CHARGE EXCHANGE-INDUCED X-RAY EMISSION OF FeXXV AND FeXXVI VIA A STREAMLINED MODEL

P. D. Mullen, R. S. Cumbee, D. Lyons, and P. C. Stancil
Department of Physics and Astronomy and the Center for Simulational Physics, University of Georgia, Athens, GA 30602, USA
Received 2015 July 3; accepted 2016 March 22; published 2016 June 8

ABSTRACT
Charge exchange (CX) is an important process for the modeling of X-ray spectra obtained by the Chandra, XMM-Newton, and Suzaku X-ray observatories, as well as the anticipated Astro-H mission. The understanding of the observed X-ray spectra produced by many astrophysical environments is hindered by the current incompleteness of available atomic and molecular data—especially for CX. Here, we implement a streamlined program set that applies quantum defect methods and the Landau–Zener theory to generate total, n-resolved, and nlS-resolved cross sections for any given projectile ion/target CX collision. By using these data in a cascade model for X-ray emission, theoretical spectra for such systems can be predicted. With these techniques, Fe25+ and Fe26+ CX collisions with H, He, H2, N2, H2O, and CO are studied for single-electron capture (SEC). These systems have been selected because they illustrate computational difficulties for high projectile charges. Furthermore, FeXXV and FeXXVI emission lines have been detected in the Galactic center and Galactic ridge. Theoretical X-ray spectra for these collision systems are compared to experimental data generated by an electron-beam ion trap study. Several λ-distribution models have been tested for Fe25+ and Fe26+ SEC. Such analyses suggest that commonly used λ-distribution models struggle to accurately reflect the true distribution of electron capture as understood by more advanced theoretical methods.

Key words: atomic data — atomic processes — line: formation — X-rays: galaxies — X-rays: general — X-rays: ISM

1. INTRODUCTION
The charge exchange (CX) process may be a large contributor to the X-ray emission of many astrophysical environments such as comets, supernova remnants, the heliosphere, astrophysical, stars, and generally, highly ionized regions of the interstellar medium (e.g., Lisse et al. 1996; Cravens 2000; Krasnopolsky et al. 2004; Bhardwaj et al. 2007; Wargelin et al. 2007; Katsuda et al. 2011; Cumbee et al. 2014). In modeling CX emission, the availability of atomic data for CX is often insufficient, thus hindering the completeness and validity of present models. Therefore, working at the interface of atomic and molecular physics with astrophysics, we have applied quantum defect methods, the Landau–Zener theory of CX, and a cascade model for X-ray emission to show that not only can CX calculations be performed but they must be considered in the X-ray spectroscopy of many astrophysical environments.

CX collisions occur when a projectile ion captures an electron from a target neutral species. In this work, we consider only single-electron capture (SEC). This process is given generally by Equation (1) where X denotes the projectile ion with charge q and Y denotes the target species,

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

while n and \( \ell \) are the principal quantum number and orbital angular momentum of the captured electron, and S and L are the total spin and total orbital electron angular momenta of the product ion.

The multichannel Landau–Zener (MCLZ) approach is applied to generate n-resolved, nlS-resolved, and total cross sections for CX. The MCLZ level of theory is not the most advanced framework when compared to other methods such as quantum-mechanical molecular-orbital close-coupling (QMOCC) (e.g., Krasnopolsky et al. 2004). However, the power of MCLZ calculations can be seen in their short computation time—relative to other techniques—and the implications and quick resolution that such a tool could bring to the current lack of atomic and molecular data necessary for the astrophysical modeling of many systems. Here, we also validate our theoretical spectra for FeXXV and FeXXVI with molecular nitrogen CX collisions by comparison to experimental spectra given in Wargelin et al. (2005, 2007). Atomic units are used throughout, unless indicated otherwise.

2. THEORY
2.1. Landau–Zener Approximations
The foundation for the MCLZ theory begins by examining the initial and final channels of the collision system. The initial channel is characterized by the interaction between the projectile ion, with charge \( q_1 \), and target species prior to collision. This interaction is modeled by Equation (2) where the potential energy of the channel is given as a function of internuclear distance \( R \),

\[ V_i = A \exp(-BR) - \frac{\alpha q_1^2}{2R^4}, \] (2)

where coefficients \( A \) and \( B \) are estimated in Butler & Dalgarno (1980). The second term represents a polarization interaction between the projectile and target, with \( \alpha \) being the dipole polarizability of the neutral target, whereas the first term accounts for the repulsive nature of the system at small internuclear distances.

The final channel \( f \) of the collision system is a Coulombic repulsive interaction because the two product species are of positive charge. Therefore, a simple Coulomb repulsion potential is used,

\[ V_f = \frac{(q_1 - 1)q_2}{R} - \Delta E_\infty, \] (3)
where \( q_1 - 1 \) is the charge of the projectile after the collision and \( q_2 \) is the final charge of the target. For SEC between an ion and a neutral, \( q_2 = +1 \). The \( \Delta E_{\infty} \) term is the energy released as a result of the CX process and is precisely the sum of (1) the difference in ionization potentials of the product ion and the target species, and (2) the excitation energy of the product ion.

The CX probability is defined in terms of the transition from the initial channel to the final channel. The internuclear distance at which this transition can occur is referred to as the avoided crossing, \( R_c \). The distances of avoided crossings are estimated by setting the initial and final potential curves equal to one another. These avoided crossings are used as input parameters in calculating the energy difference, \( \Delta V \), of the adiabatic potential at \( R_c \). We estimate \( \Delta V \) using the Olson–Salop–Taulbjerg adaptation (Olson et al. 1971; Olson & Salop 1976; Taulbjerg 1986) displayed in Equation (4):

\[
\Delta V = (9.13 f_{nl}/ \sqrt{q_i}) \exp(-1.324 R_c \beta \sqrt{q_i}),
\]

where \( \beta, q_i \), and \( f_{nl} \) are detailed in Taulbjerg (1986).

