Auger transitions to the $2p\pi$ orbital in the collisions of light atoms

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The energies of the $2p\pi$ level in a quasi molecule were determined experimentally for the first time by using the method of Auger spectroscopy.

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A quasi molecule produced by two colliding atoms can develop internal vacancies. A disintegration of vacancies by Auger transitions leads to the appearance of electrons whose energy distribution reflects the behavior of the energy $E(R)$ and width $\Gamma_A(R)$ of a level with vacancies as a result of variation of the internuclear distance R. Therefore, an analysis of Auger spectra can be used, in principle, for the spectroscopy of the levels of quasi molecules.

The probability of appearance of vacancies in the $2p\pi$ molecular orbital is high in the collisions of light atoms with $Z \leqslant 10$, since this orbital, which is formed from the vacant levels of the atoms, decreases with decreasing internuclear distance. Investigation of Auger transitions to the $2p\pi$ orbital, however, is a difficult problem which requires a measurement of the cross sections $d^2\sigma/dE_e dp$ of differential electrons with respect to energy E_e and impact parameters p. The difficulty stems from the fact that the energy spectra of electrons produced as a result of collisions in the keV range of initial energies have an intensive continuous component attributable to direct ionization of outer electrons.[1] The characteristic region for such transitions are the internuclear distances $R \approx 1$ Å. At the same time, investigation of the $2p\pi$ orbital requires that the particles be brought together to $R \approx 0.1$ Å. The ratio of the geometrical cross sections (πR^2) for these two processes is $\sim 10^2$. As a result, the continuous component associated with the direct ionization produces an intensive background that prevents Auger transitions to the $2p\pi$ orbital.

In this paper we overcome this difficulty by using the method of recording the electrons from the coincidences with the ions scattered at a fixed angle, which enables us to identify the electron collision spectra for the given impact parameters p.[2] This reduced the relative contribution of the continuous component in the spectra measured at fixed $p \approx 0.1$ Å by a factor of about 10^2 as compared with the spectrum summed over all the impact parameters $d\sigma(E_e)/dE_e$.

To study the $2p\pi$ orbital in the O—O and Ne—Ne quasi molecules, we measured the spectra of electrons produced in the O^+—O_2 and Ne^+—Ne collisions at incident ion energies $E_0 = 10$–50 keV. The experimental spectra are shown in Fig. 1. The exponents in the $d^2\sigma/dE_e dP$ spectra peak in the region $E_e \approx 80$–160 eV, whereas only the continuous component, which decreases with increasing E_e according to the exponential law, is present in the $d\sigma/dE_e$ spectra.[1] The most important argument confirming the quasi—molecular nature of the observed maxima is their shift in the direction

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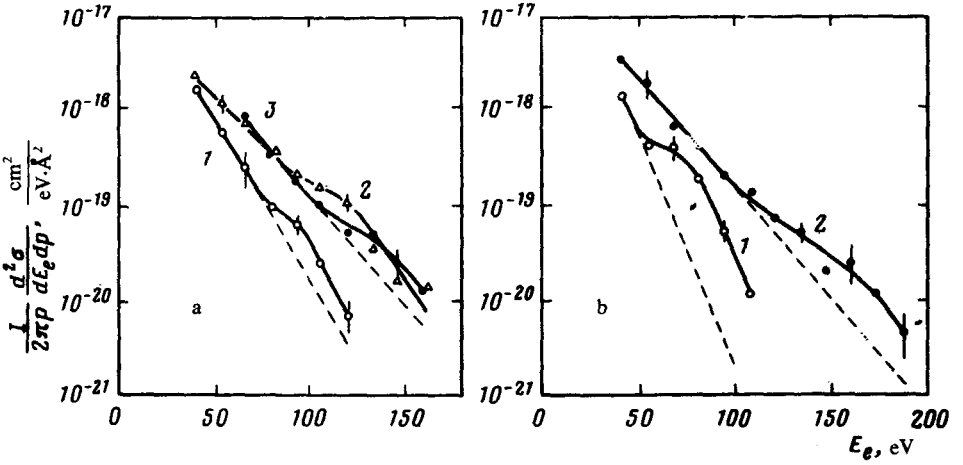

