The Kronos Database of State-Selective Charge Exchange Cross Sections

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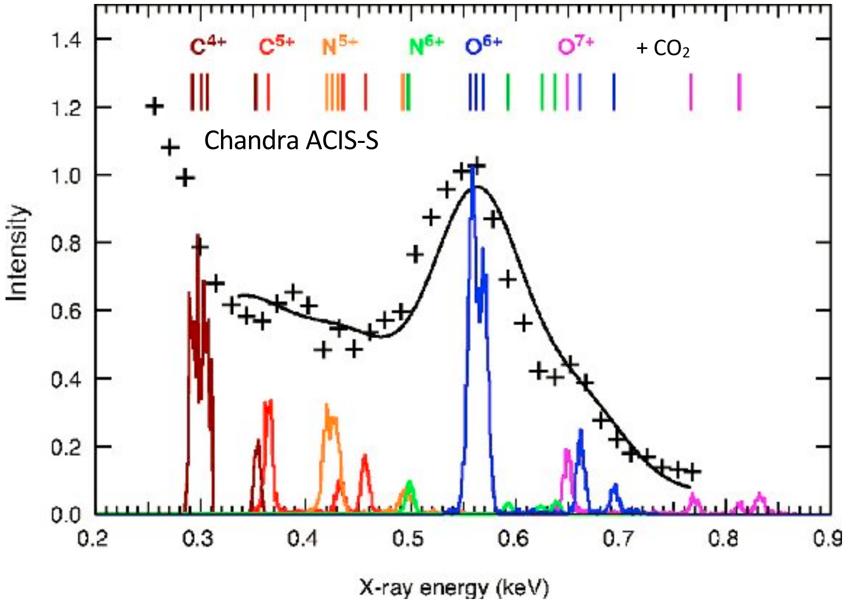
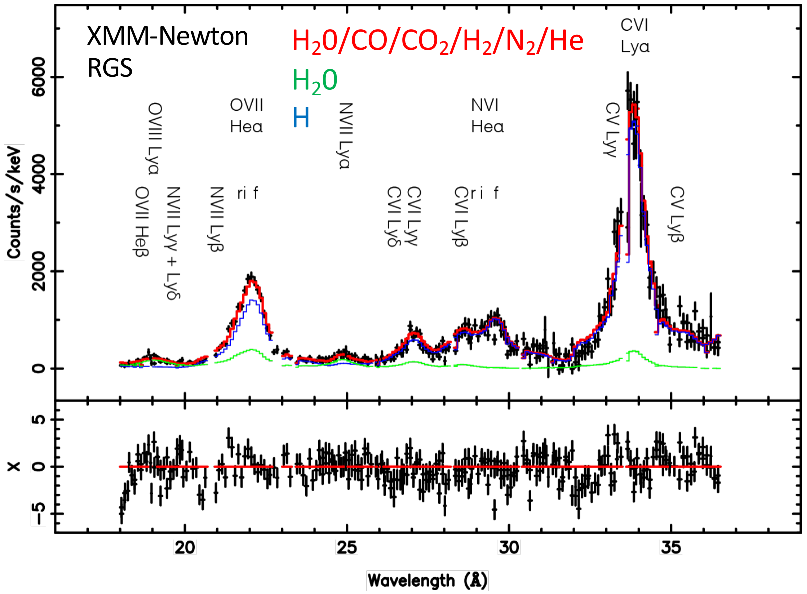
Charge Exchange -Observations

LINEAR C/1999 S4

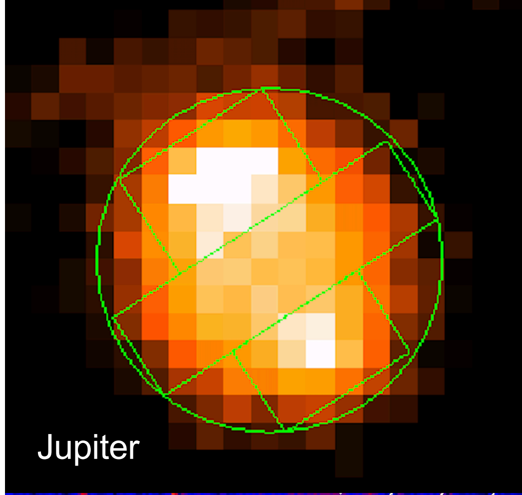


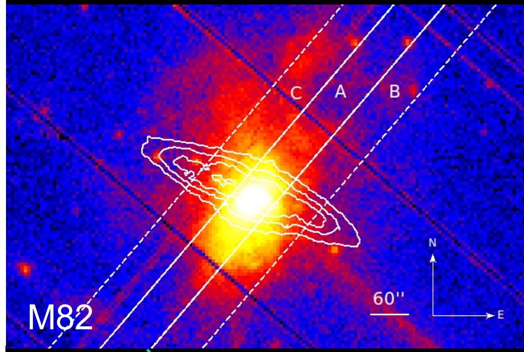
From Beiersdorfer et al. (2003).