The CX probability is thus dependent on three parameters: \( R_c, \Delta V, \) and the absolute value of the difference in slopes between the initial and final potential curves, \( |V_f' - V_i'| \). For a simple, two-channel system, the CX probability is given as

\[
\varphi_{if} = 2p_{if} (1 - p_{if}),
\]

where \( p_{if} \) is given in Butler & Dalgarno (1980) as

\[
p_{if} = \exp(-\omega_{if}),
\]

\[
\omega_{if} = \frac{4\pi^2 \Delta V^2}{\hbar v_R |V_f' - V_i'| R_c},
\]

and \( v_R \) is the radial component of the relative velocity of the collision (Butler & Dalgarno 1980).

In this work, we compute multichannel collision probabilities using the relation of Janev et al. (1983) for all allowed product ion states. The possible product states are determined following the Wigner–Wittmer rules (Wigner & Wittmer 1928; Herzberg 1950) for the angular momenta of the molecular channels and for channels connected to the initial channel via nonadiabatic radial coupling. Therefore, this computation of probabilities becomes complicated with an increasing number of product ion states, which increases with \( q_1 \), and may result in long computation times. Finally, with these probabilities, we compute cross sections for CX by considering the probability, collision energy, and all partial waves, \( J \), of the collision system,

\[
\sigma_f = \frac{\pi}{k_i^2} \sum_{J=0}^{J_{max}} (2J + 1) \varphi_{if}^J,
\]

where \( k_i \) is the wavenumber for relative motion in the initial channel \( i \).

2.2. \( \ell \)-distribution Models

For bare-ion collision systems, the product ion with a newly captured electron has \( \ell \)-states that are degenerate within a given \( n \)-state. The Landau–Zener theory requires that distances of avoided crossings are well separated. Therefore, we must apply \( \ell \)-distribution models to MCLZ \( n \)-resolved cross sections for bare-ion collision systems.

The statistical \( \ell \)-distribution discussed in Krasnopolsky et al. (2004) is given by

\[
W_{nl}^{Stat} = \frac{(2\ell + 1)/\ell!}{\ell!},
\]

and is recommended for collision energies \( \geq 10 \) keV/u. The low-energy \( \ell \)-distribution (Krasnopolsky et al. 2004, and references therein) is given by

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

and is recommended for collision energies \( \leq 10–100 \) keV/u. Two other \( \ell \)-distribution models, obtained from and adopted in the AtomDB Charge eXchange (ACX) model (Smith et al. 2014), are tested. We refer to them as the separable distribution, as displayed in Equation (11), and the modified low-energy distribution given in Equation (12):

\[
W_{nl}^{Sep} = \frac{(2\ell + 1)}{q_1} \exp \left[ -\ell (\ell + 1) \frac{1}{q_1} \right]
\]

and

\[
W_{nl}^{LowMod} = \ell (\ell + 1)(2\ell + 1) \frac{(n - 1)! (n - 2)!}{(n + \ell)!((n - \ell - 1)!}.
\]

It is interesting to note that Equation (12) gives a zero population for \( \ell = 0 \) \( (s) \) states and that Equation (11) is the only distribution dependent on incident ion charge. None of the distribution functions has an explicit dependence on collision energy.

2.3. Cascade-model for X-Ray Emission

After CX, the product ion is unstable as the electron is captured into a highly excited state. Therefore, the charged ion stabilizes by emitting a photon. The photon energies associated with such cascading events range from the extreme UV to the X-ray portion of the electromagnetic spectrum since the largest radiative probabilities correspond to decay to the ground state. Using \( nS \)-resolved cross sections, the cascade model for X-ray emission assumes that atomic levels are populated based on their relative cross sections for electron capture into associated states. Using these data alongside transition probabilities, the cascade model tracks the evolution of the electron’s cascade from its highly energetic state to stability by considering every possible transition that obeys the dipole selection rules \( \Delta \ell = \pm 1 \) and \( \Delta S = 0 \). Forbidden and intercombination transitions from the triplet \( n = 2 \) levels of He-like ions are also included. By considering all possible routes for this cascade and the initial population of states, one can compute theoretical emission lines for CX-induced X-ray emission, assuming an optically thin plasma, following the approach of Rigazio et al. (2002). In this paper, we compare such theoretical spectra for Fe XXV and Fe XXVI, which utilize the MCLZ \( nS \)-resolved cross sections, to the experimental spectra obtained with the electron-beam ion trap (EBIT) experiment of Wargelin et al. (2005, 2007).

2.4. Quantum Defect Theory

It is essential to consider all possible final channels of a given collision system and to have detailed knowledge of their excitation energies in order to properly identify locations of
avoided crossings, and ultimately, the probability relations of Janev et al. (1983). Therefore, excitation energies are gathered in order to determine the $\Delta E_\infty$ values pertinent in the estimates of avoided crossings. However, the main source for these excitation energies, the NIST Atomic Spectra Database (Kramida et al. 2014), is often missing states—especially high-lying Rydberg levels. Therefore, we have employed quantum defect theory, which basically modifies the Rydberg formula through an introduced quantum defect, $\mu$. In an effort to approximate excitation energies for all states that must be considered for CX to create He-like Fe$^{24+}$, we have devised a strategy to establish trends in quantum defect parameters. With these trends, quantum defect theory estimates energy levels via the modified Rydberg formula (see, for example, Connerade 1998), Equation (13), where the parameters of the calculation are the following: ionization potential ($E_0$), $n$-level, $\ell$-level, and $\mu_\ell$. Here, $\mu_\ell$ also depends on the parameter $\delta$, resulting in the relations

$$E_{n\ell} = E_0 \left(1 - \frac{1}{n^2}\right),$$

(13)

where

$$n^\delta = n - \mu_\ell,$$

(14)

and

$$\mu_\ell = \ell + \frac{1}{2} - \left[(\ell + 1) + 2 + \delta\right].$$

(15)

The strategy employed in estimating the unknown energy levels is by finding trends in the parameter $\delta$ from available data. We apply these trends to high-lying Rydberg levels to estimate $\delta$ and ultimately $E_{n\ell}$.

