THE ASTROPHYSICAL JOURNAL, 629:L125–L128, 2005 August 20

ON THE SIGNIFICANCE OF THE CONTRIBUTION OF MULTIPLE-ELECTRON CAPTURE PROCESSES TO COMETARY X-RAY EMISSION

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Received 2005 May 23; accepted 2005 July 12; published 2005 August 1

ABSTRACT

We report laboratory studies of the role played by multiple-electron capture (MEC) in solar wind–induced cometary X-ray emission. Collisions of Ne^{10+} with He, Ne, Ar, CO, and CO_2 have been investigated by means of the traditional noncoincident-singles X-ray spectroscopy in addition to the triple-coincidence measurements of X-rays, scattered projectile, and target recoil ions for the atomic targets. The coincidence measurements enable one to reduce the singles X-ray spectra into partial spectra originating in single-electron capture (SEC) and MEC collisions. The measurements provide unequivocal evidence of the significant role played by MEC and strongly suggest that models based solely on SEC are bound to yield erroneous conclusions on the solar wind composition and velocities and on cometary atmospheres. The experimental relative importance of MEC collisions is compared with the molecular classical-over-the-barrier model, the classical trajectory Monte Carlo technique, and the multichannel Landau-Zener method, calculations that can qualitatively reproduce the experimental trends.

Subject headings: atomic data — atomic processes — comets: general — solar wind — X-rays: general

1. INTRODUCTION

The emission of X-ray and extreme-ultraviolet (EUV) radiation from comets, first observed by Lisse et al. (1996), is now recognized as a characteristic of gassy comets. Charge exchange between highly charged solar wind (SW) minor heavy ions and cometary neutrals (suggested, e.g., by Cravens 1997) has now been established as the mechanism responsible for the observed cometary X-ray and EUV emission lines (Lisse et al. 2001; Krasnopolsky et al. 2002; Krasnopolsky & Mumma 2001). In fact, cometary X-ray emission was successfully simulated by spectra produced by charge exchange in the laboratory without the need to invoke any other X-ray production mechanism (Beiersdorfer et al. 2003). In the SW charge exchange (SWCX) mechanism, electrons are captured from cometary neutrals by the SW ions into excited states of the resulting ions, which may then decay radiatively and in the process emit X-ray and/or EUV radiation. SWCX has also been suggested as contributing to the soft X-ray background of the heliosphere (Cravens 2000; Pepino et al. 2004). The SWCX mechanism has been invoked with various degrees of sophistication to model and interpret cometary X-ray and EUV emission spectra as well as laboratory spectra, and has been recently reviewed by Cravens (2002) and Krasnopolsky et al. (2004).

Although charge exchange in collisions of slow, highly charged ions with atomic and molecular targets has been investigated both experimentally and theoretically for over 30 years (Emmons et al. 1999; Moretto-Capelle et al. 2000 and references therein), only a few of the previously reported studies are of relevance to cometary X-ray and EUV emission. Recently, however, several experimental groups have started investigating relevant collision systems (Greenwood et al. 2001; Beiersdorfer et al. 2000, 2001; Hasan et al. 2001; Gao & Kwong 2004; Bodewits et al. 2004, and references therein). Essentially all cometary X-ray and EUV emission models invoking SWCX had to rely on the limited relevant atomic data in the literature or on simple charge exchange models. In particular, all models including the most detailed ones (Kharchenko et al. 2003 and references therein) have assumed that cometary X-ray and EUV emission is the result of SEC only and ignored contributions from MEC. In this Letter, we report laboratory simulations of solar wind–comet interactions that clearly demonstrate that while the assumption of the dominance of SEC is justifiable to some extent in settings where He, or H, is the predominant target species, it is seriously flawed in the case of the many electron cometary target species such as H_2O, CO, CO_2, OH, and O.

