RESONANT TRANSFER AND EXCITATION FOR NITROGEN LIKE IONS

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ABSTRACT

The resonant transfer excitation (RTE) followed by x-ray emission (RTEX) process in ion -atom collisions is investigated. In RTEX, one of the target electrons is captured into a resonant state of the projectile which is then relaxed by radiation. In the Impulse approximation, this is related to the dielectronic recombination (DR) in electron-ion collisions. The DR cross sections are calculated for P $^{8+}$ and Fe $^{19+}$ with K-shell excitation. The RTEX cross sections for P^{8+} +He, P^{8+} + H₂, Fe $^{19+}$ +He, and Fe $^{19+}$ + H₂ collision systems are then obtained by folding the corresponding DR cross sections over the momentum distribution of the target gas in the impulse approximation. It is found that the RTEX cross section exhibits a single peak for P^{8+} and two-peak behaviour for Fe $^{19+}$.

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INTRODUCTION

Recently, much theoretical [1-5] and experimental [6,7] works has been done to understand the resonant charge transfer and excitation, RTE, in ion-atom (I/A) and ion-molecule collisions. In the RTE process, one of the electrons in the atomic helium or molecular hydrogen targets is captured by a fast highly ionized projectile and, in turn, causes an excitation to this projectile. Thus, doubly-excited intermediate states (d) of the projectile may be formed. However, the target is left as ionized ion. The RTE may be followed, as a stabilization of d state, by emission of x-rays (RTEX).

Schematically, for a target atom or molecule B, RTE and its subsequent RTEX processes can be described as

$$A^{q+}(i) + B \longrightarrow (A^{(q-1)} +)^{**}(d) + B^{+} RTE$$
 (1.1)

then

$$(A^{(q-1)+})^{**}$$
 (d) \longrightarrow $(A^{(q-1)+})^{*}$ (f)+ h RTEX (1.2)

In process (1.1), the projectile A (in its intial state i) with ionization charge (q+) captures an electron from the target B and forms an intermediate state (d) which is doubly excited (**). Regadless of the presence of the residual ion B^+ , the d state of the projectile may be relaxed by emission of x-rays with energy $h_{\mathbf{p}}$. It has to be noted that RTEX is a two-step efficient process only at relatively high projectile energy [4].

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Since RTE is a high-energy process, the effect of the target core on the excited states of the projectile is very small and can be neglected during the investigation of such process. However, this effect is important in the nonresonant transfer excitation (NTE) process which has been studied elsewhere [4,8] and was found to be of much interest only at low projectile energy range. When the RTE process takes place at high projectile energy, the conditions of the validity of the impulse approximation (IMA) may be satisfied. In The IMA, the collision velocity is assumed to be large compared to the velocity of the target electrons and the distortion of the projectile resonance state by the target nucleus is small. In other words, in the projectile rest frame, the target B is considered as a source of free electrons.

In view of these considerations in the IMA, RTE in ion-atom collisions is an identical process to resonant capture (RC) in electron-ion collisions [10]. Consquently, RTEX (a subsequent of RTE) is identical to DR (a subsequent of RC). In electron-ion (e/I) collisions, for RC and DR, we have

$$(A^{q+})$$
 (i) + $e_c \longrightarrow (A^{(q-1)+})^{**}$ (d) RC (1.3)

then

$$(A^{(q-1)+})^{**}$$
 (d) \longrightarrow (A $(q-1)+$)* (f) + h \cup DR (1.4)

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where (A^{q+}) is the target and e denotes the incident continuum electron. A comparison between this scheme and the previous one manifests that process (1.2) is identical to (1.4). Thus, the analysis of RTEX has been carried out rather sucessfully in the IMA by folding the DR cross sections over the target compton profile [10]. Direct measurements of the DR cross sections is diffcult because of their small magnitude. All of the experimental DR cross sections, involving K-shell excitation were of the RTEX type. These measurements have been found in a good agreement with the calculated values [1,4,9] e.g. Li-Like Ca $^{17+}$, Si $^{11+}$, S $^{13+}$. Unfortunatly, no experimental data are available for RTEX of N-like ions up to date. Thus, it is planned to calculate the RTEX cross section for this isoelectronic sequence. All bound-state wavefunctions used in our calculations of $\boldsymbol{\sigma}^{DR}$ are generated from the Hartree Fock (SCHF) program, while a distorted wave approximation is employed to generate the continuum wave functions. The comptom profile for the momentum distribution of the electrons in He or H_2 targets, which is used here to convert σ^{DR} into σ^{RTEX} (folding), is taken from Ref. [11]. The Author there obtained a least square fit for the experimental compton profile, and his fitting coefficients for both He and H, targets are utilized in this work. The theory behined the relationship between DR and RTEX is outlined in sec. 2. The discussion of the results is presented in sec. 3. Conclusions are summerized in sec. 4.