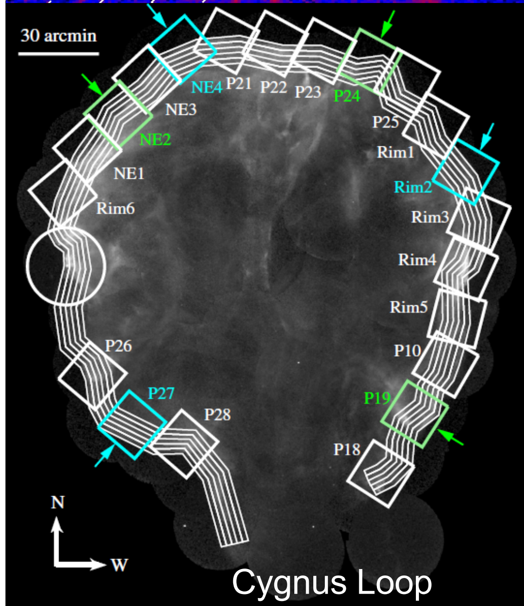
LINEAR C/2000 WM1



From Mullen et al., in Prep





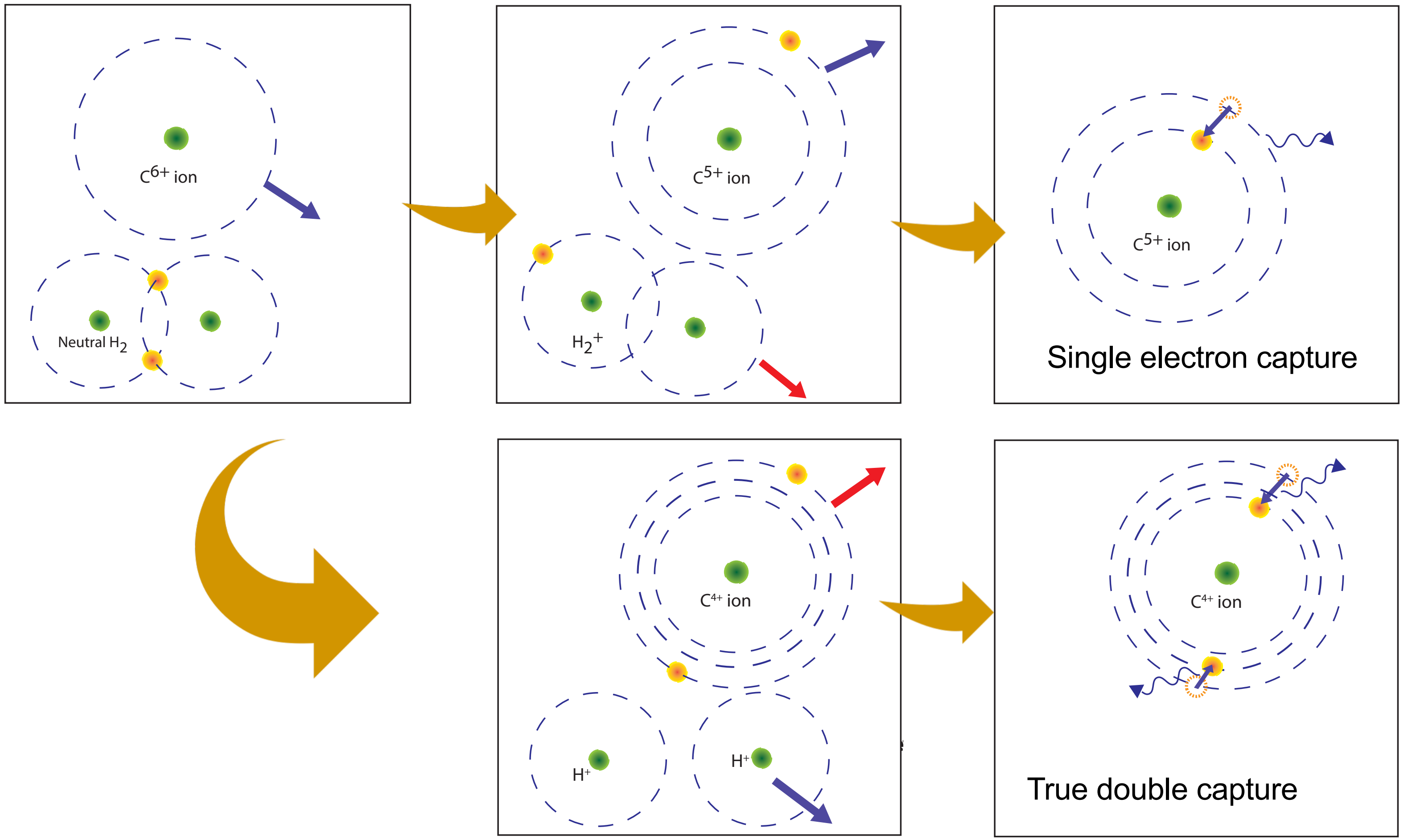


Charge Exchange Process

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

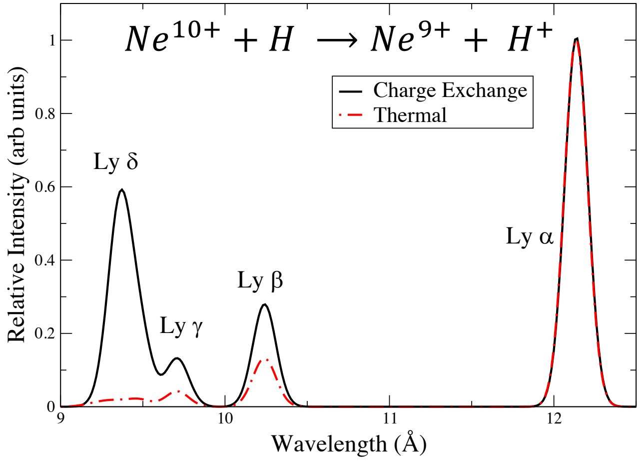
Produces highly excited, high charged state ions $X^{q-1}(nl\ ^{2S+1}L)$

