Line Ratios for Solar Wind Charge Exchange with Comets

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Abstract

Charge exchange (CX) has emerged in X-ray emission modeling as a significant process that must be considered in many astrophysical environments—particularly comets. Comets host an interaction between solar wind ions and cometary neutrals to promote solar wind charge exchange (SWCX). X-ray observatories provide astronomers and astrophysicists with data for many X-ray emitting comets that are impossible to accurately model without reliable CX data. Here, we utilize a streamlined set of computer programs that incorporate the multi-channel Landau–Zener theory and a cascade model for X-ray emission to generate cross sections and X-ray line ratios for a variety of bare and non-bare ion single electron capture (SEC) collisions. Namely, we consider collisions between the solar wind constituent bare and H-like ions of C, N, O, Ne, Na, Mg, Al, and Si and the cometary neutrals H2O, CO, CO2, OH, and O. To exemplify the application of this model, we model the X-ray emission of Comet C/2000 WM1 (linear) using the CX package in SPEX and find excellent agreement with observations made with the XMM-Newton RGS detector. Our analyses show that the X-ray intensity is dominated by SWCX with H, while H2O plays a secondary role. This is the first time, to our knowledge, that CX cross sections have been implemented into a X-ray spectral fitting package to determine the H to H2O ratio in cometary atmospheres. The CX data sets are incorporated into the modeling packages SPEX and Kronos.

Key words: atomic data – atomic processes – comets: general – line: formation – X-rays: general

Supporting material: machine-readable table

1. Introduction

With the current orbiting X-ray observatories and plans for future high-resolution X-ray missions, the need for atomic and molecular data is universally recognized by astrophysical modelers. For instance, with the possible Hitomi detection of charge exchange (CX) in the Perseus cluster or the recent Chandra observations of X-ray emission from Pluto, accurate atomic data are necessary to understand such unexpected, very recent observations (Gu et al. 2015; Lisse et al. 2016). Another interest in CX X-ray modeling is the study of comets (such as Comet C/2000 WM1 linear, Comet Tempel 1, etc.) whose primary mechanism for X-ray emission is solar wind charge exchange (SWCX). Cometary SWCX occurs when highly charged projectile ions, such as bare and H-like C, N, O, Ne, Na, Mg, Al, and Si that are present in the solar wind, capture an electron from a target neutral species, such as H2O, CO, CO2, OH, O, and H that are present in the cometary atmosphere. Although more than one electron can be captured during a CX collision, we only consider single electron capture (SEC) in this work. The SEC process is given in Equation (1) where \( X^{q+} \) denotes the projectile ion and \( Y \) denotes the collision target,

\[
X^{q+} + Y \rightarrow X^{(q-1)+} (n\ell \, 2\ell + L) + Y^+ + \Delta E,
\]

while \( n\ell \) specifies the principal quantum number and orbital angular momentum of the captured electron, \( 2\ell + L \) denotes the total spin \( S \) and total orbital angular momenta \( L \) of the product ion, and \( \Delta E \) gives the kinetic energy liberated from the collision system. During cometary SWCX, electrons are captured into highly energetic states of the solar wind ions. To stabilize, excess internal energy is emitted in the form of X-ray photons so that the captured electrons are demoted to the ground state. This CX-induced X-ray emission is observed by X-ray observatories such as Chandra, XMM-Newton, and Suzaku (e.g., Lisse et al. 1996; Cravens 2000; Krasnapolsky et al. 2004; Bhardwaj et al. 2007; Katsuda et al. 2011; Cumbee et al. 2014), but can also be detected in the laboratory through experimental apparatuses such as an electron beam ion trap (Wargelin et al. 2005, 2007). In this work, we attempt to model such observations by applying (1) the multi-channel Landau–Zener (MCLZ) theory to generate \( n\ell S \)-resolved cross sections for CX and (2) a cascade model to generate theoretical X-ray spectra and ultimately, line ratios. These line ratios can be implemented into X-ray spectral fitting packages to model cometary environments and can be used as a diagnostic for relative abundances of neutrals in cometary atmospheres while also putting constraints on solar wind composition and velocities at the comet.

We compare our theoretical atomic and molecular data to other available data in the literature, such as other cross sections obtained by different theoretical means, experimental X-ray spectra, or even available line ratios themselves. Such comparisons appear in the Appendix. These comparisons are limited, however, as this is the first time, to our knowledge, that such calculations have been performed for many of the aforementioned systems.

2. Theory

The MCLZ theory applied to generate \( n\ell S \)-resolved cross sections in this work is detailed in Mullen et al. (2016) and Lyons et al. (2017). To briefly summarize the schema, we begin
by considering all possible initial and final channels of the collision system by applying Wigner–Witmer rules (i.e., angular momentum/molecular symmetry conservation, Herzberg 1950; Wigner & Witmer 1928).

