Low-energy Electron-Ion and Ion-Atom Collisions:

Progress and needs for modeling of future NASA astrophysics observations

Phillip C. Stancil

Department of Physics and Astronomy
Center for Simulational Physics
University of Georgia

Charge

- Laboratory astrophysics review covering low energy collisions of atoms w/ atomic ions and of electrons and atomic ions for current/future NASA missions
- Cover current theoretical and experimental laboratory astrophysics work and capabilities
- Needs to meet current and future NASA astrophysics missions

Outline

- Considered processes for *lowly*-charged systems (q<5):
  - Electron Capture (charge exchange)
  - Electron-impact electronic excitation
  - Electron-impact fine-structure excitation
  - Atom-impact excitation (electronic and fine-structure)
- Applications to "*low*" temperature environments
- Survey of 2006-2010 relevant literature, researcher queries, and IAU *Reports in Astronomy, Collisional Processes*

Electron Capture (CX)

- Collision of an ion *X* of charge *q* with a neutral *Y* (*Y* = H, He, or H_2)

$$X^{q+} + Y \rightarrow X^{(q-1)+} + Y^{+}$$

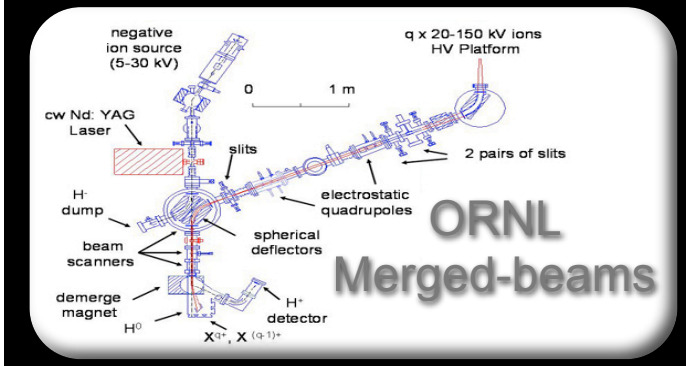
- For photoionized gas or cool environments, plays important roles in the:
  - Ionization balance (species abundances)
  - Thermal balance (Kingdon & Ferland 1998)
  - Emission Spectra
- Rate coefficients (and cross sections) available on some websites, but not comprehensive: UMIST, ORNL-UGA

Electron Capture: Methods

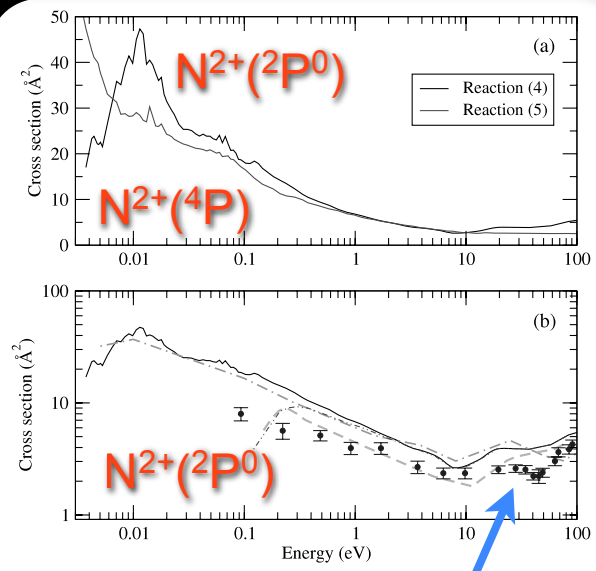
- **Experiment (total)**
- Flowing afterglow
- Ion beam-gas cell
- Ion trap
- Merged-beams
- EBIT

- **Experiment (state-resolved)**
- Trans. energy spectroscopy
- Photon spectroscopy
- Recoil ion (COLTRIMS)

- **Theory**
- Landau-Zener
- Molecular-orbital close-coupling (CC)
- Atomic-orbital CC
- Lattice methods

