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Effects of relativity on resonant transfer and excitation in collisions of U^{89+} with light targets

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The resonant transfer and excitation cross sections in collisions of U^{89+} ion with light targets have been calculated in impulse approximation using the multiconfiguration Dirac-Fock method. Effects of relativity not only shift the peak positions significantly but also change the number of peaks. Relativistic effects have been found to increase the total dielectronic recombination strength by 50%. Including Breit interaction in calculations of Auger matrix elements can enhance the resonant transfer and excitation cross sections by as much as a factor of 2.

I. INTRODUCTION

Excitation, ionization, and charge transfer are the atomic processes frequently encountered in ion-atom collisions. However, for certain projectile energies, excitation of the ion and capture of a bound target electron can occur simultaneously in a single collision to form a resonance state of the projectile. The excited state formed by this resonant transfer and excitation mechanism can stabilize either by emitting a photon (RTEX) or an Auger electron (RTEA).[1,2] Recently, several experimental investigations[1,3–6] have been carried out to study the RTEX process in ion-atom collisions. A formal theoretical treatment of simultaneous charge transfer and excitation in ion-atom collisions have also been developed.[7] Many theoretical calculations based on impulse approximation have been performed to obtain RTEX cross sections for low- and mid-z ions colliding with light atoms.[2,8–11] Recently, an experiment to measure RTEX cross section for U^{89+} in collisions with carbon target has also been attempted.[12] Most of the existing theoretical calculations were carried out in LS coupling using nonrelativistic single configuration approximation. For ion as heavy as U^{89+}, we expect that the nonrelativistic method would be inappropriate and a relativistic treatment is necessary. In this Rapid Communication, we report on the relativistic calculations of RTEX cross sections for U^{89+} ions colliding with hydrogen molecules, helium, and carbon targets, respectively. The calculations were carried out in impulse approximation.[2] Transition energies, Auger, and radiative rates were evaluated by using the multiconfiguration Dirac-Fock model (MCDF).[13,14] Effects of relativity and Breit interaction on the cross sections are also investigated.

II. THEORETICAL METHOD

Resonant electron transfer and excitation in ion-atom collisions is an atomic process analogous to dielectronic recombination (DR).[15] The DR process occurs when capture of a free electron is accompanied by simultaneous excitation of the ion to form a doubly excited autoionizing state with subsequent emission of a stabilizing photon. For a RTEX process, a weakly bound electron is captured instead of a free electron. In the impulse approximation,[2,7] the total RTEX cross section $\sigma_{\mathrm{RTE}}^{X}(i)$ for an initial state i can be obtained by folding the DR cross section with the Compton profile of the target atom

$$\sigma_{\mathrm{RTE}}^{X}(i)=\sum_{d}(M/2E)^{1/2}\Delta E\bar{\sigma}_{\mathrm{DR}}(i\rightarrow d)J(Q)\,, \qquad (1)$$

with

$$Q=(E_d-Em/M)(M/2E)^{1/2}\,. \qquad (2)$$

Here, E is the projectile energy in the laboratory frame, M is the mass of the projectile, m is the electron mass, $J(Q)$ is the Compton profile of the target atom or molecule, $\bar{\sigma}_{\mathrm{DR}}(i\rightarrow d)$ is the energy-averaged DR cross section from state i to intermediate state d with energy bin ΔE, and E_d is the energy of the intermediate state d with respect to the initial state i in the rest frame of the ion.

The energy-averaged DR cross section in isolated resonance approximation can be expressed in atomic units as

$$\bar{\sigma}_{\mathrm{DR}}(i\rightarrow d)=\frac{\pi^2}{\Delta E E_d}\frac{g_d}{2g_i}\frac{A_a(d\rightarrow i)\sum_f A_r(d\rightarrow f)}{\sum_j A_a(d\rightarrow j)+\sum_k A_r(d\rightarrow k)}\,. \qquad (3)$$

Here, g_d and g_i are the statistical weight factors for the states d and i, respectively; $A_a(d\rightarrow i)$ is the Auger rate, and $A_r(d\rightarrow k)$ is the radiative rate.

