DIFFERENTIAL CROSS SECTIONS FOR ELECTRON CAPTURE IN HIGHLY CHARGED ION
COLLISIONS WITH He AND H₂ IN THE keV REGIME*

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Abstract

Differential cross sections (DCS) for single electron-capture processes in O⁸⁺ on He and N⁷⁺ on H₂ collisions are studied using a semiclassical traveling molecular orbital expansion method. Theoretical results are in good accord with recent measurements. The influence of a double electron-capture process on the DCS is also discussed.

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A recent report by Roncin et al. (1986) of the first measurement of the differential cross section (DCS) for the processes of single and double electron capture in collisions of highly charged ions with atoms and molecules is very important since the DCS provides more detailed information, than does the total cross section, about the physical mechanism of electron capture. In addition, the DCS serves as a more stringent test for checking the validity of various theoretical approaches. Although the theoretical study of electron capture in ion-atom collisions is a subfield of atomic physics in which significant progress has been made over past a decade [see, for example, M. Kimura (1986)], we still do not have a comprehensive understanding of the detailed physical mechanisms that govern electron capture in ion-atom collisions. This report aims at providing a theoretical rationale for measured DCS for single electron capture. Also, some theoretical consideration will be given to influence the double electron capture on observed DCS.

The specific processes to be described are:

and

A semiclassical molecular orbital (MO) expansion approach, which includes molecular electron translation factors (ETF), has been employed. [See, for example, Kimura (1986).] For process (1), molecular wavefunctions, adiabatic potentials, and collision matrix elements were obtained previously using a

two-electron configuration interaction method [Kimura and Olson (1985)]. For process (2), a pseudo-potential method which treats the H_2^+ core like an atom is applied [Kimura (1986), Kimura and Lane (1987)]. The latter approach is appropriate for a distant collision, as demonstrated in studies of ion-atom collisions and has been successfully applied to the interpretation of experimental electron capture processes in highly charged ion- H_2 collisions in the keV energy regime [Kimura (1986), Kimura and Lane (1987)].

This DCS study is a more sensitive test of the adequacy of this approach. In order to keep the calculation at a reasonable level, we chose to include ten (O^{7+} : $4s$, $4p_{0,\pm 1}$, $4d_{0,\pm 1,\pm 2}$, $4f_{0,\pm 1,\pm 2}$, and initial He) and seven (N^{6+} : $5s$, $5p_{0,\pm 1}$, $4s$, $4p_{0,\pm 1}$, and initial H_2) MO states in the wave function expansion for processes (1) and (2), respectively. A Coulomb trajectory was employed to describe the heavy particle motion. The ETF of the form $\exp[\frac{1}{2} i f_i(\vec{r}, R) \vec{r} \cdot \vec{v}]$ were used. The switching functions $f_i(\vec{r} \cdot R)$ were optimized by using discrete states only. Our calculated DCS for $O^{8+} + He$ collision is displayed in Fig. 1 along with the measured values [Roncin et al. (1987)]. Relative experimental data have been normalized to the present theoretical result at $E\theta = 2$ for the comparison. It can be seen that characteristic peak of the DCS at zero degree is followed by smooth decrease of the DCS in larger angles. Also, the elbow structure apparent in the DCS at $E\theta = 3$ is similar to that seen in the DCS for electron capture in $H^+ + He$ collisions [Park (1985)]. This feature suggests that two different mechanisms govern the small and large angle scattering. At the larger angle scatterings which correspond roughly to small impact parameters, direct interaction between the projectile and the target nucleus becomes more important, while at the smaller scattering angles corresponding to large impact parameters, the projectile sees the screened target which results in weak interaction.

Another source to cause structures in the DCS may be due to so-called Stueckelberg oscillator [see, for example, Child (1974)]. The Stueckelberg oscillation results from interference of the amplitudes associated with different classical paths taken by the colliding heavy particles. Although this type of oscillatory structure has been clearly identified for certain two-channel cases [e.g., Tan et al. (1986)], it appears to be washed out in the present DCS because several channels contribute significantly to the collision dynamic.

