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L-shell resonant transfer and excitation in niobium ions

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We have calculated *L*-shell cross sections for the process of resonant transfer excitation followed by x-ray stabilization (RTEX) in collisions of Nb^{q+} ions ($q=28-32$) with H_2. The *LMn* plateau cross section is nearly constant [$(4.5-5.2)\times 10^{-20}$ cm^2] for $q=29-32$ and is consistent with the results of the recent experiment by Bernstein *et al.* [Phys. Rev. A **40**, 4085 (1989)] for $q=31$ and 32, but our results for $q=28-30$ are substantially larger than experiment. For Ne-like niobium ($q=31$), the inclusion of RTEX contributions from higher transitions (*LNn*, *LOn*, etc.) leads to good agreement with the experiment by Bernstein *et al.* in the high-energy tail. This implies that only a small contribution is possible from the uncorrelated transfer excitation process.

I. INTRODUCTION

Resonant transfer excitation followed by x-ray stabilization (RTEX) in ion-atom collisions[1] is still the main source of experimental data for dielectronic recombination (DR) in highly charged ions, as well as being of interest in its own right. For example, an electron-beam ion trap[2] (EBIT) provides a well-defined source for few-electron highly ionized atoms, but for many-electron systems it contains a mixture of several ionization stages. Analysis of the DR spectra requires the convolution of theoretical results[2] for a number of ionization stages of largely unknown abundance. Furthermore, experiments using electron coolers[3] have yet to produce results for $Z>20$ or $N>5$.

While there is good agreement between theory[4,5] and experiment[6] for *K*-shell RTEX, the case of *L*-shell RTEX is less certain.[7] The recent experimental results of Bernstein *et al.*[7] for collisions of Nb^{q+} ($q=28-32$) ions with H_2 are in substantial disagreement with the theoretical results of Hahn *et al.*[8] which were calculated (for $q=29-31$ only) in a combination of *LS*-coupling and angular-momentum-average approximations for the adjacent molybdenum ions. Furthermore, the earlier experiment by Bernstein *et al.*[9] on Ne-like niobium disagreed in the high-energy tail with the theoretical results of Hahn *et al.*[8] for *LMn* transitions. It has been proposed[10] that electron capture by the projectile nucleus together with electronic excitation by a target gas electron, uncorrelated transfer excitation, followed by x-ray stabilization (UTEX) could account for this discrepancy. The position and shape of the possible UTEX contribution is well known[10] but the magnitude is more difficult to ascertain reliably.[10] However, it is important that the RTEX contribution from *LNn*, *LOn*, and higher transitions, which contribute in the energy region of interest, should be calculated before invoking an additional process, particularly as the theoretical uncertainty for these transitions should be no worse than for the *LMn* transitions, which can be compared unequivocably with experiment.

In this paper we evaluate *LS*-coupling *L*-shell RTEX cross sections for collisions of Nb^{q+} ($q=28-32$) ions with H_2, together with an intermediate-coupling calculation for Nb^{31+}. Cross sections for *LMn* transitions are evaluated for all ions while for Nb^{31+} we also evaluate the contribution from higher transitions (*LNn*, *LOn*, etc.). The theory behind the calculation is outlined in Sec. II and the application to niobium ions is detailed in Sec. III; we present our results in Sec. IV.

II. THEORY

Using the impulse approximation,[11] the total RTEX cross section $\sigma_x(i;\mathrm{tot})$ for an initial state i may be written in terms of energy-averaged DR cross sections $\bar{\sigma}_d(i;j)$, thus

$$\sigma_x(i;\mathrm{tot})=\sum_j J(Q)\bar{\sigma}_d(i;j)\frac{\Delta E_c}{2I}\left[\frac{MI}{E}\right]^{1/2}. \tag{1}$$

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

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

E is the projectile-ion energy in the laboratory frame, E_c is the $j\to i$ Auger energy, and E_t is 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 energy of hydrogen.