The NIST Atomic Spectra Database (Kramida et al. 2014) then provides product ion excitation energies necessary for constructing the potentials associated with allowed final channels. Missing states in the NIST Atomic Spectra Database are approximated with quantum defect theory (see Mullen et al. 2016). The couplings between initial and final channels are characterized by the energy differences of the adiabatic potentials at internuclear distances between the projectile–collision pairs, at which transitions may occur (avoided crossings). The CX probability is thus dependent upon (1) avoided crossing locations $R_{\ell}$, (2) the energy differences at these $R_{\ell}$, and (3) the difference between the derivatives of the initial and final diabatic potential curves at $R_{\ell}$. We obtain the CX cross section by considering (1) the incident collision energy, (2) all partial waves of the collision system, and (3) the Janev et al. (1983) multi-channel probability relation. For bare ion collisions, the low-energy $\ell$-distribution model, as shown in Equation (2),

$$W_{\ell}^{\text{Low}} = (2\ell + 1) \frac{[(n - 1)!]^2}{(n + \ell)![(n - 1 - \ell)!]},$$

is applied (Krasnopolsky et al. 2004). Other $\ell$-distribution models may be applied (see, for example, Krasnopolsky et al. 2004; Smith et al. 2014). Non-bare ion collisions do not require the use of an $\ell$-distribution model as the product ions of CX are non-degenerate.

Using the resulting $n\ell S$-resolved cross sections to seed a cascade model for X-ray emission, we can track the network of emitted photons due to the evolution of cascading electrons to stability. Thus, with the cross sections giving an initial population of states, transition probabilities (Einstein $A$ coefficients) dictating which cascade network is most probable, and selection rules specifying allowed transitions, the cascade model yields theoretical X-ray spectra and line ratios. As an example of the cascade model output, we present the theoretical spectrum for C V emission due to the CX collision between solar wind C$^5+$ and the cometary neutral H$_2$O in Figure 1. Note that all lines are normalized to the K\(\alpha\) resonance (r) line. In this example, the strength of the forbidden (f) line is a characteristic of the CX X-ray emission process, as opposed to electron impact excitation where the resonance line typically dominates.

Special considerations are mandatory for bare ion and hydrogen-like ion collisions with OH and O. The ground electronic states for OH and O are $^3P^-$ and $^3P^+$, respectively. Because of the non-zero angular momentum of these electronic states, modifications to the initial interaction potential utilized in Mullen et al. (2016) and Lyons et al. (2017) are made so that the long-range interaction includes the quadrupole moment, $Q_{M}$, of OH and O. The potential, therefore, is of the form

$$V_{\ell}(R) = A \exp(-BR) - \frac{\alpha q^2}{2R^4} + \frac{gQ_{M}}{2R^3},$$

where coefficients $A$ and $B$ are estimated in Butler & Dalgarno (1980), $\alpha$ is the dipole polarizability of the neutral target, and $R$ is the internuclear distance between the projectile/target pair. Values for the quadrupole moments of O and OH are given by Gutsev et al. (1998) and the NIST Computational Chemistry Comparison & Benchmark Database (2016), respectively, as $Q_{M,O} = -0.95$ a.u. and $Q_{M,OH} = -3.323$ a.u.

In addition to modifications to the initial channel model, Wigner–Witmer rules, based upon momentum conservation principles, require bare ion collisions with OH to conserve the $^3\Pi$ molecular electronic symmetry; therefore, only product projectile ion states with $\ell \geq 1$ are allowed, thus requiring a renormalization of the adopted $\ell$-distribution functions. For hydrogen-like ions colliding with OH, the system must conserve the $^3\Pi$ symmetry; therefore, only singlet and triplet states with $\ell \geq 1$ are allowed for the product projectile ion. The resulting cross sections must be weighted by the approach probability $g$-factor (see Wigner & Witmer 1928 for details), which is 1/4 for $^3\Pi$ states and 3/4 for $^3\Pi$ states. These considerations for OH targets assume that CX with OH result purely from linear collisions.

For bare ion collisions with O, $^3\Sigma^-$ and $^3\Pi$ molecular electronic symmetries must be conserved and be weighted by the $g$-factors 1/3 and 2/3, respectively. For this collision, doublet states of the product projectile ion conserve the $^3\Sigma^-$ symmetry, while only doublet states with $\ell \geq 1$ conserve the $^3\Pi$ symmetry. Finally, hydrogen-like ion collisions with O conserve the $^2\Sigma^-, ^2\Pi, ^4\Sigma^-$, and $^4\Pi$ symmetries each weighted by $g$-factors 1/9, 2/9, 2/9, and 4/9, respectively. All singlet and triplet states of the product projectile ion conserve the $^2\Sigma^-$ electronic state, while only triplet states conserve the $^2\Pi$ symmetry. All singlet and triplet states with $\ell \geq 1$ conserve the $^4\Pi$ symmetry; while only triplet states with $\ell \geq 1$ conserve the $^3\Pi$ symmetry; therefore, again, the $\ell$-distribution functions must be renormalized.

