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PRODUCTION OF DOUBLY CORE EXCITED CONFIGURATIONS IN C^{4+} PROJECTILES
THROUGH RESONANT TRANSFER EXCITATION⁽¹⁾

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Projectile K-Auger electron production cross sections have been measured for C^{4+} ions in 3 to 8 MeV collisions with atomic He, Ne, and molecular Hydrogen targets at lab observation angles of 9.6° to 10.6° . The K-Auger electron spectra predominantly result from decays of Li-like excited states and are interpreted as single electron capture to the metastable $1s2s\ ^3S$ component of the incident beam. High resolution K-LL Auger spectra show that capture into $2s$ is suppressed by the presence of the $2s$ spectator electron. The formation of single and double core excited Li-like $2D$ configurations are interpreted in part as resonant transfer and excitation with the ground state and metastable components respectively. Also, the data shows a much stronger production of the $2s^22p\ ^2P$ configuration through NTE for Ne than for the He target.

1. Introduction When stripping is used to increase the charge of fast Carbon ions, excited configurations produced in the process usually decay promptly (eg. $\tau \approx 1.1 \times 10^{-12}$ sec. for $1s2p\ ^1P$ ions). However, for two-electron ions the metastable $1s2s\ ^3S$ configuration ($\tau = 2.01 \times 10^{-2}$ sec.¹) arrives on target without decay. Measurements of the fraction of vacancy bearing two-electron ions at various incident energies can be found in the literature. Their measurement is based on projectile to target K-shell vacancy transfer. $1s2s\ ^3S$ ions have been used to study partial cross sections for capture to specific n or n,l shells^{1,2} ($n \geq 2$). When our Auger electron production cross sections are divided by published values of the fraction of $1s2s\ ^3S$ ions in the incident beam¹, we find that the energy dependance of these inferred electron capture cross sections agrees with a classical Bohr-Linhardt calculation³ for capture by $C^{4+}(1s^2)$ ions. However, the data overpredict the calculation and we attribute this, in part, to differences in screening by $1s^2$ and $1s2s$ ions. The high resolution K-LL Auger spectrum is composed of decays of five Li-like configurations. Three are thought to be formed directly by electron capture into the $2p$ subshell and one by capture into the $2s$ subshell. Auger electron production from the decay of the $1s2p^2\ ^2D$ configuration exhibits a maximum intensity at a collision energy of 5 MeV, and agrees well with theoretical calculations for resonant transfer and excitation (RTE). Also, a maximum in the cross sections at 6 MeV for unresolved transitions containing capture to $n \geq 3$ as well as the doubly core excited $2s^22p\ ^2P$ and $2s2p^2\ ^2D$ configuration decaying to either $1s2s\ ^1S$ or 3S , agrees with the predicted collision energy for a maximum in the RTE cross section.

Electron transfer excitation cross sections are needed in the fields of thermonuclear fusion, heavy ion storage ring and x-ray laser design, as well as for astrophysical model calculations. In particular, RTE is closely related to dielectronic recombination - a significant energy loss mechanism in tokamak plasmas. DR, in which a fast free electron is captured by a slow ion, can be viewed as the inverse Auger process. The probability for DR depends strongly on the kinetic energy of the free electron and, if the time reversal analogy is correct, we expect this dependance to reflect the kinetic energy distribution of electrons emitted during Auger decay. The RTE process occurs in ion atom collisions when the velocity of the ion is varied so that the kinetic energy (in the ion's rest frame) of a loosely bound target electron appears to pass through a DR type resonance.

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Recently, two experimenters have reported the observation of RTE using the technique of 0° Auger spectroscopy. Swenson et. al.⁴ studied the $O^{5+} + He$ system and found resonances in the production of $1s2s2p^2$ $1D$ and $3D$ excited states. Itoh et. al.⁵ reported a similar resonance in the production of the $2p^2$ $1D$ state for the symmetric $He^+ + He$ collision system. In these experiments a target electron is captured by the ion which emerges from the collision complex in an excited configuration. Since no measurement is made on the target fragment, we know only that it is at least singly ionized, but may also be excited and multiply ionized. When the captured electron is emitted during the Auger decay, a new channel for target ionization is opened:

where $2S+1L$ is the incident ionic configuration, $2S+1L$ is the excited configuration formed through RTE, T is the target, and T^+ refers to the system composed of the remaining target electrons and nucleus. Destructive interference between this process and direct target ionization has been discussed by Swenson et. al. to explain anomalies in their K-LL Auger spectrum.

