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Heavy Particle Atomic Collisions in Astrophysics: Beyond H and He Targets

P. C. Stancil, P. S. Krstić, and D. R. Schultz

Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6372
stancil, krstic, schultz@mail.phy.ornl.gov

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Abstract. The physical conditions relating to the emission of x-rays from Jovian and cometary atmospheres and to supernova ejecta are briefly described. Emphasis is placed on elucidating the relevance and importance of atomic collision processes, the availability of data, and the outstanding data needs for modeling these environments. Some preliminary theoretical studies of electron capture for important collisions systems, involving molecular and atomic metal targets, are presented.

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INTRODUCTION

The amount of neutral atomic hydrogen and helium can be deficient in a surprising variety of astrophysical environments. In many of these situations, low-energy collisions with metal atoms (ions) and molecules can play dominant roles in establishing the excitation and ionization conditions. Unfortunately, as the focus of the atomic collision community has been primarily on H and He targets, the availability, accuracy, and comprehensiveness of the needed metal and molecular target data are wanting. Consequently, the progress in astrophysical modeling is hindered and some proposed explanations of observed phenomena may be subject to revision pending a more complete database.

As the amount of collisional data required for astrophysical applications is enormous, it is impractical to perform close-coupling (CC) investigations for each system, much less to pursue comprehensive experimental evaluations. In fact, a quantal molecular-orbital CC (MOCC) calculation of collisions involving a metal or molecular target could be considered to be near the forefront of state-of-the-art research in theoretical atomic collisions. As an alternative, we are employing a variety of approximate techniques including the quantal decay model (QDM), the classical trajectory Monte Carlo (CTMC) method, and nonadiabatic methods such as the Landau-Zener (LZ) model. A measure of the accuracy can be obtained through the consistency (or inconsistency) of the three approaches. To further gauge the reliability of the results, a program to perform *ab initio* MOCC calculations for select

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systems is in progress as well as a collaboration with benchmarking experiments at ORNL.

In this article, we describe the physical conditions and collision systems of interest for three different astrophysical environments: Jovian atmospheres, cometary atmospheres, and supernova (SN) ejecta. Some preliminary calculations of applicable total and state-selective electron capture processes are presented.

JOVIAN ATMOSPHERES

Auroral x-ray emission from Jupiter was observed by the *Einstein* satellite [1] and recently by the *Röntgen* satellite (*ROSAT*) [2]. In situ measurements by the *Voyager* spacecrafts detected energetic oxygen and sulfur ions in the Jovian Magnetosphere. Their energy spectra suggest that the oxygen and sulfur ions are of Iogenic origin and their phase space density radial gradient indicates a diffusive flux into Jupiter's atmosphere [3]. The recent *Ulysses* flyby of Jupiter also measured significant quantities of O and S ions [4]. The combined spacecraft measurements indicate an ion energy range of a few keV/u to a few MeV/u. The *Voyager* results led Horanyi et al. [5] to suggest that the auroral x-ray emission was powered by the precipitating ions, the emission being due to radiative decay from highly excited high-charge state O and S ions produced following charge exchange with neutral atmospheric species, primarily H₂. Horanyi et al. [5], and more recently Cravens et al. [6], have constructed numerical models of the ion precipitation including energy deposition, beam ionization balance, and auroral x-ray emission.

The important collisional processes for O ions are listed below. In what follows we describe the atomic data utilized by the Jovian models [5,6], new data or that not presently considered in the Jovian models, and reactions for which data is lacking. For sulfur ions, no data are available. The Jovian models have thus far assumed the cross sections are similar to the cross sections for the oxygen ions. The electron capture reactions

and

are the major processes for producing the x-ray emission and along with the projectile ionization (PrI) reaction

