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THEORY OF MOLECULAR DISSOCIATION INDUCED BY NEUTRONS.

I. DIATOMIC MOLECULES

Yu. S. SAYASOV and G. K. IVANOV

Institute of Chemical Physics, Academy of Sciences, U.S.S.R.

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A theory based on the Fermi pseudopotential method is developed for the dissociation of diatomic molecules. It is assumed that the neutron energy is of the order of the dissociation energy, and that during disintegration the molecule remains in the ground electron state. Under these assumptions, simple final formulas can be obtained for the cross sections of the processes.

1. INTRODUCTION

THE collision of a neutron with a chemically bound nucleus can be accompanied by transfer to it of momentum that is sufficient for breaking the bond, i.e., for dissociation of the molecule. This process which has not been investigated before, is of undoubted interest in radiation chemistry and biology, and also for the theory of slowing down of neutrons. Moreover, calculations of the dissociation probability of molecules by neutrons are necessary in connection with the development now being carried on of the method proposed by Gol'danskii of molecular neutronoscopy,[1] which has as its purpose the study of the different characteristics of molecules by recording neutrons scattered by them.

We shall assume that the neutrons have an energy E of the order of the molecular dissociation energy, i.e., $E \sim 10$ ev. Such energies correspond to a wavelength $\lambda_n \sim 10^{-9}$ cm. This means that the relations $\lambda_n \gg A$, $a \gg A$ hold among λ_n, the range of nuclear forces $A \sim 10^{-13}$ cm, and the characteristic molecular dimension, by which one should mean the amplitude of vibrations of nuclei in the molecule, $a \sim 10^{-9}$ cm. These relations make it possible to use the method of the Fermi pseudopotential in the case under discussion.[2]

In other words, by introducing the interaction V between neutrons and the nuclei of a molecule of type

$$V = 2\pi\hbar^2 \sum_i \frac{1}{\mu_i} A_i \delta(\mathbf{r}_n - \mathbf{r}_i) \qquad (1)$$

(here $\mu_i = m_i m/(m_i + m)$ is the reduced mass of the neutron (m) and the i-th nucleus in the molecule (m_i), $A_i = a_i + b_i(\mathbf{i}\cdot\mathbf{s})$ is the amplitude of scattering of the neutron (spin $\mathbf{s}$) by the free nucleus (spin $\mathbf{i}$), $\mathbf{i}\cdot\mathbf{s}$ is the eigenvalue of the operator $\hat{\mathbf{i}}\cdot\hat{\mathbf{s}}$), we can compute the dissociation cross section $d\sigma$ in the first Born approximation relative to V, according to the usual formulas of perturbation theory, for the probability of transition from the states of the discrete spectrum to the continuous:

$$d\sigma = \frac{k'}{k}\overline{|W|^2}\, d\varkappa_1 \ldots d\varkappa_n do. \qquad (2)$$

Here k, k′ are the wave numbers of the neutron before and after collision, $\kappa_1 \ldots \kappa_n$ are the wave vectors of particles which appear as products of the dissociation of the molecule, and do is the element of solid angle in which the neutron is scattered,

$$W = \frac{\mu}{2\pi\hbar^2}\int e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_n}\psi_0 V \psi_\varkappa^* d\mathbf{r}_n d\mathbf{r},$$

μ is the reduced mass of neutron and molecule; ψ_0 is the wave function of the initial state of the molecule, ψ_K is the wave function of the final state of the molecule which corresponds to the process of its decay of a definite type (continuous spectrum); the symbol $d\mathbf{r}$ denotes integration over all molecular coordinates; in (2), the averaging is carried out over all the energetically degenerate states.

For the neutron energies of interest to us, the formula (2) immediately admits a certain simplification, which is connected with the fact that in such cases the motion of the nuclei both in the initial and in the final state can be regarded as slow in comparison with electronic motion. Therefore, for the functions ψ_0, ψ_K, the adiabatic approximation is valid, i.e., one can represent them in the form of a product of electron wave functions and wave functions describing the motion of nuclei in a certain potential field which depends on their mutual distance.

Inasmuch as the operator V acts only on the coordinates of the nuclei, then, in accord with (2), in the adiabatic approximation, the dissociation cross section of the molecule, which is accompanied by a change in its electron state, will generally be equal to zero. Thus, it is permissible to limit ourselves to an investigation of dissociation processes for which the electron state of the molecule does not change, i.e., generally to exclude from consideration the electronic functions, considering ψ_0 and ψ_K in (2) as the wave functions of the relative motion of the nuclei corresponding to the main electron term. Nevertheless, even under these simplifying assumptions, the functions ψ_K in the general case of monatomic molecules possess a very complicated character. Therefore, we shall initially limit ourselves to the study of dissociation of diatomic molecules for which the functions ψ_K have a comparatively simple form.