2. EXPERIMENTAL

The 4.55 keV nucleon^{-1} (933 km s^{-1}) Ne^{10+} ions were provided by the University of Nevada, Reno, 14 GHz Electron Cyclotron Resonance ion source and were guided to the collision chamber where they crossed a target jet at 90°. The resulting target recoil ions were extracted at 90° relative to the incident ions and jet by an electric field and detected by a position-sensitive detector (PSD). The outgoing projectile ions were charge-analyzed electrostatically and detected by another PSD. X-rays emitted at 90° relative to the incident ions were detected by a windowless X-ray detector, opposite the recoil detector, with a resolution of 133 eV for the Ne Lyα line. The impact positions of the projectile ions on their PSD provided their final charge states, while coincident time-of-flight (TOF) measurements between projectile and recoil ions provided the recoil ion charge states. Coincidences between projectiles and X-rays ensured that all detected particles originated in the same collision event. While the targets of interest to cometary X-ray emission are mainly the molecular ones, atomic targets were used in the coincidence studies to better judge the role of MEC

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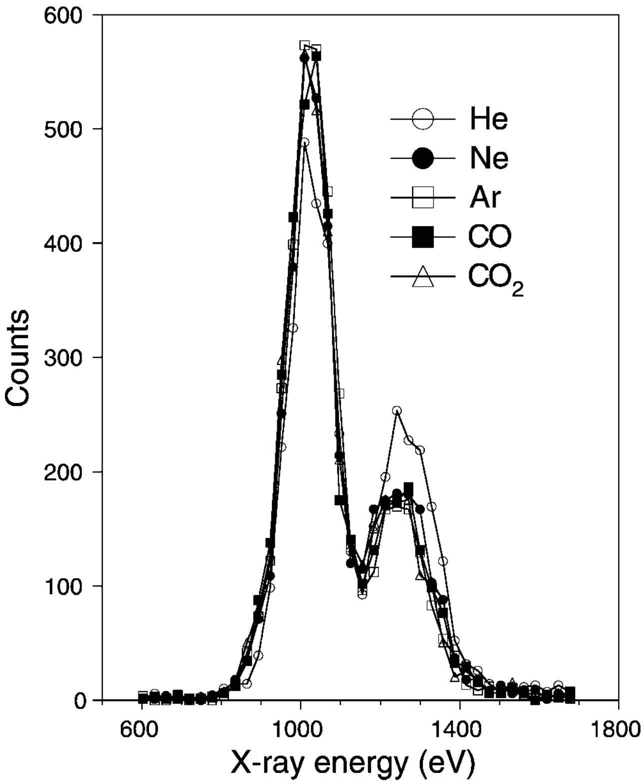

FIG. 1.—Singles X-ray spectra obtained in collisions of Ne^{10+} with He, Ne, Ar, CO, and CO_2. The spectra are normalized to the same total number of counts.

since complications would arise due to Coulomb explosions following MEC from molecular targets. Furthermore, the first few ionization potentials of Ar are close to those of the molecular targets, and electron capture processes are expected to be very similar.

3. RESULTS AND DISCUSSION

Figure 1 compares the noncoincident-singles X-ray spectra, normalized to the same total number of counts, for all targets. Surprisingly, all targets apart from He give rise to identical spectra. While the first ionization potentials of Ar (15.8 eV), CO (14.0 eV), and CO_2 (13.7 eV) are close to each other, and one might expect similar spectra assuming SEC to be dominant, that of Ne (21 eV) is much larger. The similarity of the spectra, as will become clear later, is due to the complementary roles played by SEC and MEC. This argument is further supported by the fact that the ionization potential of He (24.5 eV) is much closer to that of Ne, and yet there is a clear difference in their spectra resulting from the dominance of SEC for He as will be shown later. In fact, the He spectrum does not show the low-energy shoulder at 900 eV, a signature of MEC-induced He-like Ne^{8+} X-ray emission, that all other targets show. The higher relative intensity of Kβ, Kγ, etc., X-rays in the He target spectrum is a consequence of a number of factors. First, due to its large first ionization potential, the dominant SEC occurs at smaller impact parameters than for the other targets, and singly excited Ne^{9+} states with relatively smaller values of the angular momentum quantum number l are populated, thus increasing the probability of Kβ, Kγ, etc., emission. Second, as discussed below, MEC for the other targets populates multiply excited projectile (Ne^{8+}, Ne^{7+}, etc.) states that undergo a number of autoionization steps leading to the population of low-lying radiatively decaying states, thus reducing the probability of Kβ, Kγ, etc., emission.

