The Resonance Interaction of H-like U ion With H$_2$ and He Targets

Mona Abdel-Aziz$^1$ and H. Ramadan$^2$

$^1$Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.
$^2$Department of Basic Sciences, Faculty of Computer and Information Sciences, Ain Shams University, Cairo, Egypt.
Email:hramadan@eun.eg

Received: 2/8/2012            Accepted: 20/11/2012

ABSTRACT

Dielectronic recombination cross sections and rate coefficients for H-like U$^{91+}$, which recombines with the continuum electron to form U$^{90+}$ ion are explicitly calculated. The rate coefficients are obtained from direct evaluation of the Auger and radiative transition probabilities, which are calculated from nonrelativistic Hartree-Fock wave functions. All the available electron excitations for $\Delta n \neq 0$ are calculated. On the other hand, the resonant transfer excitation followed by X-ray (RTEX) cross sections in the collisions of highly charged Uranium ion U$^{91+}$ with H$_2$ and He are calculated. It is found that the rates peaks around 5 K Ry and has the value $3.5 \times 10^{-14}$ cm$^3$/s. Moreover, the range of the projectile energies of RTEX cross sections is between 8-17 GeV, forming three peaks, which agrees with previous experimental and theoretical works.

Key Words: Ion Atom Collision/ Dielectronic Recombination/ Hartree-Fock method.

INTRODUCTION

Dielectronic recombination (DR) is an important electron-ion collision process governing the charge balance in atomic plasmas ($^1$, $^2$). Dielectronic recombination can be viewed as a two-step process. Firstly, a free electron excites an electron in an ion X$^{z+}$, say, and a sufficient of its energy is captured to form the excited ion X$^{(z-1)+}$. The process is reversible since the total energy of the system remains conserved. However, if an electron (either the captured electron or an electron in the parent core) then makes a spontaneous radiative transition that leaves the ion in a non-autoionizing (bound) state then the recombination can be viewed as complete. Dielectronic recombination can take place via many intermediate autoionizing states—indeed, entire Rydberg series. It was the significance of the effective statistical weight of so many available states that let Burgess ($^3$) to recognize the importance of dielectronic recombination in the first place. A consequence of this is that a huge population structure model is required in principle for further progress. In astrophysics and fusion, the problem has usually been made manageable by simply summing over all final states so as to produce a total dielectronic recombination rate coefficient. In comparison with radiative recombination, this is the effective recombination coefficient from the point of view of an ionization state only the so-called coronal picture. In this picture, excited-state populations are depleted exclusively by spontaneous radiative transitions and are small compared to those of ground states with which they are in quasi-static equilibrium. Collisional processes are negligible, except with ground state targets. In turn, the ionization state is determined by balancing the effective recombination rate of (the ground state) X$^{z+}$ against the collisional ionization rate of (the intermediate state) X$^{(z-1)+}$ ($^4$). A close relationship was established not only between the reactions in electron-ion collision systems, but also among ion-atom (I-A) collisions and between electron-ion and ion-atom systems ($^5$). Thus, a unified picture of many electron-ion and ion-atom collision processes emerges if resonance dominance is assumed and when the isolated resonance approximation (IRA) and the impulse approximation (IMA) are valid. In the
resonance dominance picture, the ion-atom collision may proceed by a resonant transfer excitation (RTE) followed by either Auger (RTEA) or radiation (RTEX) emission.

\[(b + e) + A^{z+} \leftrightarrow b + (A^{(z-1)+})^{++} \rightarrow (A^{(z-1)+})^{*} + \hbar \nu + b \]  

(1)

In the resonant transfer excitation process in ion-atom collisions (Eq. (1)), the target electrons are playing important roles in exciting projectile ions \((A^{z+})\), with the transfer of one of the target electrons to the projectile. According to the energy conservation, RTEX may occur only in the vicinity of well-defined resonance energies determined by the atomic structure of the projectile ion. Each resonance in the excitation process has a width and resolution controlled by the momentum distribution of the target electrons (Compton profile).

