

perimental data.⁷ It can be seen from a comparison of the calculations that the calculations in the adiabatic approximation with the use of separable potentials reproduce the experimental data on DA cross sections somewhat better than do the calculations in the ZRP approximation, and worse than do the numerical computations without the use of the adiabatic approximation. The DA calculations for the HD and D₂ molecules are similar and are therefore not presented here. It should be noted that, by construction of the adiabatic approximation, the expected region of applicability of the model lies to the right of the point 4.48 eV, which corresponds to the dissociation energy for the H₂ molecule.

In our calculations, as the initial data, we used the two-particle *T* matrices and the wave functions corresponding to the two-particle bound states, in contrast to the other models proposed by Herzenberg, Mandi, and Firsov and Smirnov,³ in which it is necessary to know the quasistationary terms of the negative molecular ions AB⁻, terms whose determination is a fairly difficult problem. In our approach, however, these terms are determined by the imaginary zeros of the denominators of the functions *F*₁, while the complex zeros correspond to the continuation of the terms into the region of quasistationary states.²

In conclusion, I express my gratitude to V. N. Ostrovskii, who drew my attention to the possibility of obtaining an analytic solution to the Faddeev equations for a separable interaction, as well as to I. V. Komarov and S. P. Merkur'ev.

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Translated by A. K. Agyei

Absorption of optical radiation in weakly ionized gases

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(Submitted 15 December 1978)

Zh. Eksp. Teor. Fiz. **77**, 44–51 (July 1979)

The influence of atom polarization in an electromagnetic field on the photoabsorption coefficient of a weakly ionized gas is calculated. The effect turned out to be most substantial in the optical band. It is shown that for gases whose atoms have a negative scattering length the photoabsorption coefficient has a deep minimum at certain frequencies.

PACS numbers: 51.70. + f

In investigations of the properties of a weakly ionized gas in an alternating field it is customarily assumed that the field quanta are absorbed by free electrons when scattered by neutral particles, which play the role of an inert force center.^{1,2} Recent studies^{3–6} have shown, however, that in many cases an important role is played in this process by the dynamic characteristics of the neutral atoms and molecules. Namely, owing to the polarizability of the atoms and molecules in the external field, they acquire an oscillating dipole moment, and scattering by this moment changes the energy of the free electron by an amount $\hbar\omega$ (ω is the field frequency). This mechanism has explained qualitatively, in particular, the low thresholds of the optical

breakdown of alkali-metal vapor by laser radiation.⁶

An analytic formula for the cross section of the bremsstrahlung effect, with account taken of the polarization mechanism, was obtained in Ref. 6 under conditions when the Born approximation was applicable to potential scattering of an electron by an atom. In a weakly ionized gas, the Born approximation cannot be used for electrons with thermal velocities. To take into account the influence of the polarization mechanism of the absorption of radiation we therefore consider in the present paper the scattering of an electron by an atom in the short-range-potential approximation, which was applied to a similar problem earlier.^{7,8}

1. EFFECTIVE HAMILTONIAN

Let p and p' be the momenta of the electron before and after the collision with the atom. The short-range-potential approximation presupposes satisfaction of the inequalities

$$p, p' \ll \hbar/a \quad (1)$$

(a is the dimension of the atom). To satisfy these inequalities it is necessary, at any rate, that the frequency ω of the absorbed photon satisfy the inequality $\omega \ll \omega_0$, where ω_0 is the characteristic frequency of the transition of the atom from the ground state to the first excited state.

The dipole approximation is valid for the description of the electromagnetic interaction when the wavelength of the radiation greatly exceeds the deBroglie wavelength of the electrons that participate in the process. The electric field vector is in this case

$$E(t) = \text{Re} (E_0 e^{-i\omega t}),$$

E_0 is the complex amplitude. The motion of the electron in the field of the atom in the presence of radiation is described by the Hamiltonian

$$H(t) = H_a + T - Ze^2/r + \sum_{j=1}^Z e^2/|r-r_j| - eE(t) \left(r + \sum_{j=1}^Z r_j \right), \quad (2)$$

where H_a is the Hamiltonian of the free atom, T is the kinetic energy of the scattered electron, \mathbf{r} are its coordinates, \mathbf{r}_j are the coordinates of the atomic electrons, and Z is the charge of the nucleus.