### 3. Line Ratios

As our intent is to help astronomers and astrophysicists by providing atomic and molecular data for use in X-ray emission modeling, we present calculated line ratios for the various aforementioned cometary SWCX projectile–collision pairs at five characteristic collision velocities (200, 400, 600, 800, and 1000 km s$^{-1}$) in Table 1 of the Appendix. The line ratios are defined as the ratio between an emission line and the Ly$\alpha$ line.
Table 1
Charge Exchange Induced X-Ray Emission of H- and He-like C–Si

| Phot. Energy (eV) | Ion | Target | Line | Intensity 200 km s^{-1} | Intensity 400 km s^{-1} | Intensity 600 km s^{-1} | Intensity 800 km s^{-1} | Intensity 1000 km s^{-1} |
|------------------|-----|--------|------|-------------------------|-------------------------|------------------------|------------------------|------------------------|
| 298.96           | C v | N₂     | Kα f | 0.6371                  | 1.0257                  | 1.2531                 | 1.3689                 | 1.4262                 |
| 304.41           | C v | N₂     | Kα i | 0.0743                  | 0.0901                  | 0.0968                 | 0.1007                 | 0.1030                 |
| 307.90           | C v | N₂     | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | N₂     | Kβ    | 3.1379                  | 2.3855                  | 1.9549                 | 1.6592                 | 1.4604                 |
| 370.92           | C v | N₂     | Kγ    | 0.0011                  | 0.0002                  | 0.0001                 | 0.0001                 | 0.0000                 |
| 298.96           | C v | H₂O    | Kα f | 3.1488                  | 2.9681                  | 2.4518                 | 2.0284                 | 1.7915                 |
| 304.41           | C v | H₂O    | Kα i | 0.2427                  | 0.2299                  | 0.1953                 | 0.1660                 | 0.1479                 |
| 307.90           | C v | H₂O    | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | H₂O    | Kβ    | 0.4499                  | 0.7120                  | 1.2290                 | 1.5967                 | 1.7703                 |
| 370.92           | C v | H₂O    | Kγ    | 0.8395                  | 0.7724                  | 0.5980                 | 0.4360                 | 0.3298                 |
| 298.96           | C v | CO     | Kα f | 2.3460                  | 1.0689                  | 1.1178                 | 1.2206                 | 1.2946                 |
| 304.41           | C v | CO     | Kα i | 0.1977                  | 0.1031                  | 0.0977                 | 0.0981                 | 0.0992                 |
| 307.90           | C v | CO     | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | CO     | Kβ    | 2.1029                  | 2.6233                  | 2.3414                 | 2.0744                 | 1.8629                 |
| 370.92           | C v | CO     | Kγ    | 0.3719                  | 0.0653                  | 0.0264                 | 0.0153                 | 0.0107                 |
| 298.96           | C v | CO₂    | Kα f | 2.0166                  | 1.1770                  | 1.2407                 | 1.3209                 | 1.3720                 |
| 304.41           | C v | CO₂    | Kα i | 0.1724                  | 0.1065                  | 0.1011                 | 0.1010                 | 0.1017                 |
| 307.90           | C v | CO₂    | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | CO₂    | Kβ    | 2.1032                  | 2.4034                  | 2.1024                 | 1.8275                 | 1.6227                 |
| 370.92           | C v | CO₂    | Kγ    | 0.3322                  | 0.0718                  | 0.0319                 | 0.0194                 | 0.0139                 |
| 298.96           | C v | O      | Kα f | 7.1031                  | 11.7286                 | 9.4888                 | 6.8824                 | 5.6041                 |
| 304.41           | C v | O      | Kα i | 0.5514                  | 1.2741                  | 1.1028                 | 0.7808                 | 0.6037                 |
| 307.90           | C v | O      | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | O      | Kβ    | 0.3770                  | 1.3046                  | 2.4506                 | 2.6876                 | 2.6782                 |
| 370.92           | C v | O      | Kγ    | 1.1245                  | 0.8812                  | 0.4002                 | 0.1916                 | 0.1144                 |
| 298.96           | C v | OH     | Kα f | 5.7399                  | 6.2376                  | 4.8486                 | 4.0528                 | 3.7247                 |
| 304.41           | C v | OH     | Kα i | 0.3777                  | 0.5407                  | 0.4434                 | 0.3534                 | 0.3023                 |
| 307.90           | C v | OH     | Kα r | 1.0000                  | 1.0000                  | 1.0000                 | 1.0000                 | 1.0000                 |
| 354.52           | C v | OH     | Kβ    | 0.3126                  | 1.2453                  | 2.0619                 | 2.3243                 | 2.3922                 |
| 370.92           | C v | OH     | Kγ    | 1.5362                  | 1.1179                  | 0.5853                 | 0.3464                 | 0.2395                 |

