Auger emission following resonant transfer excitation in collisions of F^{8+} with H_2

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We have calculated differential cross sections for the process of resonant transfer excitation followed by Auger emission (RTEA) in collisions of H-like fluorine with H_2. At energies below the $KL\infty$ limit, our results for the *KLL*, *KLM*, and *KLN* Auger electrons agree qualitatively with the experimental results of Schulz *et al.* [Phys. Rev. Lett. **62**, 1738 (1989)] for transfer excitation (TE) that have been normalized to our *KLL* RTEA cross section at 48 Ry. Together with our RTEA results for *KLO* emission, this implies that RTE is the dominant TE mechanism at these energies for all n values measured so far although uncorrelated transfer excitation may be important at high energies. The absolute cross sections of Schulz *et al.* are about a factor of 12 smaller than theory.

I. INTRODUCTION

Resonant processes in electron-ion and atom-ion collisions have been studied in the past, in the main, by capture followed by photon emission[1-4] or excitation followed by Auger emission,[5-8] neither of which is particularly sensitive to the Auger probabilities. With the advent of projectile Auger spectroscopy[9] it has become possible, via resonant transfer excitation (RTE) in ion-atom collisions, to make comparisons between theory and experiment for individual Auger transitions; see, for example, the experiments on O^{5+} by Swenson *et al.*[10,11] and on F^{6+} by Zouros *et al.*[12] In the recent TE experiment on $F^{8+}+H_2$ collisions by Schulz *et al.*,[13] Auger emission was detected from *KLL*, *KLM*, *KLN*, and *KLO* transitions. RTE Auger emission (RTEA) is expected to peak at energies below the $KL\infty$ limit so TE Auger emission above the $KL\infty$ limit was attributed[13] to excitation of the projectile electron by a target electron and uncorrelated capture of a target electron by the projectile nucleus (UTEA). In this paper we calculate the RTEA contribution and hence, for a given energy dependence, put a bound on the UTEA contribution.

In Sec. II we outline the theory behind our calculation, in particular making allowance for the angular dependence of the Auger emission. In Sec. III we make some test comparisons with some observations in Li-like ions. In Sec. IV we describe our calculations for H-like ions, and present the results for F^{8+} in Sec. V, where we compare them with experiment. We conclude in Sec. VI.

II. THEORY

Using the impulse approximation,[14] the integrated RTEA cross section $\sigma_a(i;j;k)$ for an initial state i, an intermediate state j, and a final state k may be written in terms of an energy-averaged resonant excitation cross section $\bar{\sigma}_e(i;j;k)$, thus

$$\sigma_a(i;j;k)=J(Q)\bar{\sigma}_e(i;j;k)\frac{\Delta E_c}{2I}\left[\frac{MI}{E}\right]^{1/2}. \tag{1}$$

$J(Q)$ is the Compton profile[15] of the target gas with Q given by

$$Q=\frac{1}{2I}\left[E_c+E_t-\frac{Em}{M}\right]\left[\frac{MI}{E}\right]^{1/2}, \tag{2}$$

and E is the projectile-ion energy in the laboratory frame, E_c is the $j\rightarrow i$ Auger energy, and E_t the binding energy of the target electron, both in the rest frame of the projectile. M is the ionic mass, m the electron mass, and I is the ionization potential of the hydrogen atom.

The integrated energy-averaged resonant-excitation cross section is given by

$$\bar{\sigma}_e(i;j;k)=\frac{(2\pi a_0 I)^2}{E_c\Delta E_c}\frac{\omega(j)}{2\omega(i)}\times\frac{\tau_0\sum_{l,l'}A_a(j\rightarrow i,E_c l)A_a(j\rightarrow k,E_c' l')}{\sum_h[A_r(j\rightarrow h)+\sum_{l'}A_a(j\rightarrow h,E_c' l')]}, \tag{3}$$

where $\omega(j)$ is the statistical weight of the $(N+1)$-electron doubly excited state, $\omega(i)$ is the statistical weight of the N-electron initial state, and $(2\pi a_0)^2\tau_0=2.6741\times10^{-32}$ cm^2 sec. The autoionization rates A_a and radiative rates A_r may be evaluated in configuration-mixing LS-coupling and intermediate-coupling approximations using the AUTOSTRUCTURE (Refs. 16 and 17) package.

