KIDA '17

New calculations of radiative charge transfer and of radiative association rate coefficients

James F. Babb
ITAMP, Harvard-Smithsonian CfA
Cambridge, MA

Outline

Introduction – collision ingredients

Carbon and helium ion (C-He^+)

Carbon and proton (C-H^+)

Silicon and oxygen (Si-O)

Introduction

"Recombination with emission of photon"
"Radiative recombination"

Or "**radiative association**" for molecule formation

Atom-atom collision

A+B $\rightarrow$ AB + photon radiative association

Atom-ion collision

$A+B^+ \rightarrow AB^+$ + photon radiative association

$A+B^+ \rightarrow A^+ + B$ + photon **radiative charge transfer**

Ingredients

Scattering treatment

Potential energy curves
Long-range interactions
Transition dipole matrix elements
“oscillator strength”
Wave functions

Atom-ion C-He^+

~~$C+He^+ \rightarrow CHe^+$ + photon radiative association~~

$C+He^+ \rightarrow C^+ + He$ + photon radiative charge transfer

For modeling CO formation in SN ejecta, important to know if He^+ removed by C, S, Si, or O reactions

CO is removed by

$He^+ + CO \rightarrow He + C^+ + O$

Radiative loss cross sections

Essentially no radiative association

Use an optical potential approach for radiative charge transfer:

$$\sigma(E) \sim \frac{\pi}{k^2} \sum_J (2J+1)[1 - e^{-4\eta_J}]$$

$$\eta_{J(E)} = \frac{\pi}{2} \int_0^\infty dR \left|F_J(kR)\right|^2 A(R)$$

Cf. Babb & McLaughlin (2016)

Rate coefficients

$$\alpha(T) = \left(\frac{8}{\mu\pi}\right)^{\frac{1}{2}} \left(\frac{1}{k_B T}\right)^{\frac{3}{2}} \int_0^\infty dE\; E\; \sigma(E) e^{-E/k_B T}$$

Re-Introduction

$C + He^+ \rightarrow C^+ + He$ + photon radiative charge transfer

$C + He^+ \rightarrow C^+ + He$ nonradiative charge transfer

$C\text{-}He^+$ Kimura *et al.* (PRA 1993, PRA 1994)

$O\text{-}He^+$ Kimura *et al.* PRA (1994), Zhao et al. (2004)

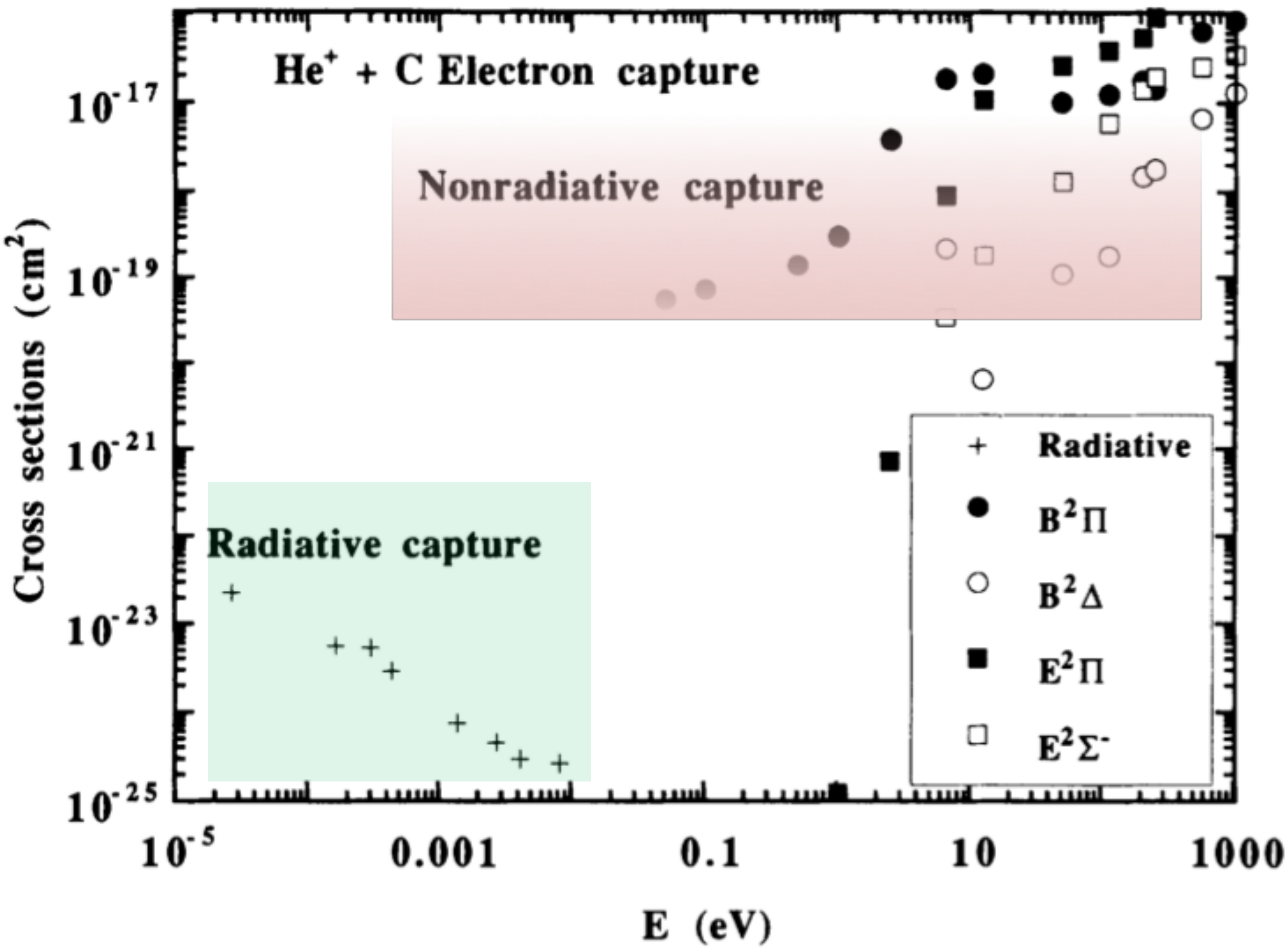
$Si\text{-}He^+$ Satta *et al.* MNRAS (2013)