Brandt (5) formulated a relation between DR and RTEX cross sections using Compton profile of the momentum distribution of electrons in atomic He or molecular H\(_2\) targets. Lee (6) has formulated the used Compton profile for both He and H\(_2\). In the last few years, RTEX cross sections were considered as indirect measurements for the DR cross sections. The relationship between RTEX and DR cross sections were confirmed by many theoretical calculations (7, 8). Many experimental work, as well, has been done (9).

In the present work, the cross sections of both DR and RTEX for U\(^{91+}\) ion as well as the rate coefficients are calculated. The only available transitions are those with (inter-shell-excitations), which reflect the importance of these transitions at high temperatures for heavy ions.

**THEORETICAL CALCULATION**

The DR process is completed in two successive steps that begins when an electron (of kinetic energy \(e_c\) and angular momentum \(\ell\)) is captured by target ion \(X_i^{(q)+}\) (here \(X_i\) stands for U\(^{91+}\)), simultaneously with excitation of a bound state elicitation. The intermediate doubly excited resonance state \(X_d^{(q-1)+}\) is formed, which may decay by emitting a photon to form a final bound state, thus completing the process of dielectronic recombination (DR). The DR process can be expressed schematically as follows:

\[e_c + X_i^{(q)+} \rightarrow X_d^{(q-1)+**} \rightarrow X_i^{(q-1)+*} + \hbar \nu \]  

(2)

Similarly, the RTEX process is a two step process in which the ion captures an electron from an atom or molecule to form an intermediate doubly excited state (d-state). This process can be represented schematically as:

\[X_i^{(q)+} + B \rightarrow X_d^{(q-1)+**} + B' \rightarrow X_i^{(q-1)+**} + B^* + X - ray \]  

(3)

DR cross sections \((\sigma^{DR})\) are calculated using the IMA within the framework of AMA to generate the RTEX cross sections \((\sigma^{RTEX})\) for the collisions of U\(^{91+}\) ion with H\(_2\) and He targets. Bound states used in the calculations are obtained using the nonrelativistic single configuration Hartree-Fock (SCHF) approximation. The continuum wave functions are obtained using the distorted wave approximation (DWA).

All doubly excited intermediate states found with \(\Delta n \neq 0\) excitations and contributing to the DR cross section are presented in Table (1).
where, $p_0$ is the momentum of the free electron, $a_o$ is Bohr radius, $\tau_o$ is the atomic unit of time which is given as $\tau_o = 2.4189 \times 10^{-17}$ sec., $V_a(i \rightarrow d)$ and $\omega(d)$ are the radiationless capture probability and fluorescence yield respectively given by:

$$V_a(i \rightarrow d) = \left( \frac{g_d}{g_e g_i} \right) \sum Aa(d \rightarrow i \ell e)$$  \hspace{1cm} (6)

$g_e$, $g_i$, and $g_d$ are the statistical factors for the continuum electron, initial state and intermediate state respectively, and

$$\omega(d) = \frac{\sum f Aa(d \rightarrow f)}{\Gamma_a(d) + \Gamma_f(d)}$$  \hspace{1cm} (7)

The Auger and radiative transition probabilities $A_a$ and $A_r$ are the basic components of the cross section given by:

$$A_a(d \rightarrow i) = \left( \frac{\gamma e}{\hbar a_o} \right) \left| \frac{1}{i} \right| \left| \frac{1}{d} \right| = \left( \frac{\gamma e}{\tau_o} \right) \left| \frac{1}{i} \right| \left| \frac{1}{d} \right|$$  \hspace{1cm} (8)

where, $\frac{1}{r_{\gamma \gamma}}$ is the electron-electron coupling operator. On the other hand, the Auger width $\Gamma_a$ is obtained by:

$$\Gamma_a(d) = [\sum_{i \ell e} A_a(d \rightarrow i \ell e) + \sum_{j \ell e} A_a(d \rightarrow j \ell e)]$$  \hspace{1cm} (9)