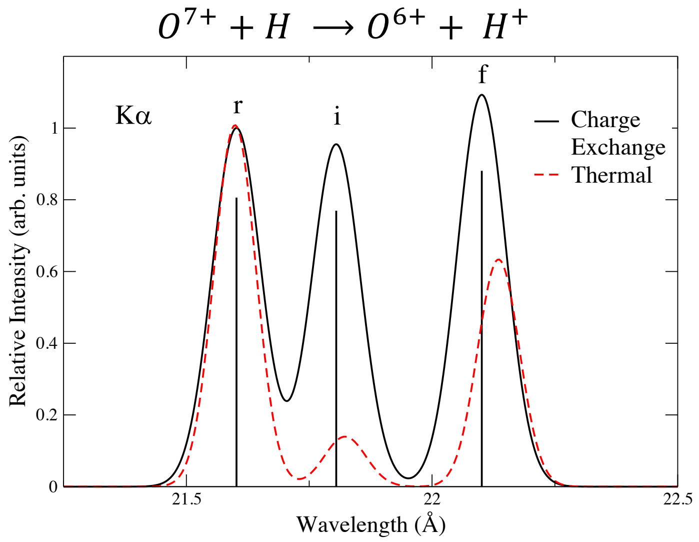
- Cascade to lowest energy
  → Produces X-rays

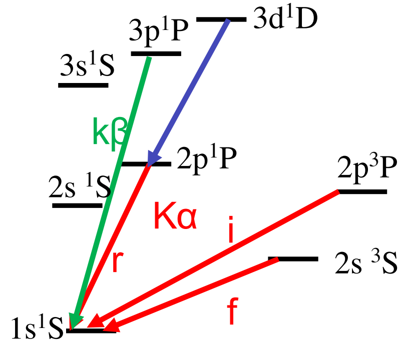


CX & Thermal Emission

- 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!







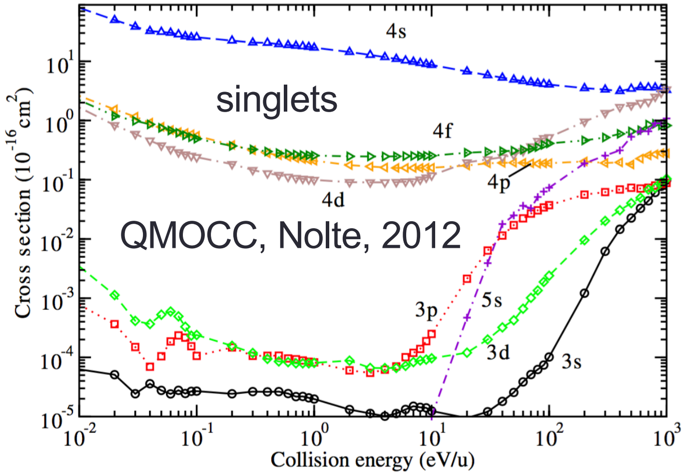
CX X-ray Emission Line Ratios (Spectra)

- 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)

Charge Exchange Cross Section

The *probability* of an electron to transfer from the neutral atom into a specific excited state (n, l, S) of the ion.

$C^{5+} + H \rightarrow C^{4+} + H^{+}$



For charge exchange calculations:

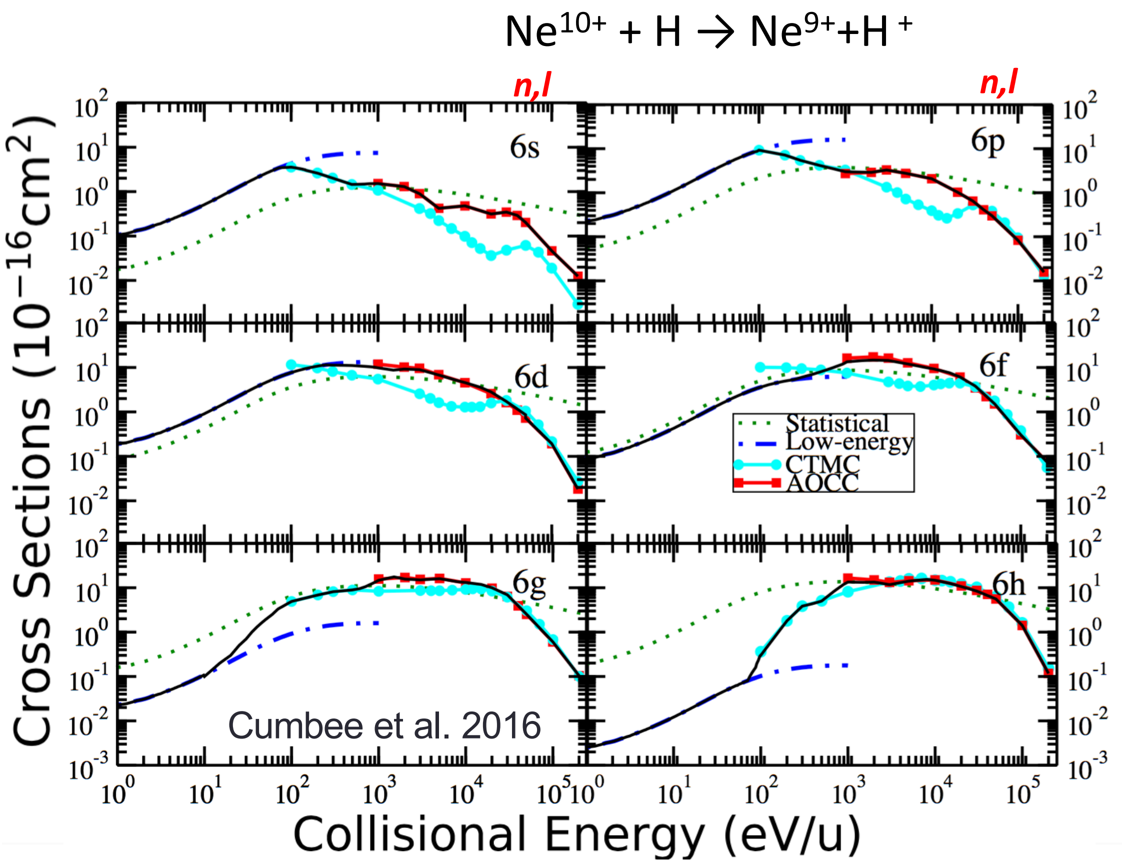
- σ depends on the
  - **n** (principle quantum number)
  - **l** (orbital angular momentum quantum number
  - **S** (spin quantum number, He-like)
  - **v** (collision velocity)
- $\boldsymbol{\sigma_{nls}(v)}$ is required to produce reliable theoretical CX X-ray emission spectra

