# Charge exchange in $C^{5+} + H$ collisions

6 October 2011

# Solar Wind Charge Exchange

- solar wind ions collide with neutral H, He
- electron is captured into an excited state of the highly charged ion
- x-ray is emitted through a K-shell transition

Applications

- heliospheric x-ray emission
- Martian and Jovian (magnetospheric, not solar wind) x-ray emission
- cometary x-ray emission
- x-ray emission from forward shock of supernova remnants (?)

# Molecular orbital close-coupling method

- gives triplet-singlet ratios; fully quantum
- total wave function is expanded in terms of adiabatic molecular orbitals:

$$\mathbf{\Psi} = \sum_j \psi_j(\mathbf{s}, \mathbf{R}) F_j(\mathbf{R})$$

- molecular orbitals are solutions of the electronic Schrödinger equation for fixed $R$:

$$[-\frac{1}{2\mu}\nabla_s^2 + V - E_j(R)]\psi_j(\mathbf{s}, \mathbf{R}) = 0$$

- coupled equations in adiabatic basis:

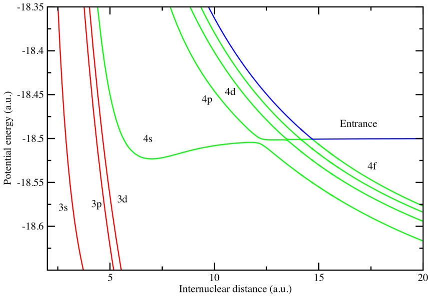
$$\left\{ \frac{\partial^2}{\partial R^2} - \frac{\mathbf{J}_i^2 - \Lambda_i^2}{R^2} - 2\mu(E_i(R) - E) \right\} RF_i(\mathbf{R}) = \sum_j [V_{ij}^R(R) + V_{ij}^C(R)] RF_j(\mathbf{R})$$

# MOCC calculations

- performed two 14-channel calculations including all $\Sigma^+$ and $\Pi$ channels for $n = 3$ and 4, for both singlets and triplets
- 5$s$ state also included to represent $n = 5$ manifold
- covered energy range $E = 0.01$ to 1000 eV/u
- CTMC and AOCC calculations performed by D. R. Schultz and Y. Hui (ORNL) for energies $E > 100$ eV/u

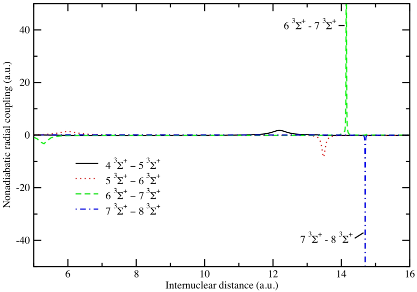
# Potentials and couplings

$^3\Sigma^+$ potentials

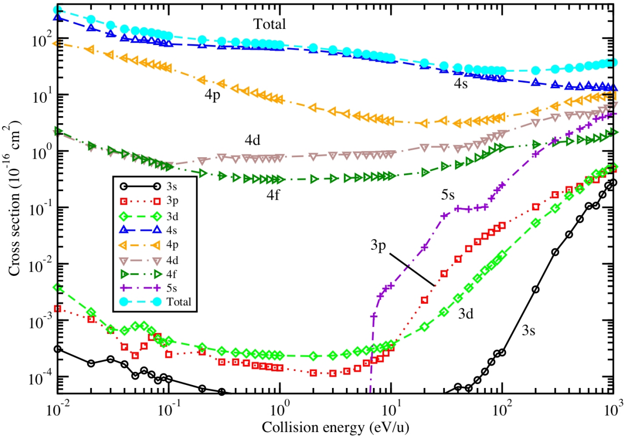



- $n = 4$ channels form dominant capture manifold due to series of avoided crossings with entrance channel