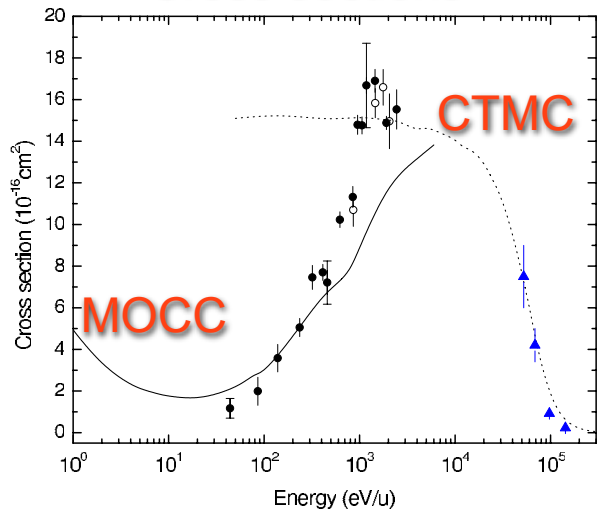


Electron Capture: Highlights

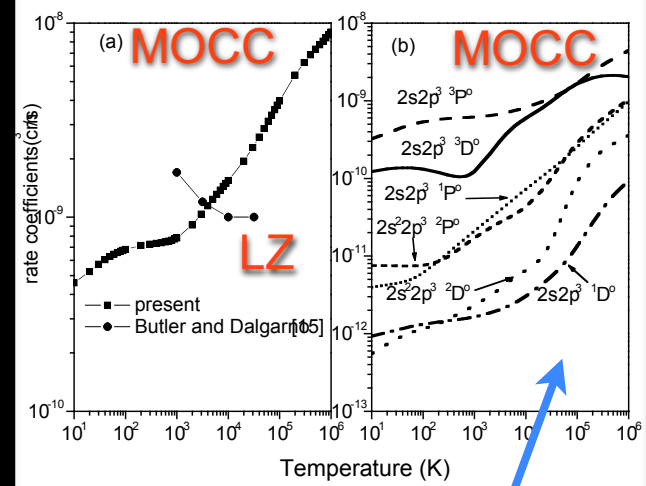


Merged-beam exp.

Cross sections



Rate Coefficients



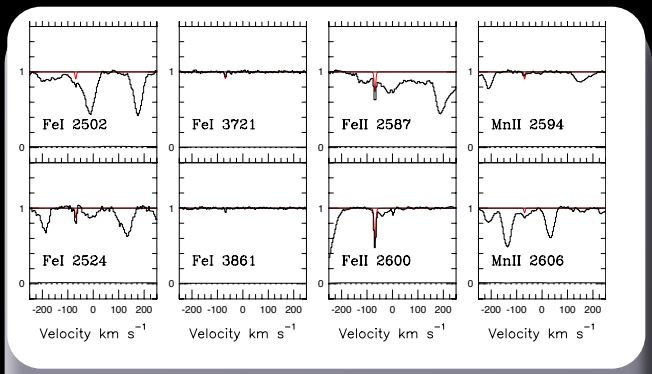
Final state-selective

N^{2+} + H, O^{2+} + H
MOCC calculations
(Barragan et al. 2006)

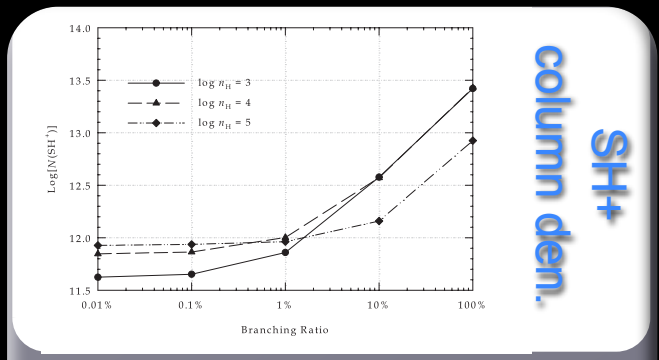
Si^{3+} + H
merged-beams
measurements
(Bruhns et al. 2008)

O^{3+} + He ➜
$O^{2+}(2s2p^3)$ + He^+
MOCC calculations
(Wu et al. 2009)

Electron Capture: Needs

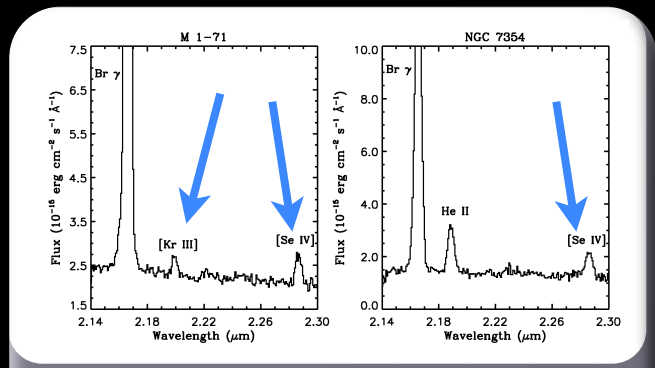


- Surprising Fe I features in Mg II absorbers
- More Fe I, than in models
- Fe + H^+ CX rate too large