"Effective area" that quantifies the likelihood of a scattering event to occur

CX Cross Sections ($\sigma_{n,l,s}$)

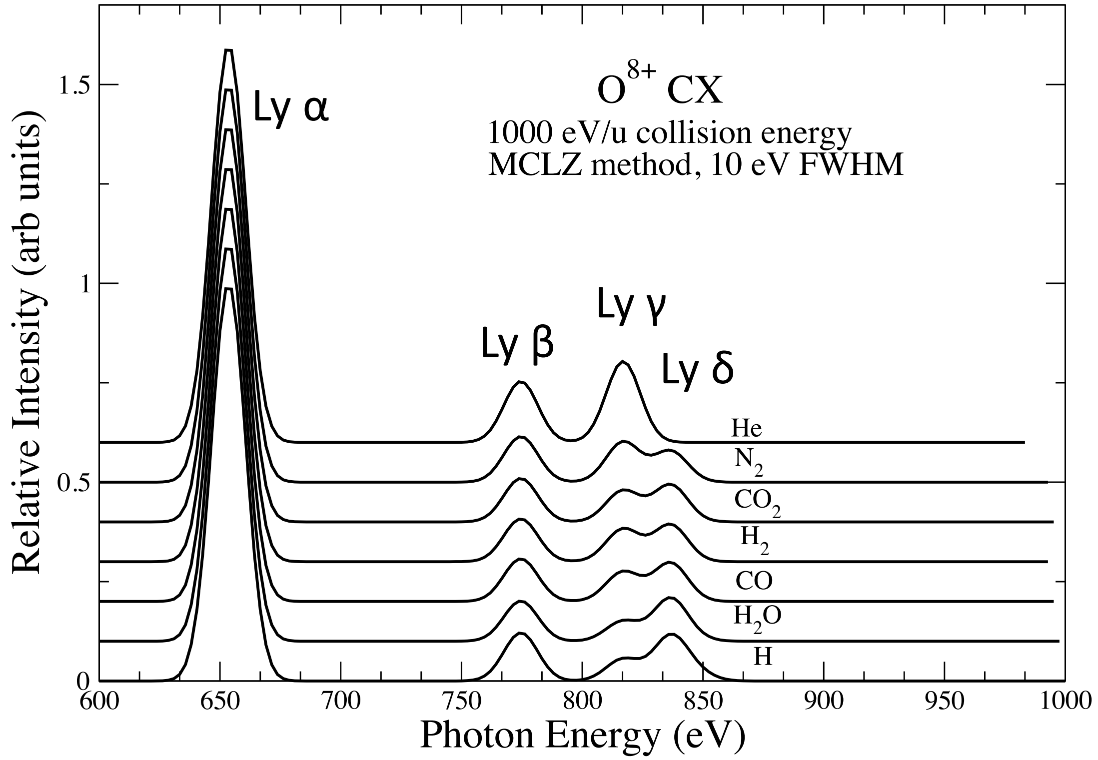
Accuracy & difficulty

- **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**



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



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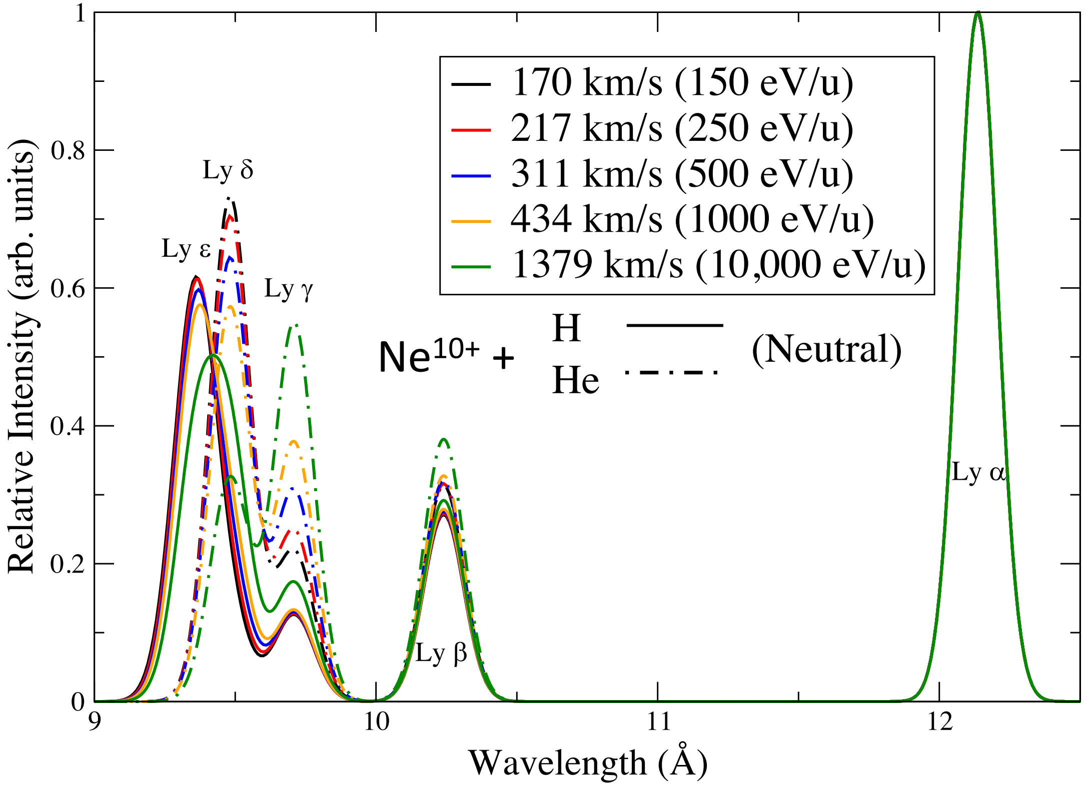
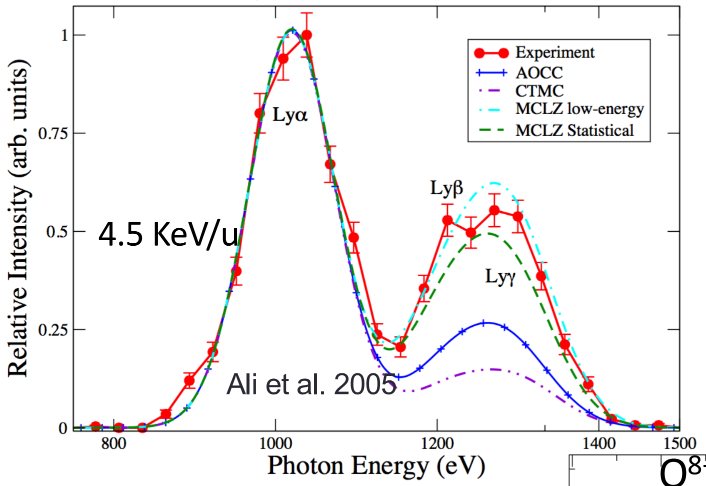
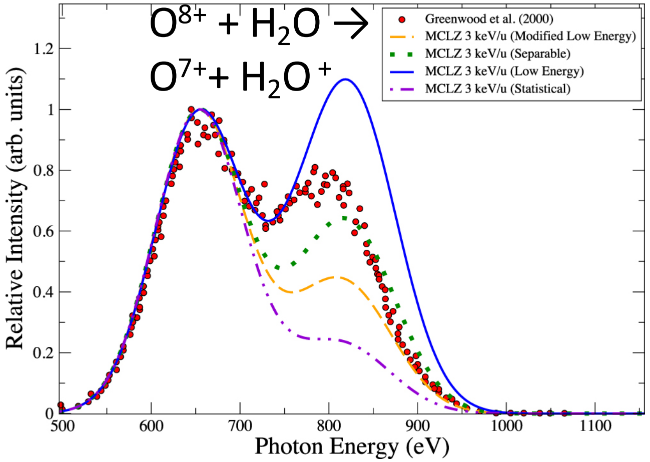