Due to interferences among different channels, apparently, no regular oscillatory structure in each partial DCS can be seen. Detailed analysis will be published elsewhere (Kimura and Lane). Although it is not possible to make a direct assessment of the relative importance of various mechanisms contributing to the DCS for double electron capture since the present treatment does not include the relevant states, a qualitative argument can be made based on adiabatic potential curves published previously [Kimura and Olson (1985)]. Energetically, the $O^{6+}(n=4, n'=3) + He^{++}$ and $O^{6+}(n=3, n'=3) + He^{++}$ levels lie below that of $O^{7+}(n=4) + He^{+}(1s)$. Consequently, the adiabatic potentials for double electron capture channels cross over that of the initial channel at smaller R . This observation combined with the absence of a forward peak in the DCS measurement suggests that sequential step-wise one-electron capture is the dominant mechanism for the double-electron capture process, as was suggested by Rocin et al. (1986).

Figure 2 compares the theoretical one-electron capture DCS for $N^{7+} + H_2$ collisions at $E = 14$ keV with the measurements of Roncin et al. (1986). Again, the relative experimental data have been normalized to the present theoretical result of $N^{6+}(n=5)$ capture at $E_0 = 0.5$. As with the previous case, a characteristic forward scattering peak for the $N^{6+}(n=5)$ channel is

apparent in both theoretical and experimental results. At larger angles, the present results for the $N^{6+}(n=5)$ channel appear to underestimate the cross section. This is probably due to our simplified treatment of H_2 in the theoretical model used to investigate this system. For the $N^{6+}(n=4)$ channel, the forward scattering peak is less prominent than that for the $N^{6+}(n=5)$ channel. This may be attributed to the fact that the avoided crossing between $N^{6+}(n=4) + H_2^+$ and the initial channel occurs around $R \sim 6$ a.u. and hence, the projectile experiences a stronger interaction during the collision which cause larger scattering angles [Kimura and Lane (1987)]. The overall agreement between our theory and the measurement for $N^{6+}(n=4)$ is unsatisfactory. This failure also may result from our simplified treatment of H_2 , which ignores its true molecular nature, since close collisions are important for their cases. In a close collision, explicit accurate representation of collision complex is necessary to describe collision dynamics correctly [Kimura (1987)]. The shape of the DCS curve for the dominant channel is very similar to that for $O^{8+} + He$ system. Thus, the previous discussions about the elbow applies here as well.

For the DCS for double electron capture, again the absence of the forward peak in the measurement suggests that the significant stepwise one-electron capture mechanism is dominant, as explained before.

In summary, we have shown that the differential cross section (DCS) measurements for one-electron capture in $O^{8+} + He$ and $N^{7+} + H_2$ collisions are well described by a model based on a molecular orbital expansion method with the inclusion of electron translation factors and with the H_2^+ core represented as an "atom" for the latter case. It is shown that the model is adequate for the dominant channel, although it gives less satisfactory agreement for the weak channel as well as for larger angle scattering, where close collisions become important. While the present model gives

satisfactorily results for the DCS for one-electron capture and provides a qualitative description for the DCS for double electron capture, it is certainly desirable to include double electron capture channels explicitly in the calculation.

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Figure Captions

Fig. 1. Differential cross section for one-electron capture in $O^{8+} + He$ collision at $E = 8$ keV.

Theory: solid line = electron capture into $O^{7+}(n=4)$ channel.

Experiment: O = Ronci et al. (1987)

normalized to the theoretical cross section at $E\theta = 2$ (keV deg).

Fig. 2. Differential cross section for one-electron capture in $N^{7+} + H_2$ collision at $E = 3.5$ keV.

Theory: solid line = electron capture into $N^{6+}(n=5)$ channel

broken line = electron capture into $N^{6+}(n=4)$ channel

Experiment: O = $N^{6+}(n=5)$ channel by Ronci et al. (1987).

X = $N^{6+}(n=4)$ channel by Ronci et al. (1987).

normalized to the theoretical cross section at $E\theta = 0.5$ (keV deg).