Note. Line ratios for X-ray emission resulting from C–Si bare and H-like ions CX collisions with N₂, H₂O, CO, CO₂, OH, and O. Note that all lines are normalized to the Lyα line and Kα resonant line for bare ion and non-bare ion collisions, respectively. Line ratios for bare ion collisions were obtained by applying the low-energy distribution (Equation (2)) to MCLZ n-resolved cross sections. For non-bare ion collisions, MCLZ nTS-resolved cross sections were used to obtain these ratios. See text for details. Line ratios for bare ion collisions applying other distribution functions are available upon request. See the included machine-readable table for complete C–Si CX data.

(This table is available in its entirety in machine-readable form.)

(for bare projectile ion collisions) or the Kα resonance line (for H-like projectile collisions). For bare projectile ion collision systems, we applied the low-energy distribution to MCLZ n-resolved cross sections before inputting them into the cascade model. Line ratios that used other distribution functions are available in the Kronos database or upon request. For H-like projectile ion collision systems, MCLZ nTS-resolved cross sections are used to generate line ratios; here, we also report forbidden, intercombination, and resonance lines for Kα emission.

The reliability of these data is tested in several ways. First, the Mullen et al. (2016) study of the high charge and computationally expensive/ extensive Fe XXV and Fe XXVI CX collision systems (with various targets) were investigated. Subsequent analyses revealed very good agreement with two electron beam ion trap studies (Wargelin et al. 2005, 2007), as well as with other theoretical calculations such as CTMC (classical trajectory Monte Carlo) given in Katsonis et al. (1991), Schultz et al. (1991), and Wargelin et al. (2007). Next, we compare MCLZ cometary SWCX calculations to available data in the literature—albeit limited. These comparisons are detailed in the Appendix.

4. Application—Comet C/2000 WM1 (Linear)
To exemplify how these results can be applied, we incorporate the CX data from this work and R. S. Cumbee et al. (2017, in preparation) into the CX package in SPEX (Gu et al. 2016) to perform a CX fitting to Comet C/2000 WM1 (linear). X-ray satellite XMM-Newton (Jansen et al. 2001) observed Comet C/2000 WM1 in 2001 December (Observation ID: 0103461101). Here, we focus on high spectroscopic resolution data taken by one XMM-Newton instrument, the Reflection Grating Spectrometer (RGS). The same RGS data have been previously fitted in Gu et al. (2016); the main difference, however, is that Gu et al. (2016) assumes only H
targets, while in this work many cometary targets have been tested (H$_2$O, CO, CO$_2$, OH, and O). Only a short period (18 ks) of exposure is analyzed. The rest of the data were collected outside the RGS field of view, which was 5 arcmin in this observation.

In the X-ray modeling package SPEX, we first implement the CX MCLZ data for bare and H-like C to Si collisions with H and H$_2$O. However, quantum molecular-orbital close-coupling data were adopted for bare and hydrogen-like C, N, and O collisions with H (Nolte et al. 2012, 2017, in preparation; Wu et al. 2011) as reported in Cumbee et al. (2014, 2017, in preparation).

To fit the spectrum, we subtract the standard model background and correct for instrumental broadening due to the spatial extent of the diffuse comet halo and its motion. The 18–36.5 Å spectrum was fitted with two SWCX components, one with atomic H targets and the other with H$_2$O targets (both naturally expected in comet spectra, Bodewits et al. 2006). The ionization temperatures of the two solar wind (SW) components are free to vary, while their collision velocities and metal abundances are assumed to be the same. As shown in Figure 2, the RGS spectrum can be reasonably fit with the model. The best-fit C statistic is 340 with 287 degrees of freedom, which is a significantly better fit than the value obtained in Gu et al. (2016). We have tried fitting the RGS data with all molecular targets from this work (H$_2$O, CO, CO$_2$, OH, and O), but the H and H$_2$O combination gives the best fit. The fit determines the H-target temperature to be 0.13 keV. For the water component, the current model prefers a two-temperature configuration at 0.22 and 0.06 keV, which might suggest the cooling of solar wind ions when they penetrate into the cometary atmosphere. The CX collision velocity is determined to be $\sim 240$ km s$^{-1}$.