$S\text{-}He^+$ …

C-He^+

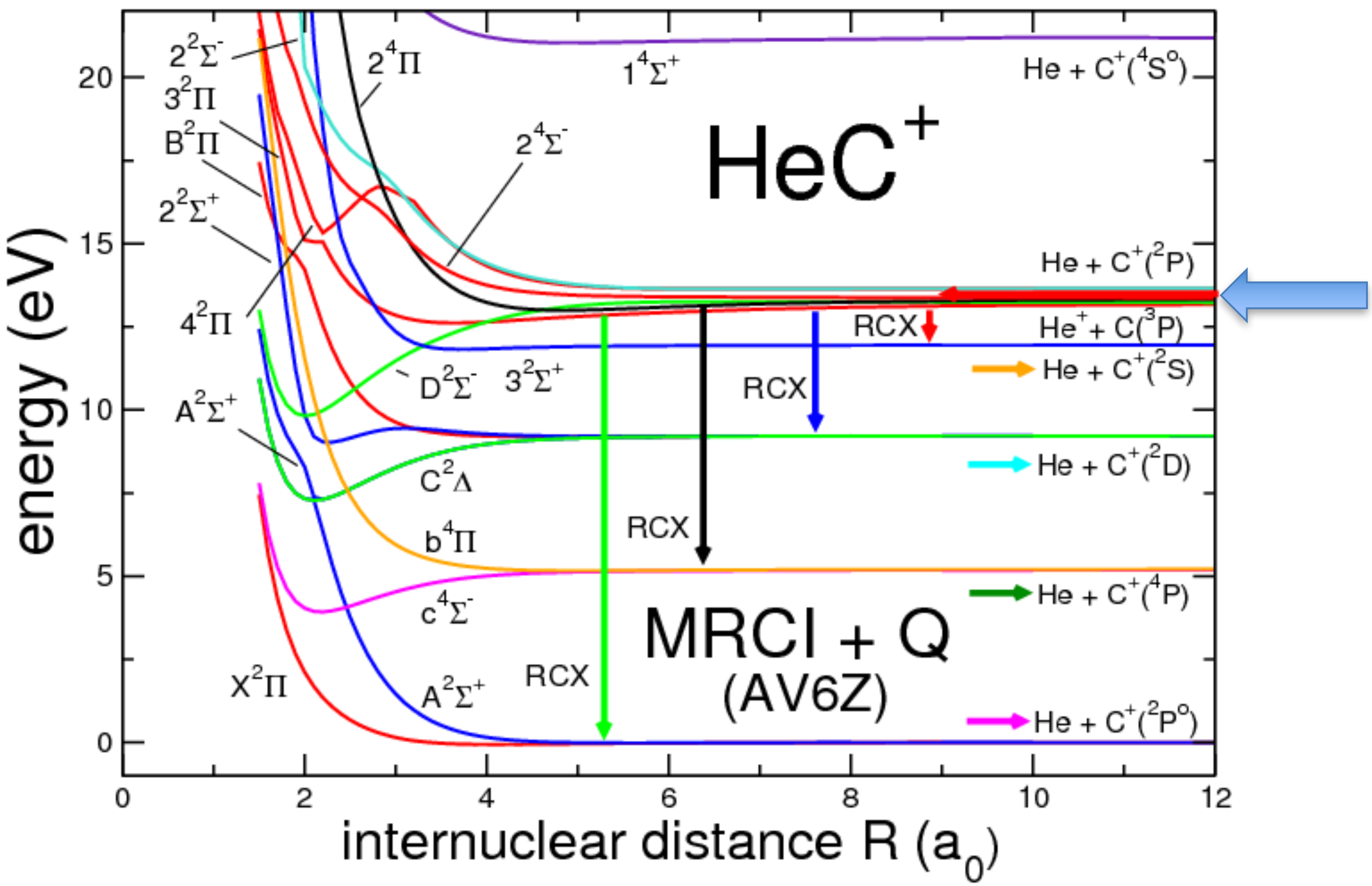
Radiative charge transfer:

Kimura, *et al.* PRA **49**, 2541 (1994)