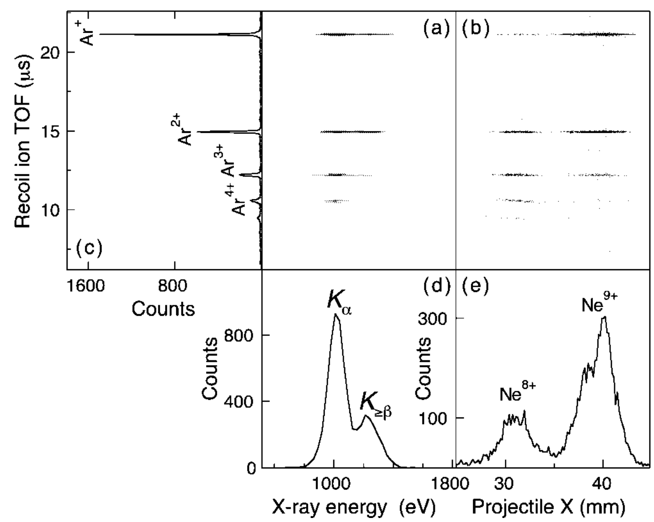

FIG. 2.—Multiparameter representation of the triple-coincidence measurements for the Ne^{10+} on Ar collision system. (*a*) Coincidences between recoil ions and X-rays. (*b*) Coincidences between projectile and recoil ions. (*c*) Recoil ion TOF spectrum. (*d*) Singles X-ray spectrum. (*e*) Final projectile charge state distribution.

Coincidence measurements have historically helped unravel the intricacies of complex atomic interactions, and the present measurements do indeed give insights relevant to cometary X-ray emission. Figure 2 is a multiparameter representation of the triple-coincidence measurements for the Ar target. Coincidences between recoil ions and X-rays are represented by the scatter plot of Figure 2*a*. Figure 2*b* represents coincidences between projectile and recoil ions. Projections onto the appropriate axes provide the recoil ion TOF spectrum (Fig. 2*c*), the singles X-ray spectrum (Fig. 2*d*), and the final projectile charge state distribution (Fig. 2*e*). It is immediately evident from Figure 2*a* that the singles X-ray spectrum resulted from processes involving the capture of up to six electrons as evidenced by the observation of Ar^{6+} target ions. It is also evident from Figure 2*b* that the projectile ions keep one or two electrons, resulting in only Ne^{9+} or Ne^{8+} final projectile ions regardless of the initial number of captured electrons. In particular, Figure 2*b* clearly demonstrates that in collisions leading to the production of Ne^{9+} ions, as many as four electrons may have been initially captured by the Ne^{10+} ions, thus forming up to quadruply excited projectile ions. These multiply excited ions must have then undergone a number of autoionization processes (see, e.g., Emmons et al. 1999) ending in singly excited Ne^{9+} ions that have subsequently decayed radiatively. To avoid confusion, "PSCC" should be used to indicate a projectile single charge-change collision, often referred to as $q, q-1$, and in what follows SEC will imply true SEC. For example, three autoionization processes take place when an Ar^{4+} target ion is produced. Such autoionization processes result in a PSCC and lead to a singly excited state population prior to the radiative transitions that is completely different from what results from SEC. Indeed, it is interesting to note that in Figure 2*a*, the higher recoil ion charge states resulting from MEC are found dominantly in coincidence with Kα X-rays. This may be due to a combination of populating lower levels on the projectile in MEC and the role played by the autoionization cascades that also feed lower levels. Both scenarios lead to the dominance of Kα emission. Therefore, in the case of many electron targets, one cannot simply assume SEC to be dominant and hope to extract accurate information through comparisons of model results with observed spectra. Accurate modeling should take into account MEC and the intermediate autoionization processes that alter the radiative state population.