- SH^+: IR diagnostic in XDRs
- Abundance depends on branching ratio

$S^{2+} + H_2 \rightarrow S^+ + H_2^+$
$\rightarrow SH^+ + H^+$



- n-capture elements are observed in PNe
- CX data are completely lacking
- Needed for q=1-5

Fe + H^+, Mg + H^+ Damped Lyman α Clouds (z~0.45) (Jones et al. 2010)

SH^+ in X-ray Dominated Regions (Abel, Federman, PCS 2008)

Se, Kr, Xe, ... + H Trans-Iron Elements in Planetary Nebulae (Sterling et al. 2007)

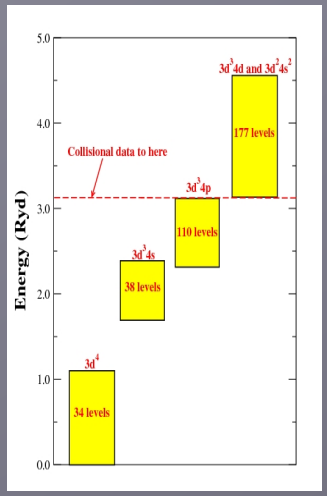
Electron Impact Electronic Excitation

- Collision of an ion *X* of charge *q* (or a neutral) with an electron $X^{q+}(nlSL) + e^- \rightarrow X^{q+}(n'l'S'L') + e^-$
- Important in a variety of environments including collisionally-ionized and photoionized gas:
  - Level populations (non-LTE emission spectra)
  - Electron density diagnostic
  - Temperature diagnostic (Osterbrock & Ferland 2006)
  - Elemental abundances
- Rate coefficients (and collision strengths) available on some websites, but not comprehensive: Cloudy, ORNL

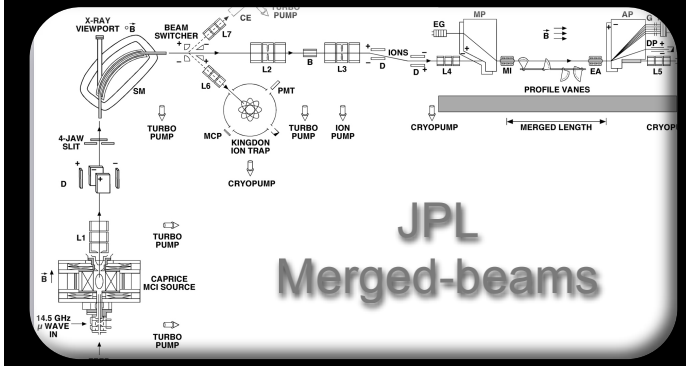
Electron-Impact Electronic Excitation: Methods

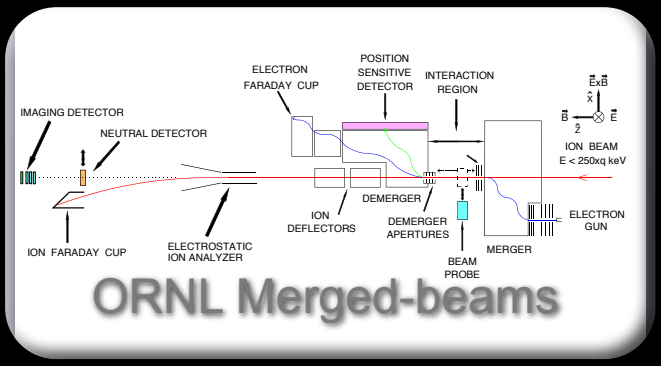
- **Experiment**
- Merged electron-ion beam energy loss (JPL & ORNL)
- EBIT