2. GENERAL FORMULAS FOR THE DISSOCIATION CROSS SECTIONS OF DIATOMIC MOLECULES

For simplicity we shall assume that the electron state of the molecules is $^1\Sigma$. Then the Hamiltonian of the relative motion of the nuclei of the molecule is identical in the adiabatic approximation with the Hamiltonian of the relative motion of two particles whose interaction is centrally symmetric; consequently, the functions ψ_K in the given case are identical with the functions $\psi_{\bar{K}}$ defined in reference 3, Sec. 113, whose asymptote for $r \rightarrow \infty$ $(\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2)$ is itself the superposition of a plane wave and a converging spherical wave:

$$\psi_{\varkappa}^{-} = \frac{1}{4\pi\varkappa r}\sum_{l=0}^{\infty} i^l(2l+1)e^{-i\delta_l}\chi_{\varkappa l}(r)P_l\left(\frac{\varkappa\mathbf{r}}{\varkappa r}\right), \qquad (3)$$

where $\chi_{\kappa l}$ are the wave functions of the equation

$$\frac{d^2\chi_{\varkappa l}}{dr^2} + \left(\varkappa^2 - \frac{2\mu_m U}{\hbar^2} - \frac{l(l+1)}{r^2}\right)\chi_{\varkappa l} = 0, \qquad (4)$$

U is the molecular potential and μ_m the reduced mass of the molecule. The functions $\chi_{\kappa l}$ are regular for r = 0 and have the asymptote

$$\chi_{\varkappa l} \sim \sqrt{2/\pi}\sin(\varkappa r - \pi l/2 + \delta_l) \quad \text{for} \quad r \rightarrow \infty.$$

The initial state of the molecule, which has a vibration number n and rotational number K can be determined in the following way:

$$\psi_0 = \frac{1}{r}\left(\frac{2}{\pi}\right)^{1/4} a^{-1/2}e^{-\xi^2}H_n(\xi)Y_{KM_K}(\theta, \varphi), \qquad (5)$$

where $\xi = (r - r_0)/a$, r_0 is the point of minimum U, $a = \sqrt{2\hbar/\mu_m\omega}$ is the amplitude of the vibrations of the nuclei in the molecule, $H_n(\xi)$ are Hermite functions, M_K is the projection of the moment of inertia of the molecule K on the axis of the molecule, θ and φ are angles which define the orientation of the molecule in the center-of-mass system (c.m.s.) of the neutron-molecule, to which all our discussions refer. Equation (2) in the case under discussion is rewritten in the following form:

$$d\sigma = \frac{k'}{k}\frac{1}{2K+1}\sum_{M_K=-K}^{K}\overline{|W_{M_K}|^2}\,d\varkappa\,do, \qquad (6)$$

where

$$W_{M_K} = \frac{\mu}{2\pi\hbar^2}\int e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_n}\psi_0 V\psi_{\varkappa}^{-*}\,d\mathbf{r}_n\,d\mathbf{r},$$

$$V = 2\pi\hbar^2\left(\frac{A_1}{\mu_1}\delta(\mathbf{r}_n - \mathbf{r}_1) + \frac{A_2}{\mu_2}\delta(\mathbf{r}_n - \mathbf{r}_2)\right). \qquad (7)$$

In (6) the averaging is carried out over orientations of the spins of the nuclei and the neutron which are assumed to be distributed randomly.

We note that the wave numbers of the neutron k, k′ and the wave number of the molecule κ are connected by a relation which follows from the law of conservation of energy:

$$k^2/2\mu - k'^2/2\mu = D_{nK}/\hbar^2 + \varkappa^2/2\mu; \qquad (8)$$

D_{nK} is the dissociation energy

$$D_{nK} = U_m - \left(n + \frac{1}{2}\right)\hbar\omega - K(K+1)\hbar^2/2\mu_m r_0^2,$$

$$U_m = -U(r_0).$$

One can transform Eq. (6) in such a way that only the characteristics of a finite state of the system are contained in it — the scattering angle of the neutron θ and the wave number of the molecule in the final state κ (see Appendix 1):

$$d\sigma_{nK} = \sqrt{\frac{\pi}{2}}\frac{k'}{k}\frac{1}{a}\left[\sum_{l=0}^{\infty}(2l+1)\sum_{L=|l-K|}^{l+K}(C_{l0K0}^{L0})^2F_{lL}\right]d\varkappa\,do,$$

$$F_{lL} = \overline{A_1^2}\frac{1}{g_1^2}\left(\frac{\mu}{\mu_1}\right)^2 J_{g_1}^2 + \overline{A_2^2}\frac{1}{g_2^2}\left(\frac{\mu}{\mu_2}\right)^2 J_{g_2}^2$$
$$+ (-1)^L\overline{2A_1A_2}\frac{\mu^2}{\mu_1\mu_2}J_{g_1}J_{g_2}\frac{1}{g_1g_2}, \qquad (9)$$

where

$$J_g = \int_0^{\infty}\frac{1}{r}e^{-\xi^2}H_n(\xi)\chi_{\varkappa l}(r)\psi_{L+1/2}(gr)\,dr,$$

$$\psi_{L+1/2}(x) = \sqrt{x}J_{L+1/2}(x), \qquad g = g_{1,2} = \frac{m_{2,1}}{m_1 + m_2}|\mathbf{k} - \mathbf{k}'|, \qquad (10)$$

C_{l0K0}^{L0} are the Clebsch-Gordan coefficients.