Benchmarking Theory to Experiments

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

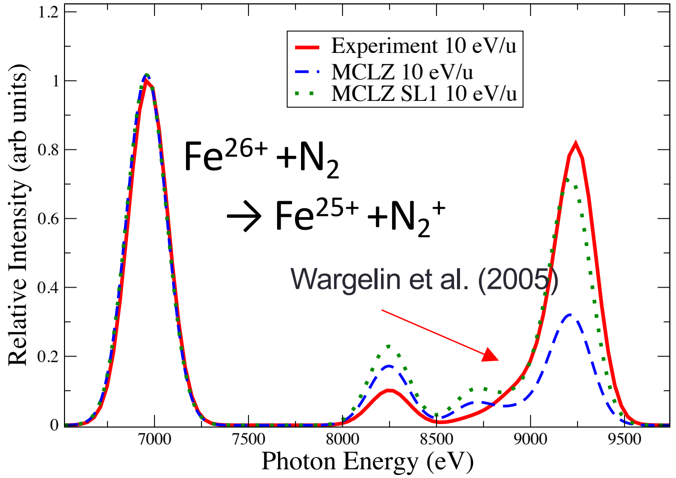


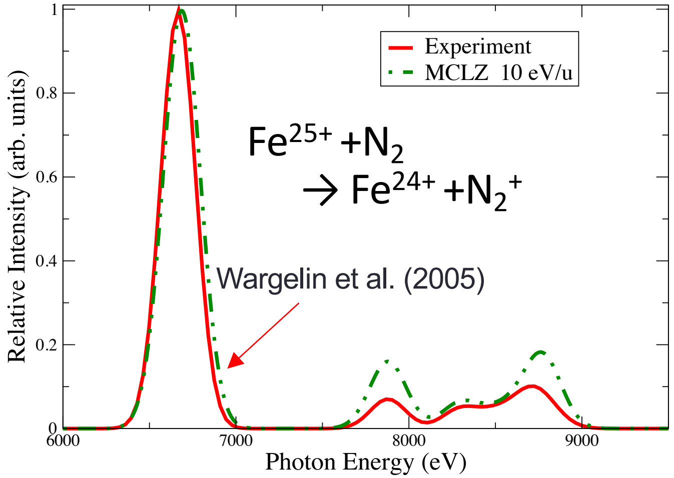
Cumbee et al. 2016



3.1 KeV/u

Muller et al. 2017

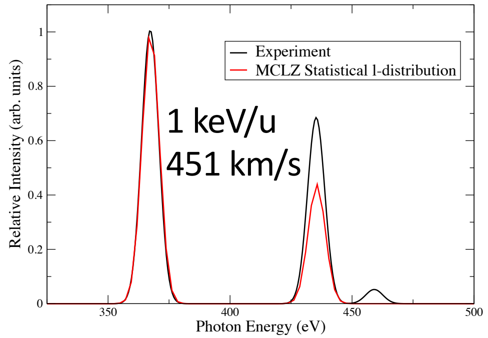




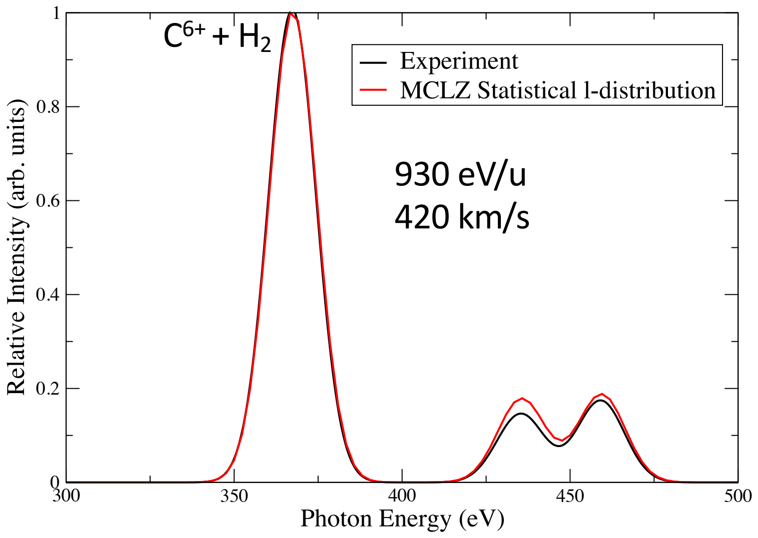
Benchmarking Theory to Experiments

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

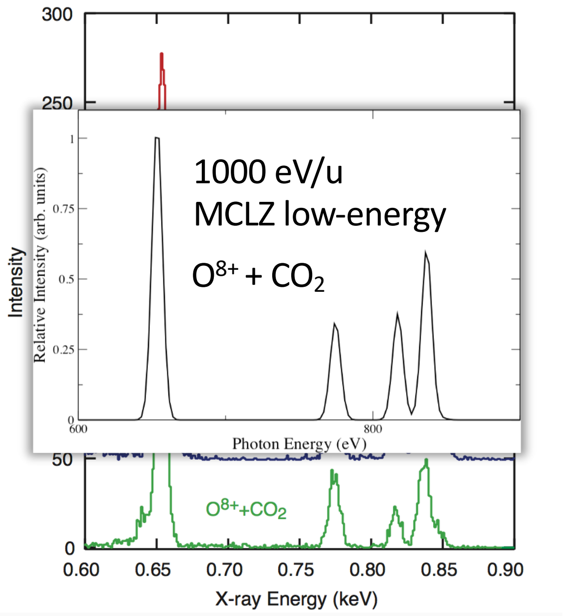
C^{6+} + He



From Defay et al. (2013)



From Fogle et al. (2014)