FIG. 1. Energy spectra of electrons produced in the collisions: a, O^+–O_2; 1, $E_0 = 25$ keV, $\theta = 8°$, $p = 0.18$ Å; 2, $E_0 = 50$ keV, $\theta = 4°$, $p = 0.16$ Å; 3, $E_0 = 50$ keV, $\theta = 9°$, $p = 0.09$ Å; b, Ne^+–Ne; 1, $E_0 = 15$ keV, $\theta = 13.3°$, $p = 0.19$ Å; 2, $E_0 = 50$ keV, $\theta = 12°$, $p = 0.09$ Å.

of large E_e with decreasing impact parameter. Such behavior is characteristic for Auger transitions to the orbital that decreases with decreasing R. Moreover, the peak electron energies differ greatly from the energies of Auger electrons produced as a result of filling the K vacancies in an isolated O atom ($\sim$470 eV) and Ne atom ($\sim$750 eV), and conversely, correspond to the energies of Auger electrons produced because of disintegration of the $2p\pi$ vacancies, which can be predicted on the basis of the correlation diagrams for Ne—Ne.[3]

The behavior of the $2p\pi$ orbital as a function of the internuclear distance can be reconstructed with an accuracy to within the binding energies of outer electrons from the energies of the Auger electrons produced at the point of greatest convergence R_0. At electron energies corresponding to the transitions in the neighborhood of R_0, the $\frac{d^2\sigma}{dE_e dP}(E_e)$ spectrum must have a peak that is described by the Airy function - $Ai(x)$[4]:

$$\frac{d^2\sigma}{dE_e dp} = 4\pi p f\, \Gamma_A\, \alpha^{-2/3}\, Ai^2\{\alpha^{-1/3}[E_e - E_e(R_0) + \frac{i}{2}\Gamma_A]\}, \quad (1)$$

where f is the number of vacancies in the orbital and α is the product of dE/dR and the acceleration d^2R/dt^2. We shall show that $\Gamma_A < 1$ eV in the investigated cases, i.e., the lifetime of the vacancies is much larger than the collision time ($\sim 10^{-16}$ sec); therefore, we can disregard a decrease in the number of vacancies due to disintegration (contribution of the imaginary part in the argument). We know that the value of $Ai^2(0)$—i.e., at the point $E_e = E_e(R_0)$—is equal to 0.44 of the maximum Airy function. The values of $E_e(R_0)$ determined in this manner are given in Table I. The connection between the scattering angel θ, p, and R_0 was calculated for the internuclear potential from Ref. 5.

Figure 2 shows the correlation diagrams of the molecular orbitals for the O—O and Ne—Ne quasi molecules. The diagram for Ne—Ne was calculated in Ref. 3 and

TABLE I.

collision	$O^+ - O_2$			$Ne^+ - Ne$	
E_0, keV	25	50		15	50
p, A	0.18	0.16	0.09	0.19	0.09
R_0, Å	0.20	0.17	0.10	0.23	0.10
$E_e(R_0)$, eV	105 ± 10	130 ± 10	155 ± 10	85 ± 10	170 ± 10

that for O—O was constructed by us by means of the scale transformation ($E \sim Z_{\text{eff}}^2$, $R \sim 1/Z_{\text{eff}}$) of the standard correlation diagrams of Ne–Ne and N–N[3]. The vertical lines in Fig. 2 represent the energies $E_{2p\pi}$ obtained from the experimental electron energies $E_e(R_0)$. The height of the vertical lines corresponds to the uncertainty of the binding energies of the outer electrons that participate in the Auger transition. The maximum (in absolute value) energy $E_{2p\pi}$ can be obtained by assuming that $2p\pi$ vacancies disintegrate via the $(2p\pi)^{-1} \rightarrow (3p\sigma)^{-2}$ transitions and the minimum energy can be obtained by assuming that they disintegrate via transitions with the participation of electrons with a zero binding energy. As seen in Fig. 2, the experimental energy $E_{2p\pi}$ is in good agreement with the calculated energy.