The energy-averaged DR cross section for a given initial state i through an intermediate state j is given by[12]

$$\bar{\sigma}_d(i;j)=\frac{(2\pi a_0 I)^2}{E_c\Delta E_c}\frac{\omega(j)}{2\omega(i)} \times\frac{\tau_0\sum_j A_r(j\to k)\sum_l A_a(j\to i,E_c l)}{\sum_h\left[A_r(j\to h)+\sum_l A_a(j\to h,E_c l)\right]}, \tag{3}$$

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. A_a and A_r may be evaluated in configuration-mixing LS-coupling and intermediate-coupling approximations using the AUTOSTRUCTURE package.[12,13]

III. APPLICATION TO NIOBIUM IONS

We describe below the transitions we consider for each niobium ion; in each case the $1s^2$ core has been suppressed.

Nb^{32+}: We consider

$$\begin{array}{ccc} 2s^22p^5+kl_c\rightleftarrows & \begin{cases} 2s2p^53l_dnl \\ 2s^22p^43l_dnl \end{cases} & \rightarrow \begin{cases} 2s^22p^53l_d+h\nu_1 \\ 2s^22p^5nl+h\nu_2 \\ 2s2p^63l_d+h\nu_3 \\ 2s2p^6nl+h\nu_4 \end{cases} \\ & \downarrow & \\ & 2s2p^6+kl'_c\ , & \end{array}$$

where $l_c,l'_c=l,l\pm1,l\pm2$, and $l_d=0,1,2$.

Nb^{31+}: We consider

$$\begin{array}{ccc} 2s^22p^6+kl_c\rightleftarrows & \begin{cases} 2s2p^6n_dl_dnl \\ 2s^22p^5n_dl_dnl \end{cases} & \rightarrow \begin{cases} 2s^2p^6n_dl_d+h\nu_1 \\ 2s^2p^6nl+h\nu_2 \end{cases} \\ & \downarrow & \\ & 2s2p^63l'_d+kl'_c & \\ & 2s^22p^53l'_d+kl'_c\ , & \end{array}$$

where $l_c,l'_c=l,l\pm1,l\pm2$; $n_d=3,4$; $l_d=0,1,\ldots,n_d-1$ and $l'_d=0,1,2$. We also consider a reduced set of configurations, viz.,

$$\begin{array}{cc} 2s^22p^6+kl_c\rightleftarrows 2s^22p^5n_dl_dnl\rightarrow & \begin{cases} 2s^22p^6n_dl_d+h\nu_1 \\ 2s^22p^6nl+h\nu_2 \end{cases} \\ \downarrow & \\ 2s^22p^5n'_dl'_d+kl'_c\ , & \end{array}$$

where $l_c=l\pm1$; $l'_c=l,l\pm1,l\pm2$; $n_d=4,5,6,7$; $l_d=0,2$; $n'_d=3,4,\ldots,n_d-1$ and $l'_d=0,1,\ldots,n'_d-1$.

Nb^{30+}: We consider

$$\begin{array}{ccc} 2s^22p^63l_d+kl_c\rightleftarrows & \begin{cases} 2s2p^63s3l'_dnl \\ 2s^22p^53s3l'_dnl \end{cases} & \rightarrow \begin{cases} 2s^22p^63l_d3l'_d+h\nu_1 \\ 2s^22p^63l_dnl+h\nu_2 \end{cases} \\ & \downarrow & \\ & 2s^22p^6nl+kl'_c\ , & \end{array}$$

where $l_c=l,l\pm1,l\pm2$ for $l_d=0$ and $l_c=l,l\pm1$ for $l_d=1,2$; $l'_c=0,1,2,3$ and $l'_d=0,1,2$.