The detailed relativistic Auger transition probability is calculated from perturbation theory using the MCDF method. The transition rate is given by[16]

$$T=\frac{2\pi}{\hbar}\left|\langle\Psi_f|\sum_{\alpha<\beta}V_{\alpha\beta}|\Psi_i\rangle\right|^2\rho(\varepsilon)\,. \qquad (4)$$

Here, Ψ_i and Ψ_f are the initial and final-state wave functions, respectively, and $\rho(\varepsilon)$ is the energy density of final states.

In the present work, the two-electron operator $V_{\alpha\beta}$ is taken to be the sum of the Coulomb and generalized Breit operator and can be expressed in atomic units by

$$V_{12}=\frac{1}{r_{12}}-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\frac{\cos(\omega r_{12})}{r_{12}}+(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2)\frac{\cos(\omega r_{12})-1}{\omega^2 r_{12}}\,, \qquad (5)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are particle positron vectors, $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$, and $\boldsymbol{\nabla}_1$ and $\boldsymbol{\nabla}_2$ are gradient operators. The $\boldsymbol{\alpha}_i$ are Dirac matrices and ω is the wave number of the exchanged virtual photon.

The relativistic radiative transition probability is also calculated from perturbation theory[17] using the MCDF method. The detailed formulation of the relativistic Auger and radiative transitions in the MCDF model has been presented in Ref. 14.

There are other transfer excitation processes in the ion-atom collisions. The same resonance states as in RTEX can be formed by collisional excitation by the target nucleus and one-electron capture in the same collision (NTE). The projectile can also be excited by collision with one of the electron in the target and the other electron can be transferred to the projectile (2*e* TE). These uncorrelated transfer excitation processes are not treated in the present work.

III. NUMERICAL CALCULATIONS

For U^{89+} ion in collisions with light targets, the resonant transfer and excitation followed by emission of a stabilizing photon can be represented by

$$\mathrm{U}^{89+}(1s^2 2s)+T \rightarrow \mathrm{U}^{88+}(1s2snln'l')+T^+$$
$$\hookrightarrow \mathrm{U}^{88+}(1s^2 2sn''l'')+h\nu\,.$$

In the present work, we include the intermediate states from the $1s2s2lnl'$ $(2 \le n \le 12$ and $0 \le l' \le 3)$ and $1s2s3l3l'$ configurations.

The atomic energy levels and bound-state wave functions were calculated using the MCDF model in the average-level scheme.[13] The calculations were carried out in intermediate coupling with configuration interaction from the same complex. The effects of quantum-electrodynamic corrections, finite nuclear size, and relaxation were included in the calculations of transition energies.

The Auger transition rates were calculated using two-electron operator [Eq. (5)] both with and without Breit interaction [second and third terms of Eq. (5)]. The radiative transition rates were evaluated for electric-dipole transition in length gauge.[17] All possible Auger channels and radiative transitions leading to stabilized bound states were included in the present calculation. Radiative transitions between autoionizing states were neglected.

In order to study the effects of relativity on the RTEX cross sections, repeated calculations for intermediate states $1s2s2lnl'$ $(2 \le n \le 8$ and $0 \le l' \le 3)$ were performed by using the nonrelativistic limit of the MCDF model. The nonrelativistic limit of the MCDF model can be achieved by increasing the velocity of light a thousandfold.[13]

In the calculations of RTEX cross sections, Compton profiles for hydrogen molecule and helium were taken from experiment.[18] For the carbon target, theoretical Compton profiles[19] were employed.