3. RESULTS AND DISCUSSION

Until this point, we have generalized the method to compute the CX cross sections and resulting X-ray spectra for a given CX collision system. Now, we will display the results in applying this methodology to the two exemplary cases of Fe$^{25+}$ and Fe$^{26+}$ CX collisions. These CX calculations were chosen for three reasons. First, the high charge of the Fe$^{25+}$ and Fe$^{26+}$ systems (i.e., $q = 25$ and $q = 26$, respectively) presents computational difficulties as more final channels (final product ion states) must be considered for the collision system. The dominant $n$-capture channel is given approximately by $n_{\text{max}} \sim q^{0.75}$, within each $n$ level, the number of $\ell$ levels is equivalent to $n$. Because MCLZ calculations typically include all product ion states from $n = 1$ to $n_{\text{max}} + 3$, the total number of channels roughly scales as $\sim n^2$ or increases with charge as $\sim q^{1.5}$. This results in the expression for the CX probability becoming much more complicated, as seen in the probability relations of Janev et al. (1983), and ultimately stress-tests the MCLZ code. Such a calculation using a more advanced method (e.g., QMOCC) would require more than 100 molecular channels and thousands of nonadiabatic coupling elements; such a calculation is not currently feasible. Second, the presence of experimental X-ray emission data for these systems made these collisions an attractive option because it presents an opportunity to compare theoretical spectra with experiment. Finally, the astrophysical relevance of Fe XXV and Fe XXVI emission in the Galactic center and ridge (Tanaka et al. 1999; Muno et al. 2004) makes these calculations useful for astrophysical modelers of these regions because CX may be a dominant process.

Therefore, it is with this motivation that total, $n$-resolved, $\ell$-resolved, and $S$-resolved cross sections were calculated for Fe$^{25+}$ and Fe$^{26+}$ collisions with H, He, H$_2$, N$_2$, H$_2$O, and CO.

3.1. Fe XXVI

To begin studying Fe$^{26+}$ bare-ion collisions, Wigner–Witmer rules are applied to determine possible product channels for the collision. These rules, based on principles of conservation of electronic angular momentum, indicate that the initial channel for Fe$^{25+}$ colliding with H is a $5\Sigma^+$ state, while for all other targets it is a $3\Sigma^+$ state. All product Fe$^{25+}$ ions are doublets with a total electron spin $S = 1/2$ (which we drop in the notation for Fe XXVI). With this information we perform Landau–Zener approximations to obtain total, $n$-resolved, and $n\ell$-resolved cross sections. First, we examine the total cross sections for the collision systems of Fe$^{25+}$ with various targets in Figure 1. One of these collision systems alone would take a several months of CPU time to calculate with more complex theories such as QMOCC—and at only one collision energy. Because of this effective Landau–Zener technique, total cross sections for Fe$^{26+}$ collisions with H, He, H$_2$, N$_2$, H$_2$O, and CO—for collision energies from 0.001 to 100 keV/u—are computed and quickly show an interesting trend, that with increasing ionization potential of the target, we see decreasing total cross sections for collision energies $\geq 10$ eV/u.

In addition to total cross sections, we can also investigate $n$-resolved cross sections. As shown in Figure 2, MCLZ calculations show that the electron capture into $n = 12, 13,$ and 14 generates the largest cross sections for Fe$^{26+}$ collisions with N$_2$ for energies applicable for the EBIT experiment, $\sim 10$ eV/u. For systems of more astrophysical relevance, such as collisions with H and He at energies around 1 keV/u, Figures 3 and 4 show that dominant capture is into $n = 11–14$ and 9–11, respectively.

\footnote{For molecular targets we consider only linear geometries and do not resolve the rotational or vibrational motion of the initial neutral or product molecular ion.}
These dominant capture results are in good agreement with the EBIT study of Wargelin et al. (2007). For instance, Wargelin et al. (2007) states that classical trajectory Monte Carlo (CTMC) calculations predict $n_{\text{max}}$ for SEC between Fe$^{26+}$ and He to be $n = 9$, whereas their experiment observed $n = 11$ and 12. As shown in the MCLZ calculations in Figure 4, around $\sim 10$ eV/u, $n_{\text{max}}$ = 11 and 12; thus, MCLZ theoretical results are in excellent agreement with experiment. Further, observed $n_{\text{max}}$ values from the EBIT study for Fe$^{26+}$ collisions with N$_2$ and H$_2$ are $n = 14$. MCLZ calculations again agree with experiment, as shown in Figures 2 and 5, respectively, with $n_{\text{max}}$ predicted to be 13 or 14.