We also attempt to fit the spectrum with two H-target only components. This yielded a worse fitting by $\Delta C = 39$. This indicates that the cometary H and H$_2$O components should both contribute to the CX emission. The emission measure of CX collisions with H$_2$O is less than 1/3 ($\sim 30\%$) of that with H. Our analyses of this fitting routine can be compared to that of Bodewits et al. (2006). For instance, Bodewits et al. (2006) predicts that the dominant target changes when the comet approaches the Sun. As seen in Figure 9 of Bodewits et al. (2006), Halley’s Comet at 1 au has more H in its cometary atmosphere than Hale–Bopp at 3.1 au due to the photodissociation of H$_2$O. Comet C/2000 WM1 (linear) is observed at around 1 au so it should behave similar to the Halley case. Based on the Halley investigation, the H$_2$O core of C/2000 WM1 (linear) has a diameter of $3 \times 10^4$ km (1.6 arcmin) in the observational frame, while H becomes more important in the outer coma ($1 \times 10^5$–3 $\times 10^5$ km). Since the RGS spectrum (which has no spatial resolution) was taken from an $R \sim 4 \times 10^7$ km region centered on the comet core, we predict that the overall emission due to CX with H is larger than that due to water.

The possibility of single-capture, multiple-collision events that eventually neutralize the solar wind ion was also tested using a model from Gu et al. (2016), but this did not improve the fit.

5. Conclusions

With current orbiting satellites, plans for future high-resolution X-ray missions underway, and the development of a streamlined MCLZ approach, CX line ratios can be applied in X-ray emission models to advance the astrophysical modeling of many environments—particularly comets. To exemplify the need and use for such data, the modeling of Comet C/2000 WM1 linear illustrates one of the most comprehensive
applications of atomic data to the astrophysical modeling of a comet to date. Subsequent analyses of this model show that there is excellent agreement between the theory and other available data, as shown in the Appendix, as well as the statistical distribution functions (see, for example, Smith et al. 2014; Mullen et al. 2016). The statistical distribution, which is expected to be applicable at very high collision energies, gives significantly less high-n emission than the experiment. However, the separable distribution function, which is the only distribution function dependent on projectile ion charge, was also tested and shows decent agreement in modeling the high-n emission peak. From Figure 3, it appears that a blend of characteristics from both the separable distribution and low-energy distributions would reproduce the experimental spectrum, but multi-electron capture (MEC) effects (not included here) might also be present in the measured spectrum (see, for example, Ali et al. 2005). The MEC process, which is a double capture followed by auto-ionization (DCAI), tends to enhance the population of lower n-states and therefore increase the relative intensity of Lyα and possibly Lyβ.

MCLZ calculations for non-bare ion collisions require no application of a distribution function as product ion states are non-degenerate. Therefore, comparisons of such collisions with available experimental data could give a better and more pure measure of MCLZ performance as opposed to the use of distribution functions. Figure 4 gives the theoretical spectra resulting from Ne9+ CX collisions with H2O compared to experimental spectra from the same Greenwood et al. (2000) study. Again, the Greenwood et al. (2000) spectrum given in Figure 4 has not been corrected for detector efficiency. Spectra for collision energies of 1, 2, and 3 keV u⁻¹ are presented while the experimental collision energy is ∼2.9 keV u⁻¹.

In Figure 4, we see a slight enhancement of high-n emission as compared to the Greenwood et al. (2000) study. This emission feature can be further investigated by looking to the theoretical line ratios; for instance, the Kβ line ratio predicted for this collision system is equal to 0.2373 while those for the Kδ and Kε lines (5p → 1s, 6p → 1s) are 0.1206 and 0.3421, respectively, for a collision energy of 1 keV u⁻¹. The reasoning behind these relatively high Kδ and Kε lines can be explained by looking into the factors that dictate their intensities: (1) their associated cross section, (2) the corresponding Einstein A coefficient, and (3) the triplet-singlet cross section ratio, which is not necessarily 3:1.
Regarding the first factor, Figure 5 gives the n-resolved cross sections for Ne\(^{9+}\) CX collisions with H\(_2\)O. At the collision energies of interest 1–3 keV u\(^{-1}\), the dominant channels are \(n = 5, 6\), which is exactly as expected by the simple formula for dominant n-capture \(q^{0.75} \sim 5.2\), where \(q\) is the charge of the projectile ion. Accompanying these large cross sections into the \(n = 5, 6\) channels, the associated Kδ and Kε Einstein A coefficients are \(\sim 5.2 \times 10^{11}\) s\(^{-1}\) and \(\sim 3.0 \times 10^{11}\) s\(^{-1}\), which are roughly of the same order of magnitude as other \(np \rightarrow 1s\) transitions for \(n\) less than \(n = 5, 6\).