Fe^{4+}: 359 levels, 2400 channels

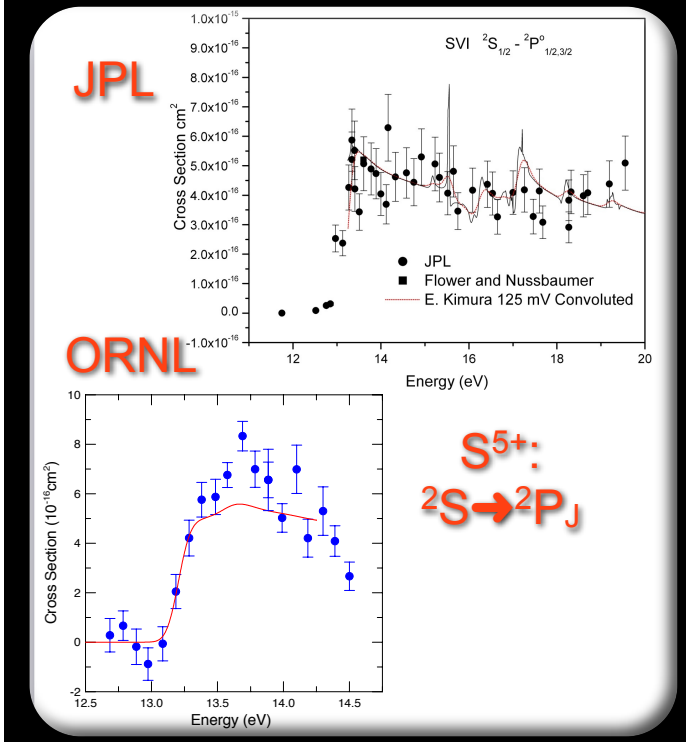


- **Theory**
- Perturbative
- R-matrix close-coupling (various flavors)
- Lattice methods

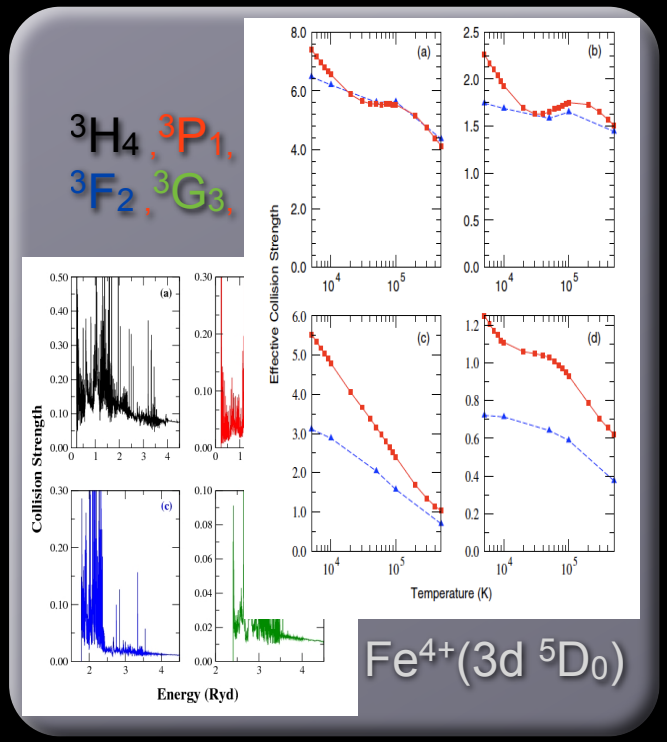




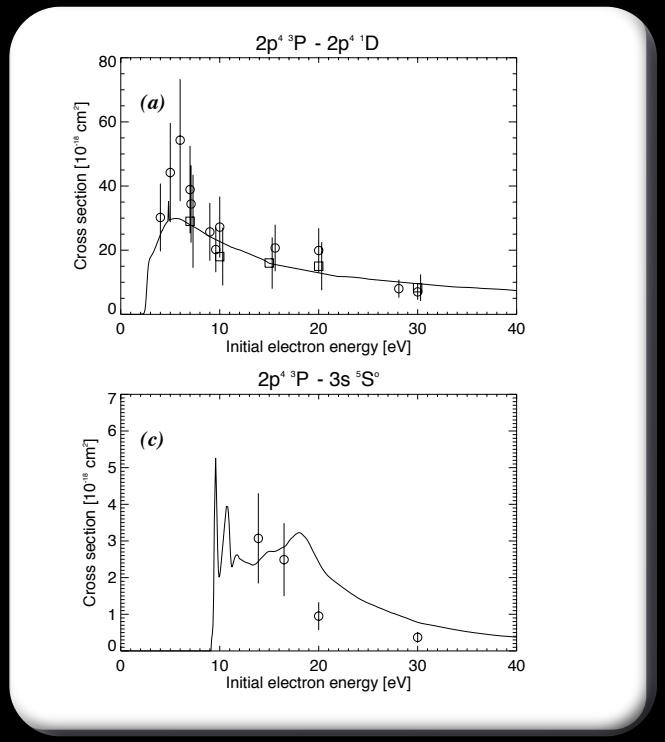
Electron Impact: Highlights



S^{5+} measurements
Wallbank et al. (2007)
Simcic et al. (2010)

