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Measurements of Inelastic Energy Loss in Single Atomic Collisions of Kr^+ on Kr at keV Energies and Large Scattering Angles

B. Fastrup and G. Hermann
Institute of Physics, University of Aarhus, DK 8000 Aarhus C, Denmark
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The inelastic energy loss Q has been measured for Kr^+-Kr single collisions at incident energies of 20 and 30 keV and scattering angles ranging from 6° to 15°. For distances of closest approach r_0 around 0.385 Å, the inelastic energy-loss distribution is triple peaked, and the differences in energy between the three peaks are independent of r_0. This structure is interpreted as being due to the production of one or two $M_{IV,V}$ vacancies.

INTRODUCTION

During the last ten years there has been great interest in inner-shell excitations in heavy ions produced by single collisions with heavy ions. Symmetric collisions, for example Ar^+-Ar, Ne^+-Ne, and Kr^+-Kr, have been studied by several groups. Afrosimov *et al.*[1] and Kessel and co-workers[2] have investigated Ar^+-Ar collisions in detail and found a triple-peaked distribution of the inelastic energy loss Q for distances of closest approach r_0 in a narrow region around 0.24 Å. The lowest Q value (Q_I) was interpreted as being due to M-shell excitation alone, and Q_{II} and Q_{III} as being due to M-shell excitation plus the formation of an $L_{2,3}$ vacancy in one or both collision partners, respectively. At small r_0 the probability of creating a vacancy in both collision partners becomes almost unity. The L vacancies decay almost exclusively by Auger processes, and LMM Auger electrons from Ar^+-Ar collisions were found by, for instance, Rudd *et al.*[3] The Ne^+-Ne case has been investigated by Kessel *et al.*,[4] who found a double-peaked structure in Q for $r_0 \lesssim 0.06$ Å. The lower Q value Q_I was attributed to L-shell excitation, and the higher one Q_{II} to L-shell excitation plus the formation of a K vacancy in one of the neon ions. The probability of creating one vacancy never exceeds 0.2, and the creation of a vacancy in both collision partners has not been observed. For this combination, KLL Auger electrons were also found.[4]

The results for these two symmetric cases have been discussed by Fano and Lichten[5] and Lichten[6] in terms of one-electron molecular orbitals. They predicted a promotion of inner-shell electrons ($L_{2,3}$ electrons for Ar and K electrons for Ne) into the outer shells for r_0 smaller than a critical value.

Also, a third symmetric case, Kr^+-Kr, has been investigated. Using a coincidence technique, Afrosimov *et al.*[7] measured both Q values and charge-state distributions at incident energies $E_0 = 25$ and 50 keV. At 25 keV and incident-particle scattering angle $\theta = 9°$, corresponding to $r_0 = 0.39$ Å, they found a sudden change in the mean Q and the degree of ionization of the collision partners. They also measured the total differential scattering cross section and found a pronounced peak at the same r_0. Coincidence measurements on Kr^+-Kr have also been performed by McCaughey *et al.*[8] using energies from 6 to 200 keV and scattering angles from 6° to 40°. At $r_0 = 0.39$ Å they found a sudden increase in the mean Q (from 60 to 230 eV) and a marked broadening in the Q distribution without resolving any structure. Moreover, electron-spectra measurements by the same authors did not show a resolved peak corresponding to fast Auger electrons.

Since our noncoincidence method (see below) gives a better resolution of the Q spectra than does the ordinary coincidence method, we studied again the Kr^+-Kr case with $E_0 = 20$ and 30 keV and $\theta = 6°-15°$. Our data clearly reveal a triple structure in the Q spectrum, due to the promotion of one or two $M_{IV,V}$ electrons in Kr.

EXPERIMENTAL METHOD

The apparatus and the experimental method have been described in detail,[9] and only a brief review will be given here. The isotopically pure Kr^+ beam is supplied by a 80-keV isotope separator. The experimental apparatus consists of a beam collimator leading into a differentially pumped chamber containing the target gas. The scattered particles are investigated by a rotatable system consisting of an exit collimator and a cylindrical electrostatic analyzer. The target-gas pressure is kept sufficiently low to ensure that single-collision conditions are fulfilled.