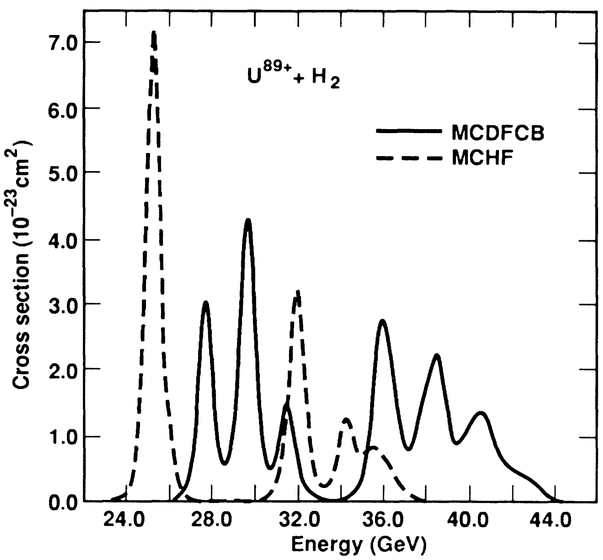

FIG. 1. RTEX cross sections for the $\mathrm{U}^{89+}+\mathrm{H}_2$ collisions as functions of projectile energy. The solid curve represents the results from the relativistic calculations, while the dashed curve indicates the nonrelativistic values.

IV. RESULTS AND DISCUSSION

For U^{88+}, effects of relativity increase the *K-LL* Auger energies by 2–18 keV and can change the individual Auger transition rates by orders of magnitude for some transitions. The total DR resonant strength converges quickly as a function of principle quantum number n along the $2lnl'$ Rydberg series. For $n=9$ to 12, it contributes only 2% of the total DR strength.

In Fig. 1, the RTEX cross sections for U^{89+} in collision

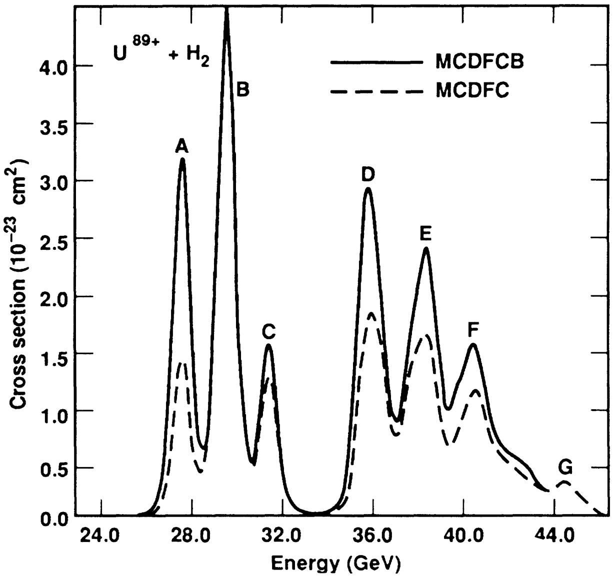

FIG. 2. RTEX cross sections for the $\mathrm{U}^{89+}+\mathrm{H}_2$ collisions as functions of projectile energy. The solid curve displays the MCDF predictions including the contributions from the generalized Breit operator. The dashed curve represents the results from the MCDF method without including Breit interaction in calculations of Auger rates. The intermediate states contributing to the peaks are A, $1s2s^2 2p_{1/2}+1s2s2p_{1/2}^2$; B, $1s2s^2 2p_{3/2}+1s2s2p_{1/2}2p_{3/2}$; C, $1s2s2p_{3/2}^2$; D, $1s2s2l3l'$; E, $1s2s2l4l'$; F, $1s2s2lnl'$ $(n \ge 5)$; and G, $1s2s3l3l'$.