Figure 2*b* clearly demonstrates that MEC collisions may also lead to the retention of two electrons by the projectile ions in what is known as projectile double charge-change (PDCC), or $q, q-2$. The weak density of events representing coincidences between Ar^{+} target ions and Ne^{8+} represent double collision events where the projectile ion retains one electron from a first collision and then retains another electron from a second collision. Double collisions in the present measurements are less than 5% and do not compromise the validity of the results and conclusions presented in this Letter. While the true double-electron capture (TDC) contributes only a small portion to PDCC, a large fraction of the capture involving more than two electrons leads to PDCC. Depending on the relaxation pathways of the multiply excited states following MEC, it is most likely that one or two X-rays are emitted in each PDCC collision. In TDC collisions, for example, PDCC is achieved through the radiative decays of both captured electrons. In triple-electron capture collisions, PDCC is achieved through one autoionization step and one or two X-ray–emitting radiative transitions depending on whether the autoionization step filled one of the original K-shell vacancies in Ne^{10+} or not. In quadruple and higher order electron capture collisions, it is unlikely that PDCC occurs through the filling of both K-shell vacancies via autoionization since the electrons are captured to high-lying energy levels and since autoionization transitions favor the smallest energy jumps. Therefore, the relaxation is expected to produce one or two X-rays. In either case, a He-like X-ray is emitted in the process of filling the second K-shell vacancy. Had Ne^{10+} been an important solar wind ion, ignoring MEC in cometary X-ray emission models would lead to overestimating the relative abundance of Ne^{9+} ions in the solar wind composition. This is because each observed He-like X-ray will be attributed to SEC by Ne^{9+}, although many of them would have been produced via MEC by Ne^{10+} ions. These same arguments hold for the more relevant O^{8+}, N^{7+}, and C^{6+} solar wind ions. For previous investigations of MEC by these ions as well as by other ions of similar charge states, the reader is referred to the excellent review by Barat & Roncin (1992) and to the work of Ali et al. (1994) and Emmons et al. (1999), and references therein.

The relative importance of SEC and MEC collisions can be obtained from recoil ion TOF spectra similar to that of Figure 2*c*, except that the spectra should be obtained from coincidence measurements of recoil ions and scattered projectiles only without regard to whether an X-ray was emitted or not. This is essential in order to account for MEC collisions that may not give rise to X-ray emission. Such TOF spectra have been measured for the He, Ne, and Ar targets and are shown in Figure 3*a*. By determining the areas under the respective peaks, the fraction of events leading to singly ionized targets (SEC) or multiply ionized targets (MEC) can be found. For the He target, SEC dominates by a large margin, and limiting the models to SEC might be easily justified in environments where He is the prevalent target, such as in the heliosphere. The case is clearly different for the Ne target where the SEC and MEC fractions are close to each other but where SEC events still outnumber MEC events. For the Ar target, however, the scenario has changed, and MEC events outnumber the SEC ones. Clearly, any model ignoring the role of MEC for Ar, or the very similar cometary neutrals, will undoubtedly lead to erroneous conclusions.

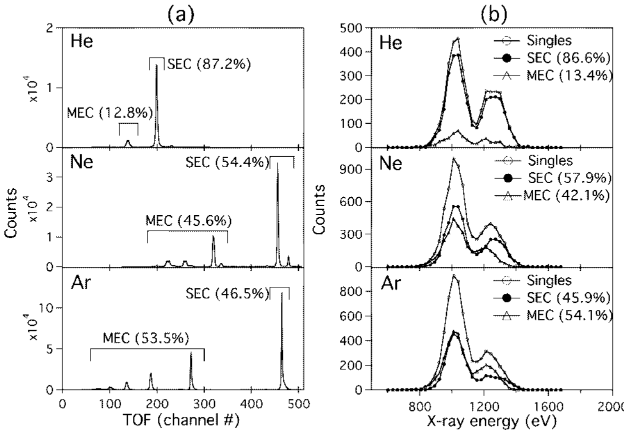

FIG. 3.—(*a*) Recoil ion TOF spectra for the Ne^{10+} on He, Ne, and Ar collision systems. The percentages represent the fraction of SEC and MEC collisions for each target. (*b*) Singles and partial X-ray spectra corresponding to SEC and MEC collisions. The percentages represent the fraction of X-rays resulting from SEC or MEC collisions.

A major advantage of the coincidence measurements is that it is possible to obtain partial X-ray spectra corresponding to any recoil charge state. For simplicity, however, we show in Figure 3*b* two partial X-ray spectra for each atomic target: one corresponding to SEC and the other corresponding to the cumulative MEC. Singles X-ray spectra, similar to those of Figure 1, which are the sum of SEC and MEC, are also shown. The percentages indicate the fraction of X-rays that resulted from either SEC or MEC collisions. We note that for He, the SEC and singles spectra are almost identical in profile, which supports the earlier argument that ignoring MEC for this target may be justified to first order in models. This is definitely not true for the Ne and Ar targets, where the SEC and the singles profiles are clearly different from each other and from MEC spectra as well. We also note that the SEC profiles for Ne and Ar are different from each other and that the same is true for the MEC profiles. Moreover, we note a shift from high-n to low-n (with $n \geq 3$) emission when comparing the MEC profiles to the SEC profiles, which confirms an earlier suggestion (Beiersdorfer et al. 2003) that strong emission from $n = 3, 4$ levels is due to double (or multiple) electron capture. Surprisingly, when added together, the SEC and MEC profiles for Ne and Ar give rise to identical singles profiles. This is unequivocal evidence for the importance of the role played by MEC in the case of the many electron targets. Assuming SEC only while attempting to model the cometary X-ray and EUV emission is definitely not justifiable.