The averaging in (9) is carried out over the directions of spins of the nuclei and of the neutron. If the nuclei in the molecule are different (see reference 3, Sec. 123), then

$$\overline{A^2_{1,2}} = a^2_{1,2} + \tfrac{1}{4} i_{1,2}(i_{1,2}+1) b^2_{1,2}, \qquad \overline{A_1A_2} = a_1a_2,$$

$i_{1,2}$ are the nuclear spins. Now if the nuclei are identical, then, as is easy to show,

$$\overline{A^2_{1,2}} = a^2 + \tfrac{1}{4} i\,(i+1)\,b^2,$$

$$\overline{A_1A_2} = a^2 + \tfrac{3}{8} b^2\,[2i\,(i+1) - I\,(I+1)],$$

I is the total spin of the system of two nuclei.

3. DISSOCIATION CROSS SECTION UNDER QUASICLASSICAL CONDITIONS

For neutron energies of interest to us, its wavelength ($\lambda_n \sim 10^{-9}$ cm) is much less than the dimensions of the molecule. Therefore, a quasiclassical approximation is generally valid for the functions $\chi_{\kappa l}$, $\psi_{L+1/2}$:

$$\chi_{\varkappa l} = \left(\frac{2}{\pi}\frac{\varkappa}{\tilde{\varkappa}}\right)^{1/2} \sin\left(\int_{r_1}^{r} \tilde{\varkappa}\,dr + \frac{\pi}{4}\right),$$

$$\tilde{\varkappa}^2 = \varkappa^2 - \frac{2\mu_m}{\hbar^2} U - \frac{l\,(l+1)}{r^2}, \tag{11}$$

$$\psi_{L+1/2} = \left(\frac{2}{\pi}\frac{g}{\tilde{g}}\right)^{1/2} \sin\left(\int_{r_2}^{r} \tilde{g}\,dr + \frac{\pi}{4}\right), \quad \tilde{g}^2 = g^2 - \frac{L\,(L+1)}{r^2}, \tag{12}$$

where r_1 and r_2 are the turning points for the functions $\tilde{\kappa}^2$ and $\tilde{g}^2$. Using (11) and (12), we can calculate J_g (10) by the method of steepest descents. We rewrite J_g in the form

$$J_g = \frac{1}{2}\operatorname{Re}\mathcal{Y}, \qquad \mathcal{Y} = \int_0^\infty b\,(r)\,e^{S(r)}\,dr,$$

where

$$b\,(r) = \frac{2}{\pi}\left(\frac{\varkappa g}{\tilde{\varkappa}\tilde{g}}\right)^{1/2}\frac{1}{r},$$

$$S = \frac{-(r-r_0)^2}{a^2} + i\left(\int_{r_1}^{r}\tilde{\varkappa}\,dr - \int_{r_2}^{r}\tilde{g}\,dr\right).$$

S(r) is a quantity of large magnitude which has a saddle point defined by the equation

$$-2\,(r_n - r_0)/a^2 + i\,(\tilde{\varkappa} - \tilde{g}) = 0. \tag{13}$$

In the general case, calculation of J_g by the method of steepest descents leads to formulas that are difficult to handle. It is easy to note, however, that in the region of values of κ and θ where the cross section $d\sigma$ is largest, the expressions for r_n and J_g are greatly simplified. We shall carry out these simplifications, assuming that the molecule is found in the ground state (i.e., n = 0, K = 0). We note that r_n is close to the point of minimum potential of U, r_0. Then, as follows directly from Eq. (13), we obtain the following expression for r_n:

$$r_n - r_0 = i\eta,$$

$$\eta = \tfrac{1}{2}a^2\,(\tilde{\varkappa}\,(r_0) - \tilde{g}\,(r_0)) = \tfrac{1}{2}a^2\left(\sqrt{\varkappa'^2 - l^2/r_0^2} - \sqrt{g^2 - l^2/r_0^2}\right),$$

$$\varkappa'^2 = \varkappa^2 - 2\mu_m\hbar^{-2}U\,(r_0) = \varkappa^2 + 2\mu_m\hbar^{-2}U_m. \tag{14}$$

As is easy to show, Eq. (14) is valid under the condition $\eta/r_0 \ll 1$ [where η is determined in (14)]. Inasmuch as

$$a^2 = \sqrt{2\hbar^2/\mu_m U''(r_0)} \sim \hbar\, r_0/\sqrt{\mu_m U_m} \sim r_0/\varkappa',$$

then the condition $\eta/r_0 \ll 1$ is equivalent to the inequality $(\kappa' - g)/\kappa' \ll 1$. Then (14) can be rewritten in the form

$$\eta \approx \frac{a^2}{4}\frac{\varkappa'^2 - g^2}{\sqrt{g^2 - l^2/r_0^2}} \approx \frac{a^2}{2}\frac{\varkappa' - g}{\sqrt{1 - l^2/l_0^2}}, \qquad l_0 = g r_0. \tag{15}$$