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determine the equilibrium ionization fractions of the precipitating ions [6]. Total single electron capture [SEC, process (1)] cross sections are available from the compilation of Phaneuf, Janev, and Pindzola [7]. As little information is available for state-selective SEC with H_2 targets, the models have adopted two schemes: (i) all captures go to $n = 2$ (80%) and $n = 3$ (20%) or (ii) all available n -states are populated equally. Since the *ROSAT* energy resolution is poor, both schemes can fit the observations reasonably well with nearly equal chi-square statistics [6]. Future observations with NASA's soon to be launched *Advanced X-ray Astrophysics Facility* (*AXAF*) and the planned Japanese *Astro-E*, however, should place serious constraints on the models as the satellites will have resolutions more than an order of magnitude smaller than *ROSAT*. As such, the need for state-selective SEC data will become more crucial.

Unlike the situation for S ions, some state-selective SEC data for O ions is available. Dijkkamp et al. [8] have measured the cross sections for capture to each of the l levels with $n = 4$ for O^{6+} collisions with H_2 at energies between 0.5 and 7 keV/u, while Beijers et al. [9] measured the $n = 3$ l -distributions from 0.04 to 1 keV/u for O^{3+} collisions with H_2 . Meng et al. [10] calculated the n -distributions for $O^{8+} + H_2$ at 50 and 100 keV/u using the CTMC method for SEC; reaction (5), transfer ionization (TI); reaction (3), double electron capture (DEC); and reaction (4), autoionization (AI). We note that the Jovian models did not consider dissociative electron capture [DiEC, process (2)], DEC, AI, or TI. We are unaware of any other available data for these processes.

There is apparently no cross sections available for projectile ionization (PrI) of O ions. Horanyi et al. and Cravens et al. adopted the C^{q+} and B^{q+} , $q = 2, 3$ results of Goffe et al. [11] and extrapolated the trends of the lower charged ions to estimate the higher charge state cross sections.

PrI, or stripping, plays a role in the ion energy loss, but target ionization (TrI) and dissociative TrI (DTrI)

are the primary energy loss processes. Cross sections for TrI and DTrI for O^{q+} , $q = 2, 3, 4$, and 5, are available from Shah and Gilbody [12]. The Jovian models extrapolated the cross section behaviors to larger and smaller charge states.

Cross section data are lacking for rovibronic and electronic target excitation (TrE)

and projectile excitation (PrE)

The models adopted the arbitrary branching ratios of 0.6 of TrI for TrE and 0.15 of PrI for PrE.

FIGURE 1. n, l distributions for $O^{7+} + H_2$ collisions at 200 keV/u. Filled circles, SEC. Open circles, TI+AI.

In preparation for future *AXAF* and *Astro-E* observations, we have begun a project to improve the modeling of auroral x-ray emission. We have initiated a program to compute an extensive database of state-selective SEC, DiEC, DEC, AI, and TI cross sections for collisions of intermediate high energy O and S ion collisions with H_2 primarily using the CTMC method. Cross sections are also being computed for H and He targets. While H and He are secondary constituents of the Jovian atmosphere, extensive theoretical and experimental data exists which can be used to test the reliability of the CTMC results. For low to intermediate energies, some MOCC calculations are also being performed.

Figure 1 presents a sample of the CTMC computations, the l -distributions for 200 keV/u collisions of O^{7+} with H_2 for select n values. As $n = 6$ corresponds to the maximum of the n -resolved cross sections, the assumption that all captures go to $n = 2$ and $n = 3$, adopted by the Jovian models, is questionable. Further, the sum of the AI and TI cross sections, processes which were neglected in the models, is greater than the SEC cross sections for most n, l levels. Use of the CTMC data should greatly improve the next generation of Jovian models for the auroral x-ray emission. Measurements of reactions (2) through (8), but particularly for S ions and reactions (2) through (5), would be useful to check the validity of theoretical calculations.