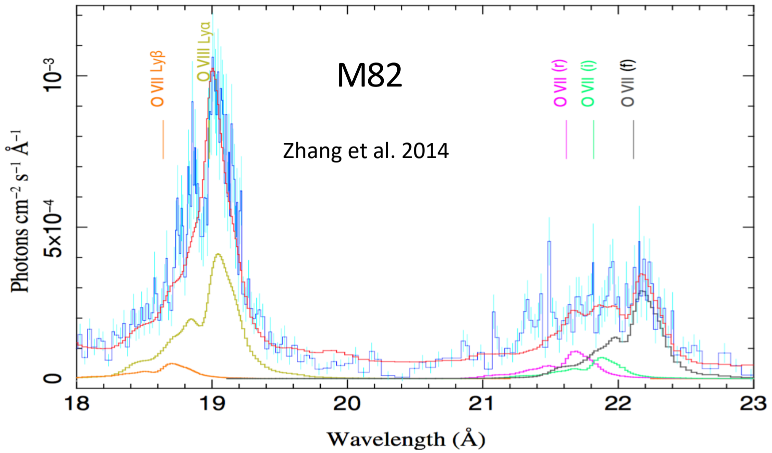
From Beiersdorfer et al. (2003)

Current CX Models and Databases

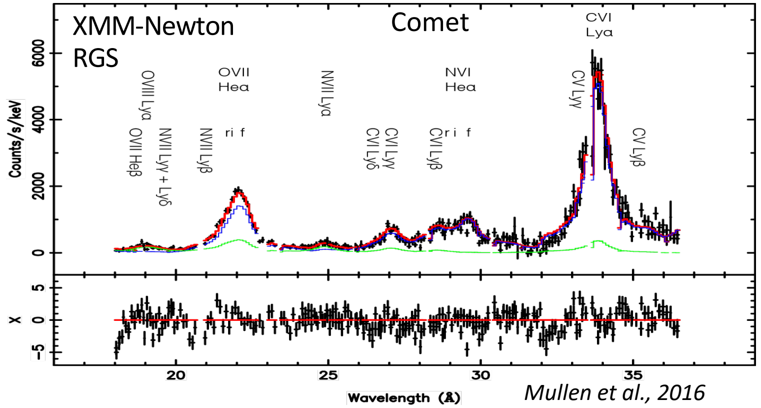
- ACX
  - Uses empirical formulae for CX cross-sections
  - Not velocity dependent
  - For use in XSPEC
- ACX2
  - Used in PyXSPEC
  - Uses MCLZ velocity-dependent cross-sections for H- and He-like ions
  - Uses ACX formulae for other cases
- SPEX-CX
  - Uses reliable cross-sections, when available in the literature
  - Uses scaling relations to estimate other cross-sections