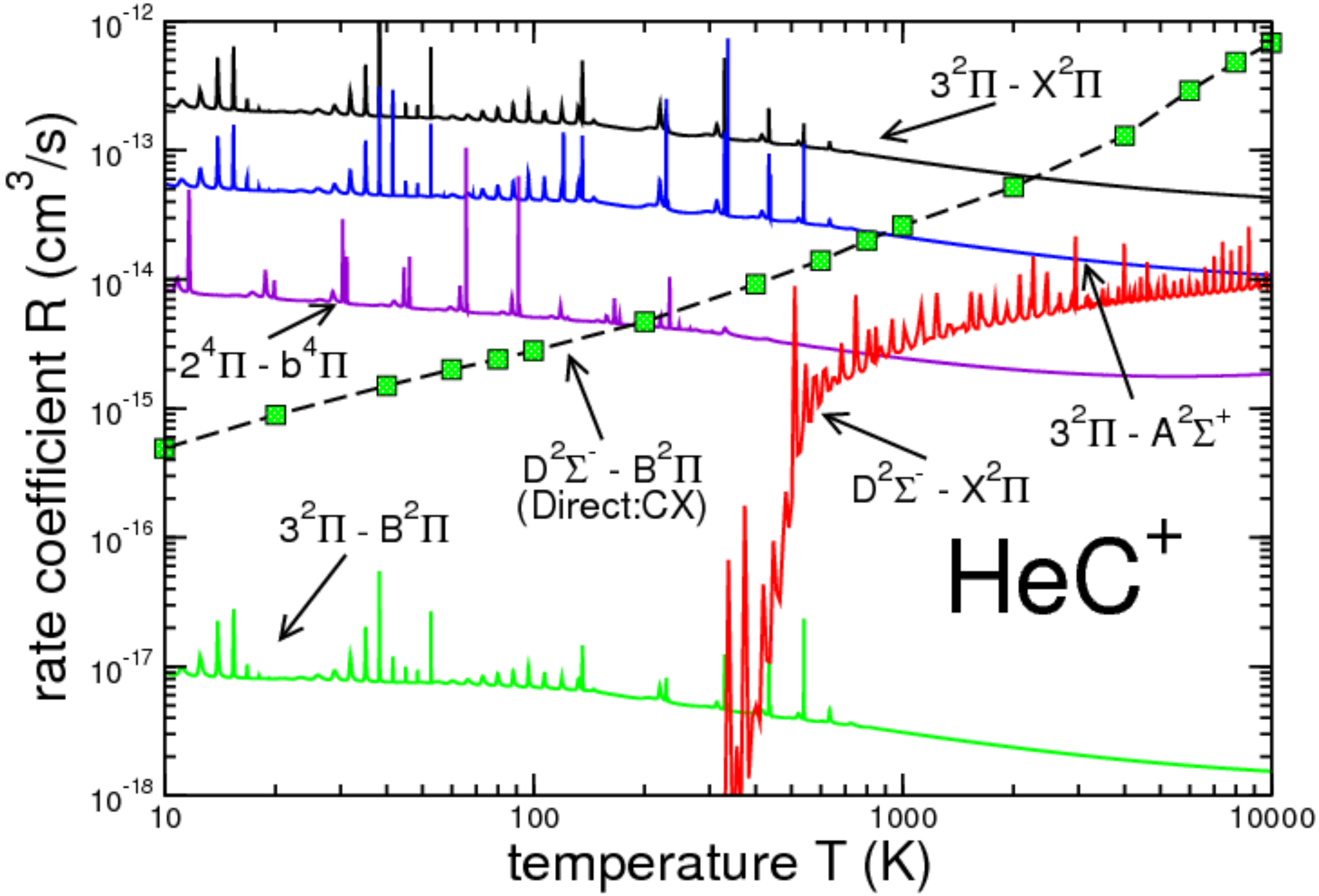
C-He$^+$ energies

MOLPRO



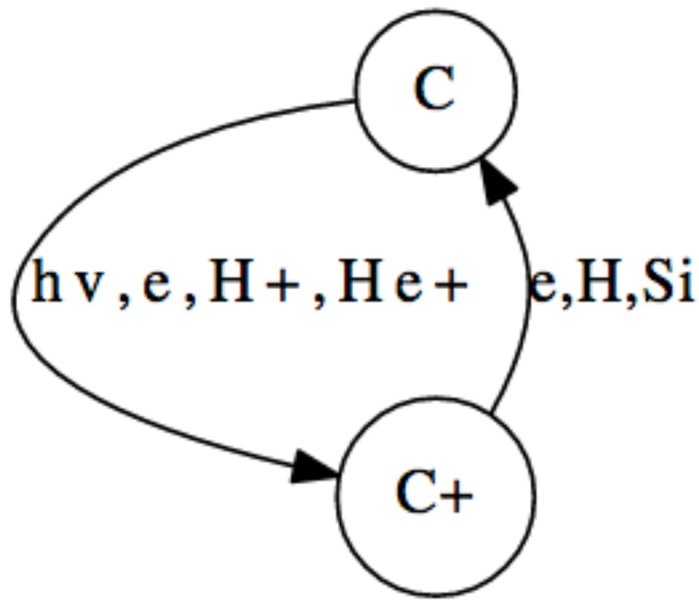
Babb & McLaughlin (2016)

C-He$^+$ rate coefficients



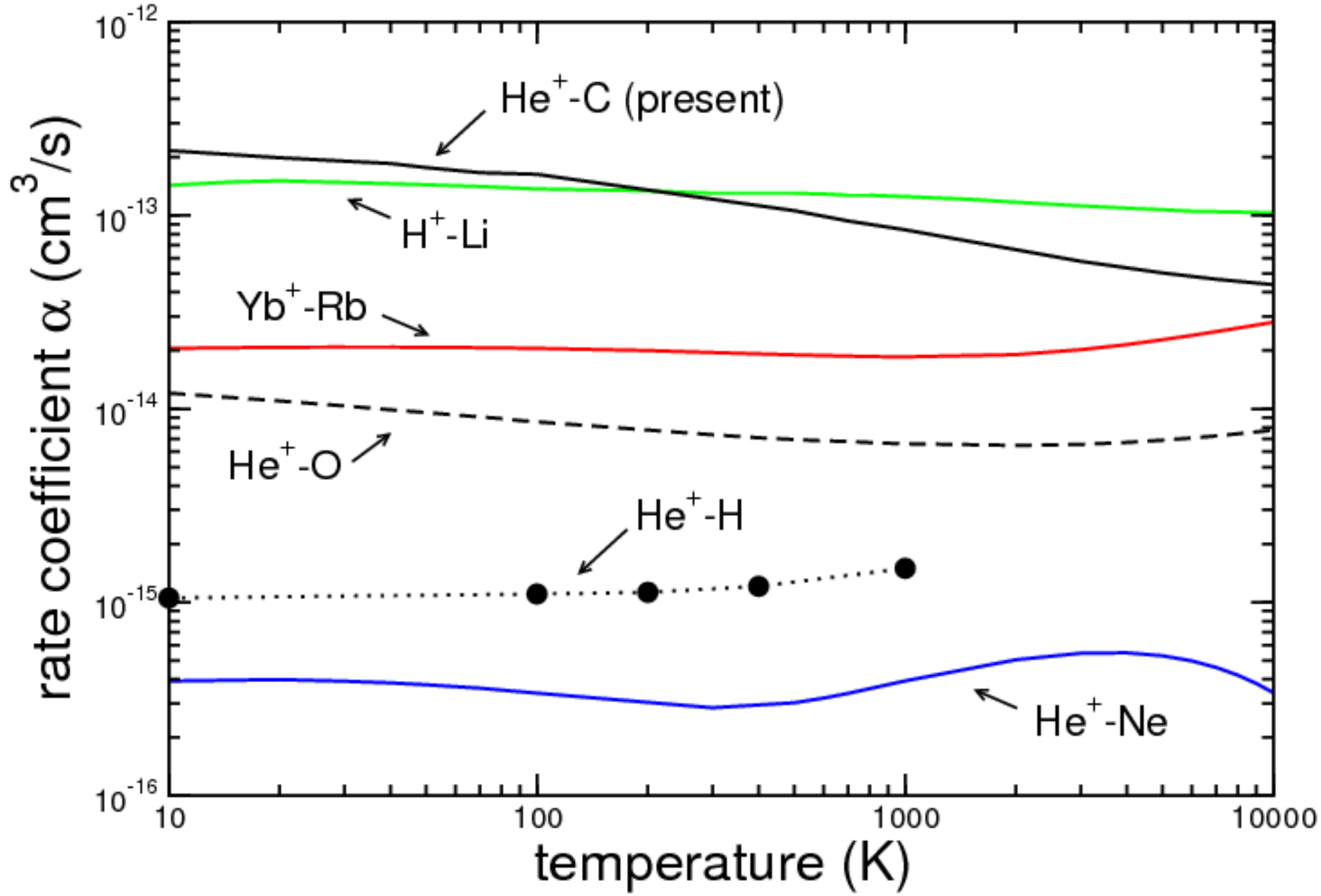
Babb & McLaughlin (2016)