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2. Theory

a) Momenta consideration in RTE

Let the momentum of a certain electron (to be captured) in the target frame is p_1 , and that of this electron relative to the projectile is p_0 . Thus, the momentum p of such electron in the projectile rest frame is given by

$$\overrightarrow{p} = \overrightarrow{p_0} + \overrightarrow{p_i}$$
 (2.1)

where

$$p_{o} = m (2E/M)^{1/2}$$
 (2.2)

E, M are the projectile energy and mass respectively, and m denotes the mass of the electron. The magnitude of p is then given by

$$p^{2} = p_{0}^{2} + p_{i}^{2} + 2 p_{0} p_{iz}$$
 (2.3)

where p_{iz} is the component of p_i parallel to p_o in z-direction. In the IMA, $\left|\overrightarrow{p_i}\right|^2 <<\left|\overrightarrow{p_o}\right|^2$ and eq. (2.3) becomes

$$p^2 = p_0^2 + 2 p_0 p_{iz}$$
 (2.4)

b) Relation between RTEX and DR cross sections

In the IMA, the RTE cross section (σ^{RTE}) for a particular resonance (d) state in I/A collisions and the RC cross section (σ^{RC}) of formation of this (d) state in e/I collisions are related by (Brandt 1983),

$$\sigma^{RTE} = \iiint_{-\infty}^{+\infty} (\sigma^{RC})_{p \mid \psi_{i}} (p_{i}) \mid^{2} d^{3}p_{i}$$
 (2.5)

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where $d^3p_i = dp_{ix} dp_{iy} dp_{iZ}$ and $(\sigma^{RC})_p$ is the RC cross section for a free electron of momentum p with respect to the ion. From (2.4) it is clear that the RC cross section depends only on the component p_{iz} of p_i parallel to p_0 . Therefore, equation (2.5) is reduced to the form

$$\sigma^{\text{RTE}} = \iiint_{-\infty}^{+\infty} (\sigma^{\text{RC}})_{\text{p}} |\psi_{\text{i}}(p_{\text{i}})|^2 d^3p_{\text{i}} \qquad (2.5)$$

where $d^3p_i = dp_{ix} dp_{iy} dp_{iZ}$ and $(\sigma^{RC})_p$ is the RC cross section for a free electron of momentum p with respect to the ion. From (2.4) it is clear that the RC cross section depends only on the component p_{iz} of p_i parallel to p_o . Therefore, equation (2.5) is reduced to the form

$$\sigma^{RTE} = \int_{-\infty}^{+\infty} \sigma^{RC} (p_{iz}) dp_{iz} \iint |\psi_{i}(p_{i})|^{2} dp_{ix} dp_{iy} (2.6)$$

$$-\infty$$

The double integration term gives the probability of finding one of the target electrons with a momentum component p_{iz} , that is the compton profile J_i (p_{iz}). Equation (2.6) can be written as

$$\sigma^{\text{RTE}} = \int_{-\infty}^{+\infty} J_{i} (p_{iz}) \sigma^{\text{RC}} (p_{iz}) dp_{iz}$$
 (2.7)

Note that, σ^{RC} peaks only at specific values of p of the captured electron which is called the resonance momentum $\{\sigma_{r}\}$. This value of momentum is related to the resonance energy (\mathcal{L}_{r}) by

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$$p_r = (2m \epsilon_r)^{1/2}$$
 (2.8)

Now, substituting from eq. (2,2) and eq. (2.8) in eq. (2.4) we get

$$2m\epsilon_r - m^2 (2E/M) = 2m (2E/M)^{1/2} p_{iz}^*$$
 (2.9)

 p_{iz}' , ϵ_r and p_r are the values of p_{iz} , ϵ and p respectively at resonance.