In the tight-binding method developed for the calculation of the cross sections for the scattering of electrons by atoms in the absence of radiation,⁹ the wave functions of the "electron + atom" system are represented as expansions in the eigenfunctions of the Hamiltonian H_a . When condition (1) is satisfied it is possible to restrict this expansion to a single term corresponding to the ground state of the atom (the "static approximation" in the terminology of electron-atom collisions). Allowance for the remaining terms leads mainly to the appearance of polarization interaction of the electron with the atom, which can be taken into account phenomenologically.

Following this procedure, we seek a solution of the Schrödinger equation with Hamiltonian (2) in the form

$$\psi(\mathbf{r}, \{\mathbf{r}_j\}, t) = \varphi(\{\mathbf{r}_j\}, t) F(\mathbf{r}, t),$$

where φ is a solution of the equation

$$i\hbar \frac{\partial \varphi}{\partial t} = [H_a - dE(t)] \varphi, \quad d = e \sum_{j=1}^Z \mathbf{r}_j, \quad (3)$$

which goes over, when the electric field is adiabatically turned on, into the stationary ground state of the atom $\varphi_0(\{\mathbf{r}_j\}, t)$ with energy ϵ_0 . We neglect here the exchange effects, whose role in the bremsstrahlung, as will be shown below, is small if condition (1) is satisfied. The equation for the function F is of the form

$$i\hbar \frac{\partial F}{\partial t} = \left\{ T - Ze^2/r + \langle \varphi(t) | \sum_{j=1}^Z e^2/|r-r_j| | \varphi(t) \rangle - eE(t) \right\} F. \quad (4)$$

The solution of equation (3) will be written in first

order of perturbation theory in terms of the field:

$$\varphi(\{\mathbf{r}_j\}, t) = e^{-i\epsilon_0 t/\hbar} \left\{ \varphi_0(\{\mathbf{r}_j\}) + \frac{1}{2} \int d\mathbf{r}_1' \dots d\mathbf{r}_z' \times [e^{-i\omega' t} G_{\epsilon_0+\hbar\omega}(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\}) dE_0' + e^{i\omega' t} G_{\epsilon_0-\hbar\omega}(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\}) dE_0] \varphi_0(\{\mathbf{r}_j'\}) \right\}.$$

Here G_ϵ is the Green's function of the atom and is a matrix element of the operator $(H_a - \epsilon)^{-1}$. After substitution in (4), with account taken of only the terms linear in the field, we obtain

$$\begin{aligned} i\hbar \frac{\partial F}{\partial t} - [T + V(\mathbf{r})] F &= [-eE(t) \\ &+ \text{Re} \langle \varphi_0(\{\mathbf{r}_j\}) | Q_e(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\}, t) | \varphi_0(\{\mathbf{r}_j'\}) \rangle] F; \quad (5) \\ V(\mathbf{r}) &= -Ze^2/r + \langle \varphi_0 | \sum_{j=1}^Z e^2/|\mathbf{r}-\mathbf{r}_j| | \varphi_0 \rangle, \\ Q_e(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\}, t) &= [e^{i\omega' t} dE_0' G_{\epsilon_0+\hbar\omega}(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\}) \\ &+ e^{-i\omega' t} d'E_0 G_{\epsilon_0-\hbar\omega}(\{\mathbf{r}_j\}, \{\mathbf{r}_j'\})] \sum_{j=1}^Z e^2/|\mathbf{r}_j' - \mathbf{r}|. \end{aligned}$$

The field-dependent operators in the right-hand side of (5) will be regarded as a perturbation. The matrix elements of these operators are determined by the region $r \sim \hbar/p$ which, owing to condition (1), is much larger than the volume of the atom. This obvious argument is confirmed by the results of calculations performed in the next section. Therefore we can choose as the unperturbed functions $F(\mathbf{r}, t)$ the asymptotic ($r \gg a$) solution of Eq. (5) without the right-hand side. The interaction $V(\mathbf{r})$ is short-range and decreases exponentially outside the region $r \sim a$,⁹ so that its role reduces only to the appearance of a nonzero s -scattering phase shift. These are precisely the arguments used in Refs. 7 and 8 in the calculations of the bremsstrahlung effect.