Because the reported experimental spectrum in Greenwood et al. (2000) was not corrected for the transmission efficiency of the Be window of their X-ray detector, we also give a comparison of our theoretical line ratios to Greenwood et al. (2000) line ratios that \(do\) correct for the detector efficiency in Tables 2 and 3. Note that the experimental line ratios presented in Tables 2 and 3 are deduced from their reported relative contributions of transitions to the total spectrum (again, after correcting for detector efficiency). Table 2 corresponds to line ratios for bare projectile ion CX collisions, while Table 3 corresponds to line ratios for hydrogen-like projectile ion CX collisions. Greenwood et al. (2000) was not able to resolve independent contributions from Ly\(\gamma\) and Ly\(\delta\) for many of the CX collisions. Therefore, in such instances, we report the sum of these. In Table 2, we report line ratios utilizing four different distribution functions: low energy, statistical, modified low energy, and separable. Greenwood et al. (2000) were also not able to resolve the intercombination and resonance lines for He-like emission, nor do the experiments observe the forbidden line due to the long lifetime of the 2\(s^2\) \(^3\)S. Therefore, for Table 3,
K = 6 + 6 + 4 = 16

40 keV u⁻¹ @ 2 keV u⁻¹

Table 3

| Transition | Greenwood et al. (2000) | MCLZ |
|------------|-------------------------|------|
| O^7+ + H₂O @ ~2.7 keV u⁻¹ | | |
| Kσ | 1.000 | 1.000 |
| Kβ | 0.186 | 0.098 |
| Kγ + Kδ | 0.243 | 0.437 |
| Hardness Ratio | 0.429 | 0.535 |
| Ne^10+ + H₂O @ ~2.9 keV u⁻¹ | | |
| Kσ | 1.000 | 1.000 |
| Kβ | 0.033 | 0.112 |
| Kγ | 0.044 | 0.050 |
| Kδ | 0.022 | 0.099 |
| Ke | 0.000 | 0.136 |
| Hardness Ratio | 0.099 | 0.397 |
| O^7+ + CO @ ~2.7 keV u⁻¹ | | |
| Kσ | 1.000 | 1.000 |
| Kβ | 0.180 | 0.141 |
| Kγ + Kδ | 0.192 | 0.507 |
| Hardness Ratio | 0.372 | 0.648 |
| Ne^10+ + CO @ ~2.9 keV u⁻¹ | | |
| Kσ | 1.000 | 1.000 |
| Kβ | 0.043 | 0.117 |
| Kγ | 0.022 | 0.069 |
| Kδ | 0.022 | 0.176 |
| Ke | 0.000 | 0.074 |
| Hardness Ratio | 0.087 | 0.436 |

Note. Same as Table 2 except comparing line ratios for He-like emission for collisions studied in Greenwood et al. (2000). Greenwood et al. (2000) was not able to resolve the intercombination and resonance lines for He-like emission or observe the forbidden line; therefore, MCLZ line ratios are normalized to the sum of Kσ, f, i, and r.

Figure 6. Comparison of theoretical MCLZ/cascade model spectrum to the Beiersdorfer et al. (2005) experimental spectrum for O^8+ collisions with N₂. Each spectrum is normalized to the maximum intensity of Lyα emission. The theoretical spectra mimic a ~10 eV FWHM resolution. Beiersdorfer et al. (2005) estimate an experimental collision energy of ~10 eV u⁻¹.

Table 4

| Transition | Greenwood et al. (2000) | MCLZ |
|------------|-------------------------|------|
| O^7+ + CO @ 2 keV u⁻¹ | | |
| Kσ | 76.20 ± 0.70 | 38.00 |
| Kβ | 23.80 ± 0.90 | 54.00 |
| Hardness Ratio | 4.00 | 9.00 |
| Ne^10+ + CO @ 2 keV u⁻¹ | | |
| Kσ | 87.00 ± 0.90 | 50.00 |
| Kβ | 13.00 ± 0.80 | 80.00 |
| Hardness Ratio | 4.00 | 6.00 |

Note. The data presented for comparison in this table are taken from the Eissa et al. (2002) study, which gathers experimental data, CTMC calculations, and Zener calculations similar to those that are computed in this work. Note that cross sections are relative, and we report the n-resolved fraction as a percentage of the total cross section.

In Figure 6, we present theoretical spectra for O^8+ collisions with N₂ at a collision energy of 10 eV u⁻¹ compared to the EBIT measurements that have an estimated collision energy of ~10 eV u⁻¹. Applying the low-energy distribution function (Equation (2)), we see an excellent agreement between the experimental and theoretical line ratios for Lyα, Lyβ, and Lyγ systems, though these collision energies are significantly larger (E_{collision} ~ 3 keV u⁻¹) than those applied in the cometary model.

Table 3 demonstrates that MCLZ nLS-resolved cross sections yield larger hardness ratios than measured in Greenwood et al. (2000). This is consistent with the findings of Figure 4 that demonstrated an enhancement of high-n emission compared to the experiment. Again, perhaps multiple electron capture could be the source of such discrepancy. We anticipate that the effect of a multiple electron capture in the experiment would enhance n = 2 → 1 emission, which would therefore decrease hardness ratios and, in turn, decrease the line ratios associated with high-n emission.