Deviding both sides by 2m, and rearranging the terms we obtain

$$p'_{iz} = [\epsilon_r - m (E/M)] (M/2E)^{1/2}$$
 (2.10)

Since the Compton profile depends on p_{iz}^{t} it may be taken out of the integration in (2.7), thus

$$\sigma^{RTE} = J_{i} (p'_{iz}) \int \sigma^{RC} (p_{iz}) dp_{iz}$$
 (2.11)

At any p_{iz} and ϵ , we may differetiate (2.10) in order to obtain

$$dC = (2E/M)^{1/2} dp_{iz}$$
 (2.12)

Thus eq. (2.11) can be written in energy space as

$$\sigma^{\text{RTE}} = J(p'_{iz}) (M/2E)^{1/2} \int_{-\infty}^{+\infty} \sigma^{\text{RC}} (\epsilon) d\epsilon \qquad (2.13)$$

Since the RC is a resonant process, thus we can restrict the intergration to an energy bin $\Delta \epsilon \to F$ (resonance width) around $\epsilon = \epsilon_r$ as follows

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$$\sigma^{\text{RTE}} = J \left(p'_{iz} \right) \left(\frac{M}{2E} \right)^{1/2} \int_{r}^{\epsilon_r} + \frac{\Delta \epsilon}{2} \sigma^{\text{RC}}(\epsilon) d\epsilon \quad (2.14)$$

$$\epsilon_r - \Delta \epsilon/2$$

Introduce the energy average RC cross section (σ^{-RC}) as

$$\sigma^{-RC} = \frac{1}{\Delta \epsilon} \int_{\epsilon_{r}}^{\epsilon_{r}} + \frac{\Delta \epsilon/2}{\sigma^{RC}} \sigma^{RC} (\epsilon) d\epsilon \qquad (2.15)$$

then eq. (2.14) will be

$$\sigma^{\text{RTE}} = J \left(p'_{12} \right) \left(M/2E \right)^{1/2} \Delta \varepsilon \sigma^{-\text{RC}} \left(\epsilon \right)$$
 (2.16)

For all i's electrons in the atomic or molecular targets, we can write

$$\sigma^{\text{RTE}} = (M/2E)^{1/2} \quad \Delta \in \sigma^{-\text{RC}} \quad \sum_{j=1}^{\infty} J(p_{j,j})$$
 (2.17)

Multipling both sides of eq. (2.17) by ω (the fluoresence yield of the d state) and making use of the facts that $\sigma^{RTEX} = \omega \, \sigma^{RTE}$ and $\sigma^{-DR} = \sigma^{-RC}$, we get the following relation between RTEX and DR cross sections,

$$\sigma^{\text{RTEX}} = (M/2E)^{-1/2} \Delta \in \sigma^{-DR}. \sum_{iz} J(p'_{iz}) \qquad (2.18)$$

The RTEX cross section is maximum at the projetile energy E $_{\rm max}$ whenever DR cross section is maximum at the resonance energy \in $_{\rm r}$ such that

$$E_{\text{max}} = \epsilon_{\text{r}} \quad M/m \tag{2.19}$$

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This is because the compton profile is maximum at $p_{iz} = 0$, which requires the vanishing of the square bracket in eq. (2.10).

In the present work, the DR cross sections are calculated in the isolated resonance approximation using the following adopted form,

$$\sigma^{-DR} = 2.68 \times 10^{-23} \cdot V_a \cdot \omega(d) / (\epsilon_c \cdot \Delta \epsilon_c)$$
 (2.20)

where $\epsilon_{\rm c}$ is the continuum electron energy, $\Delta\epsilon_{\rm c}$ is the energy bin, ω (d) is the fluorescence yield of the d state. The radiationless capture probability $\rm V_a$ for the process (1.3) to take place is calculated by

$$V_a = (g_d/2g_i) A_a$$
 (2.21)

where $\mathbf{g}_{\mathbf{d}}$ and $\mathbf{g}_{\mathbf{i}}$ are the statistical weights of the intermediate state (d) and the initial state (i) respectively. $\mathbf{A}_{\mathbf{a}}$ is the Auger rate of the decay of the state d to the state i.