As in DR, a maximum in the RTE production probability occurs when the difference between the captured electron's kinetic energy (KE) and its initial binding energy to the target (B) becomes equal to the energy difference between the excited and incident configurations: $KE - B = E(2S+1L) - E(2S+1L)$. Examination of (1) shows that this occurs when the collision energy is: $E_{\text{RTE}} = M_{\text{ion}}/m_{\text{electron}} (E_{\text{Aug}} - B)$. Brandt has shown that the momentum distribution of the bound target electron broadens the resonance as a result of orbital motion in the direction of the collision axis. This problem has been treated in the impulse approximation, and a method has been developed to relate DR to RTE using the bound electron's Compton profile⁶.

2. Experiment 10-30 μA currents of C^- were produced in a sputter ion source, and accelerated by the Triangle Universities Nuclear Laboratory model FN tandem Van de Graaff. C^{4+} ions were then formed by post acceleration stripping and selected magnetically. The distance from post stripper foil to the target cell was 9 meters. After collimation, the ions passed through a 25 mm long target cell with 2 stages of differential pumping, and were collected in a suppressed Faraday cup. Periodic checks of target current without gas in the cell showed no detectable enhancement or neutralization due to the gas. Pressure studies were done with Neon to insure single collision conditions. Projectile Auger yields were found to be linear up to 30 mTorr (39.5 μ bar).

Auger electrons were observed by the high resolution projectile electron spectrometer (HRPES). This electrostatic spectrometer has been described in detail elsewhere⁷. The normalization for absolute cross section was determined by measuring Neon K-Auger electron yields for 3 MeV H^+ collisions and comparing with a published value for Ne K-shell ionization. The length of the viewing region varied with observation angle, and is approximately 5 mm.

Typical spectra are shown in figure 1. They have been background subtracted and transformed into the rest frame of the projectile. The improved resolution in figure 1b was obtained by decelerating the electrons to 1/6 of their lab frame energy before passing through the spectrometer⁸. Since the electron pass energy was not a constant for the various collision energies, the decelerated spectra were normalized by a deceleration efficiency factor determined at each collision energy: $\epsilon_{\text{decel}} = \text{Yield}(\text{decelerated})/\text{Yield}(\text{undecelerated})$.

3. K-LL Auger Spectrum and Capture to $n=2$ Figure 2a shows the total capture cross sections into all $n \geq 2$ shells of $1s2s^3S$ ions for the various targets, and includes all K-L Auger transitions (227.5 - 299 eV). The Hydrogen data was divided by two, in order to compare with the atomic cross sections for He and Ne. Others⁹ have found the ratio for capture from molecular and atomic Hydrogen targets to be 3.89, and we do not mean to attach any special significance to our procedure. Figure 2a also shows Brandt's semiclassical calculation for the He target³ as the solid curve. As discussed above, the calculation underpredicts our data by a numerical factor of 4.5.

Ratios of cross sections for capture into specific L-S coupled configurations by $1s2s^3S$ ions are shown in table 1. They were obtained from the doubly differential high resolution spectra similar to figure 1b. Capture into the 2s sub-shell of metastable projectiles always results in the $1s2s^2 2S$, while capture into the 2p sub-shell can result in the $1s(2s2p^3P) 2P$; $1s(2s2p^1P) 2P$; or $1s2s2p^4P$. The relative strengths of the $1s(2s2p^3P) 2P$ and $1s(2s2p^1P)$ configurations indicate that

Figure 1 K-L (1a) and K-LL (1b) Auger spectrum of Carbon formed in 5 MeV collisions of C^{4+} with Helium. The Gaussian fits to the raw spectra in 1b shows improved resolution (0.5% FWHM) resulting from decelerating Auger electrons before the analyzer. The excited states shown in 1b decay to $1s^2 1S$.