CTMC calculations have been previously performed for several Fe$^{26+}$ CX collisions in Katsonis et al. (1991) and Schultz et al. (1991). As shown in Figure 3, total CTMC SEC cross sections are in excellent agreement with MCLZ total cross sections for Fe$^{26+}$ collisions with H. Similarly, in Figures 4 and 5, CTMC results are compared to MCLZ for Fe$^{26+}$ collisions with He and H$_2$, respectively. For both of these collisions, MCLZ predicts somewhat larger total cross sections than does CTMC. It is expected that the CTMC method will not be reliable for collision energies $\gtrsim 10$ keV/u due to the neglect of tunneling effects, while MCLZ calculations do not perform well for incident energies $\lesssim 5$ keV/u (Wu et al. 2011). An $nl$-resolved cross section analysis is performed in Figure 6 to compare the various $\ell$-distribution models. It is worth noting that the distributions depicted in Figure 6 apply to all Fe$^{26+}$ CX collisions with no restriction on collision energy or target. This universality is a downfall of the distribution models because they are independent of any parameters corresponding to these important factors. We see variance in each $\ell$-distribution model; therefore, it is difficult to suggest which model is recommended until these various distributions are applied to the cascade model for X-ray emission and theoretical spectra are compared with experimental data. Therefore, by applying the various $nl$-resolved cross sections to populate atomic levels, theoretical spectra are obtained and displayed in Figure 7 for Fe$^{26+}$ and N$_2$ CX collisions. In the same figure, the experimental spectrum for the system is given as extracted from the EBIT experiment (Wargelin et al. 2005).
states, but Figure 6 indicates that the low-energy distribution peaks at $\ell = 2$. All other distributions peak at even larger values of $\ell$. We postulate that, in order to get agreement with the EBIT high-$n$ emission peak, the cross sections to $p$-states should be enhanced. As a numerical experiment, we constructed an ad hoc $\ell$-distribution function $W_{\ell}^{\text{Low}}$ in which $\ell' = \ell - 1$. $W_{n,\ell=0}^{\text{Low}}$ is added to $W_{n,\ell=1}^{\text{Low}}$ to preserve the normalization, and $W_{n,\ell=n-1}^{\text{Low}} = 0$. We refer to this as the shifted low-energy (SL1) distribution. Applying SL1 in the cascade/X-ray model gives the SL1 spectrum at 10 eV/u, which is shown in Figure 7 to be in better agreement with the EBIT result. SL1 does underestimate Ly$\beta$ and Ly$\gamma$, but further manipulation of the distribution function is not warranted given the uncertainties in the experimental spectra.

Rather than presenting the spectra for all of the collision systems studied, Table 1 gives line ratios for X-ray emission resulting from SEC collisions between Fe$^{25+}$ and H, He, H$_2$, N$_2$, H$_2$O, and CO at three representative collision energies of 10, 100, and 1000 eV/u. These line ratios were obtained by applying the low-energy distribution (Equation 10) to MCLZ n-resolved cross sections and implementing the results in the X-ray cascade model. The line ratio denotes the ratio between a specific emission line and the Ly$\alpha$ line.

### 3.2. Fe $XXV$

As was discussed for Fe $XXVI$, product ion states must first be determined for the He-like Fe$^{24+}$, which is produced following CX with Fe$^{25+}$. As determined by Wigner–Witmer rules, Fe$^{25+}$ collisions with H correlate to two molecular manifolds, $1^3\Sigma^+$ and $3^2\Sigma^+$, which connect via radial couplings to molecular states of the same symmetry of the asymptotic product states of Fe$^{24+}$ + H$. As spin-changing collisions are forbidden, singlet and triplet MCLZ calculations are performed separately with the singlet cross sections weighted by a factor of 1/4, while the triplets are weighted by a factor of 3/4. In contrast, collisions with helium, molecular hydrogen, molecular nitrogen, water, and carbon monoxide correlate to doublet molecular states with both Fe$^{24+}$ singlet and triplet states considered in a single MCLZ calculation. Because both singlets and triplets must be considered, quantum defect theory is applied to estimate energies for all missing states of Fe$^{24+}$. All Fe$^{24+}$ singlet states and their corresponding energies, as calculated by our implementation of quantum defect theory, are shown in Figure 8 and compared to available NIST data as well as energies estimated by the Cloudy spectral synthesis code (Ferland et al. 2013), which also implements a version of the quantum defect method. Including all possible outgoing channels quickly makes the computation time significantly longer.

In comparing the total cross sections for Fe $XXV$ collisions for multiple targets, we again see the interesting trend that with increasing ionization potential of the target, the total cross section decreases for collision energies $\geq 10$ eV/u as shown in Figure 9.

Cross sections at the $n$-resolved level for each collision system are also computed. In Figure 10, we display the $n$-resolved cross sections for Fe$^{25+}$ collisions with N$_2$. Around $\sim 10$ eV/u, we which we again anticipate being representative of EBIT conditions, we see that dominant capture occurs into $n = 12$–14. Again, we illustrate that dominant capture occurs into states for which energies are not supplied by NIST. Thus,

![Figure 6](image-url)

**Figure 6.** Analytical $\ell$-distribution functions $W_{\ell}$ for bare-ion collisions for $q_1 = 26$.

![Figure 7](image-url)