RESULTS AND DISCUSSIONS

The DR cross sections for P^{8+} and Fe^{19+} are calculated in the isolated resonance approximation using eq. (2.20). The RTEX cross sections for these two ions are obtained by folding the DR cross sections over the Compton profile of H_2 and He targest using eq. (2.18). All the resonance states of the form $1s2s^22p^5$, $1s2s^22p^4n\ell$ with $\ell=0,1,2,3$ and $1s2s^22p^33p^2$ are included in the DR and RTEX calculations. However, the

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cascade processes reduces the DR cross section for the later state by a factor of 1. The DR cross section for this state becomes $0.18 - 10^{-21}$ cm² which represent only 2% of the state $1 \text{s2s}^2 2\text{p}^5$ alone in Fe¹⁹⁺ case. Thus the contributions of all states of the form $1 \text{s2s}^2 2\text{p}$ near n'2' to the total RTEX cross section are presumably about 1%. Such trivial contributions are neglected in the present work.

The RTEX cross sections versus the projectile energies $^{8+}$ + $^{4+}$ and $^{8+}$ + He systems are presented in figures 1 and 2 respectively. In these two figures for $^{8+}$, the RTEX cross section is represented as a single peak. However, the resonance peak for for $^{8+}$ + He is broadened (fig. 2) as compared with that for $^{8+}$ + $^{4+}$ (fig. 1), reflecting the broader momentum distribution (Compton profile) of the He atom. In other words, the effect of the target momentum distribution is evident in the more pronounced resonance peak for the $^{4+}$ case, reflecting the narrower Compton profile of molecular $^{4+}$ with respect to the broader He momentum distribution.

Specifically, for P^{8+} + H_2 (Fig. 1) we have σ_{max}^{RTEX} = 0.208 x 10^{-21} cm² at projectile energy E_{max} = 108 MeV while for P^{8+} + He (Fig 2) we have σ_{max}^{RTEX} = 0.159 x 10^{-21} cm² at E_{max} = 107 MeV. The maximum cross section σ_{max}^{RTEX} is lower for He than in H_2 case because the Compton profile for H_2 is

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broader than that for \mathbf{H}_2 target.

Figures 3 and 4 present the RTEX cross sections for Fe¹⁹⁺ + H₂ and Fe¹⁹⁺ + He systems respectively. The RTEX cross section in both figures exhibit a two-peak behaviour instead of one. In figure 3 (H₂ target), the two peaks lie at projectile energies 516 MeV and 610 Mev and their values are σ_{max}^{RTEX} (peak I) = 0.38 x 10⁻²¹ cm² and σ_{max}^{RTEX} (peak II) = 0.27 x 10⁻²¹ cm². In figure 4 (He target) the two peaks locate at 519 MeV and 604 MeV with values σ_{max}^{RTEX} = 0.28 x 10⁻²¹ cm² for peak I and 0.23 x 10⁻²¹ cm² for peak II. The first peak in both cases comes from the intermediate state 1s2s²2p⁵ and the second peak comes from states 1s2s²2p⁴n? with n \geq 3 including the high Rydberg states (HRS). It has to be noted that the extrapolation to the HRS contributions are carried out at n \geq 7 in the present work.

Since figures 3 and 4 assume the same projectile (Fe $^{19+}$), it is expected that the ratios of peaks I and II for He and H $_2$ targets must be close. Our calculations show that the ratio (peak I/peak II) equal 1.4 for H $_2$ target and 1.2 for He target. This slight difference may be attributed to the broadening effect of the Compton profile.

On the other hand, figures 1 and 3 which are drawn for the same $\rm H_2$ target and different projectiles $\rm P^{8+}$ and $\rm Fe^{19+}$

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respectively, there is a clear manifistation that the RTEX cross sections increase with the atomic number of the members in the Nitrogen isoelectronic sequence.

4. Conclusions:

The RTEX cross sections obtained by collisons of positive ions with He targets are broader than those with $\rm H_2$. As the degree of ionization of the projectile in any isoelectronic sequence increases the RTEX exhibits a two-peak behaviour and its cross section increases. The property of two-peak behaviour has been pronounced with increasing the degree of ionization in Calcium isonuclear sequence in ref. 1. Thus, it is concluded that in any isoelectronic (same N) or isonuclear (same Z) sequence the two-peak trend of RTEX must be related to the degree ionization of the ionic projectiles.