Simplifying the quantities $S(r_n)$, $S''(r_n)$, $b(r_n)$ in similar fashion, and assuming that $(\kappa' - g)/\kappa' \ll \sqrt{1 - l^2/l_0^2}$, we get

$$J_g = \frac{1}{\sqrt{\pi}}\frac{a}{r_0}\sqrt{\frac{\varkappa}{\varkappa'}}\frac{1}{\sqrt{1 - l^2/l_0^2}}\exp\left[-\frac{\rho^2}{2\,(1 - l^2/l_0^2)}\right]\cos\tau,$$

$$\rho^2 = \frac{a^2}{2}(\varkappa' - g)^2, \qquad \tau = \int_{r_1}^{r_0}\tilde{\varkappa}\,dr - \int_{r_2}^{r_0}\tilde{g}\,dr. \tag{16}$$

Upon substituting J_g in the series (9), we note that the interference terms, which contain the product of rapidly oscillating factors $\cos\tau(g_1)\cos\tau(g_2)$, vanish in the summation, i.e., the dissociation cross section is composed additively of the cross sections corresponding to the collision of the neutron with the first ($d\sigma^{(1)}$) or second nucleus ($d\sigma^{(2)}$).* Therefore, it suffices to investigate, for example, the cross section $d\sigma^{(1)}$, which is determined by the formula

$$d\sigma^{(1)} = \sqrt{\frac{\pi}{2}}\frac{k'}{k}\frac{1}{a}\overline{A_1^2}\frac{1}{g_1^2}\left(\frac{\mu}{\mu_1}\right)^2\left[\sum_{l=0}^{\infty}(2l+1)\,J^2_{g_1}\right]d\varkappa\,do. \tag{17}$$

Substituting (16) therein, and replacing the summation over l by an integration, and $\cos^2\tau'$ by its mean value ½, we get

$$d\sigma = \frac{1}{2\sqrt{2\pi}}\frac{k'}{k}a\frac{1}{\varkappa'}\frac{\mu^2}{\mu_1^2}\operatorname{Ei}(-\rho^2)\,\varkappa\,d\varkappa\,do. \tag{18}$$

Equation (18) is evidently applicable under the condition that the region of large values of l for which $(\kappa' - g)/\kappa' \sim \sqrt{1 - l/l_0^2}$ does not make an important contribution in the integration over l. Obviously, for this to happen it is necessary that for $(\kappa' - g)/\kappa$

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*If the nuclei in the molecule are identical, then $g_1 = g_2$, so that $\cos^2\tau(g)$ enters into the interference terms. Nevertheless, the interference series $\Sigma(-1)^l(2l+1)\,J_g^2/g^2$, as is easy to see, is equal to zero in this case in view of its sign alternation.

$\sim \sqrt{1 - l^2/l_0^2}$ the inequality $\rho^2/(1 - l^2/l_0^2) > 1$ be satisfied, which is possible only when $a^2\kappa'^2 \gg 1$. In Eq. (18), consequently, both large values of ρ^2, consistent with the condition $\eta/r_0 \sim (\kappa' - g)/\kappa' \ll (1 - l^2/l_0^2)^{1/2}$ and small values of ρ^2, consistent with the condition $a^2\kappa'^2 \gg 1$ can enter. For $\rho^2 > 1$, Eq. (18) has the asymptotic form

$$d\sigma = \frac{1}{2\sqrt{2\pi}} \frac{k'}{k} a \left(\frac{\mu}{\mu_1}\right)^2 \overline{A_1^2} \frac{1}{\varkappa'} \frac{e^{-\rho^2}}{\rho^2} \varkappa d\varkappa do, \tag{19}$$

while for $\rho^2 < 1$

$$d\sigma = \frac{1}{2\sqrt{2\pi}} \frac{k'}{k} a \left(\frac{\mu}{\mu_1}\right)^2 \overline{A_1^2} \frac{1}{\varkappa'} \ln(\gamma/\rho^2) \varkappa d\varkappa do \tag{20}$$

(γ is Euler's constant).

Equations (18) and (20) are inapplicable for $\rho \to 0$. Nevertheless, the difference of (20) for $\rho \to 0$ from the correct equation, in which $\ln(\gamma/\rho^2)$ must approach some finite value,* possesses only a logarithmic character; consequently, Eq. (18), having been integrated over θ and κ, must yield the correct total cross section. Actually, making use of the well-known integral

$$\int_{-\infty}^{\infty} \mathrm{Ei}(-\rho^2)\, d\rho = 2\sqrt{\pi},$$

we find that the energy spectrum of the scattered neutrons has the form

$$d\sigma^{(1)} = \pi\overline{A_1^2} \frac{\mu\mu_m}{\mu_1^2} \frac{2k'\,dk'}{k^2}, \tag{21}$$

i.e., the total cross section σ is

$$\sigma = \pi\overline{A_1^2} \frac{\mu\mu_m}{\mu_1^2} \frac{E - D}{E}. \tag{22}$$