Nb^{29+}: We consider

$$\begin{array}{ccc} 2s^22p^63s3l_d3l'_d+kl_c\rightleftarrows & \begin{cases} 2s2p^63s^23p3l''_dnl \\ 2s^22p^53s^23p3l''_dnl \end{cases} & \rightarrow \begin{cases} 2s^22p^63s3l''_d3l'''_dnl+h\nu_l \\ 2s^22p^63s3p3l''_d+h\nu_2 \end{cases} \\ & \downarrow & \\ & 2s^22p^63l'''_d3l''''_dnl+kl'_c\ , & \end{array}$$

where $l_c=l,l\pm1,l\pm2$; $l_d,l''_d=0,1,2$; $l'_c=0,1,2,3$ for $l'_d=0$ and $l'_c=0,1$ for $l'_d=1,2$.

Nb^{28+}: In principle we should consider

$$\begin{array}{ccc} 2s^22p^63s3l_d3l'_d+kl_c\rightleftarrows & \begin{cases} 2s2p^63s^23p3l''_dnl \\ 2s^22p^53s^23p3l''_dnl \end{cases} & \rightarrow \begin{cases} 2s^22p^63s3l''_d3l'''_dnl+h\nu_l \\ 2s^22p^63s3p3l''_d+h\nu_2 \end{cases} \\ & \downarrow & \\ & 2s^22p^63l'''_d3l''''_dnl+kl'_c\ , & \end{array}$$

where all $l_d=0,1,2$; $l_c=l,l\pm1,l\pm2$ and $l'_c=0,1,2,3,4$ but the preponderance of configurations with four open subshells makes this impractical and so instead we consider

$$\begin{array}{c} 2s^22p^63s^23l_d+kl_c\rightleftarrows 2s^22p^53s^23p3dnl\rightarrow 2s^22p^63s^23pnl+h\nu \\ \downarrow \\ 2s^22p^63s^2nl+kl'_c\ , \end{array}$$

where $l_c = l \pm 1$ for $l_d = 1$ and $l_c = l, l \pm 2$ for $l_d = 2$; $l_c' = 0,2$. The error likely to result from neglecting the other transitions is discussed in Sec. IV.

IV. RESULTS

In Figs. 1–6 we present our L-shell RTEX results for collisions of Nb^{q+} ($q = 28-32$) ions with H_2 and compare them with the experimental results of Bernstein and co-workers.[7,9] The energy that we plot is that of the projectile ion in the laboratory frame times m/M; see Sec. II.

A. Nb^{31+}

Our LS-coupling results for LMn transitions in Nb^{31+} are about 10% larger than those of Hahn *et al.*[8] while our intermediate-coupling results differ by less than 5% from our LS-coupling results. The effect of neglecting $\Delta n = 0$ transitions on the LMn cross section is less than 10% at all energies. Our total RTEX cross section is the sum of our intermediate-coupling cross sections for LMn transitions plus our LS-coupling cross sections, with intermediate-coupling energies, for LNn, LOn, LPn, and LQn transitions (i.e., $2 \rightarrow n, n'$; $3 \le n \le 7$, $n \le n' \le 7$). The result (see Fig. 1) lies within or just above the experimental error bars of Bernstein *et al.*[9] which measure the relative uncertainty of the experimental results; the absolute uncertainty is estimated[7] to be ±30%. The good agreement between theory and experiment at high energies is illustrated in Fig. 2 which also shows the contribution from each transition considered. The LNn results were evaluated both with the full configuration basis and the reduced configuration basis of Sec. II, both excluding $\Delta n = 0$ transitions. Cross sections from the reduced basis were 90% of those from the full basis. The effect of including $\Delta n = 0$ transitions in the reduced basis was found to be less than 1% at all energies. Thus our results for LOn and higher transitions were evaluated with the reduced basis, neglecting $\Delta n = 0$ transitions. We see that the inclusion of higher RTEX transitions than have heretofore been considered removes the discrepancy between theory[8] and experiment,[9] and that our results may need to be increased by ~10% to allow for configurations neglected by our reduced basis. Our results imply that any possible UTEX contribution must be small, <20% of the RTEX contribution, for theory to remain in agreement with experiment. We note that there is strong experimental[13] evidence for uncorrelated transfer excitation followed by Auger emission in $F^{8+} + H_2$ collisions, since in this case the theoretical resonant transfer excitation contribution[14] does not, and cannot, account for all of the experimental cross section at high energies.