Obviously, allowance for the exchange effects changes the form of the potential $V(r)$ in (5), but does not influence its short-range character. Therefore, the exchange effect, just as the polarization interaction of the electron with the atom, can be taken into account by a suitable choice of the phase shift [see formula (16) below]. The exchange effects lead also to the appearance in the right-hand side of (5) of additional operators that depend on the field. These operators, however, are also short-range and attenuate exponentially outside the region $r \sim a$ characteristic of the exchange interaction.¹⁾ Therefore the matrix elements of these operators are smaller in the terms of parameter of \hbar/pa than the matrix elements of the long-range operators written out in (5).

We note in this connection that the role of the exchange interaction is substantially different in the bremsstrahlung effect and in the "non-bremsstrahlung" scattering of an electron by an atom. The fact that when condition (1) is satisfied the exchange is immaterial for the bremsstrahlung effect does not in any way contradict the importance of exchange in "non-bremsstrahlung" scattering, for in this case it is precisely the short-range part of the potential which determines the scattering phase shift.

On the basis of the foregoing we can transform the operator Q_e in (5). Since the most essential is the region $r \gg a$, we can expand the Coulomb interaction in

powers of the parameter a/r and confine ourselves to the dipole term, which yields the longest-range non-zero contribution to the matrix element:

$$\sum_{j=1}^z e^2/|r-r_j| \approx \epsilon r d/r^2.$$

As a result we get

$$i\hbar \partial F/\partial t - [T+V(\mathbf{r})]F = [-\epsilon \mathbf{r} \mathbf{E}(t) + e\beta(\omega) \mathbf{r} \mathbf{E}(t)/r^2]F. \quad (6)$$

Here $\beta(\omega)$ is the dynamic polarizability of the atom at the frequency ω , and it is assumed for simplicity that the state φ_0 is spherically symmetrical, so that the polarizability tensor reduces to a scalar. In the general case the polarizability tensor is determined by the expression

$$\beta_{nm}(\omega) = \langle \varphi_0 | d_n G_{\epsilon_0 + \hbar\omega} d_n + d_n G_{\epsilon_0 - \hbar\omega} d_m | \varphi_0 \rangle.$$

The right-hand side of (6) is the effective Hamiltonian of the interaction of the electron with the electromagnetic field. The first term in the right-hand side corresponds to the direct action of the wave on the electron and was taken into account in Refs. 7 and 8. The second term is connected with polarization in the field of the atom, in which a dipole moment $\beta \mathbf{E}(t)$ is induced and scatters the electron. It is shown in Ref. 6 that the effective Hamiltonian (6) is obtained also under conditions when the Born approximation is valid in the region of small momentum transfers, that determine the integral cross section of the bremsstrahlung effect.

2. CROSS SECTION OF BREMSSTRAHLUNG EFFECT

In accordance with the arguments advanced in the preceding section, we write down the solution of Eq. (6) without the right-hand side in the form

$$F_{\mathbf{p}}(\mathbf{r}, t) = e^{-i\epsilon t/\hbar} \sum_l i^l (2l+1) \exp\{i\delta_l\} R_{pl}(r) P_l(\cos \theta), \quad (7)$$

$$\cos \theta = \mathbf{p}\mathbf{r}/pr, \quad \epsilon = p^2/2m,$$

where P_l are Legendre polynomials and δ_l are the scattering phase shifts. The radial functions R_{pl} take the following form

$$R_{p0}(r) = (\hbar/pr) \sin(pr/\hbar + \delta_0(p)), \quad l=0, \\ R_{pl}(r) = j_l(pr/\hbar), \quad l \geq 1,$$

where j_l are spherical Bessel functions corresponding to the free motion.

The action of the short-range potential $V(\mathbf{r})$ reduces in the considered approximation only to the appearance of a nonzero s -scattering phase shift, and the radial function R_{p0} is assumed equal to its asymptotic value.^{7,8} The phase shifts corresponding to $l \geq 1$ turn out to be must smaller than δ_0 by virtue of the inequality (1).

Let us calculate the matrix elements of the operator of the interaction of the electron with the field from the functions (7). For the first term in the right-hand side of (6), which corresponds to the direct action of the wave on the electron, we get

$$\langle F_{\mathbf{p}'}(\mathbf{r}, t) | -\epsilon \mathbf{r} \mathbf{E}(t) | F_{\mathbf{p}}(\mathbf{r}, t) \rangle = \frac{2\pi^2 i e \hbar^2}{m^2 \omega^2} \left(\frac{\mathbf{p}' \mathbf{E}_0}{p} \sin \delta_0 - \frac{\mathbf{p} \mathbf{E}_0}{p'} \sin \delta_0' \right) \delta(\epsilon + \hbar\omega - \epsilon'), \quad \delta_0 = \delta_0(p), \quad \delta_0' = \delta_0(p'). \quad (8)$$

For concreteness, we present here the amplitude of the inverse bremsstrahlung.