We take account of the angular dependence of σ_a and $\bar{\sigma}_e$ in the same manner as for nonresonant electron scattering. For an ion both initially and finally in an S state and an isolated intermediate resonance state of angular momentum L, the usual differential cross-section expression[18] simplifies immediately[19] to

$$\frac{d\bar{\sigma}_e}{d\Omega}(i;j;k)=\bar{\sigma}_e(i;j;k)\left|Y_{L0}(\theta,\phi)\right|^2, \tag{4}$$

and similarly for $\sigma_a(i;j;k)$. $Y_{L0}(\theta,\phi)$ is a spherical harmonic function and $\theta=\theta_p$ is the angle of emission of the Auger electron in the projectile frame with respect to the beam axis.

III. TESTS ON LI-LIKE IONS

Before we look at RTEA from the 1s state of H-like fluorine, it is of interest to look at RTEA for the similar

problem of a Li-like initial state, viz. $1s^2 2s + e^- \rightleftharpoons 1s2s2p\,^{2}[1,3]D$, which has been measured by Swenson *et al.*[10,11] for O^{5+} and by Zouros *et al.*[12] for F^{6+}. Both H_2 and He target gases were used, establishing the validity of the impulse approximation and the Compton profile. Since emission from individual terms was observed, we need only consider the energy-averaged resonant excitation cross section $\bar{\sigma}_e$ given by Eq. (3). We also see from Eq. (3) that there should only be a small decrease in $\bar{\sigma}_e$ on going from O^{5+} to F^{6+}, due to the increasing Auger energy, since the Auger rates change little.

From Eqs. (3) and (4) and for a bin width of 1 Ry and in units of $4\pi\times10^{-20}$ cm^2 our zero-degree energy-averaged differential resonant-excitation cross sections for F^{6+} are 115 for the ^3D term and 20.5 for the ^1D. This agrees well with those that we have extracted, via Eqs. (1)–(4), from the original results of Zouros *et al.*,[12] of 90 for the ^3D term and 22 for ^1D. Recently, Zouros *et al.*[20] revised their results downwards by a factor of 1.67 viz. 54 for the ^3D term and 13 for ^1D. Our results for O^{5+} (again at $\theta=0°$) only differ slightly, 131 for the ^3D term and 22.8 for ^1D. Those extracted from the results of Swenson *et al.*[10] are a factor of 3 smaller, 35 for ^3D and 8.7 for ^1D; however, there is some uncertainty over the normalization in this experiment.[21] Zouros *et al.*[20] repeated the O^{5+} on He experiment and obtained results about a factor of 1.5 larger than Swenson *et al.*[10] This was just within their[20] estimate of the overall experimental uncertainty. The results of Hahn[22] quoted in the paper by Swenson *et al.*[10] and the theoretical results presented by Zouros *et al.*[20] did not contain the angular factor [see our Eq. (4)]. The experimental ratios for the ^3D to ^1D RTEA cross sections are independent of the normalization. Zouros *et al.*[20] obtain an experimental ratio of 4.2 (±1.1) and a theoretical ratio of 5.4 for F^{6+} while we obtain 5.6. Swenson *et al.*[10] obtain an experimental ratio of 4 for O^{5+}, while we obtain 5.7 and Hahn[22] 6.6.

Away from 0°, the $|Y_{20}(\theta,\phi)|^2$ dependence of the differential RTEA cross section (for $1s2s2p^2\,^3D$) is confirmed by the recent relative results of Benhenni *et al.*[23] for $\theta_p=10°-90°$, following the earlier work by Swenson *et al.*[11] Only for $\theta_p>60°$, where σ_a is small and subject to interference[19] from nonresonant elastic scattering and nonresonant transfer excitation, does the $|Y_{20}(\theta,\phi)|^2$ dependence appear to fail.

We see then that there is good qualitative agreement between theory and experiment, viz. the Compton broadened RTEA cross section and the $|Y_{20}(\theta,\phi)|^2$ angular dependence. However, quantitatively, there is disagreement on the overall normalization by up to a factor of 3.

IV. APPLICATION TO H-LIKE IONS

For $n>2$ we consider

$$1s+kl_c \rightleftarrows \begin{matrix} 2snl \\ 2pnl \end{matrix} \rightarrow \begin{matrix} 1snl+\nu_1 \\ 1s2s+\nu_2 \\ 1s2p+\nu_3 \end{matrix},$$

where $l_c=l$, $l\pm1$. The σ_{KLM}, σ_{KLN}, and σ_{KLO} ($n=3$, 4, and 5, respectively) cross sections were evaluated separately, but with all possible l values ($0\le l<n$) included. The spectroscopic orbitals were evaluated in nl-dependent scaled Thomas-Fermi-Dirac-Amaldi (TFDA) model potentials.[24]