The single-electron radiative probability is given by:

$$A_r = \left( \frac{\gamma e}{\hbar} \right) \left| \langle f | \hat{D} | d \rangle \right|^2 \rho_f$$  \hspace{1cm} (10)

where, $\hat{D}$ is the photon-electron interaction operator, and $\rho_f$ is the density of final state. Moreover, the radiative width $\Gamma_r$ is given by summing all the radiative probabilities for all final states of the corresponding intermediate state:

$$\Gamma_r(d) = \sum_f A_r(d \rightarrow f)$$  \hspace{1cm} (11)

Since the Compton profile gives the probability of finding a particular target electron with a momentum $p_z$, it is utilized with the impulse approximation (IMA) to relate the RTEX cross section to the DR cross section. The relationship between DR and RTEX cross sections, following Brandt (10) is given by:
\[
\sigma^{RTEX} = \sqrt{\frac{M}{\Delta E}} \Delta \epsilon \cdot J_{R}(p_{z}) \sigma^{DR}
\]

where, \( M \) is the mass of the projectile ion of energy \( E \), \( J_{R}(p_{z}) \) is the Compton profile and \( p_{z} \) is the \( z \)-component of the momentum.

The DR cross sections are calculated for \( U^{91+} \) ion with \( \Delta n \neq 0 \) where these results are used to generate the RTEX cross sections when the Uranium ion collide with \( H_{2} \) and \( He \) targets.

**RESULTS AND DISCUSSION**

The DR cross sections for \( U^{91+} \) ion and the generated RTEX cross sections are calculated using the single configuration Hartree-Fock (SCHF) code when the angular momentum average (AMA) scheme is considered. On the other hand, the DR rates \( a^{DR} \) are calculated in the isolated resonance approximation for all intermediate states.

**DR Cross Section (\( \sigma^{DR} \))**

Table (1) shows the DR cross sections (\( \sigma^{DR} \)) (in units of \( 10^{-24} \) cm\(^2\)) vs the continuum energy \( \epsilon_{c} \) (in Ry). From the table it is found that many intermediate states have the largest contribution to the DR cross sections such as 2snp, and 2pnd state. The DR cross sections for many states can be neglected since they have very small values such as 3sns and 4sns states where they are in the range of \( 10^{-31} \) cm\(^2\).

**DR Rates (\( a^{DR} \))**

Figure (1) shows the DR rates for \( U^{91+} \) ion where, it gives a smooth variation with temperature \( kT \). From the figure it is found the rates are peaked around 5000 Ry and the peak value is \( 3.5 \times 10^{-14} \) cm\(^3\)/s. The contributions of high Rydberg states (HRS) are obtained at \( n_{c} = 6 \), i.e. the detailed calculations are stopped at \( n = 5 \), where \( A_{s} \) and \( A_{r} \) start to scale as \( 1/n^{3} \).

![Graph](image)

**Fig. (1):** The DR rate coefficients (in units of \( 10^{-14} \) cm\(^3\)/s) vs \( kT(Ry) \) for \( U^{91+} \) ion.
Table (1): The DR cross sections (in units of \(10^{14} \text{ cm}^2\)) for the calculated states at each continuum energy \(E_c\) (in Ry), the number between brackets is power of 10.