**Figure 7.** Comparison of the theoretical MCLZ/cascade model spectrum to the experimental spectrum of Wargelin et al. (2005) for Fe$^{26+}$ collisions with N$_2$. All spectra are normalized to Ly$\alpha$, and the MCLZ cross sections used the low-energy $\ell$-distribution or shifted low-energy (SL1) distribution functions. A FWHM of 150 eV was assumed for the theoretical spectra. See the text for details.
| Photon Energy (eV) | Neutral Line | Intensity |
|-------------------|--------------|-----------|
|                   |              | 10 eV/u   | 100 eV/u | 1 keV/u |
|                   |              | (43.8 km s$^{-1}$) | (138 km s$^{-1}$) | (438 km s$^{-1}$) |
| 6958              | H Lyα        | 1.0000    | 1.0000   | 1.0000   |
| 8247              | H Lyβ        | 0.1646    | 0.1693   | 0.1756   |
| 8698              | H Lyγ        | 0.0289    | 0.0607   | 0.0642   |
| 8907              | H Lyδ        | 0.0172    | 0.0304   | 0.0325   |
| 9020              | H Lyε        | 0.0114    | 0.0181   | 0.0196   |
| 9088              | H Lyζ        | 0.0583    | 0.0121   | 0.0132   |
| 9133              | H Lyη        | 0.0090    | 0.0094   | 0.0099   |
| 9163              | H Lyθ        | 0.0017    | 0.0025   | 0.0062   |
| 9185              | H Lyκ        | 0.0413    | 0.0444   | 0.0442   |
| 9201              | H Lyν        | 0.0050    | 0.0086   | 0.0060   |
| 9213              | H Lyλ        | 0.0051    | 0.0501   | 0.0875   |
| 9223              | H Lyμ        | 0.0569    | 0.1006   | 0.0806   |
| 9230              | H Lyν        | 0.1217    | 0.0728   | 0.0398   |
| 9236              | H Lyζ        | 0.0514    | 0.0219   | 0.0104   |
| 6958              | He Lyα       | 1.0000    | 1.0000   | 1.0000   |
| 8247              | He Lyβ       | 0.1884    | 0.1955   | 0.2030   |
| 8698              | He Lyγ       | 0.0714    | 0.0756   | 0.0801   |
| 8907              | He Lyδ       | 0.0370    | 0.0397   | 0.0427   |
| 9020              | He Lyε       | 0.0227    | 0.0247   | 0.0270   |
| 9088              | He Lyζ       | 0.0155    | 0.0170   | 0.0213   |
| 9133              | He Lyη       | 0.0108    | 0.0128   | 0.0372   |
| 9163              | He Lyθ       | 0.0153    | 0.0388   | 0.1026   |
| 9185              | He Lyι       | 0.0439    | 0.1335   | 0.0140   |
| 9201              | He Lyκ       | 0.1721    | 0.1378   | 0.0826   |
| 9213              | He Lyλ       | 0.0973    | 0.0387   | 0.0181   |
| 9223              | He Lyμ       | 0.0085    | 0.0030   | 0.0013   |
| 9230              | He Lyν       | 0.0002    | 5.2E-5   | 2.2E-5   |
| 9236              | He Lyζ       | 2.5E-7    | 8.5E-8   | 3.6E-8   |
| 6958              | H Lyα        | 1.0000    | 1.0000   | 1.0000   |
| 8247              | H Lyβ        | 0.1680    | 0.1744   | 0.1816   |
| 8698              | H Lyγ        | 0.0600    | 0.0635   | 0.0676   |
| 8907              | H Lyδ        | 0.0299    | 0.0321   | 0.0346   |
| 9020              | H Lyε        | 0.0178    | 0.0193   | 0.0211   |
| 9088              | H Lyζ        | 0.0118    | 0.0129   | 0.0143   |
| 9133              | H Lyη        | 0.0093    | 0.0098   | 0.0108   |
| 9163              | H Lyθ        | 0.0019    | 0.0047   | 0.0129   |
| 9185              | H Lyι        | 0.0473    | 0.0415   | 0.0558   |
| 9201              | H Lyκ       | 0.0044    | 0.0309   | 0.0804   |
| 9213              | H Lyλ       | 0.0292    | 0.0963   | 0.0971   |
| 9223              | H Lyμ       | 0.1137    | 0.0954   | 0.0586   |
| 9230              | H Lyν       | 0.0855    | 0.0385   | 0.0186   |
| 9236              | H Lyζ       | 0.0173    | 0.0066   | 0.0029   |
| 6958              | N2 Lyα-Low   | 1.0000    | 1.0000   | 1.0000   |
| 8247              | N2 Lyβ-Low   | 0.1688    | 0.1760   | 0.1840   |
| 8698              | N2 Lyγ-Low   | 0.0604    | 0.0644   | 0.0690   |
| 8907              | N2 Lyδ-Low   | 0.0302    | 0.0326   | 0.0355   |
| 9020              | N2 Lyε-Low   | 0.0180    | 0.0197   | 0.0218   |
| 9088              | N2 Lyζ-Low   | 0.0119    | 0.0132   | 0.0151   |
| 9133              | N2 Lyη-Low   | 0.0093    | 0.0099   | 0.0129   |
| 9163              | N2 Lyθ-Low   | 0.0021    | 0.0058   | 0.0207   |
| 9185              | N2 Lyι-Low   | 0.0471    | 0.0418   | 0.0657   |
| 9201              | N2 Lyκ-Low   | 0.0054    | 0.0439   | 0.0842   |
| 9213              | N2 Lyλ-Low   | 0.0390    | 0.0996   | 0.0890   |
| 9223              | N2 Lyμ-Low   | 0.1171    | 0.0866   | 0.0511   |
| 9230              | N2 Lyν-Low   | 0.0763    | 0.0333   | 0.0159   |
| 9236              | N2 Lyζ-Low   | 0.0149    | 0.0056   | 0.0025   |
| 6958              | N2 Lyα-SL1   | 1.0000    | 1.0000   | 1.0000   |
| 8247              | N2 Lyβ-SL1   | 0.2248    | 0.2371   | 0.2515   |
| 8698              | N2 Lyγ-SL1   | 0.0955    | 0.1037   | 0.1136   |
| 8907              | N2 Lyδ-SL1   | 0.0532    | 0.0589   | 0.0660   |
we see that, through the quantum defect method, we can rapidly estimate the energies of these high-lying Rydberg states that assume vital roles in the Fe$^{25+}$ CX process. For astrophysical conditions $\sim 1$ keV/u, Figures 11 and 12 display $n$-resolved cross sections for Fe$^{25+}$ collisions with H and He, respectively. Dominant capture for these processes occurs into $n = 11-14$ and $9-11$, respectively.

CX collisions with H-like projectile ions result in non-degenerate product ions. Thus, the use of $\ell$-distribution functions is neither required nor recommended. However, it is commonplace for astrophysical modelers to incorporate such distribution functions for all CX collisions—even those with multielectron product ions—due to the general lack of such data (Smith et al. 2014). Therefore, in Figure 13, we compare the results from $n\ell S$-resolved cross sections via MCLZ to $n\ell$-resolved distribution functions for Fe$^{25+}$ collisions with N$_2$.

In this figure, the three dominant $n$-levels for the collision are shown at three different energies. After comparing the distributions, we see that the low-energy distribution function compares best to the explicit MCLZ calculations. When performing similar analyses of the distributions resulting from Fe$^{25+}$ CX collisions with H, He, H$_2$, H$_2$O, and CO, some of the distributions tend toward the low-energy modification function or the separable function. However, again, although it is not recommended, if one does use a distribution function for non-bare projectile ion CX collisions, we suggest using the low-energy distribution function, as given by Equation (10), in most cases.