Another study that we compare our theoretical data to is that of Beiersdorfer et al. (2005) who used the same microcalorimeter spectrometer originally designed for the Astro-E mission. In Figure 6, we present theoretical spectra for O^8+ collisions with N₂ at a collision energy of 10 eV u⁻¹ compared to the EBIT measurements that have an estimated collision energy of ~10 eV u⁻¹. Applying the low-energy distribution function (Equation (2)), we see an excellent agreement between the experimental and theoretical line ratios for Lyα, Lyβ, and Lyγ...
emission that the microcalorimeter had no difficulty in resolving. However, again for high-\(n\) emission, the theory predicts a much higher contribution to the spectra than the EBIT measurement. Therefore, we look to other distribution functions—namely the modified low-energy distribution and the separable distribution (note that this collision energy is so small that the statistical distribution is not considered). Both the separable and modified low-energy distribution model Ly\(\delta\) well. However, it is worth noting that the low-energy distribution function models Ly\(\alpha\), Ly\(\beta\), and Ly\(\gamma\) most accurately and would be expected to be valid at this low collision energy.

We benchmark MCLZ cross sections directly to other available theoretical data and extrapolations from experiment as seen in Table 4. Eissa et al. (2002) shows agreement between relative \(n\)-resolved cross sections for various systems with previous Landau–Zener (LZ) calculations (see Eissa et al. 2002 for details) and CTMC calculations. For instance, MCLZ calculations for \(\text{N}^7+\) collisions with CO at collision energies of 2 keV u\(^{-1}\) are in almost perfect agreement with previous LZ calculations and are comparable to CTMC calculations. Interestingly, all theoretical methods predict that \(\sigma_{\text{N}^7+} > \sigma_{\text{N}^5+}\) whereas experiment suggests that \(\sigma_{\text{N}^5+}\) comprises nearly 75% of the total cross section. Identical behavior is seen for \(\text{N}^7+\) collisions with CO\(_2\) at collision energies of 2 keV u\(^{-1}\)—namely, MCLZ is in agreement with CTMC and previous LZ calculations whereas experiment suggests a different dominant channel than all theoretical calculations. This disagreement in dominant channels between theory and experiment is not universal. When comparing MCLZ \(n\)-resolved cross sections for Ne\(^{10}\)+ + \(\text{H}_2\text{O}\) collisions at \(\sim 10\) keV u\(^{-1}\) to the Rigazio et al. (2002) study that extracts populations from X-ray measurements, both sets of data agree that the dominant channels are \(n = 6, 7\).

As previously mentioned, few theoretical CX calculations for systems involving cometary molecules have been performed. Therefore, Table 4 lacks CTMC and previous LZ calculations for all \(\text{O}^+\) collisions. However, MCLZ calculations for the \(\text{O}^+ + \text{H}_2\text{O}\) CX collisions at 2 keV u\(^{-1}\), which is a particularly important solar wind/cometary gas interaction, are in excellent agreement with the experiment. However, we note