In the present measurements, only the scattered incident particles are investigated, and for a given E_0 the scattering angle θ and the energy of the scattered ions E_1 are measured for each charge state $m > 0$. From these values the inelastic energy loss Q can be calculated,

$$Q = 2\gamma(E_0E_1)^{1/2}\cos\theta - (1+\gamma)E_1 + (1-\gamma)E_0 , \qquad (1)$$

where γ is the ratio of incident to target masses. This method,[9] the so-called scattered-particle method, cannot give as detailed information as can the coincidence method, but it has the advantage of providing better-resolved Q spectra. The reason for this is that the broadening of the energy spectra of the scattered incident particles caused by the thermal motion of the target atoms is almost negligible.[9] This may be illustrated by an example where $E_0 = 20$ keV and $\theta = 11°$. For the scattered-particle method, the contribution δQ_T of the thermal target motion to the observed half-width at $1/e$ height ($\sqrt{2}$ times the standard deviation) is ≤ 9 eV, whereas for the conventional coincidence method the corresponding δQ_T is 45 eV.

A complication in the present measurements is that while the incident beam contains mass number 84 only, the target gas consists of four significant isotopes. The resulting distribution in γ contributes to the width of the measured Q distribution. From Eq. (1) we obtain

$$\delta Q_\gamma = E_2 \delta\gamma \simeq E_0 \sin^2\theta\delta\gamma , \qquad (2)$$

where E_2 is the recoil energy and equal to $E_0 - (E_1 + Q)$. At large scattering angles, this broadening seriously degrades our resolution. For Kr, $\delta\gamma$ equal to $\sqrt{2}$ times the standard deviation of γ is approximately 0.022. For example, for $E_0 = 20$ keV and $\theta = 11°$, this results in $\delta Q_\gamma \simeq 16$ eV.

DATA AND RESULTS

A triple-peaked energy spectrum of the scattered incident particles corresponding to $E_0 = 20$ keV, $\theta = 11.9°$, and $m = 2$ is shown in Fig. 1. From such spectra, the Q values Q_j^m and the probabilities P_j^m corresponding to charge state m and peak j ($j = I$, II, and III) can be obtained. From these basic data we derive $\overline{Q}_j$, the mean Q for peak j weighted over charge-state distribution, the excitation probability P_j of exciting Q_j, and $\overline{m}_j$, the mean-charge state for Q_j-excited scattered incident particles. For more details concerning the data treatment, see Ref. 9.

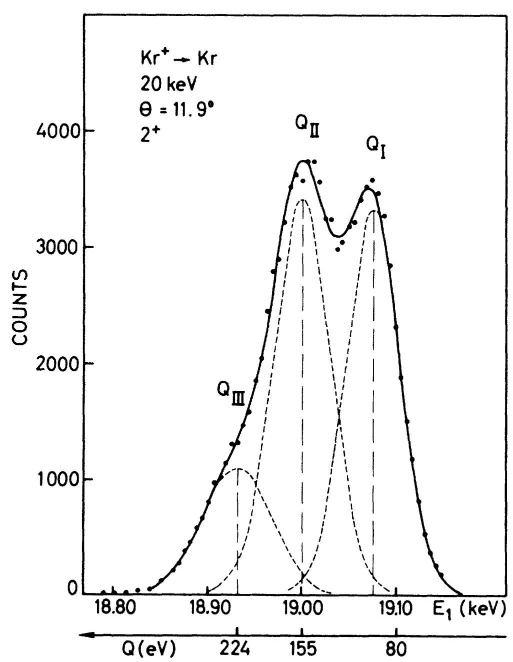

FIG. 1. Triple-peaked energy spectrum of scattered 2+ krypton ions from Kr^+-Kr collisions with $E_0 = 20$ keV and $\theta = 11.89°$.

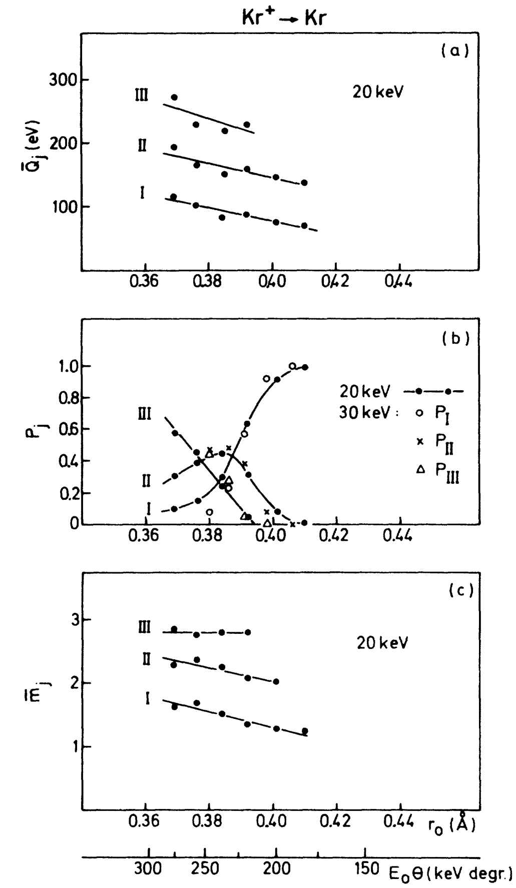

FIG. 2. (a) Weighted mean inelastic energy loss $\overline{Q}_j$ at $E_0 = 20$ keV. (b) Excitation probabilities P_j at $E_0 = 20$ and 30 keV. The curves are drawn through the 20-keV points. (c) Mean-charge states $\overline{m}_j$ at $E_0 = 20$ keV.

