CHARGE EXCHANGE OF Xe^{3+} *AND* Xe^{4+} *IN NEON*

G. N. OGURTSOV and I. P. FLAKS

Leningrad Physico-technical Institute, Academy of Sciences, U.S.S.R.

Submitted to JETP editor October 12, 1961

J. Exptl. Theoret. Phys. (U.S.S.R.) **42**, 721-724 (March, 1962)

The cross sections for electron capture in single collisions between Xe^{3+} or Xe^{4+} ions and Ne atoms are measured. For accelerating voltages from 2 to 30 kV the capture cross sections σ^{32} and σ^{43} are large and reach values of the order 10^{-15} cm^2. The absolute magnitude of σ^{32} is greater than that of σ^{43} and its maximum is reached at the relative ion velocity v $\approx 10^7$ cm/sec. The cross section σ^{43} increases with Xe^{4+} kinetic energy over the entire investigated range. The experimental results are compared with calculations based on the Landau-Zener method of the pseudo-crossing of potential energy curves. Satisfactory agreement is found between the calculated and experimental curves for $\sigma^{32}(v)$ and $\sigma^{43}(v)$.

INTRODUCTION

WE have previously[1,2] investigated charge exchange occurring in collisions between fast I^{n+} ions (n = 1, 2, 3) and inert gas atoms. In the range of accelerating voltages from 2 to 30 kV the cross sections for endothermic and exothermic charge exchange differ greatly. For example, for the endothermic charge exchange $Xe^{2+} + Ne \rightarrow Xe^{+} + Ne^{+}$ ($\Delta E \approx -0.36$ eV) the cross section σ^{21} was almost two orders of magnitude smaller than for the exothermic process $Kr^{2+} + Ne \rightarrow Kr^{+} + Ne^{+}$ ($\Delta E \approx 3.0$ eV); in the latter case σ^{21} exceeded 10^{-15} cm^2. For the exothermic charge exchange of Ne^{3+} in Kr ($\Delta E \approx +50$ eV) the cross section σ^{32} reached 4 $\times 10^{-15}$ cm^2, with a maximum indicated at ion kinetic energy T < 9 keV.

In order to account for the foregoing results it was suggested that in the exothermic charge exchange of multicharged ions a pseudo-crossing of the potential energy curves of the system before and after collision can occur at moderate values of the internuclear distance R_X. In this case the probability of electron transfer is not determined by the internal energy difference ΔE of the system at infinity, but rather by the internal-energy difference $\Delta U(R_X)$ at the closest approach of the potential energy curves. It should be noted, however, that for Ne^{3+} in Kr the absolute value of σ^{32} and the shape of the $\sigma^{32}(T)$ curve could be determined both by pure charge exchange and by exothermic ionization with capture. In the latter case the energy liberated by electron capture is expended for further ionization.[3] The ions Xe^{3+} and Xe^{4+} in Ne were the most suitable objects for both the experimental and theoretical investigations of charge-exchange processes.

In collisions of Xe^{3+} and Xe^{4+} ions with Ne atoms the reduction of ion charge results practically entirely from pure charge exchange:

$$Xe^{3+} + Ne \rightarrow Xe^{2+} + Ne^{+} \quad (DE = +10{,}54\text{eV}), \quad (1)$$
$$Xe^{4+} + Ne \rightarrow Xe^{3+} + Ne^{+} \quad (DE = +23{,}94\text{eV}), \quad (2)$$

since ionization with capture in the processes

$$Xe^{3+} + Ne \rightarrow Xe^{2+} + Ne^{2+} + e,$$
$$Xe^{4+} + Ne \rightarrow Xe^{3+} + Ne^{2+} + e$$

is endothermic and the cross sections σ_{02}^{32} and σ_{02}^{43} make only small contributions to the measured total cross sections σ^{32} and σ^{43}.

For relatively small values of ΔE pseudo-crossing of the potential curves will occur at distances R_X of only a few atomic units. In these cases we can attempt a theoretical calculation of the cross sections for single-electron charge exchange by the Landau-Zener method.

An additional reason for selecting the Xe^{4+}—Ne system was the possibility of producing a fairly intense Xe^{4+} beam, thus enabling us to extend our previous measurements of charge-exchange cross sections to this higher ion charge. As in our earlier work the range of accelerating voltages was 2—30 kV.