COMETARY ATMOSPHERES

In 1996 an unexpected observation was made by *ROSAT*; Lisse et al. [13] detected strong x-ray emission from comet C/1996 B2 (Hyakutake). Subsequent searches of the *ROSAT* all-sky survey archival data found that four other comets had also been serendipitously observed emitting x-rays [14]. Additionally, x-ray emission has been recently detected from C/1996 Q1 (Tabur) [15], from 6P/d'Arrest with the *Extreme Ultraviolet Explorer* (*EUVE*) [16], and from C/1995 O1 (Hale-Bopp) with *BeppoSAX* [17].

A number of models have been put forth to explain the x-ray emission. Schemes which invoke fluorescent emission and scattering of solar x-rays in the comet's coma [18] or bremsstrahlung [19] and inner-shell excitation of oxygen atoms [20] due to energetic electrons predict x-ray fluxes which are orders of magnitude smaller than observed. Only two models appear to reproduce the observed magnitude of the x-ray flux: scattering of solar x-rays by small dust particles in the coma [21] and electron capture of heavy solar wind ions to highly excited states following collisions with cometary neutrals [22,23]. Mumma et al. [16] have analyzed the observed x-ray brightness offset (i.e., the distance from the comet nucleus along the comet-sun vector), maximum brightness, and x-ray production rates for four comets and concluded that the electron capture model is favored over the dust mechanism. Conversely, Owens et al. [17] argue that the x-ray emissions are consistent with dust scattering of solar x-rays, but inconsistent with the electron capture scenario as the models of Häberli et al. [23] predict that intense narrow lines at energies greater than 0.28 keV which are not observed in their *BeppoSAX* measurements of Hale-Bopp. Further, Owens et al. point out that x-rays were not observed from the dust deficient comet Bradfield 1979X. However, their arguments can be disputed by considering the comet 6P/d'Arrest and the uncertainties in the models of Häberli et al. The dust and gas production rates in the coma of 6P/d'Arrest are 30% smaller and three times larger, respectively than observed for Bradfield 1979X, though an x-ray flux one-tenth that of Hale-Bopp was measured by the *EUVE* [24] suggesting no correlation of x-ray emission with dust. While the models of Häberli et al. include an elaborate three-dimensional magnetohydrodynamic simulation of the cometary plasma environment, their treatment of the atomic collision processes, as admitted by the authors, is perhaps too simplistic, owing to the lack of available collision data. The primary process for producing the x-rays is the SEC reaction

where A is a heavy solar wind ion and X a cometary neutral. Häberli et al. considered only $A = \text{C}, \text{O}, \text{and Ne}$ and $X = \text{H}_2\text{O}, \text{OH}, \text{O}, \text{H}, \text{and CO}$. Since SEC data are only available for H targets, they adopted the H total SEC cross sections of Phaneuf et al. for $X = \text{O}$ and H_2 target cross sections for $X = \text{H}_2\text{O}, \text{OH}, \text{and CO}$. A constant cross section of $4 \times 10^{-15} \text{ cm}^2$ was utilized for all Ne ions with all neutral targets. For n, l distributions, they assumed that the n distribution was

maximum for $n \propto q^{3/4}$ and for intermediate n levels, that the capture takes place to high l .

The x-ray emission models due to electron capture can be improved if cross sections for the actual neutrals are utilized. Neutral production rates due to sublimation from the surface of the comet nucleus as inferred from numerous measurements (e.g. Ref. [25]) suggest that the coma is composed of $\gtrsim 75\%$ H_2O and its photodissociation products OH, O, and H; $\sim 15\%$ CO; and $\sim 5\%$ CO_2 . Traces of complex hydrocarbons have also been observed: CH_4 ($\sim 1\%$), C_2H_2 ($\sim 0.5\%$), and C_2H_6 ($\sim 0.5\%$). In addition to C, O, and Ne ions, the solar wind also contains significant quantities of N, Si, S, and Fe ions.