Figure 2 Inferred cross sections for capture into all sub-shells with $n \geq 2$ by $1s2s \ ^3S$ ions from H_2 , He , and Ne targets is shown in 2a. (Auger production cross sections were divided by the fraction of metastables at each collision energy). Figure 2b shows the $1s2p^2 \ ^2D - 1s^2 \ ^1S$ Auger production cross section as well as various production schemes (Auger production cross sections were divided by the fraction of ground state ions at each collision energy). Table 1 Intensity fraction of metastable ions in the incident beam at the various collision energies (values were taken from reference 1, and statistical errors were $\sim \pm .06$). Also, experimental Auger production ratios for three configurations formed by capture into the $n=2$ shell of C^{4+} in collisions with He .

capture into the empty $2p$ sub-shell is statistical. From tables of fractional parentage coefficients¹⁰:

$$(2) \quad |< 1s2s \ ^3S, 2p | 1s (2s2p \ ^1P) \ ^2P >|^2 = 3 |< 1s2s \ ^3S, 2p | 1s (2s2p \ ^3P) \ ^2P >|^2$$

and

$$|< 1s2s \ ^3S, 2p | 1s 2s2p \ ^4P >|^2 = \frac{4}{3} |< 1s2s \ ^3S, 2p | 1s (2s2p \ ^1P) \ ^2P >|^2$$

This equation gives the statistical ratios for coupling the $1s2s \ ^3S$ preparent and $2p$ coparent to either $1s2s2p \ ^2P$ or $1s2s2p \ ^4P$ postparents. Specifying either the $(2s2p \ ^1P)$ or $(2s2p \ ^3P)$ intermediate coupling removes any ambiguity in the $1s2s2p \ ^2P$ postparent. The director $(|)$ leads from lower symmetry to higher symmetry. We find that the experimental ratio for capture into the different $1s2s2p \ ^2P$ configurations is nearly equal to the ratio of 3:1 as predicted above.

The excited $1s2p^2 \ ^2D$ configuration cannot be formed directly by single electron capture to either component of the incident projectile beam. Instead, it is formed when a target electron is captured and an additional projectile electron is excited into a $2p$ orbital during the same collision. The situation becomes even more complex when we consider that the excitation may result from the time varying potential of either the target nucleus, or the target electrons. The $1s2p^2 \ ^2D$ configuration can be formed from $1s2s \ ^3S$ Carbon ions when capture into the $2p$ orbital is accompanied by $2s-2p$ excitation. This channel is shown in figure 2b as the monotonically decreasing curve. The probabilities $P_{2s-2p}(b)$ and $P_{1s-2p}(b)$ were calculated analytically in the semiclassical approximation with individually screened hydrogenic wave functions¹¹. The calculation assumes a straight line trajectory for the projectile, and no target recoil. $P_{capt}(b)$ was formulated by Brandt³ based on a two step Bohr-Lindhardt model. In the first step, an electron is released by the target when the target binding potential is overcome by the attractive potential of the projectile. Capture by the projectile can then occur if the distance from the projectile at the time of release is smaller than $R_C = 2q/(v_{proj})^2$ (that is if the electron's kinetic energy is smaller than its potential energy in the field of the projectile). The TE curve is then calculated according to:

$$(3) \quad \sigma_{TE}(1s2s \ ^3S \rightarrow 1s2p^2 \ ^2D) = 2\pi \int P_{exc}^{2s-2p}(b) P_{capt}^{2p}(b) b db \quad \text{where} \quad P_{capt}^{2p}(b) \approx \frac{1}{2} P_{capt}(b)$$

Since the calculation does not give partial probabilities for capture into specific orbitals of the projectile, we have used the $1/n^3$ scaling law in (3) and assume that capture into $2s$ is negligible to estimate that $\sim 1/2$ of all capture is into a $2p$ orbital.

