The Kronos Database of State-Selective Charge Exchange Cross Sections

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Charge Exchange Observations

**LINEAR C/1999 S4**

![Graph showing X-ray energy vs. intensity with various ion species labeled.]

*From Beiersdorfer et al. (2003).*

**LINEAR C/2000 WM1**

![Graph showing wavelength vs. count rate with spectral lines labeled.]

*From Mullen et al., in Prep.*
Charge Exchange Process

\[ X^{q^+} + Y \rightarrow X^{q-1}(nl \ 2S+1L) + Y^+ \]

- Produces highly excited, high charged state ions \( X^{q-1}(nl \ 2S+1L) \)
  - Cascade to lowest energy
  - Produces X-rays

Single electron capture

True double capture

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CX & Thermal Emission

- X-ray emission from charge exchange produces a very distinct spectrum compared to thermal emission.
- With high resolution spectra, it is plausible to disentangle CX from thermal emission!

\[ \text{Ne}^{10+} + H \rightarrow \text{Ne}^{9+} + H^+ \]

\[ O^{7+} + H \rightarrow O^{6+} + H^+ \]
CX X-ray Emission Line Ratios (Spectra)

- Two steps are required to produce a CX X-ray emission spectrum:
  - 1) Calculate cross-sections
    - $\sigma_{nl(S)}(v)$
      - Highly dependent on ion, neutral target, and velocity
    - Not simple
  - 2) Radiative cascade
    - Transition probabilities (Einstein A Coefficients)
    - Transition Energies
    - More Simple (FAC, AUTOSTRUCTURE, etc)
The probability of an electron to transfer from the neutral atom into a specific excited state \((n, l, S)\) of the ion.

For charge exchange calculations:
- \(\sigma\) depends on the
  - \(n\) (principle quantum number)
  - \(l\) (orbital angular momentum quantum number)
  - \(S\) (spin quantum number, He-like)
  - \(v\) (collision velocity)
- \(\sigma_{nls}(v)\) is required to produce reliable theoretical CX X-ray emission spectra

"Effective area" that quantifies the likelihood of a scattering event to occur
Recommended Cross-sections for the n=6 quantum levels

- Multi-channel Landau-Zener
  - Statistical l-distribution
  - Low energy l-distribution
- Classical Trajectory Monte Carlo
- Atomic Orbital Close Coupling
- Quantum Mechanical Molecular orbital Close Coupling
- All available cross-sections for H-like and He-like CX collisions are implemented in Kronos Database

Ne\textsuperscript{10+} + H → Ne\textsuperscript{9+} + H\textsuperscript{+}

Cumbee et al. 2016

Cross Sections (10\textsuperscript{-16} cm\textsuperscript{2})

Accuracy & difficulty

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CX as a diagnostic

- CX is highly dependent on:
  - Ion stage (O\(^{8+}\), O\(^{7+}\))
  - Neutral target (H, He, CO\(_2\))
  - Velocity of the collision

![Graph showing relative intensity vs. photon energy for various elements and collision energies, with peaks at Ly \(\alpha\), Ly \(\beta\), Ly \(\gamma\), and Ly \(\delta\).]

1000 eV/u collision energy
MCLZ method, 10 eV FWHM
CX as a diagnostic

CX is highly dependent on:
- Ion stage (O^{8+}, O^{7+})
- Neutral target (H, He, CO_{2})
- Velocity of the collision
Benchmarking Theory to Experiments

Ne^{10+} + He $\rightarrow$ Ne^{9+}+He^+

[Graph showing relative intensity vs. photon energy for Ne^{10+} + He reaction with peaks at 4.5 KeV/u and labels](Cumbee et al. 2016)

O^{8+} + H_2O $\rightarrow$ O^{7+}+ H_2O^+

[Graph showing relative intensity vs. photon energy for O^{8+} + H_2O reaction with peaks at 3.1 KeV/u and labels](Mullen et al. 2017)

Fe^{26+} + N_2 $\rightarrow$ Fe^{25+} + N_2^+

[Graph showing relative intensity vs. photon energy for Fe^{26+} + N_2 reaction with peaks at 5.3 KeV/u and labels](Wargelin et al. 2005)

Fe^{25+} + N_2 $\rightarrow$ Fe^{24+} + N_2^+

[Graph showing relative intensity vs. photon energy for Fe^{25+} + N_2 reaction with peaks at 3.1 KeV/u and labels](Wargelin et al. 2005)
Benchmarking Theory to Experiments