In particular, if the neutron collides with a proton in a heavy molecule, then $\mu_1 = m/2$, $\mu = \mu_m = m$ and, consequently, $\mu\mu_m/\mu_1^2 = 4$, i.e.,

$$\sigma = \sigma_0 (E - D)/E, \tag{23}$$

where $\sigma_0 = 4\pi\overline{A_1^2}$ is the cross section of scattering of the neutron by a free proton. In accord with (23), σ at $E \gg D$, as was to have been expected, is identical with σ_0. We now consider the angular distribution of the scattered neutrons from the basis of Eqs. (18) and (19). The maximum of $d\sigma$ is evidently obtained for the angle $\theta = \theta_0$ for which $\rho = 0$, i.e., $\kappa' = g$. We assume that $ak' \gg 1$. Then, as is easy to see, the angle θ_0 is determined from the relation

$$\varkappa' \approx \sqrt{\frac{\mu_m}{\mu}(k^2 - k'^2)} = g_1 = \frac{m_2}{m_1 + m_2}\sqrt{k^2 + k'^2 - 2kk'\cos\theta},$$

with accuracy up to a quantity of order $1/a^2k'^2$, i.e.,

$$\cos\theta_0 = [(\nu + 1)\, p'^2 - (\nu - 1)\, p^2]/2pp',$$
$$p = k\hbar, \qquad p' = k'\hbar, \qquad \nu = m_1(m_1 + m_2 + m)/mm_2. \tag{24}$$

It can be shown that θ_0 has the meaning of the angle at which the neutron will be scattered by a free nucleus initially at rest with mass m, in the set of coordinates which we have used, i.e., one connected with the center of mass of the neutron-molecule system. It is very easy to establish this by the example of the collision of a neutron with a proton in a heavy molecule, i.e., for $m_2 \gg m_1 = m$. Then $\nu \approx 1$ and, in accord with (24), $\cos\theta_0 = p'/p$ in correspondence with the given determination of θ_0 (the set of coordinates in this case is identical with the laboratory set).

We shall assume that the angle θ is close to θ_0, i.e., $\theta = \theta_0 + \vartheta$, $\vartheta \ll \theta_0$. Then (for $\nu = 1$) we have, in first approximation in ϑ, $\rho = \vartheta/\vartheta_0$, $\vartheta_0 = \sqrt{2}/ak' \ll 1$. In this case Eq. (18) is simplified:

$$d\sigma = \frac{\sigma_0}{\sqrt{2\pi}} \left(\frac{p'}{p}\right)^2 \mathrm{Ei}\left(-\frac{\vartheta^2}{\vartheta_0^2}\right) \frac{1}{p_0}\, dp'\, d\vartheta. \tag{25}$$

It is important to emphasize that in accord with (25) the cross section for the neutron scattering accompanied by dissociation of the molecule does not depend on the detailed form of the molecular potential, but only on the frequency of vibration of the nuclei in the molecule, ω. Moreover, inasmuch as for $\vartheta > \vartheta_0$, $\mathrm{Ei}(-\rho^2)$ is proportional to $\exp(-\vartheta^2/\vartheta_0^2)$, then one can show that all the scattered neutrons with final momentum p′ are contained in the small range of angles

$$\vartheta \sim \vartheta_0 = \sqrt{2}\, p_0/p_1, \qquad p_0 = \sqrt{m\hbar\omega}.$$

The angle ϑ_0 is in order of magnitude the difference of the scattering angles of the neutron by a free proton initially at rest and by a free proton possessing a momentum p_0 before the collision. This means that the dissociation process of the molecules by the neutrons can be described in general terms by means of a very simple model, in which the chemically associated nuclei are considered as free but possessing the same scatter of momenta as nuclei in the molecule.*

We now note that for scattering of the neutron not by a proton but by a heavy nucleus, $\nu \gg 1$, i.e., in accord with (24), $\cos\theta_0 \sim -\nu D/E$ and, consequently, the region of the maximum of the angular distribution $\theta \sim \theta_0$ in this case, with neu-

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*As can be shown, as $\rho \to 0$, $\ln(\gamma/\rho^2)$ must be replaced by a finite quantity of the order of $\ln(ak')$.

*This model of the dissociation process, which is undoubtedly valid even in the case of the collision of a neutron with a polyatomic molecule, was pointed out to us by V. I. Gol'danskiĭ.

tron energies on the order of the dissociation energy D, is generally not achieved. Therefore the dissociation total cross section, which corresponds to collision with this nucleus, should be exponentially small.

In conclusion, attention should be called to the fact that all the results obtained here, which are introduced under the assumption that $K = 0$, are valid also for $K \neq 0$, if only K is not too large ($K \sim 1$). Actually, the summation in the series (9) is carried out over a large number of terms corresponding essentially to the largest values of l, but for $l \gg 1$ and $K \sim 1$, the difference between L and l can be neglected, i.e., $d\sigma_K \approx d\sigma_0$.