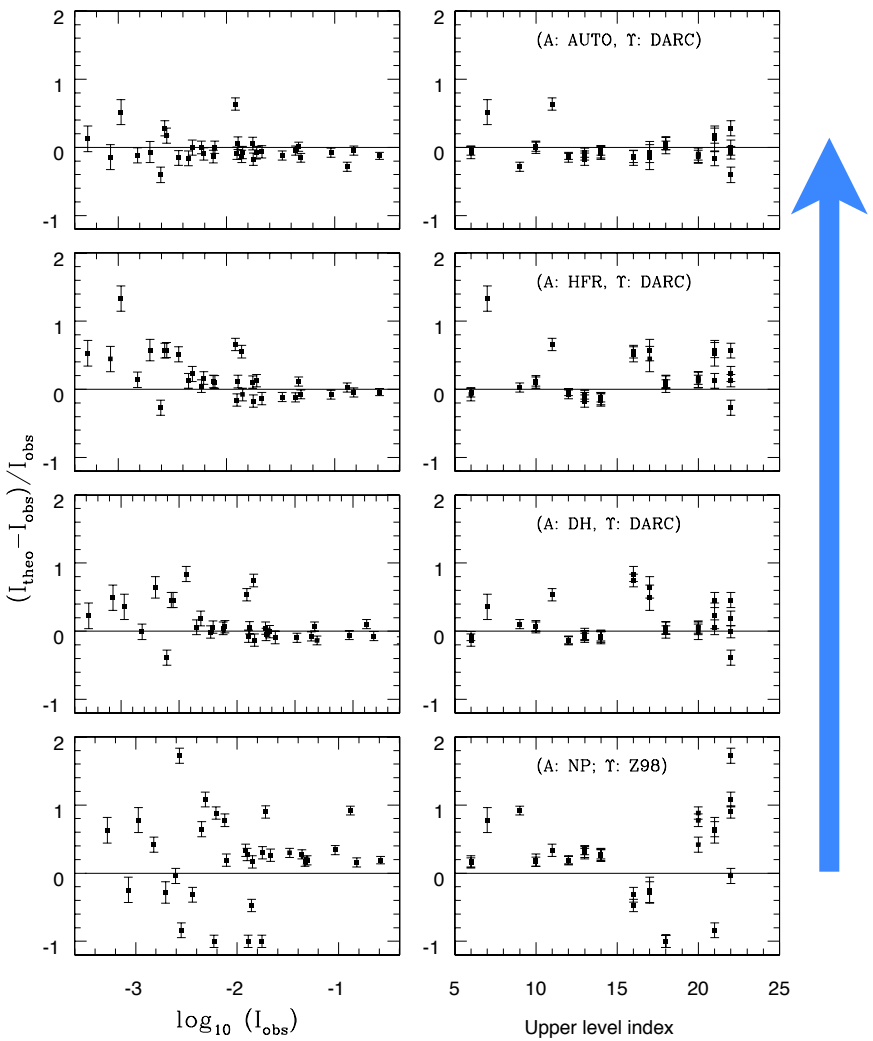


Fe^{4+} R-matrix calculations
(Ballance et al. 2008)
new=359 levels,
previous=80 levels



O($2p^4$,3s,3p) R-matrix calculations
(Barklem 2006)

Electron Impact: Needs



Bautista et al. 2010

- Combined atomic data/modeling study of Fe III in the Orion Nebula
- New Dirac-Fock A-values
- New Dirac R-matrix collision strengths
- Dramatic improvement over previous atomic data