The $1s2p^2 \ ^2D$ can also be formed in collisions with $1s^2$ ground state projectiles. In this case, a $1s-2p$ excitation accompanies capture into the $2p$ orbital. This process has been considered before and is known as non resonant transfer excitation (NTE). Since the incident ion is now in the $1s^2$ state, the statistical ratio of capture into $2p$ to capture into all $n \geq 2$ is 1/3:

$$(4) \quad \sigma_{NTE}(1s^2 \ ^1S \rightarrow 1s2p^2 \ ^2D) = 2\pi \int P_{exc}^{1s-2p}(b) P_{capt}^{2p}(b) b db \quad \text{with} \quad P_{capt}^{2p}(b) = \frac{1}{3} P_{capt}(b)$$

The NTE calculation is shown in figure 2b and peaks at a collision energy of ~ 3 MeV.

One final mechanism for producing the $1s2p^2 \ ^2D$ configuration is through RTE. This production mechanism is similar to NTE in that a $1s-2p$ excitation occurs when a $1s^2 \ ^1S$ ion captures an electron into a $2p$ orbital. However, the excitation is now the result of internal conversion of the captured electron's kinetic energy. As shown in figure 2b, a maximum in the RTE production for the $C^{4+}(1s^2 \ ^1S) + He$ collision system is predicted at ~ 5 MeV in agreement with the data. The RTE calculation was provided by McLaughlin¹², and uses the method outlined by Brandt⁶ for folding the target electron's Compton profile with calculated DR cross sections.

4. Hyper-Satellites and Capture to $n \geq 3$ High resolution spectra for Carbon K-Auger electrons with energy greater than 250 eV are shown in figure 3. They are the result of 4 MeV collisions of C^{4+} with He (3a) and Ne (3b). Each peak is labeled and identified in table 2. As shown there, the excited configurations are formed chiefly by capture into $n \geq 3$ shells of $1s2s^3S$ ions. As n increases, it becomes more difficult to resolve the various transitions. Capture into 3s and 3p (peak 1) is resolved from capture into 3d (peak 2). However, for capture into $n=4$, we are unable to resolve capture into the various 4l subshells (peak 4). Also, capture into shells with $n \geq 5$ (region 6) are essentially unresolved. The Auger electron energy for the $(1s2s^3S)nl$ series limit to $1s^2 1S$ decay occurs at ~ 299 eV¹⁴. Also identified in table 2 are the hypersatellite Auger transitions corresponding to $2s^2 2p^2 P$ and $2s^2 2p^2 D$ configurations decaying to either $1s2s^1S$ or $1s2s^3S$ (peaks 3,4,5). The energies for these transitions were calculated by Chung¹³, and are reported here for the first time.

Peak Number	Excited - Final Configuration	Energy (eV)
1	$(1s2s^3S)3s^2S - 1s^2 1S$	269.6
	$(1s2s^3S)3p^2P - 1s^2 1S$	271.9
2	$(1s2s^3S)3d^2D - 1s^2 1S$	274.3
	$2s^2 2p^2 P - 1s2s^1S$	275.8
3	$(1s2s^1S)3s,p,d - 1s^2 1S$	< 279
	$2s^2 2p^2 P - 1s2s^3S$	281.3
4	$(1s2s^3S)4s,p,d,f - 1s^2 1S$	< 286
	$2s^2 2p^2 D - 1s2s^1S$	282.4
5	$(1s2s^1S)4s,p,d,f - 1s^2 1S$	< 291
	$2s^2 2p^2 D - 1s2s^3S$	287.9
6	$(1s2s^3S)nl$ series limit - $1s^2 1S$	< 299

Figure 3 High resolution Auger electron production spectra of Carbon formed in 4 MeV collisions of C^{4+} with He (3a) and Ne (3b). **Table 2** Identification of Auger transitions for figure 3a and 3b. The transitions in bold script are thought to be formed through RTE or NTE with incident $C^{4+}(1s2s^3S)$, and their Auger decay energies were calculated by Chung¹³, and are identified in reference 14.

Figure 4 shows inferred capture cross sections into all $n \geq 3$ shells of metastable C^{4+} ions. They were obtained by dividing production cross sections for all Auger electrons having energies between ~ 269 eV and 299 eV by the metastable fractions given in table 1. Although all of the excited configurations contributing to Auger production in this range of emission energies result from capture into metastables, the hypersatellite transitions also fall in this range. The doubly core excited configurations can be formed by $n=2$ capture into metastable ions accompanied by $1s - 2s$ or $1s - 2p$ excitation such as occurs in either RTE or NTE. Indeed, the data shows an increase for all targets near the RTE resonance collision energy.