4. THE DISSOCIATION CROSS SECTION CLOSE TO THRESHOLD

If the wave number κ is very small, so that $\kappa r_0 < 1$, then the quasiclassical approximation (11) for the function $\chi_{\kappa l}$ is not applicable over the whole region of variation of r. This fact, which holds for energies of the neutron close to the dissociation D, requires special consideration, which will be given below.

For low energies of the scattering molecule $\hbar^2\kappa^2/2\mu_m$, the dissociation cross section should depend essentially on whether the molecule has a discrete level ϵ close to zero. We shall first assume that this level is sufficiently deep that $E - D \ll \epsilon$. In this case, one can investigate the behavior of the functions $\chi_{\kappa l}$ by a method similar to that used in the investigation of slow collisions (see reference 3, Sec. 108), i.e., in the region $r \sim r_0$, (where $\kappa^2 \ll -2\mu_m U/\hbar^2$ and which gives the principal contribution to the integrals $J_{g_{1,2}}$) $\chi_{\kappa l}$ is represented in the form $\chi_{\kappa l} = C_l(\kappa)\chi_l$; χ_l is the solution of the equation

$$\frac{d^2\chi_l}{dr^2} - \left(\frac{2\mu_m}{\hbar^2}U + \frac{l(l+1)}{r^2}\right)\chi_l = 0,$$

for which the quasiclassical approximation is valid. The coefficient $C_l(\kappa)$ is chosen under the condition that, for $r \to \infty$, the correct transition is obtained to the asymptote

$$\chi_{\varkappa l} \sim \sqrt{2/\pi}\sin(\varkappa r - \pi l/2 + \delta_l).$$

Thus we find that $C_l \sim \kappa^{l+1}$ (see reference 3, Sec. 108), i.e., in the series (9), only terms can be left corresponding to $l = 0$:

$$d\sigma_{nk} = \sqrt{\frac{\pi}{2}}\frac{k'}{k}\frac{1}{a}(C_{00K0}^{K0})^2 F_{0K}d\varkappa\, do,$$

$$F_{0K} = \overline{A_1^2}\frac{\mu^2}{\mu_1^2}\frac{1}{g_1^2}J_{g_1}^2 + \overline{A_2^2}\frac{\mu^2}{\mu_2^2}\frac{1}{g_2^2}J_{g_2}^2 + (-1)^K 2\overline{A_1A_2}\frac{\mu^2}{\mu_1\mu_2}\frac{1}{g_1g_2}J_{g_1}J_{g_2}. \qquad (26)$$

The coefficient $C_0(\kappa)$ entering into $J_{g_{1,2}}$ is essentially independent of the form of the potential U, in particular, independent of its behavior at infinity.

As shown in Appendix 2, if $U \sim U_0e^{-\alpha r}$ for $r \to \infty$, then

$$\chi_0 = \frac{\varkappa}{\alpha\cos q}\left(\frac{2\alpha}{\tilde{\varkappa}_0}\right)^{1/2}\sin\left(\int_{r_1}^{r}\tilde{\varkappa}_0\,dr + \frac{\pi}{4}\right), \qquad (27)$$

where

$$\tilde{\varkappa}_0^2 = -\frac{2\mu_m U}{\hbar^2}, \qquad q = \int_{r_1}^{\infty}\tilde{\varkappa}_0 dr, \qquad U(r_1) = 0$$

(it is assumed that U depends on r through the variable αr). Substituting (27) in the integrals $J_{g_{1,2}}$, and finding them as before by the method of steepest descents, we obtain the threshold formula for the dissociation cross section of a heavy hydrogen-bearing molecule in the ground state ($n = K = 0$), which is valid for $\sqrt{2\mu_m(E-D)}/\hbar\alpha \ll 1$:

$$d\sigma = \frac{1}{\sqrt{2\pi}}\sigma_0\frac{a}{r_0^2\alpha}\frac{\cos^2\tau}{\cos^2 q}\frac{k'\varkappa^2}{k^4}d\varkappa do, \qquad (28)$$

where

$$\tau = \int_{r_1}^{r_0}\tilde{\varkappa}_0 dr - gr_0.$$

The total dissociation cross section corresponding to (28) is given by the formula

$$\sigma = \frac{1}{2}\left(\frac{\pi}{2}\right)^{3/2}\sigma_0\frac{a}{\alpha r_0^2}\left(\frac{E-D}{D}\right)^2\frac{\cos^2\tau}{\cos^2 q}. \qquad (29)$$

We note that the quadratic dependence of the cross section close to the threshold D on the excess energy $E - D$ is the general property of reactions accompanied by the production of three slow particles the interaction among which bears a short-range character[4] (in our case these are the neutron and the two atoms which are produced upon decay of the molecule).