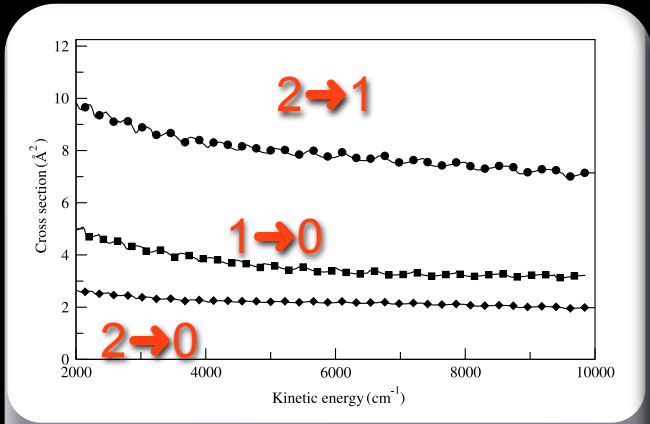
Sterling et al. (2010)

- To model planetary emission lines of n-capture elements, collision strengths are needed for many ions
- $Se^{1,2+}$, $Se^{4,5+}$, Kr^{+}, Kr^{5+}, Xe^{+},Xe^{5+}, Br^{q+}, Rb^{q+}, ...

Fine-Structure Excitation

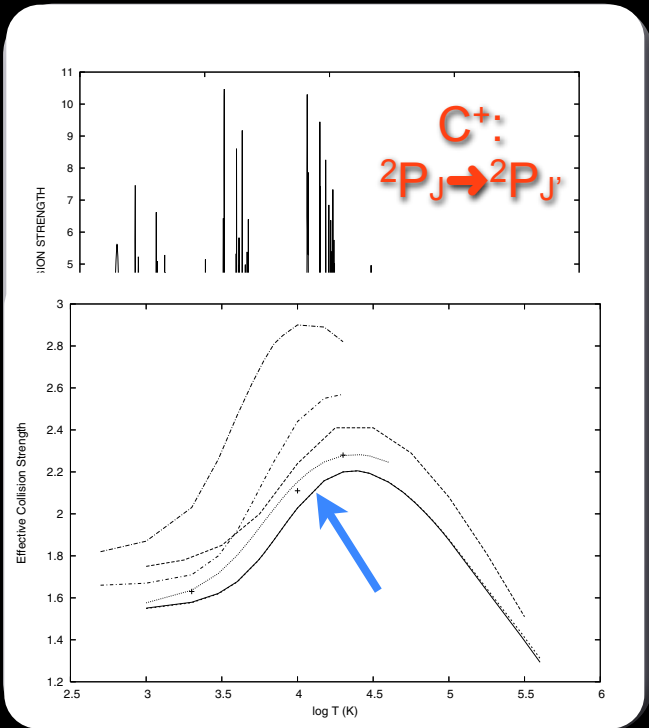
- Collision of an ion X of charge q (or a neutral) with an electron or H atom $$X(nlLJ) + Y \rightarrow X(nlLJ') + Y$$
- Important in a variety of cool and molecular environments:
  - Level populations (non-LTE emission spectra)
  - Radiative cooling
  - Temperature, density, radiation diagnostics
  - Many lines observable by *Spitzer, SOFIA, Herschel*
- No comprehensive data compilation