EXPERIMENTAL TECHNIQUE AND RESULTS

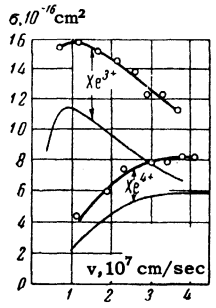
The charge-exchange cross sections σ^{32} and σ^{43} were determined by measuring the primary fast-ion current and the current of fast ions with charged reduced by one unit. A detailed descrip-

tion of the technique and apparatus can be found in [1,2]. Charge-exchange cross sections were determined from the formula

$$\sigma^{nm} = (kT_0/pl)\,[\,(N_{ni}/N_n)_p - (N_{mi}/N_n)_r\,], \qquad (3)$$

where N_n is the intensity of the primary ion beam entering the collision chamber, N_m is the intensity of the secondary ion beam, p and T_0 are the gas pressure and temperature in the collision chamber, and k is the Boltzmann constant. The subscripts p and r denote measurements at the operating pressure of the investigated gas in the collision chamber and in the residual gas. The operating pressure never exceeded 2×10^{-4} mm Hg, thus insuring single collisions. The residual gas pressure was under 5×10^{-6} mm. The total error in the cross sections did not exceed 15%.

The heavy curves in the accompanying figure represent the charge-exchange cross sections σ^{32} and σ^{43} determined from (3) as functions of the velocity of the primary Xe^{3+} and Xe^{4+} ions. The maximum of σ^{32} was close to 1.6×10^{-15} cm at $v \approx 10^7$ cm/sec; this cross section decreases at higher velocities. The cross section σ^{43} is smaller than σ^{32}; its initial rapid increase with velocity becomes a slower gradual approach to $\sim 8 \times 10^{-16}$ cm^2 at $v \approx 4 \times 10^7$ cm/sec.



Cross section for single-electron charge exchange of Xe^{3+} and Xe^{4+} in Ne as functions of velocity v. Heavy curves—experimental; thin curves—calculated.

DISCUSSION OF RESULTS

In order to account for the observed $\sigma^{32}(v)$ and $\sigma^{43}(v)$ curves and the large charge-exchange cross sections at relatively low ion velocities we calculated the cross sections for single-electron charge exchange using the theory of Landau [4] and Zener. [5] Bates and Moiseiwitsch [6] and Dalgarno [7] have performed similar calculations for the charge exchange of doubly- and triply-charged ions in atomic hydrogen; Boyd and Moiseiwitsch [8] have calculated charge exchange in helium. Our calculation was simplified by considering only states where the projection of the orbital angular momentum was zero. The cross sections for processes (1) and (2) are then given by

$$\sigma = 4\pi R_x^2 \int_1^\infty e^{-\eta x}\left[1 - e^{-\eta x}\right] x^{-3} dx, \qquad (4)$$

where R_x is the internuclear distance at which pseudo-intersection of the potential curves occurs. The value of η is given by

$$\eta = 247\,(n-1)\,\mu^{1/2}[\Delta U\,(R_x)\,]^2/T^{1/2}\,(\Delta E)^2, \qquad (5)$$

where μ is the reduced mass, n is the multiplicity of ion charge, T is the ion kinetic energy, ΔE is the resonance defect, and $\Delta U(R_x)$ is the separation of the potential curves at the point R_x.

The internuclear distance R_x can be determined from the energy balance equation at the crossing point of the curves:

$$-E_1 - ne^2/R_x - \alpha n^2 e^2/2R_x^4 = -E_2 - e^2/R_x, \qquad (6)$$

where α is the polarizability of the neon atom. We neglect the polarization of ions formed in the reaction, since the contribution of polarization corrections is substantially reduced with decreased ion charge and increased ionization energy. [9] Representing the difference $E_2 - E_1$ at infinity by ΔE, we obtain

$$\Delta E = (n-1)\,e^2/R_x + \alpha n^2 e^2/2R_x^4. \qquad (7)$$

The ground-state values of E_1 and E_2 were used in calculating R_x, since transitions to excited levels result either in endothermic reactions or in the crossing of levels at very large distances. We calculated $\Delta U(R_x)$ from the perturbation formula [6]

$$\Delta U\,(R_x) = \frac{2\,|\,H_{if}\,(R_x) - S_{if}\,(R_x)\,H_{ff}\,(R_x)\,|}{1 - |\,S_{if}\,(R_x)\,|^2}, \qquad (8)$$