5. Discussion The experimental ratios for production of the $1s(2s2p^1P)^2P$ to $1s(2s2p^3P)^2P$ configurations at the various collision energies are given in table 1. The $1s2s2p^2P$ is formed directly when a Helium electron is captured into the 2p orbital of a metastable ion. As discussed in the text, fractional parentage coefficients show that this ratio is 3.0 when a 2p

Figure 4 Inferred capture cross sections into all sub-shells with $n \geq 3$ by $1s2s^3S$ projectiles. Capture cross sections are obtained by dividing Auger production cross sections by the fraction of metastable ions in the incident projectile beam at each collision energy.

electron is coupled into a $1s2s\ ^3S$ ion, and 1/3 when coupled into a $1s2s\ ^1S$ ion. Our measured ratios range from 2.0 to 2.89 and indicate that 80% to 96% of the incident metastables are $1s2s\ ^3S$.

Also shown in table 1 are the experimental production ratios for $1s2s^2\ ^2S$ and $1s(2s2p\ ^1P)\ ^2P$ configurations. Based merely on the number of 2s and 2p vacancies in the incident $1s2s\ ^3S$ ions (one for 2s, and six for 2p) and since 3/8 of all 2p capture into these ions results in the $1s(2s2p\ ^1P)\ ^2P$ a ratio of $1s2s^2\ ^2S$ to $1s(2s2p\ ^1P)\ ^2P$ production of .444 is expected. The experimental values are lower than .444 indicating that capture into the half full 2s subshell is strongly suppressed at low collision energies. This suppression is the result of the repulsive potential between the spectator and captured electrons. The data indicates that the repulsion becomes less important as the collision velocity is increased. At 3 MeV the collision velocity is about equal to the Bohr orbital velocity of the 2s electron, while at 15 MeV it is about $2.84\ v_{2s}$.

Since the spin-orbit interaction is negligible for Carbon, the orientation of the total spin vector (S) for electrons in the incident ion and that of the captured electron (s) should not effect the capture probability. For capture into a 2p orbital of $1s2s\ ^3S$ ions, $1s2s2p\ ^4P$ and $1s2s2p\ ^2P$ configurations should be produced with equal probability. Since the $1s2s2p\ ^4P - 1s^2\ ^1S$ decay requires a spin flip, its mean life (eg. $t=117\ \text{nsec}$ for $4P_{5/2}^{15}$) is greater than the transit time for ions over the spectrometer viewing region and only a fraction of the $4P$ ions produced in this region decay before the ion exits. This is clearly shown in figure 1b where the $1s2s2p\ ^4P - 1s^2\ ^1S$ appears as the weakest transition. In order to obtain absolute production cross sections, the measured intensity for this transition must be divided by an efficiency factor calculated at each collision energy:

$$(5) \quad \epsilon_{1s2s2p\ ^4P - 1s^2\ ^1S} = \int_{x_0}^{x_0+x_1} \frac{(1 - e^{-x/v\tau})}{x_1} dx$$

where x_0 is the distance from the entrance aperture of the target cell to the start of the viewing region, x_1 is the length of the viewing region and v is the collision velocity. Using calculated values for $4P_{5/2,3/2,1/2} - 1S_0$ lifetimes¹⁵ and assuming a statistical population for the multiplets, this correction gives experimental $4P$ production cross sections that are significantly larger than $2P$ production cross sections. This indicates that the $1s2s2p\ ^4P$ may be fed by cascades. Work is in progress to account for this.