The values of Γ_A were estimated on the basis of expression (1). The experimental values of $f\Gamma_A$ for O^+—O_2 and Ne^+—Ne are equal to 1×10^{14} and 5×10^{14} sec^{-1}, respectively. The number of vacancies f was estimated from the statistical consider-

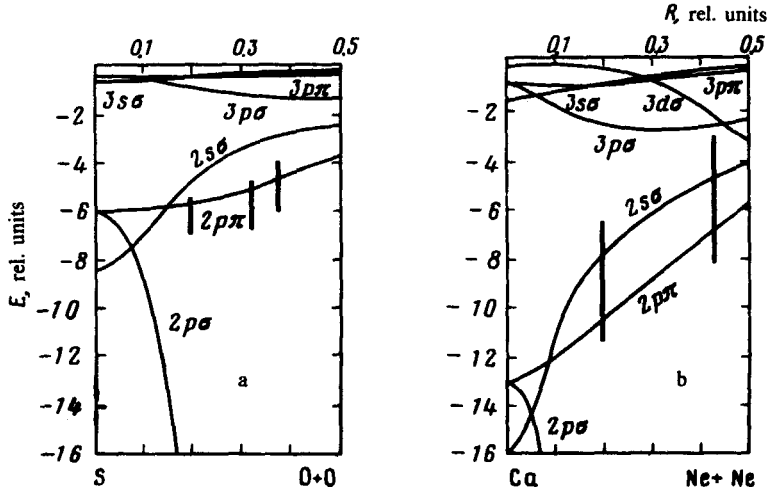

FIG. 2. Correlation diagrams of quasi molecules; a, O–O; b, Ne–Ne.

ations. The probability of the existence of m vacancies in the $2p\pi$ orbital is determined by the number of combinations of the $2p$ vacancies, which are present in the atoms prior to the collision, in the orbitals formed from the $2p$ levels. The average number of vacancies is $f = \Sigma_m m(C^m_{n_v} C^{4-m}_{n_e} / C^4_n)$, where n_e and n_v are the number of electrons and vacancies in the $2p$ levels prior to collision and $n = n_v + n_e$. The average number of vacancies in the investigated O^+—O_2 and Ne^+—Ne is 1.67 and 0.33, respectively.

According to an estimate, $\Gamma_A \sim 10^{14}$ sec^{-1} ($\sim$0.1 eV) for the O—O quasi molecule and $\sim 10^{15}$ sec^{-1} ($\sim$1 eV) for Ne—Ne. Both values are close to the probabilities of Auger decay of the $2p$ vacancies in the combined atoms: S($Z = 16$) and Ca($Z = 20$). The calculated values[6] of Γ_A for the S and Ca atoms are equal to 1.0×10^{14} and 3.3×10^{14} sec^{-1}, respectively.

It should be noted that the value of Γ_A in the investigated cases differs from that in the Kr—Kr quasi molecule.[7] The probability of Auger transitions to an orbital identified as $4p\pi$ in the case of Kr^+—Kr turned out to be $\sim 10^{16}$ sec^{-1}, which is more than an order of magnitude higher than the transition probability characteristic of isolated atoms. The reasons for an increase of Γ may be that the number of electrons in a quasi molecule, in contrast to an isolated atom, may increase in the upper levels that participate in the Auger transitions and the wave functions of the states between which the transition occurs may overlap.

One of the objectives of our study was to determine how common is the increase of Γ_A in a quasi molecule. The results show that the conditions leading to an increase of Γ_A do not exist in every quasi molecule, i.e., in contrast with isolated atoms an increase of Γ_A in them is not compulsory.

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