4. THEORETICAL CONSIDERATIONS

Theoretically, a quantum mechanical treatment of collisions involving more than two electrons and highly charged ions is prohibitively difficult due to the large number of channels involved. To account for MEC, Niehaus (1986) developed a molecular classical over-the-barrier model (MCBM) that has been subjected to several critical tests (Hasan et al. 1999 and references therein). Next in order of sophistication is the more elaborate classical trajectory Monte Carlo (CTMC) technique (Olson & Salop 1977). Another approach widely used in astrophysical applications is the multichannel Landau-Zener (MCLZ) approximation (Butler & Dalgarno 1980; Janev et al.

1983). In order to theoretically assess the importance of MEC collisions, we have used the MCBM and the CTMC technique for all three atomic targets while the MCLZ method was used for the He target only.

Six valance electrons have been considered for both the MCBM and CTMC (see references in Wang et al. 2002) calculations for the Ne and Ar targets. In the CTMC calculations, initial electron orbitals were simulated with the standard microcanonical ensemble, while the electron-nuclear charge interaction of the target was described by an effective charge. For the Ne and Ar target models, the microcanonical distributions were filtered to remove all but the valance *p* orbitals (otherwise a statistical mixture of *s* and *p* orbitals would have resulted). A variety of other CTMC models were also considered, but they gave results generally within several percent of those presented here. At the conclusion of the time propagation for each trajectory, the binding energies of the electrons were examined to determine whether a SEC or MEC event had occurred. For the MCLZ method, the multichannel probability approach of Janev et al. (1983) was adopted with radial couplings estimated for monoelectronic transitions following Olson & Salop (1976) and dielectronic transitions following Fremont et al. (1994). Further details concerning the MCLZ and CTMC methods as well as final-state-selective results will be presented in a later paper. Theoretical results for the three methods are presented in Table 1 and generally show qualitative agreement with experiment in predicting the fraction of MEC events. Both the MCBM and CTMC results predict that the percentage of MEC increases with decreasing binding energy of the target, but both underestimate the significant contrast of He with respect to the other targets. Surprisingly, the MCLZ method gave the best agreement for the He target. Nevertheless, while the comparison given here suggests that these methods can be used to give qualitative estimates of the importance of MEC processes, it appears that more elaborate approaches (e.g., close-coupling) will be necessary to make accurate, quantitative predictions as we pointed out in our earlier study of *n*-resolved cross sections for SEC (Hasan et al. 2001).

TABLE 1
PERCENTAGE OF MEC EVENTS[a]

Target	Exp. (%)	CTMC (%)	MCBM (%)	MCLZ (%)
He	12.8	21	40	11
Ne	45.6	33	57	...
Ar	53.5	38	65	...

[a] In 4.55 keV nucleon^{-1} (933 km s^{-1}) Ne^{10+} on He, Ne, and Ar collisions.

5. CONCLUSIONS

We have presented unequivocal evidence for the significant role played by MEC processes in cometary X-ray emission. The evidence strongly suggests that models should take into account MEC in order to extract reliable information on the solar wind composition and velocities and on cometary atmospheres. The experimental relative importance of MEC collisions is compared with CTMC, MCBM, and MCLZ calculations, and it is found that these methods can give qualitative predictions of the fraction of MEC collision events but that more elaborate quantal methods are required for quantitative comparisons.

This work was supported by NSF grant PHY-0099592 and NASA grant NAG5- 11453. Work done at ORNL was supported by a NASA Planetary Atmospheres Program, the US DOE, OFES, through grants to the ORNL managed by UT-Battelle, LLC under contract DE-AC05-00OR22725. Work at the University of California Lawrence Livermore National Laboratory was performed under the auspices of the US DOE under contract W-7405-ENG-48 and supported by NASA's Planetary Atmospheres Program under work order W-19,938.

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