C-He$^+$ network



Bovino et al. A&A 590 (2016)

Comparisons: radiative charge transfer

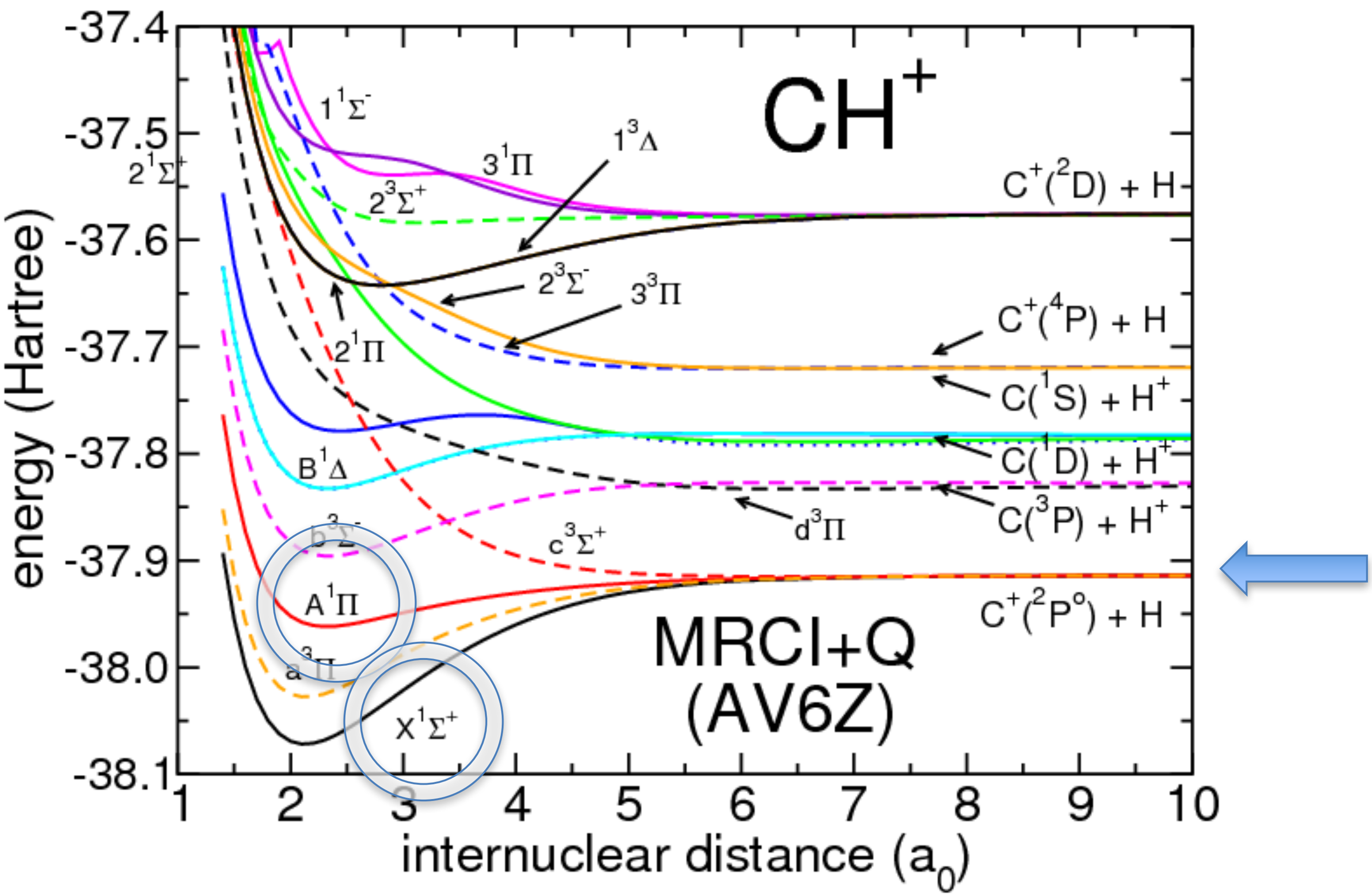


Babb & McLaughlin (2016)

CH^+ prior work radiative association

Many papers over decades, explored for formation of CH^+.

Now other mechanisms/reactions. All singlet transitions (A→X).