Equation (29) is clearly found to be inapplicable if q is close to $\pi(n + 1/2)$, with n an integer. But the equality

$$q = \frac{1}{\hbar}\int_{r_1}^{\infty}\sqrt{-2\mu_m U}\,dr = \pi\left(n + \frac{1}{2}\right)$$

is identical with the quasiclassical condition for the existence of a discrete level very close to zero (see reference 3, Sec. 48). Thus the inapplicability of (29) is connected with the fact that in this case (in the decay of the molecule) resonance phenomena take place which arise from the fact that the dissociating molecule decays into a state which, even though it refers to the region of continuous spectra, is quasi-stationary because of its nearness to the level ϵ. We limit ourselves to the study of these phenomena for a special choice of potential

$$U = U_0 \left[\exp\{-2\alpha(r - r_0)\} - 2\exp\{-\alpha(r - r_0)\}\right]$$

(the Morse potential). The function χ_0, having the correct asymptote as $r \to \infty$ and $r \to 0$ can be determined now by the formula

$$\chi_0 = \frac{2\sqrt{2\pi\varkappa}}{[\cos^2(\pi\lambda) + \pi^2\varkappa^2/\alpha^2]^{1/2}\,\alpha\,(\lambda - 1/2)\,\Gamma(\lambda - 1/2)}\,\xi^{-1/2}\,W_{\lambda,\mu}(\xi),$$

$$\lambda = \sqrt{2\mu_m U_0}/\alpha\hbar, \qquad \mu = i\varkappa/\alpha, \quad \xi = 2\lambda\exp\{-\alpha(r - r_0)\}, \tag{30}$$

$W_{\lambda,\mu}$ is the Whittaker function. In the region $r \sim r_0$, (30) is simplified

$$\chi_0 = \varkappa\left[\cos^2(\pi\lambda) + \pi^2\frac{\varkappa^2}{\alpha^2}\right]^{-1/2}\sqrt{\frac{2\alpha}{\tilde{\varkappa}_0}}\sin\left(\int_{r_1}^{r}\tilde{\varkappa}_0\,dr + \frac{\pi}{4}\right),$$

$$\pi\lambda = \int_{r_1}^{\infty}\tilde{\varkappa}_0\,dr = q. \tag{31}$$

For $\cos(\pi\lambda) \gg \pi\kappa/\alpha$, (31) is identical with (29). In accord with (31), the dissociation cross section corresponding to the same assumptions as in the derivation of (29) has the form

$$d\sigma = \frac{1}{\sqrt{2\pi}}\sigma_0\frac{a}{r_0^2\alpha}\,\frac{\cos^2\tau}{\cos^2 q + \pi^2\varkappa^2/\alpha^2}\,\frac{k'\varkappa^2}{k^4}\,d\varkappa do. \tag{32}$$

If $\cos q = 0$ (such an assumption corresponds, as is easy to see, to the condition $E - D \gg \epsilon$), then in accord with (32) the total cross section is

$$\sigma = \frac{1}{\sqrt{2\pi}}\sigma_0\frac{a\alpha}{r_0^2 k_m^2}\,\frac{E - D}{D}\cos^2\tau, \qquad k_m^2 = \frac{2\mu_m D}{\hbar^2}. \tag{33}$$

Thus in this case the cross section increases linearly with the energy of the neutron E. As was pointed out to us by A. I. Baz', such a growth of the threshold cross section with energy is a general law for processes in which two slow particles arise in the collision of two particles, one of which slow particles (in our case the dissociating molecule) is in a quasi-stationary state.

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APPENDIX 1

Integrating in (7) over the coordinate of the neutron r_n, we have

$$W_{M_K} = A_1\frac{\mu}{\mu_1}J_1 + A_2\frac{\mu}{\mu_2}J_2,$$

$$J_{1,2} = \int\exp\{\pm i\mathbf{g}_{1,2}\mathbf{r}\}\,\psi_0\psi_{\varkappa}^{-*}\,d\mathbf{r}, \qquad \mathbf{g}_{1,2} = \frac{m_{2,1}}{m_1 + m_2}(\mathbf{k} - \mathbf{k}'). \tag{1a}$$

We choose the z axis so that its direction in the set of coordinates which we have used for the neutron-molecule coincides with the fixed direction of the vector $\mathbf{g}$, i.e., $\mathbf{g}_1$ or $\mathbf{g}_2$. The direction $\mathbf{r}$ in the set of coordinates specialized in this fashion is defined by the angles θ, φ and the direction κ by the angles γ, 0. The angle between κ and $\mathbf{r}$ is denoted by θ'. The elements of volume in $\mathbf{r}$ and κ space will be, respectively,

$$d\mathbf{r} = r^2\,dr\sin\theta d\theta\,d\varphi, \qquad d\boldsymbol{\varkappa} = \varkappa^2\,d\varkappa\,do_{\varkappa}.$$

The Legendre polynomials entering into (3), $P_l(\cos\theta')$, can be transformed by means of the well-known theorem for the superposition of spherical functions (see reference 3, Sec. 113).