<table>
<thead>
<tr>
<th>state</th>
<th>(\ell_c)</th>
<th>(\sigma_{DR})</th>
<th>state</th>
<th>(\ell_c)</th>
<th>(\sigma_{DR})</th>
<th>State</th>
<th>(\ell_c)</th>
<th>(\sigma_{DR})</th>
</tr>
</thead>
<tbody>
<tr>
<td>2s3s</td>
<td>7420</td>
<td>2.81(-4)</td>
<td>4s5s</td>
<td>7606</td>
<td>1.23(-7)</td>
<td>3p3d</td>
<td>6610</td>
<td>5.85(-2)</td>
</tr>
<tr>
<td>2s4s</td>
<td>5837</td>
<td>1.73(-4)</td>
<td>n ≥ 6</td>
<td>7841</td>
<td>2.22(-7)</td>
<td>3p4d</td>
<td>7013</td>
<td>3.42(-2)</td>
</tr>
<tr>
<td>2s5s</td>
<td>6022</td>
<td>9.56(-5)</td>
<td>4s3d</td>
<td>7012</td>
<td>2.32(-3)</td>
<td>3p5d</td>
<td>7198</td>
<td>1.27(-2)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>6257</td>
<td>1.94(0)</td>
<td>4s4d</td>
<td>7420</td>
<td>1.59(-3)</td>
<td>n ≥ 6</td>
<td>7433</td>
<td>4.07(-2)</td>
</tr>
<tr>
<td>2s2p</td>
<td>4268</td>
<td>3.09(-1)</td>
<td>4s5d</td>
<td>7607</td>
<td>6.98(-4)</td>
<td>4p5s</td>
<td>7607</td>
<td>1.25(-2)</td>
</tr>
<tr>
<td>2s3p</td>
<td>5440</td>
<td>7.80(-1)</td>
<td>n ≥ 6</td>
<td>7842</td>
<td>4.90(-3)</td>
<td>n ≥ 6</td>
<td>7842</td>
<td>5.77(-2)</td>
</tr>
<tr>
<td>2s4p</td>
<td>5839</td>
<td>3.76(-2)</td>
<td>2p3s</td>
<td>5439</td>
<td>5.57(-1)</td>
<td>4p3</td>
<td>7419</td>
<td>2.00(-2)</td>
</tr>
<tr>
<td>2s5p</td>
<td>6122</td>
<td>7.98(-1)</td>
<td>2p4s</td>
<td>5838</td>
<td>2.32(-1)</td>
<td>4p5p</td>
<td>7607</td>
<td>2.01(-2)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>6357</td>
<td>1.61(-2)</td>
<td>2p5s</td>
<td>6022</td>
<td>1.03(-1)</td>
<td>n ≥ 6</td>
<td>7482</td>
<td>1.18(-1)</td>
</tr>
<tr>
<td>2s4d</td>
<td>5840</td>
<td>2.09(-2)</td>
<td>n ≥ 6</td>
<td>6257</td>
<td>1.42(-3)</td>
<td>4p4d</td>
<td>7420</td>
<td>1.08(-2)</td>
</tr>
<tr>
<td>2s5d</td>
<td>6023</td>
<td>1.34(-2)</td>
<td>2p2</td>
<td>4296</td>
<td>3.05(0)</td>
<td>4p5d</td>
<td>7607</td>
<td>5.21(-3)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>6258</td>
<td>2.71(-6)</td>
<td>2p3p</td>
<td>5441</td>
<td>1.03(-1)</td>
<td>n ≥ 6</td>
<td>7482</td>
<td>2.57(-2)</td>
</tr>
<tr>
<td>3s2</td>
<td>6608</td>
<td>1.69(-6)</td>
<td>2p4p</td>
<td>5839</td>
<td>4.25(-1)</td>
<td>3d5s</td>
<td>7197</td>
<td>1.40(-3)</td>
</tr>
<tr>
<td>3s4s</td>
<td>7010</td>
<td>3.85(-6)</td>
<td>2p5p</td>
<td>6023</td>
<td>2.36(-1)</td>
<td>n ≥ 6</td>
<td>7432</td>
<td>1.06(-2)</td>
</tr>
<tr>
<td>3s5s</td>
<td>7196</td>
<td>2.60(-6)</td>
<td>n ≥ 6</td>
<td>6258</td>
<td>2.53(-2)</td>
<td>3d4p</td>
<td>7012</td>
<td>2.36(-2)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>7431</td>
<td>5.27(-1)</td>
<td>2p3d</td>
<td>5445</td>
<td>4.45(-1)</td>
<td>3d5p</td>
<td>7197</td>
<td>7.77(-3)</td>
</tr>
<tr>
<td>3s3p</td>
<td>6606</td>
<td>1.71(-2)</td>
<td>2p4d</td>
<td>5841</td>
<td>1.94(-1)</td>
<td>n ≥ 6</td>
<td>7432</td>
<td>1.25(-3)</td>
</tr>
<tr>
<td>3s4p</td>
<td>7011</td>
<td>5.81(-2)</td>
<td>2p5d</td>
<td>6023</td>
<td>8.30(-2)</td>
<td>3d2</td>
<td>6614</td>
<td>6.08(-3)</td>
</tr>
<tr>
<td>3s5p</td>
<td>7200</td>
<td>7.54(-2)</td>
<td>n ≥ 6</td>
<td>6258</td>
<td>8.55(-2)</td>
<td>3d4d</td>
<td>7014</td>
<td>4.81(-3)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>7435</td>
<td>8.32(-2)</td>
<td>3p4s</td>
<td>7011</td>
<td>5.26(-2)</td>
<td>3d5p</td>
<td>7198</td>
<td>3.32(-3)</td>
</tr>
<tr>
<td>3s3d</td>
<td>6609</td>
<td>6.58(-3)</td>
<td>3p5s</td>
<td>7196</td>
<td>2.85(-2)</td>
<td>n ≥ 6</td>
<td>7433</td>
<td>9.16(-3)</td>
</tr>
<tr>
<td>3s4d</td>
<td>7013</td>
<td>3.49(-3)</td>
<td>n ≥ 6</td>
<td>7432</td>
<td>2.09(-1)</td>
<td>4d5s</td>
<td>7607</td>
<td>6.16(-4)</td>
</tr>
<tr>
<td>3s5d</td>
<td>7197</td>
<td>2.42(-3)</td>
<td>3p2</td>
<td>6608</td>
<td>1.09(-1)</td>
<td>n ≥ 6</td>
<td>7842</td>
<td>2.84(-3)</td>
</tr>
<tr>
<td>n ≥ 6</td>
<td>7432</td>
<td>4.90(-3)</td>
<td>3p4p</td>
<td>6903</td>
<td>8.36(-2)</td>
<td>4d4</td>
<td>7421</td>
<td>1.02(-3)</td>
</tr>
<tr>
<td>4s2</td>
<td>7420</td>
<td>2.55(-8)</td>
<td>3p5p</td>
<td>7197</td>
<td>5.82(-2)</td>
<td>4d5d</td>
<td>7608</td>
<td>1.50(-3)</td>
</tr>
</tbody>
</table>