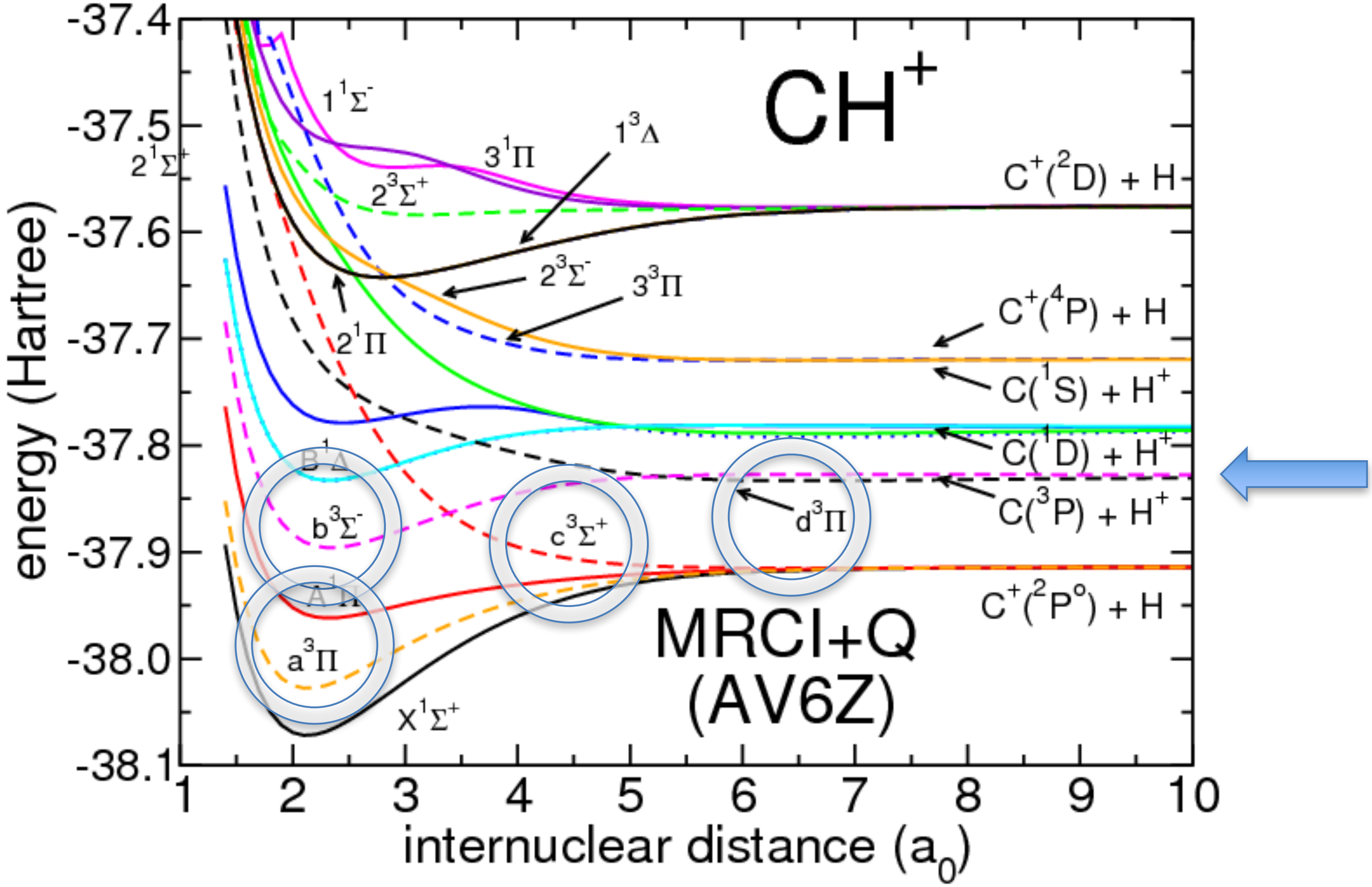
Radiative association cross sections

$$\sigma(E) \sim g \sum_{J} \sum_{v} \sigma_{vj}(E)$$

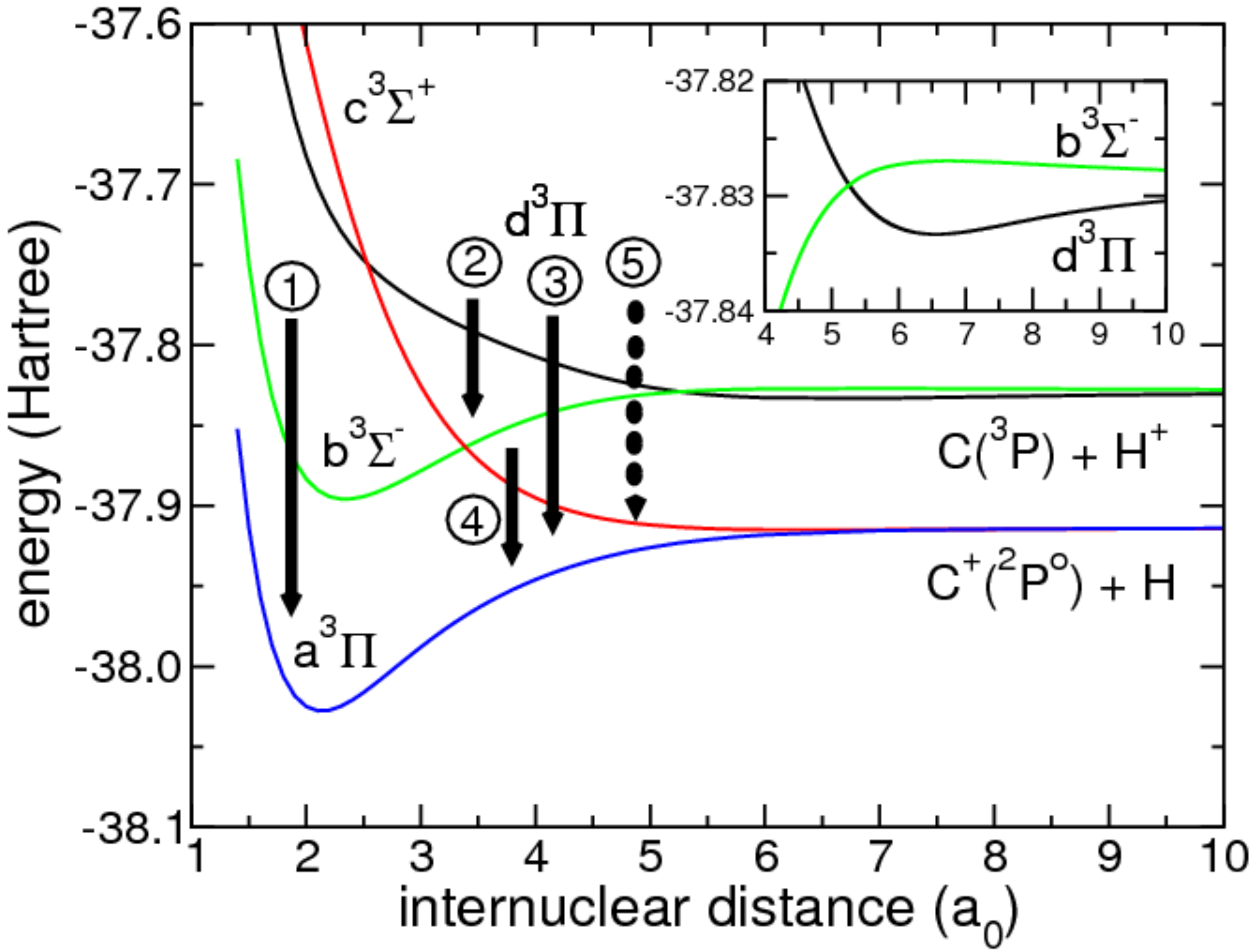
$$\sigma_{vJ}(E) \sim \frac{(h\nu)^3}{E} |\langle vJ|D(R)|k\rangle|^2$$