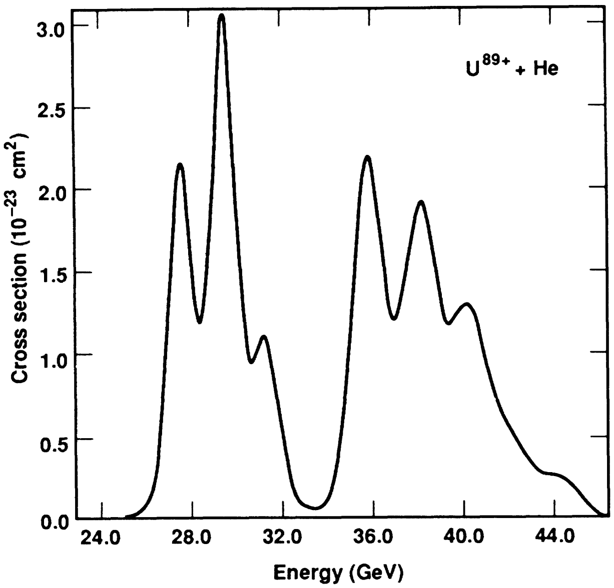

FIG. 3. RTEX cross sections for the $U^{89+}+He$ collisions as a function of projectile energy.

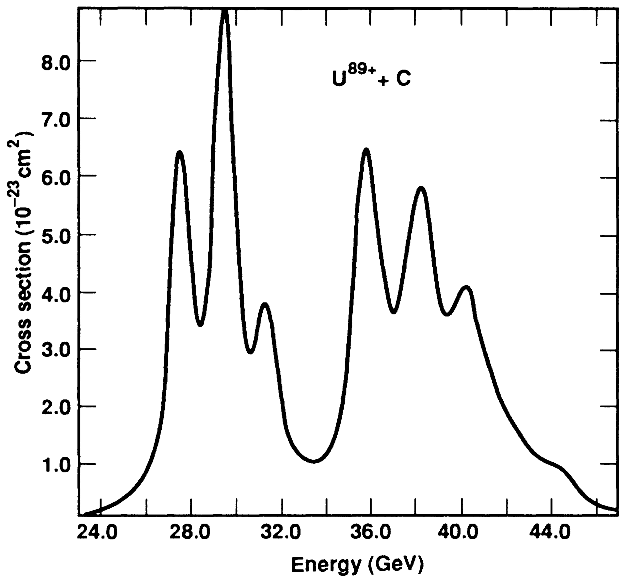

FIG. 4. RTEX cross sections for the $U^{89+}+C$ collisions as a function of projectile energy.

with H_2 from nonrelativistic calculations (MCHF) are compared with results from the MCDF model including Breit interaction in calculations of Auger rates (MCDFCB). There are six peaks in the relativistic spectra contributed from the $1s2s2lnl'$ intermediate states and only four in the corresponding nonrelativistic case. The effects of relativity shift the peaks to higher energies and split the first peak arising from the $1s2s2l2l'$ intermediate states into three peaks. The splitting of the first peak is mainly caused by the inclusion of the spin-orbit interaction in the present relativistic calculations. The total DR resonance strength is increased from 1.60×10^{-19} cm^{2}eV to 2.43×10^{-19} cm^{2}eV due to the effects of relativity.

The RTEX cross sections for $U^{89+}+H_2$ system from the MCDF calculations with and without Breit interaction in the Auger operator are compared in Fig. 2. There are seven distinct peaks in the energy range $26 \leq E \leq 46$ GeV. The first three peaks arise from the intermediate states $1s2s^22p_{1/2}$ (90%)$+1s2s2p_{1/2}^2$ (10%), $1s2s^22p_{3/2}$ (19%)$+1s2s2p_{1/2}2p_{3/2}$ (81%), and $1s2s2p_{3/2}^2$, respectively. The last four peaks come from $1s2s2l3l'$, $1s2s2l4l'$, $1s2s2lnl'$ ($n\geq5$), and $1s2s3l3l'$ configurations, respectively. Including Breit interaction in the calculations of Auger matrix elements can increase the cross sections at some projectile energies by as much as a factor of 2. Breit interaction has little effect on the $1s$-$2p_{1/2}2p_{3/2}$ Auger transitions (peak *B* in Fig. 2) which is consistent with the findings for the corresponding transitions in the neutral atoms.[20]