Inferred cross sections for capture into $n \geq 2$ shells of K-vacancy bearing ions in collisions with H_2 , He and Ne targets are shown in figure 2a. The average ratio of these cross sections for Ne and He is 5.6 indicating an approximate scaling of capture with the number of target electrons ($N_{Ne}/N_{He}=5$). The trend with energy of the data agrees with the semiclassical calculation for He electron capture by C^{4+} ions, but the calculation had to be multiplied by 4.5. This is expected since the data represents capture into $1s2s\ ^3S$ configurations and the calculation assumes a structureless projectile with nuclear charge of 4+ which underestimates the true projectile potential in the region between the projectile nucleus and the spectator electron. As a result, the calculation systematically underpredicts the capture probability for small impact parameters. Other failures of the calculation are the assumption of a straight line trajectory for the projectile in the rest frame of the Helium atom, and the inability to predict partial cross sections for capture into particular nl orbitals. A calculation which would predict partial capture cross sections would be very useful in the various transfer excitation calculations shown in figure 2b.

The primary sources of systematic error in our data are uncertainty in the value of the fraction of metastable ions in the incident beam and the assumption of isotropic Auger electron emission. Isotropic emission is assumed in transforming our measured projectile Auger electron yields into absolute production cross sections. Since our measurements were taken at $\sim 10^\circ$ with respect to the ion beam emerging from the target cell ($\sim 20^\circ$ in the projectile rest frame) any alignment of excited configurations with the collision axis would result in our cross sections being too large. Preliminary angular studies of the Auger decay of excited states formed through RTE for the $O^{5+} + He$ system show a strong decrease in intensity as the observation angle is increased. We estimate that the absolute uncertainty in the metastable fraction values given in table 1 to be $\pm 10\%$.

In figure 2b we show the $1s2p^2\ ^2D - 1s^2\ ^1S$ Auger production cross sections and various calculations for capture into $2p$ accompanied by excitation. A maximum in the data at 5 MeV is present for all targets and agrees with the RTE resonance collision energy: $E_{RTE} = E_{Aug}(1s2p^2\ ^2D - 1s^2\ ^1S) M_C/m_e = 5.3\ \text{MeV}$. The resonance width of the scaled RTE calculation describes the Helium target data well, showing that the impulse approximation⁶ is valid for the Carbon - Helium collision system. Near the 4 MeV collision energy the RTE and NTE probabilities are nearly equal and the measured cross section seems to be significantly lower than that predicted by summing the various calculations. It would be interesting to obtain more data in this region to see if there is destructive interference between RTE, NTE, and TE.

In the case of $1s2s\ ^3S$ ions, electron capture into $n=2$ accompanied by $1s-2p$ excitation results in either a $2s2p^2\ ^2P$ or $2s2p^2\ ^2D$ doubly core excited configuration. The calculated Auger electron energies for the hypersatellite transitions that result when these ions decay to either $1s2s\ ^1S$ or $1s2s\ ^3S$ are shown in bold print in table 2. A maximum in the production of the doubly core excited configurations through RTE would be expected at: $E_{RTE}(^2P) = (M_C/m_e) (275.8\ \text{eV}) = 6.1\ \text{MeV}$ and $E_{RTE}(^2D) = (M_C/m_e) (282.4\ \text{eV}) = 6.2\ \text{MeV}$. Inclusive cross sections for capture into $n \geq 3$ of $1s2s\ ^3S$ ions as well as capture into $n=2$ accompanied by $1s-2s$ or $1s-2p$ excitation (RTE and NTE) are shown in figure 4. An increase in the data near 6 MeV is seen for all targets and is thought to be due to RTE. The spectra shown in figure 3a (Helium target) and 3b (Neon target) were measured at a collision energy of 4 MeV. At this collision energy, the probability for production of doubly core excited configurations through NTE is maximum. For both targets, nearly all of the intensity in peaks 3 and 4 are due to

hypersatellite decays to $1s2s\ ^1S$. The only other likely source of Auger electrons at these energies would be from decays of $(1s2s\ ^1S)3l$ or $(1s2s\ ^1S)4l$ to $1s^2\ ^1S$. This is unlikely since those excited configurations are formed by electron capture into $n=3$ or $n=4$ of $1s2s\ ^1S$ projectiles and we already know that only $\sim 10\%$ of the incident metastables are $1s2s\ ^1S$. Finally, a propensity for forming $2s^22p\ ^2P$ ions for collisions with Neon is seen (peaks 2 and 3).

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