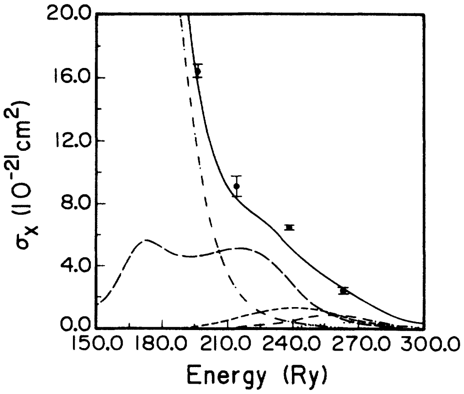

FIG. 2. L-shell RTEX cross sections for $\mathrm{Nb}^{31+} + H_2$. ——, total; —··—, LMn transitions; — — —, LNn transitions; ----; LOn transitions; —·—·—, LPn transitions; · · · ·, LQn transitions; all this work. ♦, experimental points from Bernstein *et al.* (Ref. 9).

B. Nb^{q+} ($q = 28, 29, 30, 32$)

As a result of our detailed calculations for Nb^{31+} and because of the sparse experimental data, our results for these ions (Figs. 3–6) were calculated in LS coupling and for LMn transitions only, neglecting $\Delta n = 0$ transitions. Our results for Nb^{32+} (see Fig. 3) were slightly smaller than experiment,[7] while our results for Nb^{31+} were slightly larger. The good agreement for $q = 32$ may be fortuitous since the experimental results may also include

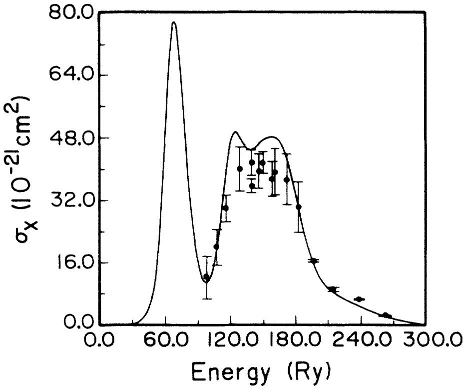

FIG. 1. L-shell RTEX cross sections for $\mathrm{Nb}^{31+} + H_2$. ——, theory; this work. ♦, experimental points from Bernstein *et al.* (Ref. 9).

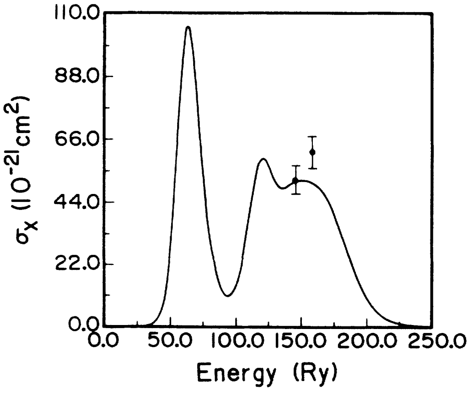

FIG. 3. L-shell RTEX cross sections for $\mathrm{Nb}^{32+} + H_2$. ——, theory; this work. ♦, experimental points from Bernstein *et al.* (Ref. 7).

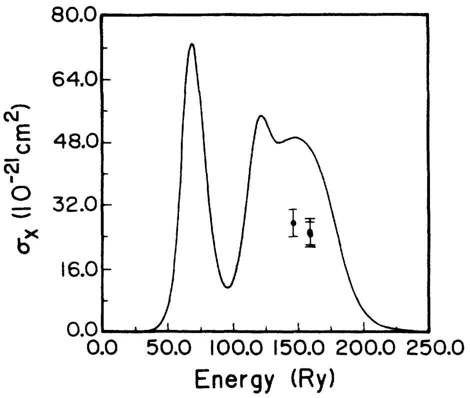

FIG. 4. As in Fig. 3, but for Nb^{30+}.