For $n=2$ we consider

$$1s+kl_c \rightleftarrows \begin{matrix} 2s^2+2s3\bar{s} \\ 2s2p+2s3\bar{p} \\ 2p^2+2p3\bar{p}, \end{matrix} \rightarrow \begin{matrix} 1s2s+\nu_1 \\ 1s2p+\nu_2 \end{matrix}$$

where $3\bar{s}$ and $3\bar{p}$ denote screened hydrogenic correlation orbitals, again determined by minimizing a weighted sum of eigenenergies.[24] The correlation configurations were included to take account of spectroscopic configurations omitted from the eigenfunction expansion.[24] We found our results for the case of $n=2$ to be particularly sensitive to the structure that we used. We evaluated all of our cross sections in *LS* coupling; intermediate-coupling effects were found to be small ($\le1\%$) for this degree of ionization and these low-lying states.[25]

V. RESULTS

We now turn to the $F^{8+}+H_2$ TE experiment of Schulz *et al.*[13] The Auger emission was observed at $\theta_L=9.6°$ with respect to the beam axis in the laboratory frame,[13] $\theta_p=19.2°$ in the projectile frame.[9] In Figs. 1–4 we present our differential RTEA cross sections for the *KLL*, *KLM*, *KLN*, and *KLO* transitions described in Sec. IV and compare them with the experimental TE results of Schulz *et al.*[13] The $KL\infty$ limit is at 62 Ry, where the energy we plot is that of the projectile ion in the laboratory frame times m/M (see Sec. II).

It would appear from an initial comparison that there is good quantitative as well as qualitative agreement between theory and experiment.[13] However, although it is not stated explicitly in their paper, it turns out[26] that Schulz *et al.*[13] multiplied their differential cross sections by 4π. Thus, in fact, there is again a large discrepancy ($\sim4\pi$) between theory and experiment concerning the overall normalization. We note that DePaola[27] has recently carried out the same experiment for *KLL* transitions and obtained a substantially larger normalization than Schulz *et al.*[13] It would appear then that there is a large uncertainty in the overall experimental normalization. Assuming that the overall normalization is independent of energy and the transition involved, we can still make a useful comparison between our theoretical results and the experimental results of Schulz *et al.*,[13] if we normalize them to our theoretical *KLL* RTEA cross section at 48 Ry.

From Figs. 1 and 2 we see that our theoretical results for the *KLL* and *KLM* Auger transitions agree with the normalized experimental results below the $KL\infty$ limit (excepting the lowest *KLM* point), but diverge above. At these higher energies the experimental results were attributed[13] to uncorrelated transfer excitation (UTE), (i.e., capture of a target electron by the projectile nucleus and excitation of the projectile electron by a target electron. Thus the UTEA channel opens up at the $KL\infty$ limit but

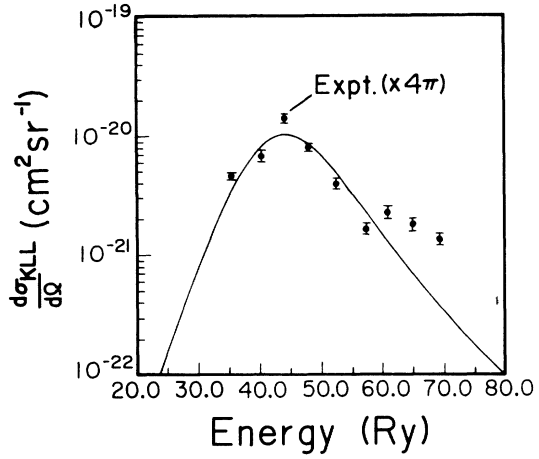

FIG. 1. Differential RTEA cross sections ($\theta_L = 9.6°$) for *KLL* transitions in $F^{8+} + H_2$ collisions. ——, theory from this work; ↧, experimental results from Schulz *et al.* (Ref. 13) multiplied by 4π.

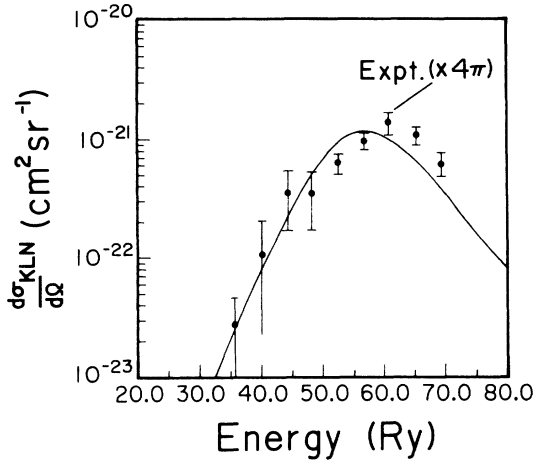

FIG. 3. Same as Fig. 1, but for *KLN* transitions.

is Compton broadened to contribute below. Excitation by the target nucleus and electron capture by the projectile nucleus, i.e., nonresonant transfer excitation (NTE, is only important at low energies.[28] There may be some evidence of NTE in the lowest energy experimental data points for *KLL* and *KLM* transitions seen in Figs. 1 and 2.