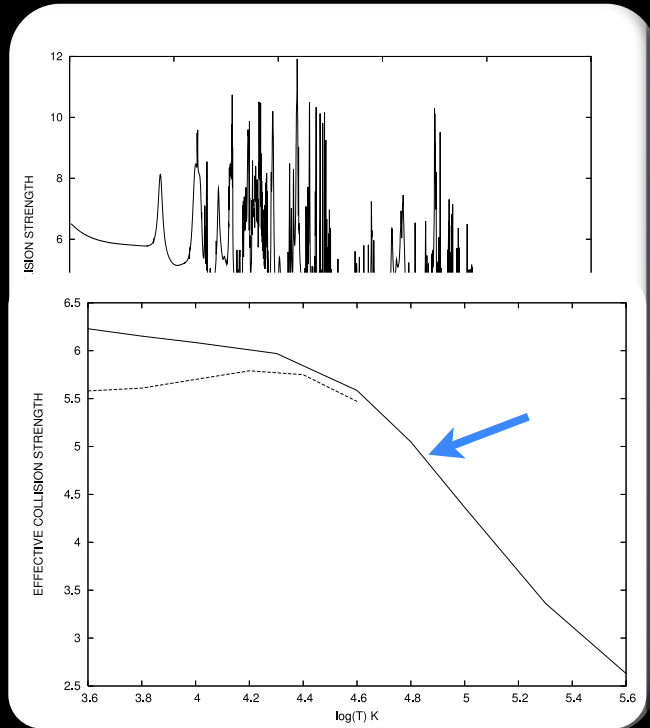
Fine-structure excitation: Highlights



O: $^3P_J \rightarrow {}^3P_{J'}$

- Larger by factors of 2-4 compared to previous calculations



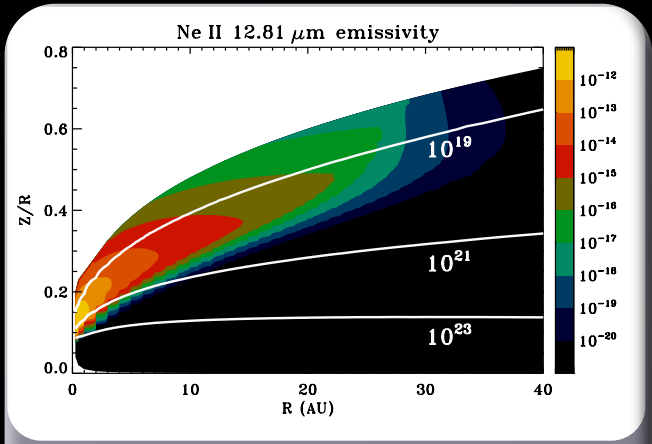


O + H, C+H MOCC Calculations Abrahamsson et al. (2007)

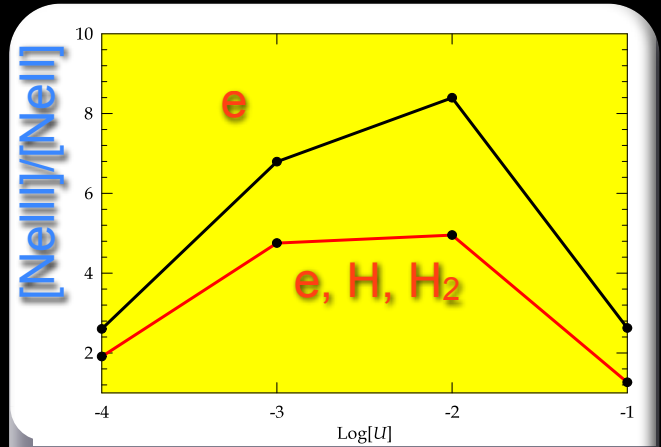
C^+ + e R-matrix calculations Tayal (2008)

Si^+ + e R-matrix calculations Tayal (2008)

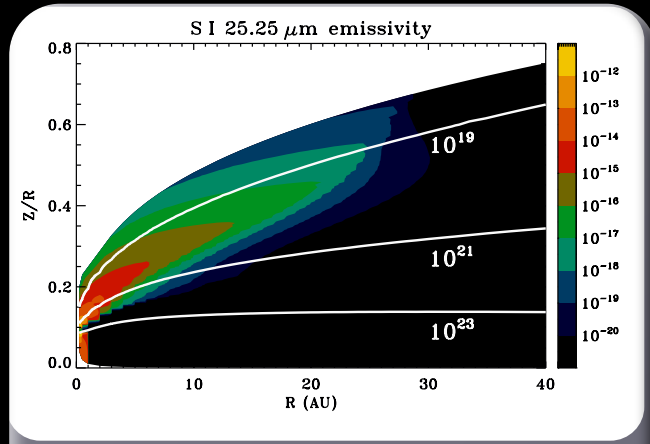
Fine-structure excitation: Needs



- [NeIII] and [NeII] lines observed in protoplanetary disks with *Spitzer*
- H collisional rates needed



- [NeIII]/[NeII] ratio used as a diagnostic of AGNs
- Usually only e-collisions considered



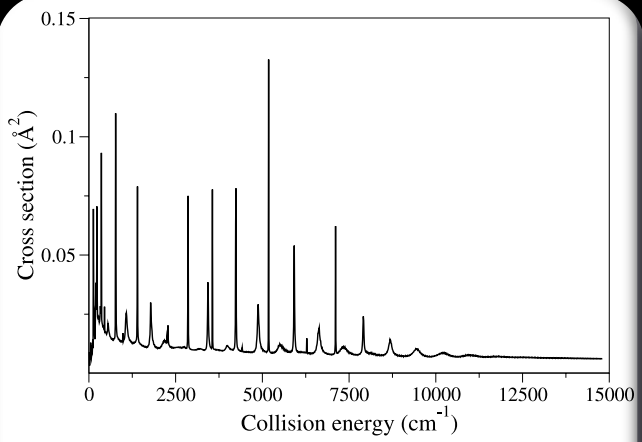
- [SI] observed in proto-planetary disks
- H collisional rates needed