Radial couplings for adjacent $n = 4$ $^3\Sigma^+$ channels

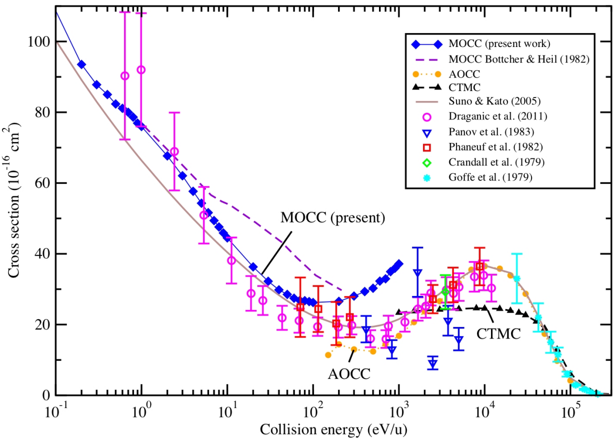


# Total cross sections



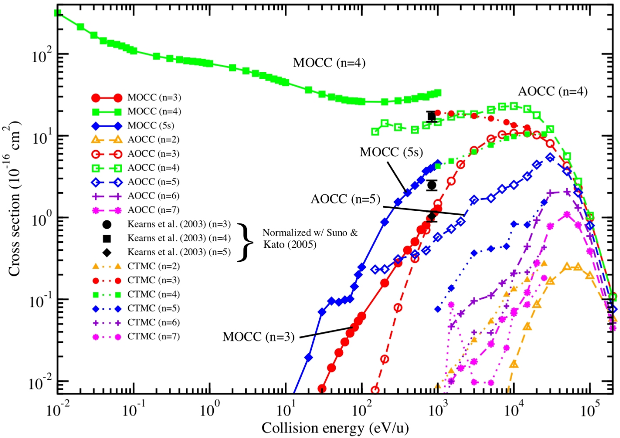

- 4*s* dominates across entire energy range
- increase in $n = 3$ channels at $\sim 10$ eV/u as approach of 4*s* to $n = 3$ manifold becomes energetically accessible
- sharp increase in 5*s* at 7 eV/u

# Comparison with previous data



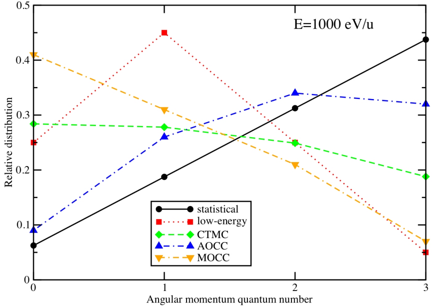

- good agreement for MOCC results below 100 eV/u
- MOCC results diverge for $E > 100$ eV/u
- AOCC fits well for $E > 5000$ eV/u
- CTMC fits well for $E > 50000$ eV/u

# $n$-resolved cross sections




- MOCC, AOCC, and Kearns et al. agree in ordering of $n = 4$, $n = 3$ cross sections
- MOCC alone in showing dominance of $n = 5$ over $n = 3$ above 300 eV/u

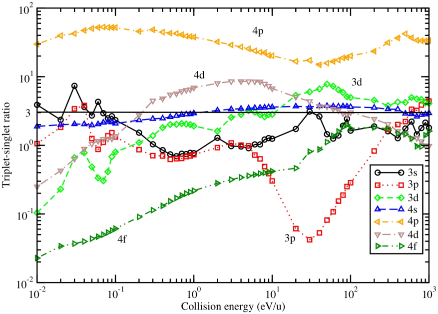
# $l$-distribution (1000 eV/u):



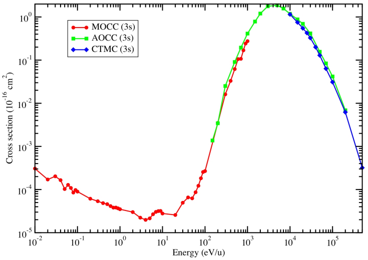

$$W_{nl}^{stat} = (2l+1)/n^2$$

$$W_{nl}^{l.e.} = (2l+1)\frac{[(n-1)!]^2}{(n+l)!(n-l-1)!}$$

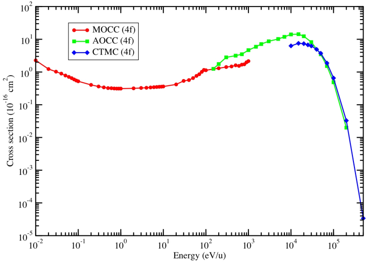
# Triplet-singlet ratios:

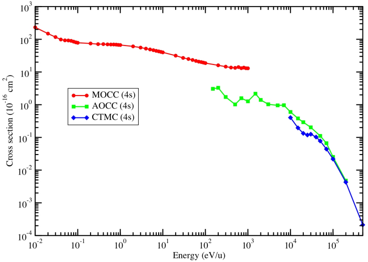


# Recommended fits




- MOCC: lowest energies → $10^2$-$10^3$ eV/u
- AOCC: $10^2$-$10^3$ eV/u → $10^5$ eV/u
- CTMC: all higher energies
- Triplet-singlet ratios extrapolated from MOCC beyond 1 keV/u to approach 3:1



# Future work

- construction of fits for $n, l, S$-resolved cross sections based on MOCC, AOCC, and CTMC data
- extension of MOCC calculations to other charge exchange systems
- modeling of x-ray spectra

# Acknowledgments

Collaborators:
Phillip Stancil (UGA), Heinz-Peter Liebermann (Wuppertal), Robert Buenker (Wuppertal), David Schultz (ORNL), Yawei Hui (ORNL), Ilija Draganić (ORNL), and Charles Havener (ORNL).

This work was partially supported by NASA grant NNX09AV46G.