It is seen that the amplitude of the transition vanishes if we set equal to zero the scattering phase shifts δ_0 and δ_0' . It is known that this fact reflects the impossibility of photon absorption by a free electron. However, the second term in the right-hand side of (6) (we shall henceforth call it the "polarization" term) has nonzero matrix elements also for transitions between plane-wave states of the electron, inasmuch as the force acting on the electron is not constant in space in this case. Of course, this does not contradict the impossibility of photon absorption by a free electron, since the very appearance of this force is due to the presence of the scattering particle.

It can be shown that allowance for the phase shifts δ_0 leads to the appearance of small quantities in the bremsstrahlung amplitude that is due to the polarization term in (6). For this estimate it is convenient to write down the wave function of the electron in the field of the atom in the scattering-length approximation¹¹:

$$F_{\mathbf{p}}(\mathbf{r}, t) \approx (e^{i\mathbf{p}\mathbf{r}} - r^{-1} L e^{i\mathbf{p}'\mathbf{r}}) e^{-i\epsilon t/\hbar}, \quad (9)$$

L is the scattering length and $\sin \delta_0 \approx -pL/\hbar$. As a result of simple calculations with the functions (9) we easily obtain

$$\langle F_{\mathbf{p}'}(\mathbf{r}, t) | e\beta(\omega) \frac{\mathbf{r} \mathbf{E}(t)}{r^3} | F_{\mathbf{p}}(\mathbf{r}, t) \rangle \\ = 4\pi^2 \hbar e \beta(\omega) \left\{ i\hbar \frac{\mathbf{E}_0 \mathbf{q}}{q^2} - \frac{L}{3} \left[\frac{\mathbf{E}_0 \mathbf{p}}{p'} {}_2F_1\left(\frac{1}{2}, 1; \frac{5}{2}; \frac{p^2}{p'^2}\right) + \frac{\mathbf{E}_0 \mathbf{p}'}{p} {}_2F_1\left(\frac{1}{2}, 1; \frac{5}{2}; \frac{p'^2}{p^2}\right) \right] \right\}. \quad (10)$$

Here $\mathbf{q} = \mathbf{p} - \mathbf{p}'$ is the momentum transfer and ${}_2F_1$ is a hypergeometric function. Since $L \sim a$, the terms in the square bracket in (10) are smaller by a factor $Lq/\hbar \ll 1$ that the first term, thus proving the foregoing statement.

It is also seen from (10) that the matrix elements of the long-range operators are determined by a region with dimensions $\sim \hbar/p$, thus justifying the approximations introduced in the preceding section.

Summing expression (9) and the principal term from (10), we write down the total amplitude of the inverse bremsstrahlung in the form

$$A_{\mathbf{p}\mathbf{p}'}(\omega) = 4\pi^2 i e \hbar^2 (\mathbf{M} \mathbf{E}_0) \delta(\epsilon + \hbar\omega - \epsilon'), \quad (11)$$

$$\mathbf{M} = \frac{\hbar}{2m^2 \omega^2} \left(\frac{\mathbf{p}'}{p} \sin \delta_0 - \frac{\mathbf{p}}{p'} \sin \delta_0' \right) + \frac{\mathbf{q}}{q^2} \beta(\omega).$$

The photon-absorption probability per electron and per atom is

$$dW = \frac{e^2 m}{\hbar^2} p' |\mathbf{M} \mathbf{E}_0|^2 d\Omega_{\mathbf{p}'}. \quad (12)$$

We shall show that this expression does not depend on the polarization of the radiation. We introduce for this purpose the polarization field-density matrix

$$\rho_{ij} = |\mathbf{E}_0|^{-2} E_{0i} E_{0j}^*,$$

with the aid of which we rewrite (12) in the form

$$dW = \hbar^{-2} e^2 m p' |\mathbf{E}_0|^2 \rho_{ij} M_i M_j d\Omega_{\mathbf{p}'}. \quad (13)$$

We have used here the fact that the vector amplitude \mathbf{M} is real. Directing the z axis along the radiation wave

vector, we obtain

$$dW = \frac{e^2 m}{\hbar^2} p' |\mathbf{E}_0|^2 \left\{ \frac{1}{2} (M_x^2 + M_y^2) - l M_x M_y \sin 2\varphi + \frac{l}{2} (M_x^2 - M_y^2) \cos 2\varphi \right\} d\Omega_p, \quad (13)$$

where L is the degree of linear polarization of the radiation, and φ is the angle between the x axis and the direction of the maximum linear polarization.¹² After averaging over this angle we arrive at the statement made above.