Using the cascade model and $n\ell S$-resolved cross sections, we obtain theoretical X-ray spectra as given by Figure 14 for Fe$^{25+}$ collisions with N$_2$ with a FWHM of 150 eV. These theoretical spectra are shown alongside the Fe $\text{xxv}$ EBIT experiment.
Wargelin et al. (2005). We see reasonable agreement between theoretical and experimental spectra; however, all theoretical models overestimate the experimental intensity of the Kβ and higher lines, with the overestimation increasing slightly with collision energy. As the Kβ and higher lines originate only from Fe24+ singlet states, the comparison suggests that the MCLZ calculation predicts cross sections to nP1 with n ∼ 12–14 that are somewhat too large.

Again, we include line ratios for the various Fe25+ collision systems. MCLZ nS-resolved cross sections were applied in the X-ray cascade model to obtain these ratios. Table 2 gives the line ratios for X-ray emission resulting from SEC collisions between Fe25+ and H, He, H2, N2, H2O, and CO at the same representative collision energies as used in Table 1. Here, the line ratios denote the ratio between a specific emission line and the Kα resonant line.

Another useful diagnostic is the G-ratio, which is the ratio of the sum of the intensities of the forbidden and intercombination lines to that of the resonant line (Porter & Ferland 2007; Porquet et al. 2010; Foster et al. 2012). Figure 15 displays the G-ratios as a function of collision energy for emission resulting from the studied Fe25+ SEC processes. Also included in Figure 15 are the G-ratio results presented in Foster et al.
pertaining to electron impact excitation (EIE, or so-called thermal excitation) for a plasma in collisional ionization equilibrium (CIE), as well as the G-ratio for photoionization equilibrium (PIE) or a recombining photoionized plasma (Bautista & Kallman 2000; Porter & Ferland 2007). MCLZ CX cross sections and their implementation in the X-ray cascade model yield similar G ~ 0.8 among He, H₂, N₂, H₂O, and CO targets with only a slight increase with collision energy. These fall near the maximum EIE G-ratio, which occurs for electron temperatures of ∼10⁷ K (Foster et al. 2012). Conversely, the G-ratio for Fe²⁵⁺ and H CX is ∼3.7, similar to the values obtained for a recombining plasma (PIE) with an electron temperature of 10⁷ K (Bautista & Kallman 2000; Porter & Ferland 2007).

Unfortunately, the resolution of the EBIT measurement was insufficient to resolve the individual Kα components to determine a G-ratio. However, it is possible to estimate the G-ratio from knowledge of the Kα line centroid. For Fe²⁵⁺ collisions with N₂ at 10, 100, and 1000 eV/u, the centroids using the MCLZ cross sections are predicted to be 6686.3, 6685.3, and 6684.0 eV, respectively. These can be compared to the measured values for CX, 6666 ± 5 eV (EBIT beam off), and EIE, 6685 ± 2.5 eV (EBIT beam on) (Wargelin et al. 2005). From the experimental centroid, we estimate G = 1.2–2.65, depending on the assumed relative intensities of forbidden and intercombination lines. This is somewhat larger than the computed G-ratios from the MCLZ calculations of 0.82, 0.92, and 1.05 for 10, 100, and 1000 eV/u, respectively.
Table 2
Normalized Line Ratios for Fe xxv for Charge Exchange X-Ray Emission