CH^+ prior work radiative association

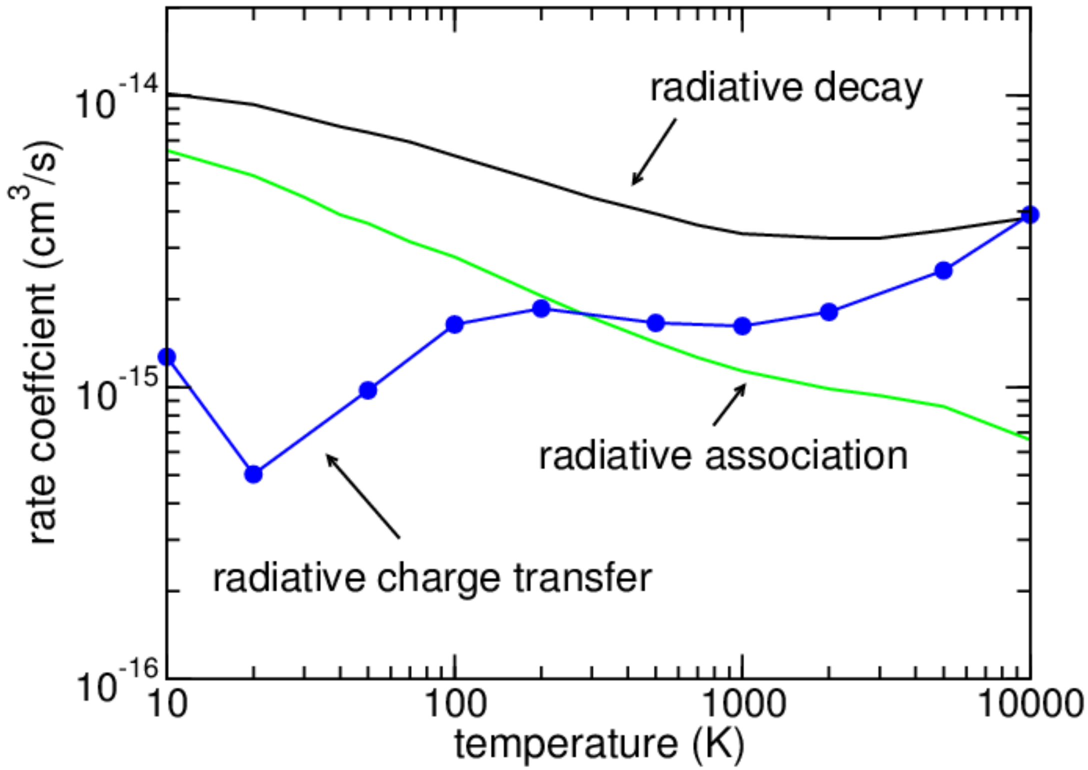
Consider, triplet transitions (d→ a), (d→ b), (d→ c), (c→ a), (b→ a)



C-H^+ radiative association / radiative charge transfer



$$C + H^+ \rightarrow CH^+ + h\nu$$
$$C + H^+ \rightarrow C^+ + H + h\nu$$



$$C + H^+ \rightarrow CH^+ + h\nu$$

rate coefficient about 100× that for

$$C^+ + H \rightarrow CH^+ + h\nu$$

… though need "C"

SiO - prior work radiative association

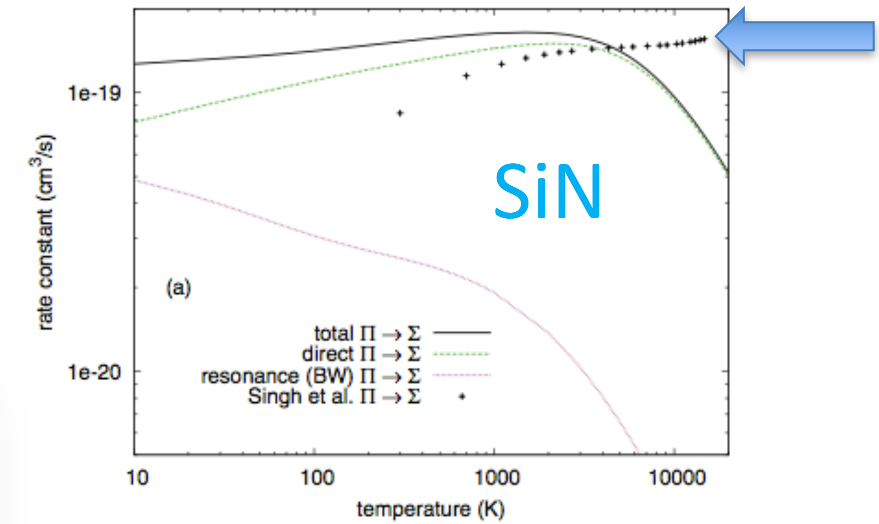
Found in Supernova 1987a "ejecta" (as was CO)

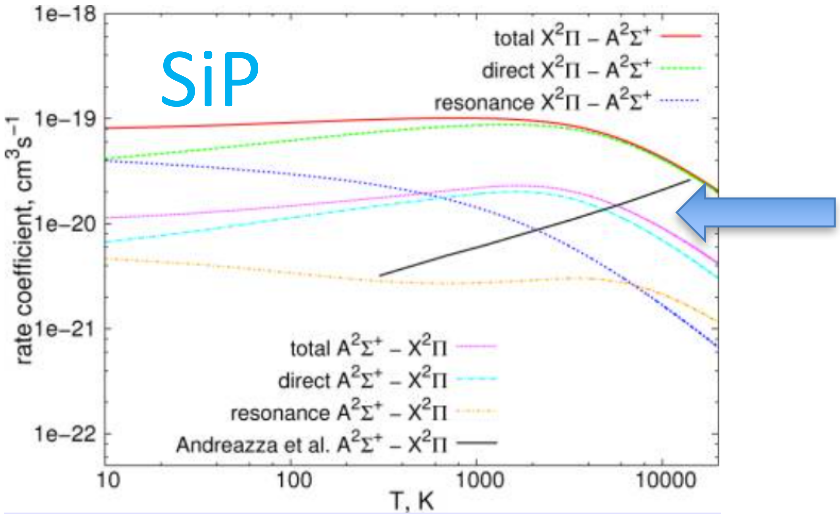
Calculations: Si+O → SiO + photon

Andreazza *et al*. ApJ (1995)

Problems?