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**Table 5**

| Phot. Energy (eV) | Ion Line | Rel. Diff. |
|------------------|----------|------------|
|                  |          | 200 km s\(^{-1}\) | 400 km s\(^{-1}\) | 600 km s\(^{-1}\) | 800 km s\(^{-1}\) | 1000 km s\(^{-1}\) |
| 298.96           | C \(\text{V}\) K\(\alpha\) \(f\) | 0.422 | 0.296 | 0.456 | 0.596 | 0.729 |
| 304.41           | C \(\text{V}\) K\(\alpha\) \(i\) | 0.392 | 0.366 | 0.608 | 0.723 | 0.802 |
| 307.90           | C \(\text{V}\) K\(\alpha\) \(r\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 354.52           | C \(\text{V}\) K\(\beta\) | 0.381 | 1.001 | 1.445 | 1.539 | 1.505 |
| 370.92           | C \(\text{V}\) K\(\gamma\) | 0.733 | 1.113 | 1.055 | 0.956 | 0.820 |
| 367.49           | C \(\text{VI}\) L\(\text{Y}\alpha\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 435.55           | C \(\text{VI}\) L\(\text{Y}\beta\) | 1.114 | 0.891 | 0.929 | 1.045 | 1.078 |
| 459.37           | C \(\text{VI}\) L\(\text{Y}\gamma\) | 1.307 | 1.178 | 1.122 | 1.207 | 1.239 |
| 470.39           | C \(\text{VI}\) L\(\text{Y}\delta\) | 1.575 | 1.868 | 1.927 | 1.910 | 1.879 |
| 419.80           | N \(\text{VI}\) K\(\alpha\) \(f\) | 1.351 | 1.208 | 1.013 | 0.856 | 0.748 |
| 426.32           | N \(\text{VI}\) K\(\alpha\) \(i\) | 0.627 | 0.630 | 0.559 | 0.492 | 0.463 |
| 430.70           | N \(\text{VI}\) K\(\alpha\) \(r\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 497.97           | N \(\text{VI}\) K\(\beta\) | 0.441 | 0.118 | 0.409 | 0.698 | 0.865 |
| 521.58           | N \(\text{VI}\) K\(\gamma\) | 1.042 | 1.209 | 1.267 | 1.344 | 1.386 |
| 532.65           | N \(\text{VI}\) K\(\delta\) | 1.756 | 1.895 | 1.913 | 1.881 | 1.986 |
| 500.28           | N \(\text{VII}\) L\(\text{Y}\alpha\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 592.93           | N \(\text{VII}\) L\(\text{Y}\beta\) | 0.676 | 1.016 | 1.046 | 1.089 | 1.146 |
| 625.35           | N \(\text{VII}\) L\(\text{Y}\gamma\) | 1.195 | 1.514 | 1.478 | 1.424 | 1.404 |
| 640.36           | N \(\text{VII}\) L\(\text{Y}\delta\) | 0.823 | 1.246 | 1.263 | 1.309 | 1.343 |
| 560.99           | O \(\text{VII}\) K\(\alpha\) \(f\) | 0.801 | 0.637 | 0.714 | 0.772 | 0.875 |
| 568.59           | O \(\text{VII}\) K\(\alpha\) \(i\) | 0.100 | 0.005 | 0.103 | 0.168 | 0.285 |
| 573.95           | O \(\text{VII}\) K\(\alpha\) \(r\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 665.62           | O \(\text{VII}\) K\(\beta\) | 0.671 | 0.920 | 0.889 | 0.953 | 0.896 |
| 697.80           | O \(\text{VII}\) K\(\gamma\) | 0.880 | 1.415 | 1.513 | 1.523 | 1.487 |
| 712.72           | O \(\text{VII}\) K\(\delta\) | 1.037 | 1.486 | 1.556 | 1.608 | 1.608 |
| 653.56           | O \(\text{VIII}\) L\(\text{Y}\alpha\) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 774.59           | O \(\text{VIII}\) L\(\text{Y}\beta\) | 1.042 | 0.945 | 0.959 | 1.028 | 1.113 |
| 816.95           | O \(\text{VIII}\) L\(\text{Y}\gamma\) | 1.276 | 1.397 | 1.475 | 1.521 | 1.554 |
| 836.55           | O \(\text{VIII}\) L\(\text{Y}\delta\) | 1.529 | 1.486 | 1.477 | 1.531 | 1.565 |
| 847.20           | O \(\text{VIII}\) L\(\text{Y}\epsilon\) | 0.539 | 0.025 | 0.123 | 0.023 | 0.339 |

**Note.** Relative difference between MCLZ line ratios for CX collisions with H\(_2\)O and Bodewits et al. (2007) ratios for CX collisions with H (i.e., \(2|X_{\text{Bodewits}} - X_{\text{MCLZ}}|/|X_{\text{Bodewits}} + X_{\text{MCLZ}}\)). In many models, the latter ratios are applied to model cometary CX no matter the target. Differences between the ratios symbolize the significant effect of target dependence in CX data. All relative differences for the K\(\alpha\) resonance \((r)\) line and Ly\(\alpha\) are zero because the hydrogen-like and helium-like emission data sets are normalized to these lines, respectively. Theoretical calculations for bare ion collisions via MCLZ apply the low-energy distribution.
again that the current work considers only SEC, while the effects of multiple capture from multi-electron targets at SW velocities are not well understood.

Finally, we compare MCLZ line ratios for bare and H-like C, N, and O collisions with H2O to Bodewits et al. (2007) in Table 5. The Bodewits et al. (2007) data corresponds to collisions with H, not H2O. This comparison emphasizes the target dependence of not just CX cross sections but the resulting line ratios themselves. Thus, we suggest that X-ray modelers consider, when available, the dependencies of (1) projectile ion, (2) target, and (3) collision energy. This is now possible due to the fact that all data presented here and in R. S. Cumbee et al. (2017, in preparation) are available in Kronos and SPEX. Furthermore, scripts are available to generate line ratios in XSPEC format using the recommended cross sections from Kronos. In these scripts, each X-ray emission line (i.e., Lyα or Lyβ) is put in separately as a Gaussian parameter. Energies from 200 eV u−1 (∼200 km s−1) to 5000 eV u−1 (∼1000 km s−1) can be chosen, and ions from C to Si can be considered, using the best available cross sections for a given ion-neutral interaction. Additional details are given in R. S. Cumbee et al. (2017, in preparation).

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