 (3)	4.099 (3)	3.955 (3)
0.004	3.180 (3)	3.008 (3)	2.912 (3)	2.764 (3)
0.005	2.467 (3)	2.296 (3)	2.199 (3)	2.052 (3)
0.006	1.992 (3)	1.820 (3)	1.724 (3)	1.577 (3)
0.007	1.653 (3)	1.482 (3)	1.385 (3)	1.238 (3)
0.008	1.399 (3)	1.228 (3)	1.132 (3)	9.846 (2)
0.009	1.201 (3)	1.030 (3)	9.344 (2)	7.874 (2)
0.01	1045.0	873.9	787.8	629.9
0.02	334.9	167.7	83.6	-69.2
0.03	101.3	-60.1	-142.2	-287.2
0.04	13.2	-183.0	-246.7	-
0.05	-79.2	-234.0	-	-
0.06	-121.1	-	-	-
0.07	-149.0	-	-	-

Note. $a(n)$ denotes $a \cdot 10^n$.

1] are cut off in the region of the field strengths $\log B \approx 12.6-12.8$. This cutoff is due to the fact that at such fields the levels discussed no longer exist as discrete energy states since they are crowded out of the potential well of the given molecular ion into the continuum (see Ref. 7).

As a whole we can see in these figures that the probabilities of the nuclear reactions discussed depend substantially on the magnetic field strength. The dependence on the vibrational quantum numbers is also rather strong.

It is interesting to mention that a still more substantial

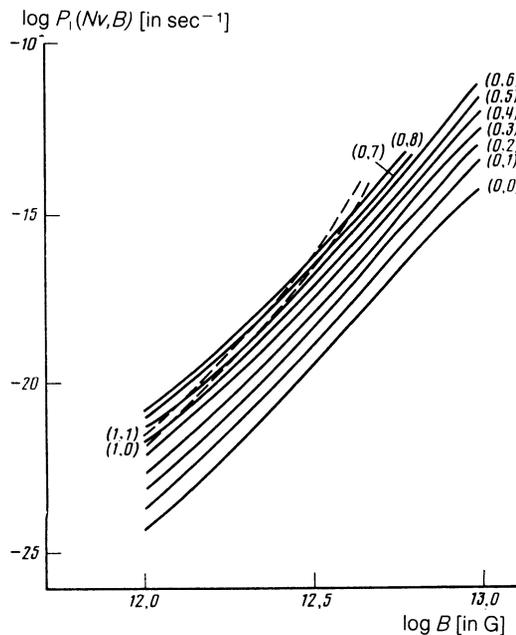


FIG. 1. Probability of nuclear reaction I in the molecular ion HD^+ as a function of the magnetic field. In parentheses beside the curves we have given the rotational and vibrational quantum numbers (N, v) .

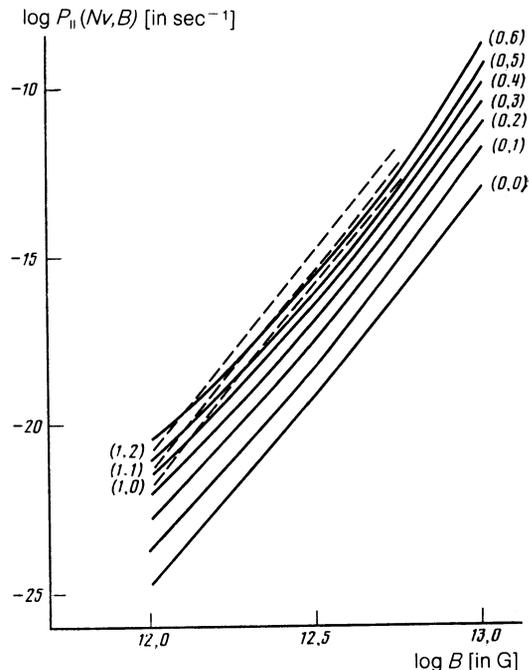


FIG. 2. Probability of the nuclear reaction II in the molecular ion D_2^+ as a function of the magnetic field. The notation is the same as in Fig. 1.

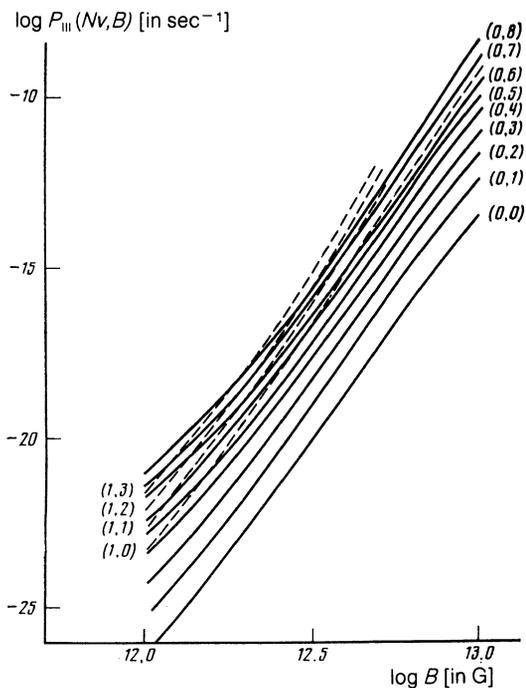


FIG. 3. Probability of the nuclear reaction III in the molecular ion DT^+ as a function of the magnetic field. The notation is the same as in Fig. 1.

acceleration of nuclear reactions in a strong magnetic field can be expected in the neutral molecules HD, D_2 , and DT. In

fact, the decisive factor affecting the penetrability of the potential barrier separating the nuclei is its width. In neutral molecules containing two binding electrons, the width should be significantly smaller than in molecular ions. Calculations carried out for the H_2 molecule for the case in which the axis of the molecule coincides with the direction of the magnetic field⁹ have shown that this is actually the case. Consequently the probabilities of nuclear reactions in neutral molecules can be higher than the values calculated in the present work by several orders of magnitude. However, in order to carry out corresponding calculations it is necessary to have data on the shape of the potential surfaces and on the structure of the energy levels of these molecules. At the present time there is no detailed information of this type.

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