The quantity of charge transfer data for heavy ion collisions with cometary neutrals is sparse. We briefly summarize what is currently available. For the dominant neutral species, H_2O , total SEC due to He^{2+} (4-113 keV/u) [26] and O^+ (0.01-7 eV/u) [27] have been measured. We are not aware of any data for OH targets, but total and state-selective SEC impact-parameter calculations have been performed for O^+ (6-600 eV/u), O^{2+} (20 eV/u), S^+ (16-300 eV/u), S^{2+} (0.3-300 eV/u), and S^{3+} (20 eV/u) with O [28]. Numerous data are available for H targets [7,29]. Total SEC measurements for CO targets are available for H^+ (5-150 keV/u) [30,31], He^+ (1-88 keV/u) [32], He^{2+} (0.3-113 keV/u) [26,33], and Ar^+ (0.002-0.15 eV/u) [34]. Thermal SEC rate coefficient measurements for N^{2+} [35], O^{2+} [36], Ne^{2+} [37], and Kr^{2+} [37] for CO gas have also been performed. For CO_2 targets, total SEC measured cross sections are available for H^+ (5-150 keV/u) [31], He^+ (1-88 keV/u) [32], and He^{2+} (4-113 keV/u) [26] and thermal SEC rate coefficients for Ne^{2+} [37], Ar^{2+} [38], and Kr^{2+} [37]. Some data are available for the trace constituent target CH_4 with H^+ (0.05-150 keV/u) [31,39], He^+ (1-88 keV/u) [32], He^{2+} (4-113 keV/u) [26], C^{4+} (0.7-300 eV/u) [40], Ne^{2+} [37], Ar^{2+} [38], and Kr^{2+} [37]; C_2H_2 with H^+ (0.1-7 keV/u) [41]; and C_2H_6 with C^{4+} (0.7-300 eV/u) [40]. While the low charge state ions will not produce x-rays, the cross sectional data may be useful for testing future theoretical calculations or investigating ejected electron induced processes and the overall ionization structure.

To ascertain whether charge transfer is a viable mechanism for the production of cometary x-rays, detailed total and state-selective SEC as well as DEC, DiEC, TI, and AI cross sections are needed primarily for H_2O , but also for OH, O, CO, and CO_2 . We are currently in the process of extending the CTMC and MOCC calculations for H_2 targets discussed in the previous section to the cometary neutrals. Measurements of these collision systems would be highly desirable.

SUPERNOVA EJECTA

Type Ia Supernovae

The ionization balance in the ejecta of a SN is strongly affected by charge transfer reactions. However, since the abundances of hydrogen and helium are negligible in

the core regions due to inefficient mixing of the elements, the important reactions involve metal atoms and metal ions, systems which have received little attention in the atomic collision community. For example, the iron core of a Type Ia SN is composed primarily of Fe, Co, and Ni with charge states of $q = 1 - 3$ and neutrals. Liu, Jeffery, and Schultz [42] have found that the iron ionization structure is controlled by SEC

and electron impact ionization. Similar processes determine the Co and Ni ionization structures. The SEC rate coefficients utilized in this model were estimated from QDM and CTMC calculations assuming that DEC would be negligible [43]. The only guidance as to the reliability of this assumption are SEC and DEC measurements of Mg^{2+} collisions with Mg and Zn [44]. While these measurements are limited to energies $\gtrsim 50$ eV/u, they suggest, however, that for smaller energies DEC will dominate. This is due to the resonant or quasis resonant conditions for DEC with both targets. To test the validity of our methods, we show in Figure 2 cross sections for SEC in Mg^{2+} collisions with Mg computed with QDM, CTMC, and LZ [43] in comparison with the measurements. Two types of LZ calculations are presented; one using the Olson-Salop [45] empirical (model) radial coupling and the other utilizing a radial coupling deduced from an *ab initio* computation of the Mg_2^{2+} potentials. The QDM and CTMC results overestimate the low energy SEC cross section as they assume a quasi-resonant situation exists when in actuality only two exit channels exist which are exoergic by 7.4 and 3 eV. The LZ method, which accounts for non-resonant interactions, gives good agreement with the experiment if an accurate estimate of the coupling can be obtained. On the other hand, LZ calculations which apply empirical couplings, constructed for H and He targets, to metal targets may be inappropriate [46]. The *ab initio* LZ calculations further suggest that SEC will be unimportant for the $\text{Mg}^{2+} + \text{Mg}$ system [43].