Figure 2 shows $\overline{Q}_j$, P_j, and $\overline{m}_j$ as a function of r_0 and $E_0\theta$, where r_0 is calculated from an exponentially screened Coulomb potential. It should be noticed here that we do not detect the neutrals, so that minor corrections could be applied to some of the data. From Fig. 2 it is seen that the differences between the three Q values are independent of r_0 and that $\overline{Q}_{III} - \overline{Q}_{II} = 74 \pm 15$ eV, $\overline{Q}_{II} - \overline{Q}_I = 72 \pm 15$ eV. The P_j curves show the same general behavior as in the Ar^+-Ar case[1,2]: P_I is unity at high r_0 and decreases rapidly at lower r_0, where P_{II} and P_{III} increase.

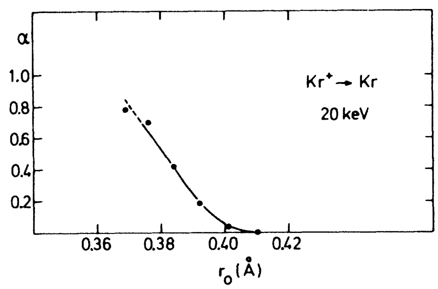

FIG. 3. One-electron promotion probability α as a function of r_0 for $E_0 = 20$ keV.

P_{II} reaches a maximum of about 0.5 at $r_0 = 0.385$ Å, where both P_I and P_{III} have values of about 0.25. P_{III} becomes dominant at small r_0. Unfortunately the isotope-broadening effect mentioned earlier [see Eq. (2)] makes it impossible to resolve the energy spectra at large scattering angles or small r_0. Consequently, it is not possible to decide whether P_{III} at small r_0 reaches a maximum value of approximately unity or whether it reaches a maximum value substantially less than unity. P_j values for both 20 and 30 keV are shown in Fig. 2. The fact that the 30-keV data fit the 20-keV curves very well indicates that velocity effects are not significant. Correction for the neutrals will only give a negligible change in the P_j shown. The $\bar{m}_j$ curves show that $\bar{m}_{III} - \bar{m}_{II} = 0.5 \pm 0.1$ and $\bar{m}_{II} - \bar{m}_I = 0.75 \pm 0.1$. Correction for the neutrals estimated from Refs. 7 and 8 will lower the shown $\bar{m}_I$ and $\bar{m}_{II}$ values by about 0.1 and 0.05 charge units, respectively.

Measurements of the energy spectrum of the electrons emitted from Kr^+-Kr collisions were included in the present investigation in order to find $M_{IV,V}NN$ Auger electrons with estimated energies around 60–70 eV. The data showed no distinct Auger group, which is in agreement with the earlier observations by McCaughey *et al.*[8] The reason for this is probably twofold: First, the energy width of the Auger group is large owing to the many decay channels with different transition energies. Second, the electron "background" spectrum due primarily to auto-ionization processes in the outer shell extends beyond the Auger group, making a separation of Auger electrons and background electrons ambiguous.

DISCUSSION

The Kr^+-Kr data presented here show the same general behavior as the earlier Ar^+-Ar data that were discussed successfully within the Fano-Lichten model.[5,6] It is therefore natural to base the discussion of the Kr^+-Kr data on the same model. The ionization energy of the $M_{IV,V}$ shell in krypton is approximately 90 eV, i.e., it is a little higher than the observed values for $\bar{Q}_{III} - \bar{Q}_{II}$ and $\bar{Q}_{II} - \bar{Q}_I$. Since the ionization energy of the M_{III} shell is as high as 215 eV, the data suggest that the triple-Q structure is due to promotions of one or two $M_{IV,V}$ electrons.

In the Ar^+-Ar case, Kessel and co-workers[2] introduced a one-electron promotion probability $\alpha(r_0)$. If it is assumed that the two electrons are promoted independently of each other, it is easy to see that the excitation probabilities P_j are given by $P_I = (1-\alpha)^2$, $P_{II} = 2\alpha(1-\alpha)$, and $P_{III} = \alpha^2$. An analysis of the Kr^+-Kr data results in an $\alpha(r_0)$ curve which is unambiguously determined within the experimental uncertainty. Figure 3 shows $\alpha(r_0)$ for $E_0 = 20$ keV. This result suggests that the two electrons are independently promoted in Kr^+-Kr collisions, as was also found for the Ar^+-Ar case.