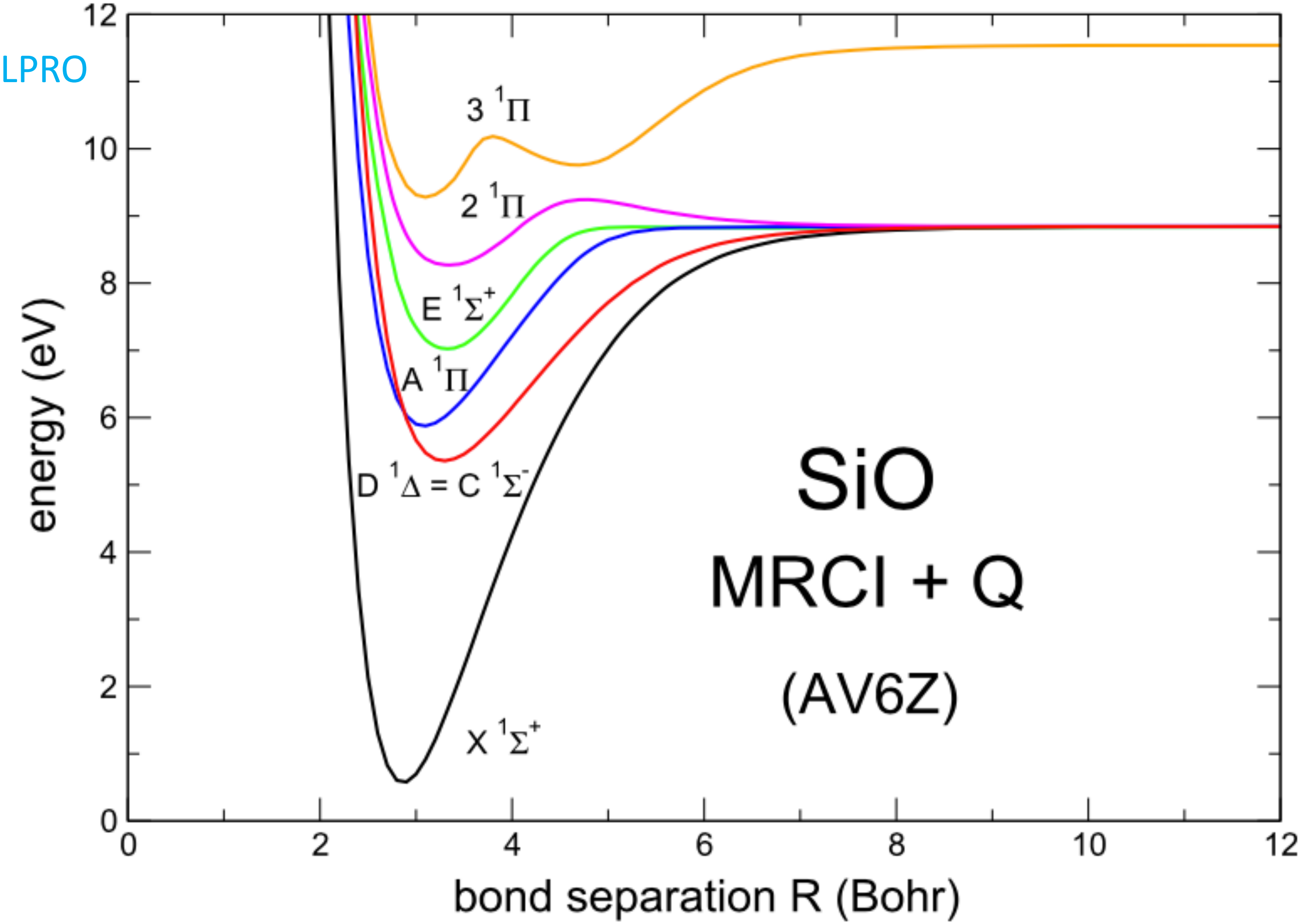
- Potential energy data
- Inconsistencies vs. Andreazza+ ApJ (2006)
- SiN — Gustafsson *et al.* JCP (2012) SiP — Golubev *et al.* JPCA (2013)