However, compared to the simple $3s^2$ configuration of Mg, the iron-group elements of interest for Type Ia SNe have complicated valence structures ($3d^6 4s^2$ for Fe) as well as large angular momenta and spin. This results in many low-lying atomic excited states and a multitude of molecular states for the interacting iron-group pair. As an example, consider the molecular states of Fe_2^{2+} which correlate to the ground states of Fe and Fe^{2+} . The Wigner-Witmer rules predict that there are a total of 15 molecular states from Σ_g^+ to Γ_g for each of five multiplicities $2S + 1 = 1, 3, 5, 7, 9$, for a total of 75 molecular states. A large number of these should be easily capable of coupling to a number of lower-lying exoergic channels correlating to $\text{Fe}^+ + \text{Fe}^{+*}$. It would appear that for the iron-group elements, the quasi-resonance conditions would be satisfied and that SEC would be at least as important as DEC in the low energy regime. A study is currently underway to compute *ab initio* potential curves and perform MOCC calculations for some of these iron-group systems to verify if the quasi-resonance condition exists.

FIGURE 2. SEC for $\text{Mg}^{2+} + \text{Mg}$.

Type II Supernovae

In 1987 molecular emission from a SN was detected for the first time in the type II object SN1987a [47,48]. The emissions originate from vibrational bands of CO, SiO, and possibly CS [49]. Emission features near $2.3 \mu\text{m}$ in the low resolution spectra of SN1995ad are also thought to be due to the first overtone band of CO [50]. Since the discovery of molecular emission from SN1987a, a number of groups have attempted to model the emission of CO (see Ref. [51] for a review) with fair success. As the density is below the critical value, the vibrational populations will depart from local thermodynamic equilibrium (LTE). The model of Liu et al. [52] assumes that the vibrational levels are populated by electron impact excitation

for which only the $v'' = 0$ to $v' = 1$ cross section has recently been measured by Allan [53] and calculated by Morgan [54]. This is thought to be a good approximation as the ejecta is ionized with an electron fractional abundance as high as 10^{-2} . To estimate the rate coefficients for $\Delta v = 1$ transitions for other vibrational levels, Liu et al. [52] assumed these were proportional to the absorption oscillator strengths. As no experimental or theoretical electron impact data for SiO are available, Liu and Dalgarno [55] estimated the excitation rate coefficients using the Born approximation and the available Einstein A -coefficients. Liu [57] made the same approximation for CS excitation.

However, the most abundant species in the zone of the ejecta where the molecules are formed is atomic oxygen suggesting that excitation due to O impacts

may play a role. Adopting the vibrational excitation rate coefficient of CO due to H collisions from Hollenbach and McKee [58], but scaled by the O-CO collision system reduced mass suggests that the rates for electron and O impact excitation of CO are comparable. Therefore, to improve models of molecular emission from Type II SNe, experimental and theoretical data are needed for electron and O impact excitation of CO, SiO, and CS.

CONCLUSIONS

Three astrophysical environments have been described in which atomic collisions with metal and molecular targets are important. Much of the necessary data to model these environments are unavailable. The major processes of interest are total and state-selective electron capture due to multiply charged ion collisions with H₂, H₂O, OH, O, CO, and CO₂ and collisions of iron-group ions with iron-group neutrals. Other processes of interest include projectile and target ionization and excitation due to oxygen and sulfur ion collisions with H₂ and vibrational excitation of CO, SiO, and CS due to O collisions.

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