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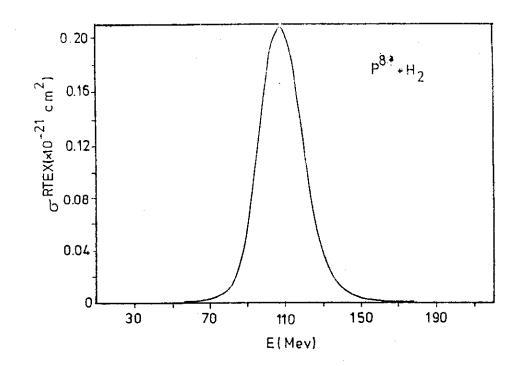


Figure 1. The RTEX cross sections in ${\rm cm}^2$ vs the projectile energy in MeV for the ${\rm P}^{8+}$ + ${\rm H}_2$ collision system with k-shell excitation.

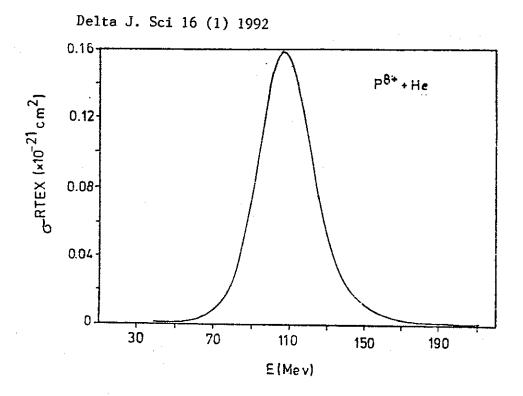
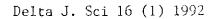
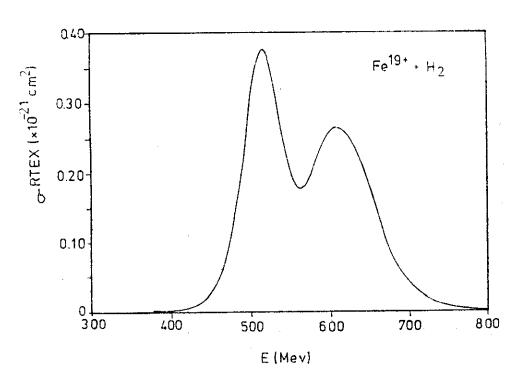


Figure 2. Same as in figure 1 but for He target.





igure 3. The RTEX cross sections in ${\rm cm}^2$ vs the projectile energy in MeV for the collision of Fe $^{19+}$ with H $_2$ target.

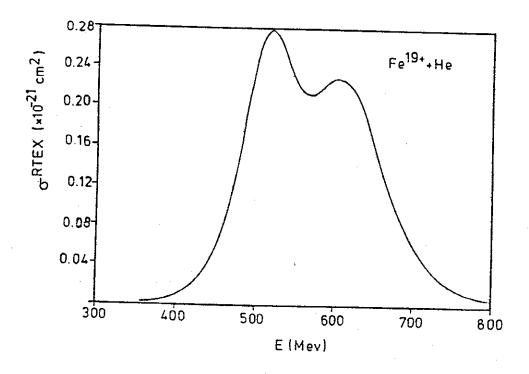


Figure 4. Same as figure 3 but for He target.

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الانتقال الرنيني المثير للايونات الشبيهسه بالنتروجين

جابب عمسسر قسم الغيزياء _ بكلية العلسوم _ جامعسة عين شمسس العباسيسة _ القاهسرة _ مصسر

وفي عملية RTEX يتم أسر أحد الكترونات الهدف (جزئ الهيدروجين أو درة الهيليسوم) بواسطة المقدوف الذي يتار ثم تنبعث أشعة اكس عند استقراره٠

وفى التغريب الدفعى تكون عملية RTEX مما علم لعملية أعادة الاتحساد الالكترونسى (DR) فى تصادم الالكترونات بالايونات ولذلك فقد حسبت المقاطع المستعرضسة لعملية (DR) لايونات Fe¹⁹⁺, P⁸⁺ المتارة فى قشرنها الايونسات ومنها تم استنتاج المقاطع المستعرضسة لعملية RTEX لهذان الايونسسات عند تصادم كل منهما مع أهداف الهيدروجين والهيليسوم