Integrating the terms remaining in (13) with respect to $d\Omega_p$, and averaging over the orientations of the initial electron momentum p , we obtain a formula for the integral absorption cross section

$$\sigma_\omega(v) = \frac{16}{3} \pi^2 \alpha \frac{v'}{v} \left\{ \frac{\hbar^2}{2m^2 \omega^3} \left(\frac{v'^2}{v^2} \sin^2 \delta_0 + \frac{v^2}{v'^2} \sin^2 \delta_0' \right) + \frac{\beta^2 \omega}{vv'} \ln \frac{v'+v}{v'-v} - \frac{\hbar \beta}{m\omega} \left[\frac{1}{v} \sin \delta_0 + \frac{1}{v'} \sin \delta_0' \right] + \frac{\hbar \omega}{m v v'} \left(\frac{1}{v} \sin \delta_0 - \frac{1}{v'} \sin \delta_0' \right) \ln \frac{v'+v}{v'-v} \right\}, \quad (14)$$

$$v = p/m, \quad v' = (v^2 + 2\hbar\omega/m)^{1/2}, \quad \alpha = e^2/\hbar c \approx 1/137.$$

Putting $\beta = 0$ in (14) we obtain from this formula the result of Ref. 7. For estimates we can put $\sin \delta_0 \approx pL/\hbar$, $\sin \delta_0' \approx p'L/\hbar$. It is then easily seen that all the terms in (14) are of the same order of magnitude at $v \approx 10^7$ cm/sec and in the optical frequency band $\omega \approx 10^{15}$ Hz.

3. NUMERICAL RESULTS

The coefficient of absorption of radiation by a weakly ionized gas is determined by the relation

$$k_\omega = N_e N_a \langle v \sigma_\omega(v) \rangle, \quad (15)$$

where N_e and N_a are the densities of the electrons and atoms, and the averaging is over the electron distribution function. The determination of the numerical values of the absorption coefficient from formulas (14) and (15) entails no difficulty if the scattering phase shift δ_0 is known. In the low-energy approximation of O'Malley, Spruch, and Rosenberg⁹

$$p \operatorname{ctg} \delta_0 = -\frac{\hbar}{L} + \frac{\pi \alpha c m \beta}{3 \hbar L} p + \frac{2 \alpha c m \beta}{3 \hbar^2 L} \ln \frac{\alpha c m \beta p^2}{16 \hbar^2}. \quad (16)$$

Such an expression for the phase shift was used, in particular in Ref. 13 to calculate the absorption coefficient of a weakly ionized gas in the low-frequency region of the spectrum, using formulas derived in Ref. 7 and 8.

Figures 1 and 2 show the behavior of the quantity $\langle v \sigma_\omega(v) \rangle$ as a function of the radiation frequency for neon and argon. A Maxwellian electron distribution was assumed, with the absolute temperature marked in the figures. The scattering lengths were chosen to be¹¹ $L = 0.106 \text{ \AA}$ for neon and $L = -0.875 \text{ \AA}$ for argon. At a frequency ω much lower than the natural atom absorption frequency, the dynamic polarizability can be set equal to the static value. We have therefore assumed¹⁴ $\beta = 0.4 \text{ \AA}^3$ for neon and $\beta = 1.64 \text{ \AA}^3$ for argon.