where H_{if} and H_{ff} are matrix elements of the Hamiltonian operator, and S_{if} is the integral for the transition between the initial and final states:

$$S_{if} = \int_\tau \Phi_i^* \Phi_f d\tau. \qquad (9)$$

In the calculation of S_{if} the stationary functions Φ_i and Φ_f were Slater hydrogen-like wave functions, [10] which are sufficiently good approximations in problems concerning the transfer of a single outer electron from any atom. These functions are

$$\Phi_{nl} = Cr^{n^*-1}e^{-(Z-s)r/n^*}Y_{lm}\,(\vartheta,\ \varphi), \qquad (10)$$

where n* is the effective principal quantum number, Z is the charge of the atom or ion, s is the screening constant, and C is the normalizing factor. The integrals in the expression for $\Delta U(R_x)$ were computed in elliptic coordinates and the solution was obtained as a function of the internuclear distance R.

Process	ΔE, eV	R_x/a_0	S_{if}	$\Delta U(R_x)$, eV
(1)	10.54	5.35	$1.78 \cdot 10^{-2}$	1.3
(2)	23.94	3.8	−0.35	5.3

The calculated values of R_X (in atomic units), S_{if} and $\Delta U(R_X)$ (in eV) are given in the table. The calculated cross sections σ^{32} and σ^{43} as functions of the relative velocity v are the thinner curves in the figure, where a good correspondence between the experimental and calculated curves is seen. The measured and calculated maxima are located at approximately identical velocities, but the absolute measured cross sections are about 1.5 times larger than the calculated cross sections. This discrepancy can be accounted for by experimental and calculating errors and by defects of the Landau-Zener theory, which have been thoroughly discussed by Bates.[11] In particular, the hypothesis that electron transfer can occur only in a very narrow region near the crossing of levels is apparently not confirmed in our case. According to Bates, the width ΔR_a of the transition zone at the kinetic energy corresponding to the maximum transfer probability can be obtained from the formula

$$\Delta R_a \cong 0.245 \, |\Delta U(R_x)| \, R_x^2. \qquad (11)$$

For our processes (1) and (2) we have

$$\Delta R_a \cong \frac{0.245}{\sqrt{n-1}} \left| \Delta U(R_x) \right| R_x^2. \qquad (12)$$

Substituting the calculated values of $\Delta U(R_X)$ and R_X in (12), we obtain $\Delta R_a \approx 6.4$ atomic units for process (1) and $\Delta R_a \approx 10.8$ for process (2).

Our analysis shows that the theory of pseudocrossing of the potential energy curves provides a good explanation of the observed cross sections for the charge exchange of Xe^{3+} and Xe^{4+} in Ne. The same theory can probably also account for the exothermic charge exchange of multicharged ions which we investigated previously.

In conclusion the authors wish to express their deep appreciation to O. B. Firsov for valuable comments in a discussion of the results, and to N. V. Fedorenko and V. M. Dukel'skiĭ for their continuous interest.

[1] I. P. Flaks and E. S. Solov'ev, ZhTF **28**, 599 and 612 (1958), Soviet Phys.-Tech. Phys. **3**, 564 and 577 (1958).

[2] I. P. Flaks and L. G. Filippenko, ZhTF **29**, 1100 (1959), Soviet Phys.-Tech. Phys. **4**, 1005 (1959).

[3] Flaks, Ogurtsov, and Fedorenko, JETP **41**, 1438 (1961), Soviet Phys. JETP **14**, 1023 (1962).

[4] L. D. Landau, Sow. Phys. **1**, 88 (1932); **2**, 46 (1932).

[5] C. Zener, Proc. Roy. Soc. (London) **A137**, 696 (1932).

[6] D. R. Bates and B. L. Moiseiwitsch, Proc. Phys. Soc. (London) **A67**, 805 (1957).

[7] A. Dalgarno, Proc. Phys. Soc. (London) **A67**, 1010 (1954).

[8] T. J. M. Boyd and B. L. Moiseiwitsch, Proc. Phys. Soc. (London) **A70**, 809 (1957).

[9] N. F. Mott and I. N. Sneddon, Wave Mechanics and its Applications, Oxford Univ. Press, 1948.

[10] J. C. Slater, Phys. Rev. **36**, 57 (1930).

[11] D. R. Bates, Proc. Roy. Soc. (London) **A257**, 22 (1960).

Translated by I. Emin
115