EXCITATION CROSS SECTION OF He *ATOM IN SLOW COLLISIONS WITH* He

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Starting from the existence of a region of pseudo-intersection of the terms at small internuclear distances, we calculate the cross section for the transition of the He atom into the $2s^1S_0$ state following a collision with He. In the pseudo-intersection region ($R = 1.1a_0$), the term separation equals 2.84 eV. The cross section calculated in the 100–500 eV region of relative energy in the laboratory frame amounts to $\sim 2 \times 10^{-17}$ cm^2.

MANY recent experimental and theoretical papers are devoted to inelastic interactions of atoms at low energies ([1-5] and others). Whereas the experimental papers give values for the cross sections (cf., e.g.,[3]), the theory is still being discussed at the level of the general[4] or particular[5] analysis of various models. A concrete calculation of the cross sections, which is necessary for both experiment and theory, is therefore quite timely.

Since it has been shown in[3] that for inert gases the ionization rate in atom-atom collisions is determined mainly by the rate of excitation of the atom to the level closest to the ground level, we shall calculate the excitation cross section of the simplest system in the reaction

$$\mathrm{He}(1s^2\,{}^1S_0) + \mathrm{He}(1s^2\,{}^1S_0) \to \mathrm{He}(1s^2\,{}^1S_0) + \mathrm{He}(1s2s\,{}^1S_0).$$

Out of the two possible singlet states of the excited HeHe* quasimolecule, we are naturally interested in the state having the same symmetry as the ground state, i.e., $^1\Sigma g$.

Comparison of the terms of the ground and excited states calculated in[6,7] indicates that in the region of small internuclear distances, at $R = 1.1a_0$, there is a pseudo-intersection "point" $U_R = 1.64\ e^2/a_0$, reckoned from the ground state of the He-He system. An analysis of the behavior of the terms of the same quasimolecule, performed in[5], confirms convincingly the existence of pseudo-intersections in the region of small R[1]. In this case the transition probability is written in the form

$$W = P_1(1-P_1)[1 + (1-P_2)^2 + P_2^2(1-P_3)^2 + P_2^2P_3^2(1-P_4)^2 + \ldots], \quad (1)$$

where

$$P_i = \exp(-2\pi V_{min}^2/\hbar v|F_n - F_m|)$$

is the transition probability for a single passage of the i-th pseudo-intersection point, corresponding to the Landau-Zener problem. In the region of the maximum of W, we can approximate (1) by means of the expression

$$W = P_1(1-P_1) \quad (2)$$

with accuracy ~50% in the worse variant. However, since P_2 corresponds to a transition between the S- and P-states, we can hope that at the maximum of W the value of P_2 will be not smaller than $\frac{1}{2}$. In this case, the error amounts to ~25%. Obviously, with increasing velocity, the accuracy of formula (2) will increase.

The cross section of the transition with allowance for (2) was calculated from the formula

$$\sigma = 2\pi R_1 \int_1^\infty e^{-\eta x}(1 - e^{-\eta x})x^{-3}\,dx, \quad (3)$$

where $\eta = \pi\Delta U/\hbar v\Delta F$, v—radial velocity, ΔF—difference of the forces at the point of pseudo-intersection, and the separation of the terms is

$$\Delta U = 2\frac{S_{ff}H_{if} - S_{if}H_{ff}}{S_{ff}^2 - S_{if}^2}.$$

Here

$$S_{if} = \int \Psi_i^*\Psi_f\,d\tau, \quad S_{ff} = \int \Psi_f^*\Psi_f d\tau,$$

$$H_{if} = \int \Psi_i^*\hat{H}\Psi_f\,d\tau, \quad H_{ff} = \int \Psi_f^*\hat{H}\Psi_f d\tau,$$

where $\hat{H}$ is the total Hamiltonian of the He-He system, and Ψ_i and Ψ_f are the fully-symmetrized wave functions of the ground and excited states of the He-He system, similar to those used in[7]. The necessary matrix elements were calculated with an electronic computer, and the term separation for the region $R = 1.1a_0$ of interest to us is $\Delta U = 2.84$ eV.

The cross section for the excitation of He atoms by collisions with He, calculated from formula (3) for the kinetic energy of relative motion in the laboratory coordinate frame, are as follows:

E_∞^{lab}, eV:	100	150	200	300	500
σ, 10^{-17} cm^2:	2.23	2.3	2.1	1.89	1.72

The calculation was performed starting with $E_\infty^{l.s.} = 100$ eV, which in our case is the lower limit of the applicability of the Landau-Zener formula[9].

The figures following the decimal points are given only to indicate the maximum of the cross section, without claiming, of course, an accuracy higher than that indicated.

Unfortunately, we do not know the experimental cross sections of the reaction considered above. However, the ionization cross sections in He-He$^+$ collisions amount to $(2.4–2.6) \times 10^{-17}$ cm^2 in the energy region 100–400 eV[10], and the cross sections for the excitation of Ar, Kr, and Xe, extrapolated to the same energy interval, are respectively $(0.4–4) \times 10^{-17}$, (0.5–5)

[1] We note that at $R \approx 3a_0$ there exists a non-adiabaticity region due to the "break" of the adiabatic terms [8] made up of the He$^+$-He and He-He* ($1s2s\ ^1S_0$) terms. Here, however, we shall disregard this non-adiabaticity.

$\times 10^{-17}$, and $(0.8-7) \times 10^{-18}$ cm[2][3]. These data confirm, albeit indirectly, the assumed model of the excitation reaction. We note that the approximation of the cross section in the threshold region by means of a linear function of the energy, $\sigma = C(E - E^*)$[1-3], in analogy with excitation by electron impact, can apparently be explained by means of the model proposed in[8], but when the energy is increased the contribution to the cross section from the quasi-intersection region becomes fundamental and is determined entirely by the model assumed here. Naturally, in this case with increasing kT there should be observed a change in the threshold energy E*, from ~23.5 eV (region of the "kink") to ~44.6 eV (region of the non-adiabatic transitions considered here).

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