| Photon Energy (eV) | Neutral Line | Intensity |
|-------------------|--------------|-----------|
|                   |              | 10 eV/u   | 100 eV/u | 1 keV/u |
|                   |              | (43.8 km s\(^{-1}\)) | (138 km s\(^{-1}\)) | (438 km s\(^{-1}\)) |
| 6637              | H Kα f       | 0.50760   | 0.57366  | 0.65399 |
| 6676              | H Kα i       | 3.17116   | 3.19627  | 3.23542 |
| 6700              | H Kα τ       | 1.00000   | 1.00000  | 1.00000 |
| 7881              | H Kβ         | 0.17851   | 0.19549  | 0.21538 |
| 8296              | H Kγ         | 0.06863   | 0.07711  | 0.08720 |
| 8487              | H Kδ         | 0.03492   | 0.03965  | 0.04536 |
| 8591              | H Kε         | 0.02053   | 0.02345  | 0.02700 |
| 8653              | H Kζ         | 0.01358   | 0.01557  | 0.01803 |
| 8694              | H Kη         | 0.00964   | 0.01110  | 0.01292 |
| 8722              | H Kθ         | 0.00722   | 0.00835  | 0.00993 |
| 8742              | H Kι         | 0.00565   | 0.00656  | 0.01133 |
| 8757              | H Kλ         | 0.00458   | 0.00636  | 0.03785 |
| 8787              | H Kµ         | 0.05162   | 0.09783  | 0.08323 |
| 8774              | H Kν         | 0.09310   | 0.06116  | 0.03303 |
| 8790              | H Kξ         | 0.03029   | 0.01401  | 0.00640 |
| 6637              | He Kα f      | 0.14153   | 0.16738  | 0.20431 |
| 6676              | He Kα i      | 0.64585   | 0.72242  | 0.81582 |
| 6700              | He Kα τ      | 1.00000   | 1.00000  | 1.00000 |
| 7881              | He Kβ        | 0.20136   | 0.22302  | 0.24269 |
| 8296              | He Kγ        | 0.07725   | 0.08848  | 0.09933 |
| 8487              | He Kδ        | 0.03880   | 0.04517  | 0.05164 |
| 8591              | He Kε        | 0.02258   | 0.02654  | 0.03072 |
| 8653              | He Kζ        | 0.01486   | 0.01758  | 0.02063 |
| 8694              | He Kη        | 0.01055   | 0.01254  | 0.01854 |
| 8722              | He Kθ        | 0.00792   | 0.01160  | 0.06140 |
| 8742              | He Kι        | 0.01271   | 0.08175  | 0.14309 |
| 8757              | He Kλ        | 0.12915   | 0.13032  | 0.08885 |
| 8787              | He Kµ        | 0.05882   | 0.02949  | 0.02449 |
| 8774              | He Kν        | 0.00177   | 0.00078  | 0.00036 |
| 6637              | H2 Kα f      | 0.12842   | 0.15124  | 0.18180 |
| 6676              | H2 Kα i      | 0.66993   | 0.74032  | 0.82185 |
| 6700              | H2 Kα τ      | 1.00000   | 1.00000  | 1.00000 |
| 7881              | H2 Kβ        | 0.18355   | 0.20067  | 0.22028 |
| 8296              | H2 Kγ        | 0.06988   | 0.07857  | 0.08873 |
| 8487              | H2 Kδ        | 0.03505   | 0.03992  | 0.04572 |
| 8591              | H2 Kε        | 0.02035   | 0.02335  | 0.02699 |
| 8653              | H2 Kζ        | 0.01332   | 0.01536  | 0.01789 |
| 8694              | H2 Kη        | 0.00938   | 0.01087  | 0.01274 |
| 8722              | H2 Kθ        | 0.00698   | 0.00813  | 0.00973 |
| 8742              | H2 Kι        | 0.00543   | 0.00635  | 0.01035 |
| 8757              | H2 Kλ        | 0.07156   | 0.09828  | 0.05238 |
| 8787              | H2 Kµ        | 0.09921   | 0.06030  | 0.10122 |
| 8774              | H2 Kν        | 0.08392   | 0.09491  | 0.06742 |
| 8790              | H2 Kξ        | 0.06273   | 0.03467  | 0.01756 |
| 6637              | N2 Kα f      | 0.13302   | 0.15832  | 0.19328 |
| 6676              | N2 Kα i      | 0.68604   | 0.76220  | 0.85266 |
| 6700              | N2 Kα τ      | 1.00000   | 1.00000  | 1.00000 |
| 7881              | N2 Kβ        | 0.18756   | 0.20578  | 0.22713 |
| 8296              | N2 Kγ        | 0.07190   | 0.08120  | 0.09236 |
| 8487              | N2 Kδ        | 0.03617   | 0.04140  | 0.04783 |
| 8591              | N2 Kε        | 0.02104   | 0.02427  | 0.02832 |
| 8653              | N2 Kζ        | 0.01378   | 0.01599  | 0.01882 |
| 8694              | N2 Kη        | 0.00971   | 0.01133  | 0.01343 |
| 8722              | N2 Kθ        | 0.00723   | 0.00848  | 0.01167 |
| 8742              | N2 Kι        | 0.00563   | 0.00673  | 0.02290 |
| 8757              | N2 Kλ        | 0.00455   | 0.01457  | 0.06817 |
| 8768              | N2 Kµ        | 0.01584   | 0.07397  | 0.10060 |
| 8777              | N2 Kν        | 0.09111   | 0.09026  | 0.06079 |
| 8784              | N2 Kξ        | 0.05685   | 0.03048  | 0.01531 |
4. TOTAL FEXV AND FEXVI SPECTRA

The total theoretical spectrum, the sum of Fe xxv and xxvi, is compared to the total EBIT experimental spectrum in Figure 16. This total theoretical spectrum utilizes the shifted low-energy (SL1) distribution as discussed for Fe25+ collisions with N2 and the nS-resolved cross sections for Fe25+ collisions with N2. By summing the two theoretical spectra and eliminating any need for extraction of the associated product ion’s contribution to the emission, we see excellent agreement between theory and experiment. Figure 17 compiles all theoretical total and individual spectra with corresponding emission lines and the total experimental spectra with associated FeXXV and extracted Fe XXVI from Wargelin et al. (2005). From this figure, we can see each ion’s contribution, theoretically and experimentally, to the overall spectra and the very good agreement overall for this system of two highly charged ions.

5. CAVEATS

A number of approximations were required in both the calculations of cross sections and the models of X-ray spectra. They are of such a magnitude that it is not meaningful to
spectra from Wargelin et al. result in the Fe XXVI components with corresponding emission lines, and total experimental avoided crossings (approximations are inherent in the current MCLZ calculations: attempt to estimate the theoretical uncertainty. Six main approximations are inherent in the current MCLZ calculations: (i) the splitting in the adiabatic potentials at the locations of avoided crossings (Equation (4)); (ii) the adoption of the SEC MCLZ probability formalism of Janev et al. (1983); (iii) for H-like product ions, the adoption of an \( \ell \)-distribution model; (iv) for He-like product ions, the estimation of missing Rydberg energies with the quantum defect approach; (v) the neglect of multielectron capture (MEC) processes; and (vi) the applicability of MCLZ calculations in the high-energy regime. Of these, it is likely that item (i) has the largest impact on all state-resolved cross sections. For the case of the multichannel probability model (ii), only long-range avoided crossings are considered. The model of Janev et al. (1983) cannot treat short-range avoided crossings, which are usually highly endoergic. As a consequence, the cross sections for the highest \( n \), those which fall off as \( E^{-1/2} \) for all energies, will be lower limits for the highest collision energies. MEC processes (v) also cannot be treated with the SEC MCLZ probability model. There exists no analytic MEC formula valid for all ions—each CX collision system must be treated individually and therefore such calculations are not amenable to our streamlined program set. However, Wargelin et al. (2005) argue that MEC processes do not play a significant role in the Fe\(^{25+}\) and Fe\(^{26+}\) systems. On the other hand, in a combined experimental/theoretical study of Ne\(^{10+}\) collisions with He, Ne, and Ar, Ali et al. (2005) find that MEC could contribute from \( \sim 10\% \)–\( 50\% \) of the X-ray spectrum, with the fraction increasing with the number of electrons in the target. Finally, the performance of the multichannel calculations in a molecular representation, such as the MCLZ method, was suggested by Wu et al. (2011) to break down for incident energies \( \gtrsim 5 \) keV/u. At such high incident energies, other channels (ionization, excitation, dissociation) become important and eventually dominant. This leads to the interpretation that MCLZ CX cross sections are upper limits in the high-energy regime. MCLZ calculations are compared to CTMC data (more applicable at higher collision energies) in Figures 3–5 and show good agreement, thus meriting their use as a base approximation for such high collision energies.