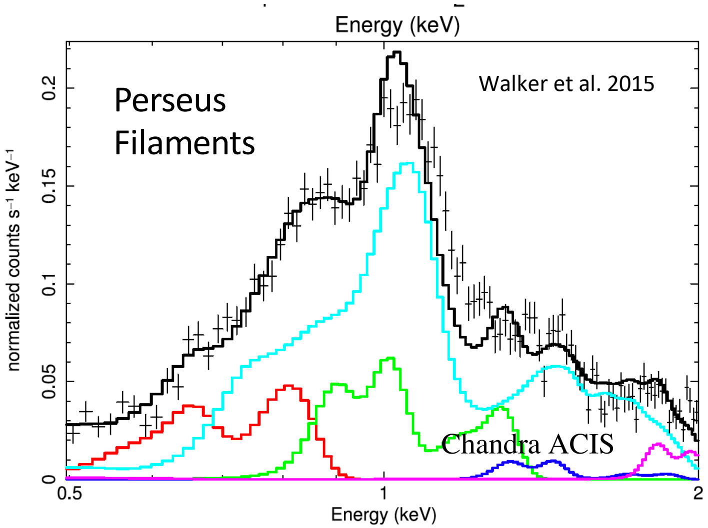
Charge exchange Models

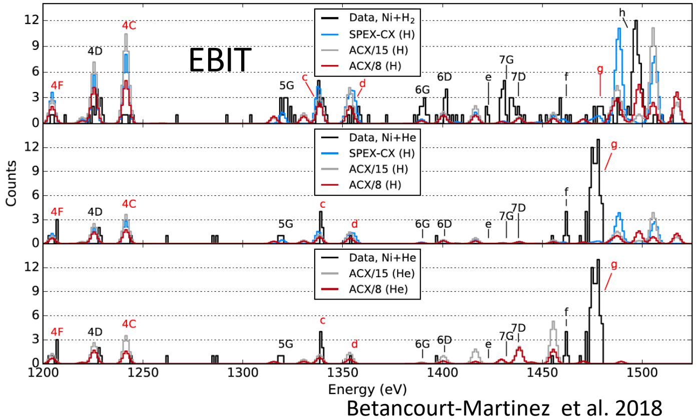
AtomDB CX
ACX2.0



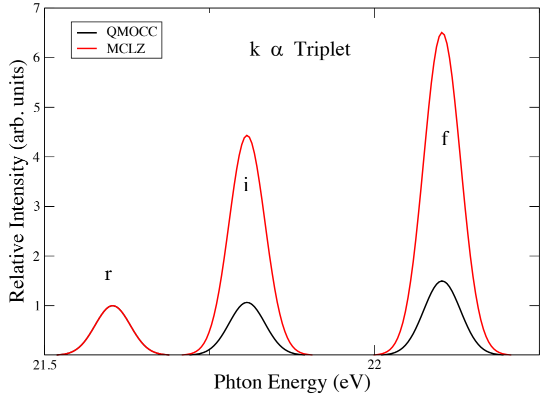
SPEX

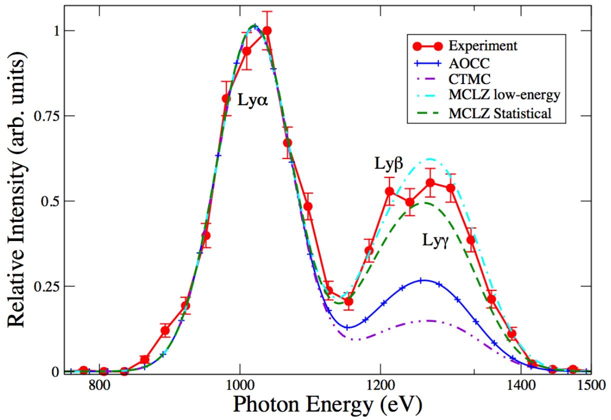




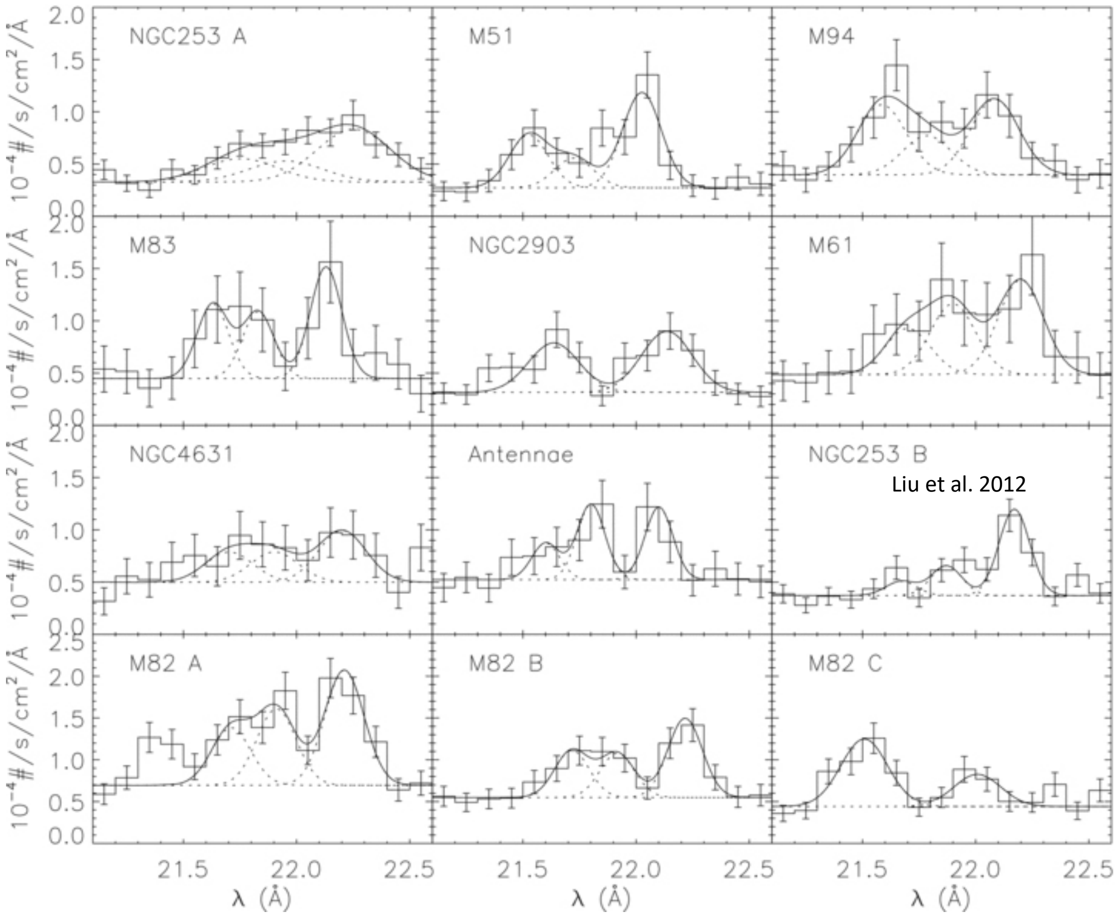


Kronos CX Database





O^{7+} Triplet of Star Forming Galaxies



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- SPEX-CX
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- Kronos
  - Database of n,l,S resolved cross-sections
  - Cross-sections $\sigma_{nl(S)}(v)$
    - ***Ions***: H- and He-like C, N, O, Ne, Mg, Al, Si
    - ***Neutrals***: H, He, H_2, H_2O, 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 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