Ne^{+} + H, Ne^{2+} + H
protoplanetary disks
(Meijerink et al. 2007)

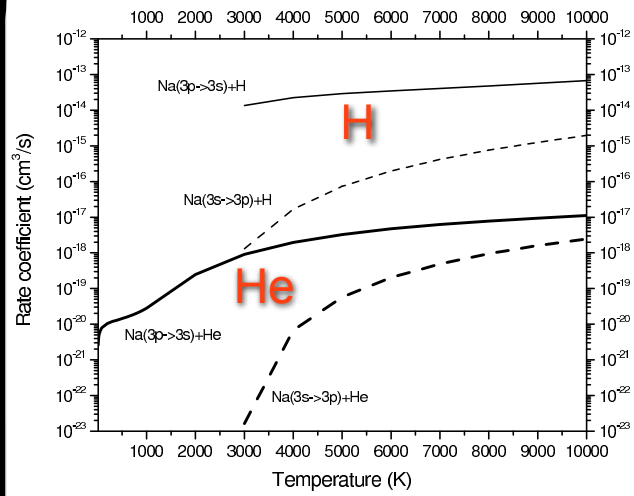
Ne^{+}+H,H_2,
Ne^{2+} + H,H_2 in XDRs
(Abel 2008)

S + H
protoplanetary disks
(Meijerink et al. 2007)

Electronic excitation: Highlights



O: $^1D \rightarrow {}^3P$



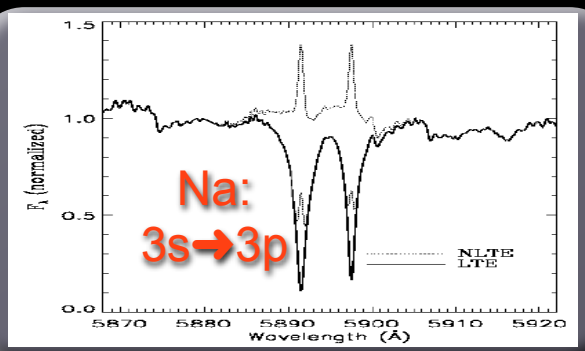
Na: 3s➜3p

- Na I was the first detected atomic feature in an extrasolar planet
- Barman et al. (2002) suggest Na is in non-LTE
- Collisions with H_2, He, and H should dominate electrons
- Similar for K and Rb

PHOENIX Na EGP model

O + H MOCC calculations
Krems et al. (2006)

Na + He MOCC calculations
Lin et al. (2008)



Summary - Needs

- Electron capture (charge transfer):
  - State-selective low-E measurements
  - Improvements in molecular energies for MOCC calcs.
  - Lattice-methods - 2-electron (6D), lower-energy
  - Measurements/calculations of n-capture elements (q=1-5)
  - H^+ with 3rd and 4th row elements (Fe, Mg, Se, ...)
  - Select ions (q<5) up to Zn only have Landau-Zener rates
- Electron impact electronic excitation:
  - n-capture elements (q=1-5)

Summary - Needs

- Fine-structure excitation:
  - Measurements are generally lacking
  - Calculations for S, S^+, Ne^+, Ne^{2+} due H (He)
  - Calculations for Ne^+ and Ne^{2+} due to H_2
  - Improvements for select electron collisions
- Electronic excitation by neutral collisions:
  - Measurements are generally lacking
  - Na due H_2; K, Rb by H_2, He, and H, ...
- Compilations

Acknowledgements

- Funding from NASA:
  - Astronomy and Physics Research and Analysis (APRA)
  - Origins of Solar Systems Program (OSS)
  - Astrophysics Data Program (ADP)
  - Astrophysics Theory Program (ATP)
- Contributions from collaborators and colleagues:
  - Brendan McLaughlin, Ara Chutjian
  - Nick Abel, Mark Bannister, Steven Federman, Gary Ferland, Charlie Havener, Dave Schultz, Nick Sterling, Yong Wu, ...