**RTEX Cross Sections (\(\sigma_{RTEX}\))**

\(\sigma_{RTEX}\) cross sections are generated by folding the DR cross sections over the Compton profile of H\(_2\) molecule and He atom under the validity of impulse approximation (IMA). The results are shown in Fig. (2), where it is found that there are three peaks at the energies 10, 12.5 and 13.5 GeV. It has to be noted that, the RTEX cross sections for U\(^{91+}\) + He is broader than that with H\(_2\) target, which reflects the effect of the momentum distribution of electron in H\(_2\) and He target. Accordingly, the peak value of RTEX cross section for U\(^{91+}\) + H\(_2\) is higher by a factor of 1.4 than that of U\(^{91+}\) + He. The results of the RTEX cross sections partially agree with the results given in reference (ii), since both results have three peaks for the collision of U\(^{91+}\) + H\(_2\).
CONCLUSION

The present theoretical results for the DR cross sections, DR rate coefficients and RTEX cross sections of H-like U$^{91+}$ ion forming He-like U$^{90+}$ ion are calculated using the angular momentum average (AMA) scheme. The study is performed for $\Delta n \neq 0$ excitation, where it is found that the dominant states affecting on the DR cross sections are 2snp, 2pnp and 2pnd states. Moreover, the states 3sns and 4sns have almost no contribution in the DR cross sections. It is also found that the rates are varying in a smooth way with the temperature $kT$. The rates ($a_{DR}^{DR}$) are peaked at 5000 Ry with a value of $3.5 \times 10^{-14}$ cm$^3$/s. The RTEX cross sections $\sigma_{RTEX}$ with H$_2$ and He targets have three peaks which agree with reference [11]. In addition, the RTEX cross section for U$^{91+}$ He is broader than the RTEX cross section for U$^{91+}$ H$_2$, and the ratio between the peak values is 1.4 higher for H$_2$ than for He.

REFERENCES

(3) A. Burgess; APJ.; 139, 776 (1964).