In the cascade/X-ray emission models, we have assumed a low-density plasma environment in which only single-collision events occur and the plasma is optically thin. Optical depth effects and/or multiple collisions may become important, thus modifying the predicted line ratios in high-density environments. In addition, as detailed above, the cross sections were only computed for SEC, so no MEC effects are included in the X-ray spectra or line ratios.

6. CONCLUSIONS

Fe\(^{25+}\) and Fe\(^{26+}\) CX collisions with multiple targets were studied because of their astrophysical relevance in the Galactic center, the Galactic ridge, and other environments; the computational difficulty that such highly charged systems entailed, and the presence of experimental data for comparison. Theoretical studies using quantum defect theory and the MCLZ approach were able to compute, with ease, \( n\ell S \)-resolved cross sections for Fe\(^{25+}\) and Fe\(^{26+}\) collisions with H, He, H\(_2\), N\(_2\), H\(_2\)O, and CO. This is the first time, to our knowledge, that MCLZ calculations have been performed for these systems. Further, to our knowledge, this is the first time that such calculations have been performed altogether for Fe\(^{25+}\) collisions with N\(_2\), H\(_2\)O, and CO and Fe\(^{26+}\) collisions with all targets considered in this work. With these new data and approach, comparisons of total Fe XXV and Fe XXVI theoretical spectra to total experimental EBIT spectra demonstrate very good agreement. Through the simplicity of the MCLZ method, these data were generated quickly and robustly, thus allowing interesting trends to be identified. Namely, with increasing ionization potential of the target, we see decreasing total cross sections for collision energies \( \gtrsim 10 \) eV/u. Further, several \( \ell \)-distribution models have been tested for Fe\(^{25+}\) and Fe\(^{26+}\) SEC. Such analysis suggests that commonly used \( \ell \)-distribution models struggle to accurately reflect the true distribution of electron capture as understood by more advanced frameworks of theory. However, if there is no other recourse, then the so-called low-energy distribution function is preferred. Ultimately, we have shown through extensive theoretical studies, agreement between theory and experiment, and the complexity of the Fe XXV and Fe XXVI systems that the quantum defect/MCLZ approach is an excellent tool to quickly provide accurate CX data, for any system, to experimentalists, astrophysical modelers, and astronomers and to aid in bringing resolution to the current lack of atomic and molecular data for such a vital process.
This work was partially supported by NASA grants NNX09AC46G and NNX13AF31G. We thank Brad Wargelin for providing the experimental EBIT spectra and for helpful discussions.

REFERENCES

Ali, R., Neill, P. A., Beiersdorfer, P., et al. 2005, ApJL, 629, L125
Bautista, M. A., & Kallman, T. R. 2000, ApJ, 544, 581
Bhardwaj, A., Elsner, R. F., Gladstone, G. R., et al. 2007, P&SS, 55, 1135
Butler, S. E., & Dalgarno, A. 1980, ApJ, 241, 838
Connerade, J. P. 1998, Highly Excited Ions (Cambridge: Cambridge Univ. Press)
Cravens, T. E. 2000, ApJL, 532, L153
Cumbee, R. S., Henley, D. B., Stancil, P. C., et al. 2014, ApJL, 787, L31
Ferland, G. J., Porter, R. L., van Hoof, P. A. M., et al. 2013, RMxAA, 49, 137
Flower, D. R. 1990, Molecular Collisions in the Interstellar Medium (Cambridge: Cambridge Univ. Press)
Foster, A. R., Smith, R. K., & Brickhouse, N. S. 2012, ApJ, 756, 128
Herzberg, G. 1950, Spectra of Diatomic Molecules (2nd ed.; New York: Van Nostrand-Reinhold)
Janev, R. K., Belić, D. S., & Bransden, B. H. 1983, PhRvA, 28, 3
Katsuda, S., Tsunemi, H., Mori, K., et al. 2011, ApJ, 730, 24
Kramida, A., Ralchenko, Yu., Reader, J. & NIST ASD Team 2014, NIST Atomic Spectra Database (ver. 5.2), [Online].Available: http://physics.nist.gov/asdD [2015, June 10]. National Institute of Standards and Technology, Gaithersburg, MD
Krasnopolsky, V. A., Greenwood, J. B., & Stancil, P. C. 2004, SSRv, 113, 271
Lisse, C. M., Dennerl, K., Englhauser, J., et al. 1996, Sci, 274, 205
Muno, M. P., et al. 2004, ApJ, 613, 326
Olson, R. E., & Salop, A. 1976, PhRvA, 13, 1312
Olson, R. E., Smith, F. T., & Bauer, E. 1971, ApOpt, 10, 1848
Porquet, D., Dubau, J., & Grosso, N. 2010, SSRv, 157, 103
Porter, R. L., & Ferland, G. J. 2007, ApJ, 664, 586
Rigazio, M., Kharchenko, V., & Dalgarno, A. 2002, PhRvA, 66, 064701
Schultz, D. R., Meng, L., Reinhold, C. O., & Olson, R. E. 1991, PhSyS, T37, 89
Smith, R. K., Foster, A. R., Edgar, R. J., & Brickhouse, N. S. 2014, ApJ, 787, 77
Tanaka, Y., Miyaji, T., & Hassinger, G. 1999, AN, 320, 181
Taulbjerg, K. 1986, JPhB, 19, L367
Wargelin, B. J., Beiersdorfer, P., & Brown, G. V. 2007, CaJPh, 86, 151
Wargelin, B. J., Beiersdorfer, P., Neill, P. A., Olson, R. E., & Scofield, J. H. 2005, ApJ, 643, 687
Wigner, E., & Witmer, E. 1928, ZPhy, 51, 859
Wu, Y., Stancil, P. C., Liebermann, H. P., et al. 2011, PhRvA, 84, 022711