The result $\bar{m}_{III} - \bar{m}_I = 1.25$ needs some comment. If we assume the same value for the recoils, it shows that, as an average, a promotion and the following Auger process raise the charge state by more than unity. This result may be explained by promotion into the continuum or by Auger processes emitting more than one electron.[10] Similar results have been found for Ar^+-Ar collisions.[9,11]

ACKNOWLEDGMENTS

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Infinite-Channel Close-Coupling Approximation in the Second Born Approximation. II. Treatment of Charge Polarization in Elastic Scattering by Use of the *T*-Matrix Formalism*

R. A. Bonham

Department of Chemistry, Faculty of Science, University of Hokkaido, Sapporo, Japan and Department of Chemistry, Indiana University, Bloomington, Indiana 47401

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An operator expansion of the T matrix is shown to lead to an equation for describing charge polarization on elastic scattering similar to that reported previously by use of the infinite-channel close-coupling approximation in the second Born approximation. The resulting equations are used to calculate the charge-polarization corrections for elastic electron scattering from H and He at incident electron energies of 100 eV, 500 eV, and 40 keV over the angular range of 0° to 50°. The results agree well with those of Bromberg and LaBahn and Callaway for elastic scattering from He with an incident electron energy of 500 eV.

In the first paper in this series[1,2] it was shown that an old approach to the problem of describing the effects of charge polarization on the elastic cross section was capable of yielding results in excellent agreement with experiment at incident energies as low as 500 eV, providing certain reasonable assumptions were made concerning the choice of the one adjustable parameter present in the theory. This approach called the infinite-channel close-coupling approximation in the second Born approximation (ICCCA) was also found to compare favorably with the results of the extended polarization potential method of LaBahn and Callaway.[3] Other theoretical approaches, which in principle can be used to attack this same problem but where detailed calculations are not yet available for the case of He at 500 eV, are versions of the coupled-channel partial-wave theory,[4] the method of equivalent potentials,[5] and the phase-grating approximation.[6] Recently two studies have appeared which apply the nuclear independent-particle model[7] to the calculation of charge polarization in elastic electron scattering for the case of He at incident energies of 100 to 500 eV with excellent results. This last approach can in some sense be considered a variant of the approach outlined in Ref. 5.

The purpose of this paper is to investigate the use of the T-matrix formalism for the description of charge polarization. This approach depends only on an operator expansion and bypasses the necessity of using closure as an approximation.

I. *T*-MATRIX DESCRIPTION OF CHARGE POLARIZATION

In the nonrelativistic T-matrix formalism, the exact elastic scattering amplitude can be written as[8]

$$f(\theta)=f^{\mathrm{Born}}(\theta)+\frac{1}{4\pi}\times\left\langle \psi_0\left| e^{-i\vec{k}_s\cdot\vec{r}_0}\, V\bar{\mathrm{A}}\frac{1}{H-E-i\epsilon}\, Ve^{i\vec{k}_i\cdot\vec{r}_0}\right|\psi_0\right\rangle , \quad (1)$$

where

$$f^{\mathrm{Born}}(\theta)=(1/4\pi)\,\langle\psi_0|e^{-i\vec{k}_s\cdot\vec{r}_0}\,V\bar{\mathrm{A}}\,e^{i\vec{k}_i\cdot\vec{r}_0}\,|\psi_0\rangle \quad ,$$

and ψ_0 is the ground-state wave function of the target; $\vec{k}_i$ and $\vec{k}_s$ are the wave vectors of the incident and scattered electron; V is the interaction potential between the incident electron and the target; and H is the complete Hamiltonian with E the total energy. The operator $\bar{\mathrm{A}}$ is an antisymmetrizer acting to the left which permutes the coordinates of the incident electron $\vec{r}_0$, with those of the target electron in such a way that the overall matrix element is antisymmetric with respect to electron exchange.[9] The procedure to be followed here[10] is to express V in the Fourier form

$$V=\frac{1}{\pi^2}\int\frac{d\vec{q}}{q^2}\,e^{i\vec{q}\cdot\vec{r}_0}\times\left(\sum_{n=1}^{M}Z_n e^{-i\vec{q}\cdot\vec{R}_n}-\sum_{\nu=1}^{N}e^{-i\vec{q}\cdot\vec{r}_\nu}\right) \quad , \quad (2)$$