It was suggested[13] that UTEA dominates the TE process for high n at all energies. We see from Fig. 3 that our RTEA results for *KLN* transitions still agree with the normalized experimental results below the $KL\,\infty$ limit and are significant at 61 Ry where Schulz *et al.*[13] fitted their estimate of the theoretical UTEA cross section to their experimental results. Our RTEA results show that the UTEA results at this energy point must be at least a factor of 2 smaller than was assumed, but do not invalidate the energy dependence derived by Schulz *et al.*[13] It is noted, however, that there was some uncertainty[13] in the magnitude of their calculated UTEA cross section, hence the fitting to the data at 61 Ry for the *KLN* transitions. We see from Fig. 4 that even for the *KLO* Auger transitions, our theoretical RTEA results still dominate the TE cross section below the $KL\,\infty$ limit, and again, that there is the characteristic experimental peak above the limit.

For all of these Auger transitions, it is possible that the various *KLn* states could also be populated by capture to a high n state and then radiatively cascade down to a lower level. However, the fluorescence yields are of the order 10^{-3}–10^{-4} and so this effect is negligible. We emphasize again that these comparisons depend on there being no energy or transition dependence in the normalization of the experimental results to our theoretical *KLL* RTEA cross section at 48 Ry. Indeed, it is quite possible that UTEA has not, in fact, been observed.

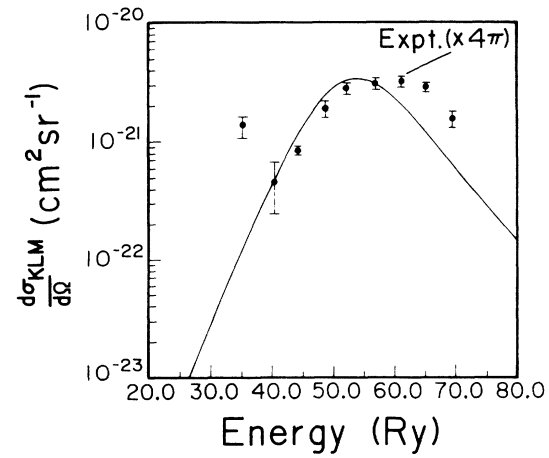

FIG. 2. Same as Fig. 1, but for *KLM* transitions.

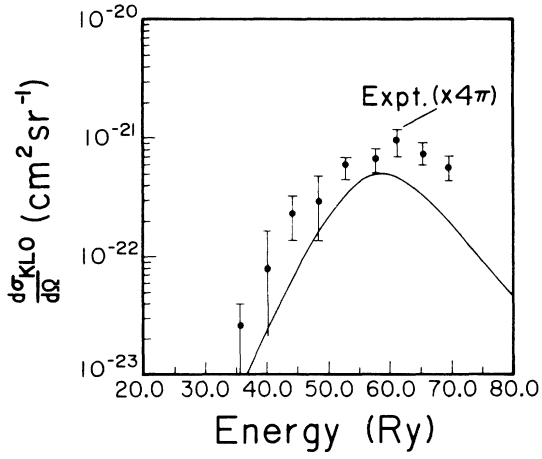

FIG. 4. Same as Fig. 1, but for *KLO* transitions.

VI. CONCLUSION

We have calculated differential cross sections for resonant transfer excitation followed by Auger emission in $F^{8+}+H_2$ collisions. Our results for *KLL*, *KLM*, and *KLN* transitions agree qualitatively with experiment[13] at energies below the $KL\infty$ limit and, together with our results for *KLO* transition, show that RTEA dominates TE at these energies for all n values measured so far. Any other TE process that is followed by Auger emission (e.g., UTEA) is only of secondary importance for energies below the $KL\infty$ limit, but may be an important process at high energies. The caveat being that we have normalized the experimental results of Schulz *et al.*[13] to our calculated *KLL* RTEA cross section at 48 Ry. It is desirable that the overall normalization of Auger spectroscopy experiments be determined, first, to gain repeatability by different experimental groups and, second, to enable absolute comparisons to be made with the results of theoretical calculations.

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