Multi-electron Capture

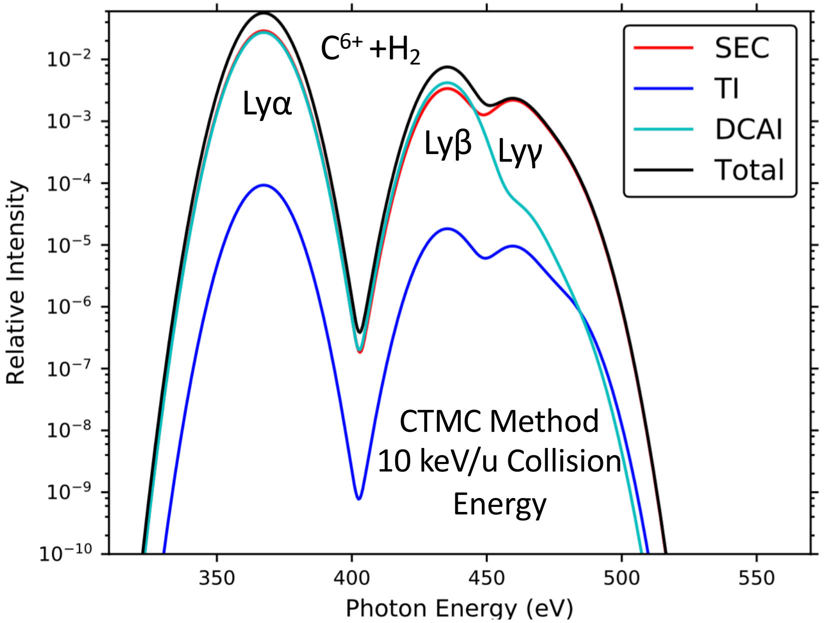
Single Electron Capture: $C^{6+} + H_2 \rightarrow C^{5+}(n\ell) + H_2^+$

Transfer Ionization: $C^{6+} + H_2 \rightarrow C^{5+}(n\ell) + 2H^+ + e^-$

True Double Capture: $C^{6+} + H_2 \rightarrow C^{4+}(n\ell, n'\ell') + 2H^+$

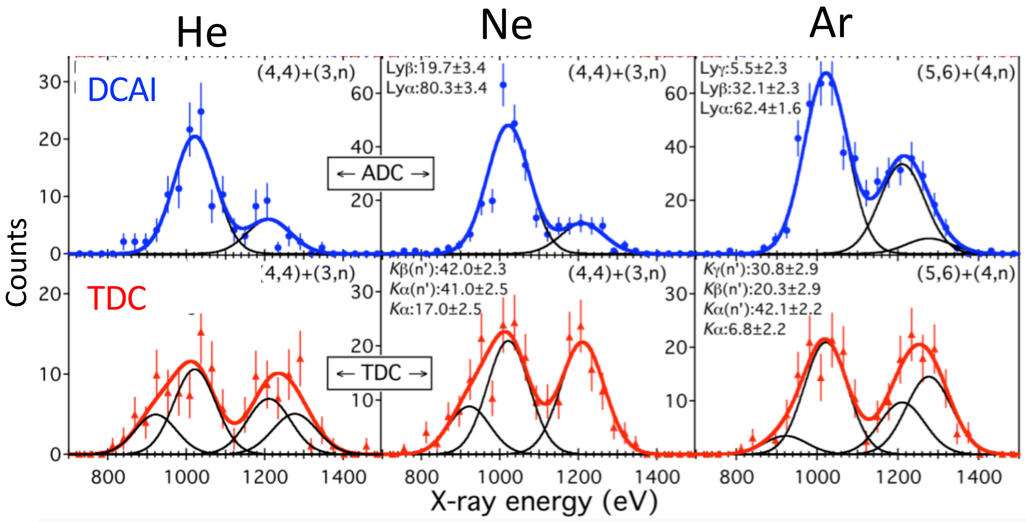
Double Capture Autoionization: $C^{6+} + H_2 \rightarrow C^{4+}(n\ell, n'\ell') + 2H^+$
$\rightarrow C^{5+}(n''\ell'') + 2H^+ + e^-$

CTMC Theory



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

Ne^{10+} +



From Ali et al. 2016

Experiment

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.

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