The solid lines in the figures correspond to calculation of the cross section by formula (14), and the dashed lines correspond to calculation without allow-

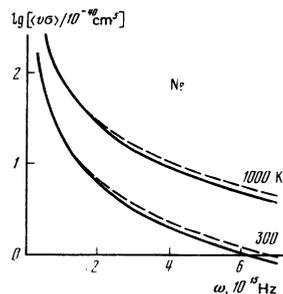


FIG. 1. Frequency dependence of the reduced photoabsorption coefficient of electrons in neon.

ance for the polarizability of the atom in formula (14), but with account taken of the influence of the polarizability on the phase shift in (16). It is seen that in the case of neon the influence of the polarization interaction of the electron with the radiation is negligible, but for argon the absorption curve changes strongly. This is due to the fact that argon has a negative scattering length, so that destructive interference takes place between the contributions made to the bremsstrahlung amplitude effect by the two terms in the Hamiltonian of the interaction between the electron and the field. We recall that the negative scattering length in argon leads also to the Ramsauer effect, which was observed in neon. However, the minimum of the photoabsorption curve is not connected directly with the Ramsauer effect, since the frequency corresponding to the photoabsorption minimum is much higher in this case than the width of the Ramsauer dip. This fact is seen also in Fig. 2: the dashed lines calculated with account taken of the Ramsauer effect in the scattering phase shifts remain monotonic. At $\hbar\omega \gg kT$ the position of the minimum on the absorption curve is determined at $L < 0$ by the approximate formula $\omega_{\min} \approx \hbar |L| / m\beta$.

We discuss now the influence of the unaccounted-for small effects on the noted singularity of the absorption coefficient, which is connected with the mutual cancel-

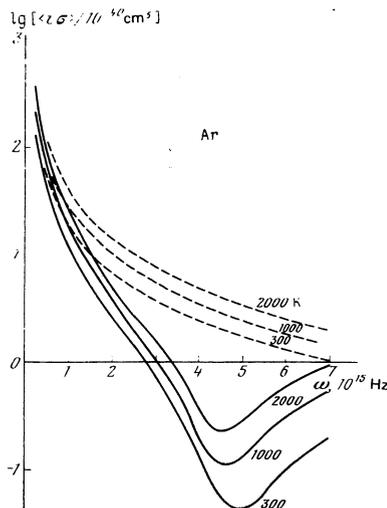


FIG. 2. Frequency dependence of the reduced photoabsorption coefficient of electrons in argon.

lation of the principal terms. If we make the natural assumption that the small quantities have a smooth dependence on the radiation frequency, then the small corrections, by interfering with the principal terms, lead to a shift of the calculated minimum. On the other hand, if the small corrections give an additive increment to the absorption cross section, then the entire frequency dependence of the absorption coefficient shifts upwards with practically no deformation. Thus, the qualitative conclusion that the absorption coefficient has a deep minimum remain unchanged.

The author thanks V. M. Buřmistrov for remarks and V. N. Kolesnikov for interest in the work.

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Translated by J. G. Adashko

Interaction potential of He(2^3S_1) atoms with H₂ molecules at thermal energies

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(Submitted 22 January 1979)
Zh. Eksp. Teor. Fiz. **77**, 52-59 (July 1979)

Optical orientation of the atoms was used to investigate the ionization of H₂ molecules by He(2^3S_1) atoms. The temperature dependence of the reaction rate constant $\bar{C}(T)$ is determined in the interval 77-400 K. Analytic expressions for $\bar{C}(T)$ are obtained within the framework of the classical treatment of the chemo-ionization process for the case of an exponential representation of the real and imaginary parts of the complex interaction potential $V^* - i\Gamma/2$. This has made it possible to obtain for this potential parameters that agree with the obtained experimental $\bar{C}(T)$.

PACS numbers: 82.20.Pm, 82.20.Kh, 82.30.Cf, 34.20.Be

INTRODUCTION

The excitation energies of metastable helium atoms, 19.8 eV for 2^3S_1 and 20.6 eV for the 2^1S_0 state, are sufficient for the ionization of most atoms (with the exception of helium and neon in the ground state) and molecules. The investigation of the ionization reactions with participation of metastable helium atoms has received much attention of late.¹⁻⁷ The simplest molecule that can be ionized by a helium atom in a metastable state is hydrogen. In the case of He*(2^3S_1), this reaction proceeds via the following channels:



where (1a) is Penning ionization and its contribution is >80%⁸; (1b) is associative ionization with a contribution ~3%⁸; (1c) is ionization with restructuring, with a contribution ~15%⁸; (1d) is dissociative ionization with the smallest contribution, <1%.¹

The total ionization cross section σ_{H_2} , which is the sum of the cross sections of all the channels of the reaction (1), was determined in experiment by investigating a decaying plasma⁹⁻¹¹ using atomic and molecular beams^{12,13} as well as with the aid of optical orientation of atoms.¹⁴⁻¹⁶