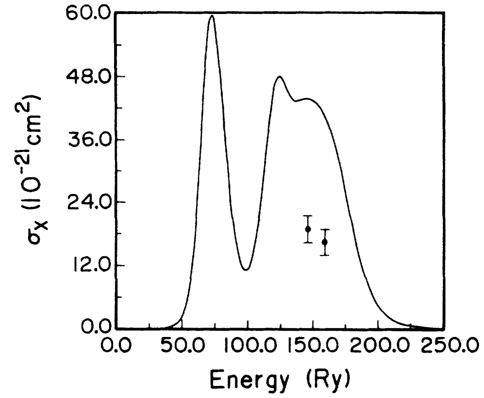

FIG. 5. As in Fig. 3, but for Nb^{29+}.

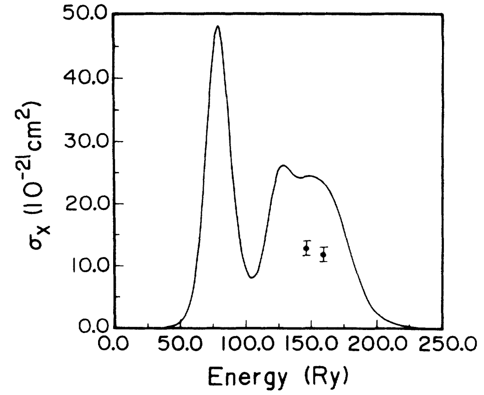

FIG. 6. As in Fig. 3, but for Nb^{28+}.

a contribution from direct electron capture followed by emission of an *L*-shell x ray.[7] However, our results for Nb^{q+} ($q=28$, 29, and 30) in Figs. 4–6 are consistently larger than experiment, by a factor of 2 ($q=28,30$) or 3 ($q=29$). The experimental results of Bernstein *et al.*[7] show a monotonic decrease in the value of the plateau cross section with decreasing ionization which is not borne out by the results of our calculations. We find only a small variation for $q=29-32$; Hahn *et al.*[8] obtained a similar result for $q=29-31$. Only for $q=28$ do our theoretical results drop substantially, by factor of 2, but they still remain a factor of 2 above experiment. For $q=28$ we used a smaller configuration basis than we would have liked; see Sec. III. However, on the basis of our results for the other ions we estimate that the contribution from 2*s* excitations would be no more than 10% of our existing results as would that from outer electron stabilization ($n>3$). The neglect of all autoionizing transitions into excited states increases our results for $q=29$ and 30 by 20% and 10%, respectively; there are no such $\Delta n=1$ transitions for $q=31$ and 32, while for $q=28$ the neglect of those transitions that we do include (see Sec. III) increases our results by 30%. The effect of autoionization into excited states which involve a 3*s* electron should be smaller.

The reason for the disagreement between theory and experiment for $q=28-30$ is not clear. At the experimental energies of Bernstein *et al.*[9] the cross section is dominated by *LMn* ($n<10$) RTEX transitions only and so should be insensitive to environmental effects. We note that our calculations have assumed that only levels of the ground term are populated; for this degree of ionization it is unlikely that a significant fraction of the ion beam remains in the metastable levels. All in all, it would be helpful to have experimental results over a wider range of energies for these ions, in particular, including the *LMM* peak.

V. CONCLUSION

We have calculated *L*-shell RTEX cross sections for collisions of Nb^{q+} ($q=28-32$) ions with H_2. For Ne-like niobium our results are in good agreement with the experimental results of Bernstein *et al.*,[9] including the high-energy tail which is dominated by *Lmn* ($m>M$, $n\geq m$) transitions and this implies that any contribution from UTEX is small compared to the RTEX contribution. For the remaining ions, apart from Nb^{32+}, there is substantial disagreement with experiment, which is surprising given the good agreement between theory[4,5] and experiment[6] for *K*-shell RTEX. Further experimental results over a wider range of energies are desirable for these ions.

ACKNOWLEDGMENTS

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