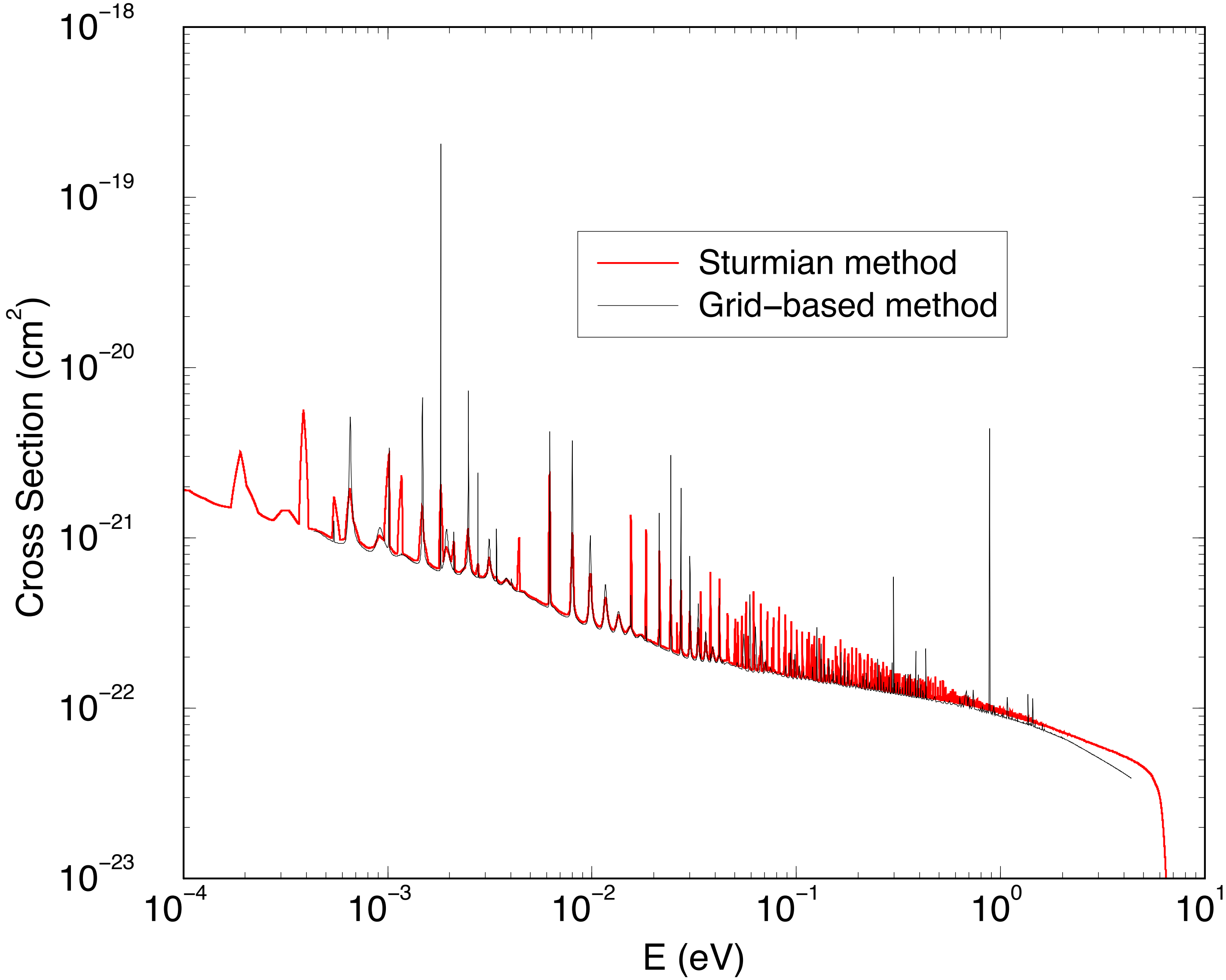
Potential energy data

MOLPRO



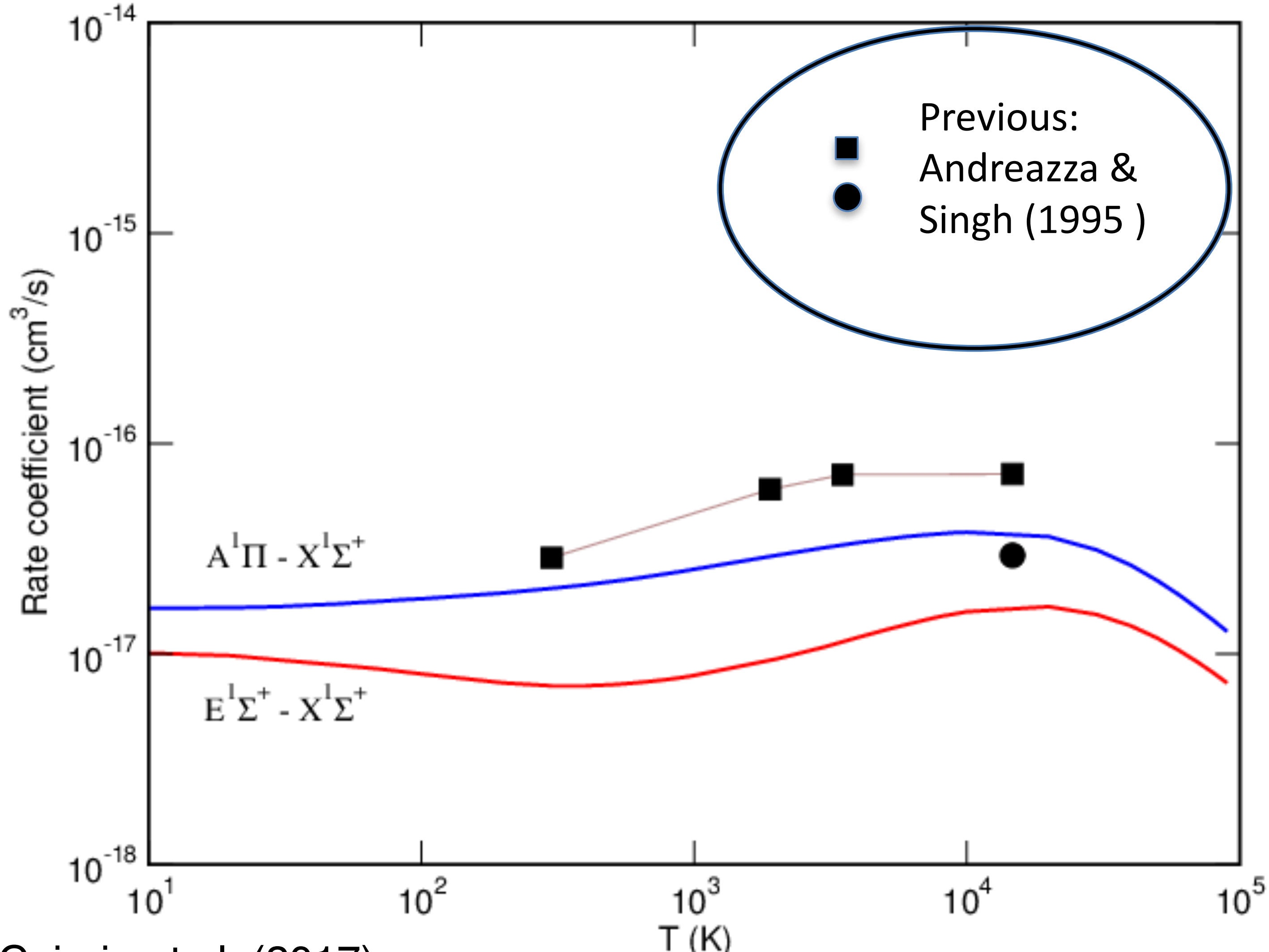
Forrey et al. (2016)

Cross sections: Two methods



Forrey et al. (2016); Cairnie et al. (2017)

Rate coefficients



Cairnie et al. (2017)

Postdoctoral fellowship in theoretical astrochemistry.

Research areas include, but are not limited to, primordial chemistry, and atomic and molecular processes in interstellar space and exoplanet atmospheres.

Applications deadline November 17, 2017.

Interested applicants are encouraged to visit itamp.harvard.edu for further information and access the online application process.

Acknowledgments

B. McLaughlin (Queen's U. Belfast)

P. Stancil (U. Georgia), SiO

R. Forrey (Penn State Berks), SiO

ITAMP (NSF)

If you have ideas for workshops or visits ...
itamp.harvard.edu