In the calculation of the integrals $J_{1,2}$, one can use the fact that in the products $P_l^*(\cos\theta') \times Y_{KM_K}(\theta, \varphi)$ only those terms make a non-vanishing contribution which contain the product $Y_{lM_K}^*(\theta, \varphi)\,Y_{KM_K}(\theta, \varphi)$, which with the aid of well-known formulas of the vector superposition of moments (see reference 2, p. 614) can be written in the form

$$Y_{lM_K}^* Y_{KM_K} = (-1)^{M_K}\sum_{L=-(l-K)}^{l+K}\left[\frac{(2l+1)(2K+1)}{4\pi(2L+1)}\right]^{1/2}$$
$$\times C_{l0K0}^{L0}\,C_{l-M_K\,KM_K}^{L0}\,Y_{L0}(\theta), \tag{2a}$$

C_{l0K0}^{L0}, $C_{l-M_KK0}^{L0}$ are Clebsch-Gordan coefficients. Substituting (2a) in J_1, and making use of the well-known formula

$$\int_0^{\pi}P_L(\theta)\exp\{ig_1 r\cos\theta\}\sin\theta d\theta = \sqrt{2\pi}\,\frac{i^L}{g_1 r}\,\psi_{L+1/2}(g_1 r),$$

we get

$$J_1 = \left(\frac{2K+1}{2}\right)^{1/2}\frac{1}{2\varkappa g}\sum_l(2l+1)\,e^{i\delta_l}(-i)^l\left[\frac{(l-M_K)!}{(l+M_K)!}\right]^{1/2}$$
$$\times P_l^{M_K}(\cos\gamma)\sum_{L=|l-K|}^{l+K}C_{l0K0}^{L0}\,C_{l-M_K\,KM_K}^{L0}\,i^L J_{g_1}, \tag{3a}$$

where

$$J_{g_1} = \int_0^{\infty}\frac{1}{r}\,e^{-\xi^2}H_n(\xi)\,\chi_{\varkappa l}(r)\,\psi_{L+1/2}(gr)\,dr.$$

The integral J_{g_2}, which is transformed in similar fashion, differs from J_{g_1} only in that the sum in it

$$\sum C_{l0K0}^{L0}\,C_{l-M_K\,KM_K}^{L0}\,i^L J_{g_1}$$

is replaced by

$$\sum C_{l0K0}^{L0}\,C_{l-M_KKM'_K}^{L0}\,i^{-L}J_{g_2}.$$

Making use in Eq. (6) of the expression (3a) for J_{g_1} which is similar to the expression for J_{g_2}, and the well-known property of the orthogonality of the Clebsch-Gordan coefficients, we get Eq. (9) shown in the text.

APPENDIX 2

To find the correct form of the function χ_0, which is determined by the equation

$$d^2\chi_0/dx^2 + f(x)\chi_0 = 0, \quad f(x) = -2\mu_m U/\hbar^2, \quad x = \alpha r$$

in the region $r \sim r_0$, we make use of the method of standard equations.[5] Let $f(x) \to de^{-x}$ as $x \to \infty$. We choose as a standard equation

$$d^2\varphi/ds^2 + de^{-s}\varphi = 0,$$

i.e.,

$$\varphi = Z_0(\eta), \quad \eta = 2d^{1/2}e^{-s/2}.$$

According to the general formula we have

$$\chi_0 = (de^{-s}/f(x))^{1/4} Z_0(\eta),$$

where the variable s is connected with x by the expression

$$\eta = \int\limits_s^\infty d^{1/2}e^{-s/2}\,ds = 2d^{1/2}e^{-s/2} = \int\limits_x^\infty f^{1/2}\,dx,$$

i.e., $s \to x$ as $x \to \infty$. If $Z_0(\eta)$ is chosen in the form

$$Z_0(\eta) = C\,[e^{-i\eta_0}H_0^{(1)}(\eta) - ie^{i\eta_0}H_0^{(2)}(\eta)],$$

$$\eta_0 = \int\limits_{x_1}^\infty f^{1/2}\,dx, \qquad f(x_1) = 0$$

and we use the asymptote $H_0^{(1),(2)} \sim \sqrt{2/\pi\eta} \times \exp\{\pm i(\eta - \pi/4)\}$, then in the region where $\eta \gg 1$, χ_0 is reduced to the form

$$\chi_0 = \frac{2i}{\sqrt{\pi}} C f^{-1/4} \sin\left(\int\limits_{x_1}^{x} f^{1/2}\,dx + \frac{\pi}{4}\right).$$

On the other hand, $x \to s$ and $\eta \to 0$ as $x \to \infty$, and, by using the asymptote $Y_0(\eta) \to (2/\pi)\ln(2/\eta)$, we get $\chi_0 \approx \pi^{-1} C\, 2xi \cos\eta_0$. In order that this asymptote go over into $\chi_0 \sim \sqrt{2/\pi}\,\sin(\kappa r + \delta_0)$ for $\kappa r < 1$, it is necessary to choose C by the formula

$$C = \sqrt{\pi/2}\,i\varkappa/\alpha\cos\eta_0,$$

which also gives in the region $r \sim r_0$

$$\chi_0 = \frac{2^{1/2}\varkappa}{\alpha\cos\eta_0} f^{-1/4} \sin\left(\int\limits_{x_1}^{x} f^{1/2}\,dx + \frac{\pi}{4}\right).$$

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