The RTEX cross sections for U^{89+} in collisions with helium and carbon are shown in Figs. 3 and 4. Similar peak structure as in the $U^{89+}+H_2$ collisions is obtained. The cross sections for the $U^{89+}+C$ collisions are about a factor of 2 larger than those for the $U^{89+}+H_2$ and $U^{89+}+He$ systems due to the fact that there are six electrons in a carbon atom and the *K*-shell electrons in the carbon atom contribute little to the RTEX cross sections.

V. CONCLUSIONS

We have calculated the RTEX cross sections for U^{89+} ion in collisions with light targets in impulse approximation using fully relativistic MCDF method. We have demonstrated that the effects of relativity can change the peak positions, and number of peaks, as well as the peak heights. We conclude that the relativistic effects should be included in the calculations of RTEX cross sections in heavy-ion collisions.

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[1] J. A. Tanis, S. M. Shafroth, J. E. Willis, M. Clark, J. Swenson, E. N. Strait, and J. R. Mowat, Phys. Rev. Lett. **47**, 828 (1981).

[2] D. Brandt, Phys. Rev. A **27**, 1314 (1983).

[3] J. A. Tanis, E. M. Berstein, W. G. Graham, M. Clark, S. M. Shafroth, B. M. Johnson, K. W. Jones, and M. Meron, Phys. Rev. Lett. **49**, 1325 (1982).

[4] J. A. Tanis, E. M. Berstein, M. P. Stockli, M. Clark, R. H. McFarland, T. J. Morgan, K. K. Berkner, A. Schlacter, and J. W. Stearns, Phys. Rev. Lett. **53**, 2551 (1984).

[5] J. A. Tanis, E. M. Berstein, M. W. Clark, W. G. Graham, R. H. McFarland, T. J. Morgan, J. R. Mowat, D. W. Mueller, A.

Muller, M. P. Stockli, K. H. Berkner, P. Gohil, R. J. McDonald, A. S. Schlacter, and J. W. Stearns, Phys. Rev. A **34**, 2543 (1986).

[6] M. Schulz, R. Schuch, S. Datz, E. L. B. Justiniano, P. D. Miller, and H. Schöne, Phys. Rev. A **38**, 5454 (1988).

[7] J. M. Feagin, J. S. Briggs, and T. M. Reeves, J. Phys. B **17**, 1057 (1984).

[8] D. J. McLaughlin and Y. Hahn, Phys. Lett. **112A**, 389 (1985).

[9] D. J. McLaughlin and Y. Hahn, Phys. Rev. A **37**, 3587 (1988).

[10] C. P. Bhalla and K. R. Karim, Phys. Rev. A **39**, 6060 (1989).

[11] N. R. Badnell, Phys. Rev. A **40**, 3579 (1989).

[12] W. G. Graham *et al.*, in *Proceedings of the Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, New York, 1989,* Abstracts of Contributed Papers, edited by A. Dalgarno *et al.* (XVI ICPEAC Program Committee, New York, 1989).

[13] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).

[14] M. H. Chen, Phys. Rev. A **31**, 1449 (1985).

[15] M. J. Seaton and P. J. Storey, in *Atomic Processes and Applications,* edited by P. G. Burke and B. L. Moisewitsch (North-Holland, Amsterdam, 1976), p. 133.

[16] W. Bambynek *et al.*, Rev. Mod. Phys. **44**, 716 (1972).

[17] I. P. Grant, J. Phys. B **7**, 1458 (1974).

[18] J. S. Lee, Chem. Phys. **66**, 4906 (1977).

[19] F. Biggs, L. B. Mendelsohn, and J. B. Mann, At. Data. Nucl. Data Tables **16**, 201 (1975).

[20] M. H. Chen and B. Crasemann, Phys. Rev. A **28**, 2829 (1983).