- Microcalorimeter detectors produce high-resolution spectra
  - Useful for benchmarking Theory

- From Fogle et al. (2014)
  - $930 \text{ eV/u}$
  - $420 \text{ km/s}$

- From Defay et al. (2013)
  - $1 \text{ keV/u}$
  - $451 \text{ km/s}$

- From Beiersdorfer et al. (2003)
  - $1000 \text{ eV/u}$
  - MCLZ low-energy
  - $O^{8+} + CO_2$

- Benchmarking Theory to Experiments

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Current CX Models and Databases

• ACX
  • Uses empirical formulae for CX cross-sections
  • Not velocity dependent
  • For use in XSPEC

• ACX2
  • Used in PyXSPEC
  • Uses MCLZ velocity-dependent cross-sections for H- and He-like ions
  • Uses ACX formulae for other cases

• SPEX-CX
  • Uses reliable cross-sections, when available in the literature
  • Uses scaling relations to estimate other cross-sections
Charge exchange Models

- **AtomDB CX ACX2.0**
- **SPEX**

**Chandra ACIS**

**Perseus Filaments**

**EBIT**

**XMM-Newton RGS**

**Comet**

**M82**

Zhang et al. 2014

**Mullen et al., 2016**

**Walker et al. 2015**

**Betancourt-Martinez et al. 2018**

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Kronos CX Database

O$^+$ Triplet of Star Forming Galaxies

<table>
<thead>
<tr>
<th>NGC253 A</th>
<th>M51</th>
<th>M94</th>
</tr>
</thead>
<tbody>
<tr>
<td>MB3</td>
<td>NGC2903</td>
<td>M61</td>
</tr>
<tr>
<td>NGC4631</td>
<td>Antennae</td>
<td>NGC253 B</td>
</tr>
</tbody>
</table>

Liu et al. 2012

Relative Intensity (arb. units)

Photon Energy (eV)

$\lambda$ (Å)
Current CX Models and **Kronos** Database

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- **Kronos**
  - Database of $n,l,S$ resolved cross-sections
  - Cross-sections $\sigma_{nlt(S)}(v)$
    - **Ions**: H- and He-like C, N, O, Ne, Mg, Al, Si
    - **Neutrals**: H, He, H$_2$, H$_2$O, CO, CO$_2$, N$_2$
  - **Collision Energies**: 0.01eV/u - ~100 keV/u
  - **Methods**: AOCC, CTMC, MCLZ, QMOCC, Recommended
  - Transition probabilities (Einstein A Coefficients)
  - Transition Energies
  - X-ray line ratios following radiative cascade
Limitations

• In comets, more ionization stages (other than \( \text{H-like} \) and \( \text{He-like} \)) are significant

• Multi-electron capture, in which 2 or more electrons is transferred can be significant for collisions with neutrals with more than 1 electron
Multi-electron Capture


M. Rakovic and D. R. Schultz (2012)

Single Electron Capture: \( C^{6+} + H_2 \rightarrow C^{5+} (n\ell) + H_2^+ \)
Transfer Ionization: \( C^{6+} + H_2 \rightarrow C^{5+} (n\ell) + 2H^+ + e^- \)
True Double Capture: \( C^{6+} + H_2 \rightarrow C^{4+} (n\ell, n'\ell') + 2H^+ \)
Double Capture Autoionization: \( C^{6+} + H_2 \rightarrow C^{5+} (n\ell, n'\ell') + 2H^+ + e^- \)

CTMC Theory

CTMC Method 10 keV/u Collision Energy

M. Rakovic and D. R. Schultz (2012)

Experiment


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• Current theory needs to be benchmarked to experiment for a variety of collision energies.

• MCLZ is relatively easy to calculate, but requires more approximations than QMOCC or AOCC.
Summary

• Kronos Database
  • H-like and He-like C, N, O, Ne, Mg, Al, and Si
  • H and He targets
  • 200-1000 km/s
  • QMOCC, AOCC, CTMC, and MCLZ methods

• Limitations
  • In comets, more ionization stages (other than H-like and He-like) are significant
  • Multi-electron capture, in which 2 or more electrons is transferred can be significant for collisions with neutrals with more than 1 electron
  • Current theory needs to be benchmarked to experiment for a variety of collision energies
  • MCLZ is relatively easy to calculate, but requires more approximations than QMOCC or AOCC.
  • Some data available in AtomDB CX and SPEX packages

All data available in Kronos Database
https://www.physast.uga.edu/research/stancil-group/atomic-molecular-databases/kronos
Google search: UGA Stancil Kronos