The University of Georgia

Computation of Rovibrationally-Resolved Photodissociation Cross Sections for interstellar, circumstellar, and stellar atmospheric environments

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Who Did the Work

UGA

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Past Funding: NASA NSF

Main Points

- Photodissociation from excited rovibrational (RV) levels (v,J) - not just from v=0,J=0
- In ``high density'' environments, photodissociation (PD) from a thermal (LTE) distribution may be most relevant
- Electronic transitions to high-lying electronic states - even beyond the Lyman limit
- Photoionization may be important when threshold is near the Lyman Limit (H_2)
- Diatomic PD cross sections are relatively straight-forward

Outline

- Photodissociation processes
- Calculation details
- New cases: NH and SH^+
- Survey of prior results
- Summary

Photodissociation Processes

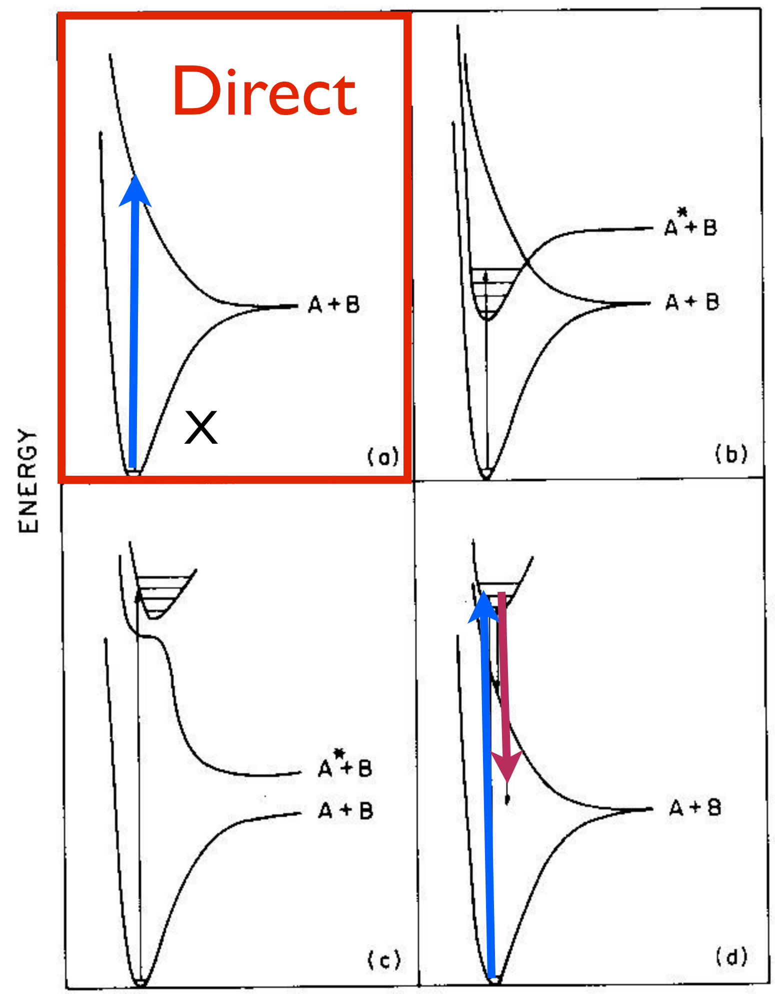
- Photodissociation due to UV photons is the primary destruction process for most molecules
- Two processes are usually dominant
- Direct photodissociation:

$$AB + h\nu \rightarrow A + B$$

- UV absorption followed by fluorescence to the continuum (Solomon process) - H_2, CO:

$$AB + h\nu \rightarrow AB^*$$

$$AB^* \rightarrow A + B + h\nu'$$



From van Dishoeck (1993)

Photodissociation Processes

- The direct photodissociation rate for molecule AB

  given by $$\Gamma_{AB}(A_V) = 4\pi \int_{\lambda_{min}}^{\lambda_{max}} J_\lambda(A_V)\sigma_{AB}(\lambda)d\lambda$$

- where J_λ is the mean intensity of radiation at depth A_V
- σ_{AB} is the photodissociation cross section given by

$$\sigma_{AB}(E_{ph}) \propto E_{ph}|\langle\chi_{fk'J'}(R)|D_{fi}(R)|\chi_{iv"J"}(R)\rangle|^2$$

Our Approach

- Start with accurate molecular potentials and transition dipole moment (TDM) functions: MRCI-Q, if available
- Shift potentials to match experimental asymptotic atomic energies, known dissociation energies, ...
- Obtain accurate rovibrational (RV) energies of the ground electronic state (X) - Numerov
- Extend TDMs to separated- and united-atom limits
- Compute matrix elements with 2-channel Fermi Golden rule approximation (neglect nonadiabatic couplings)

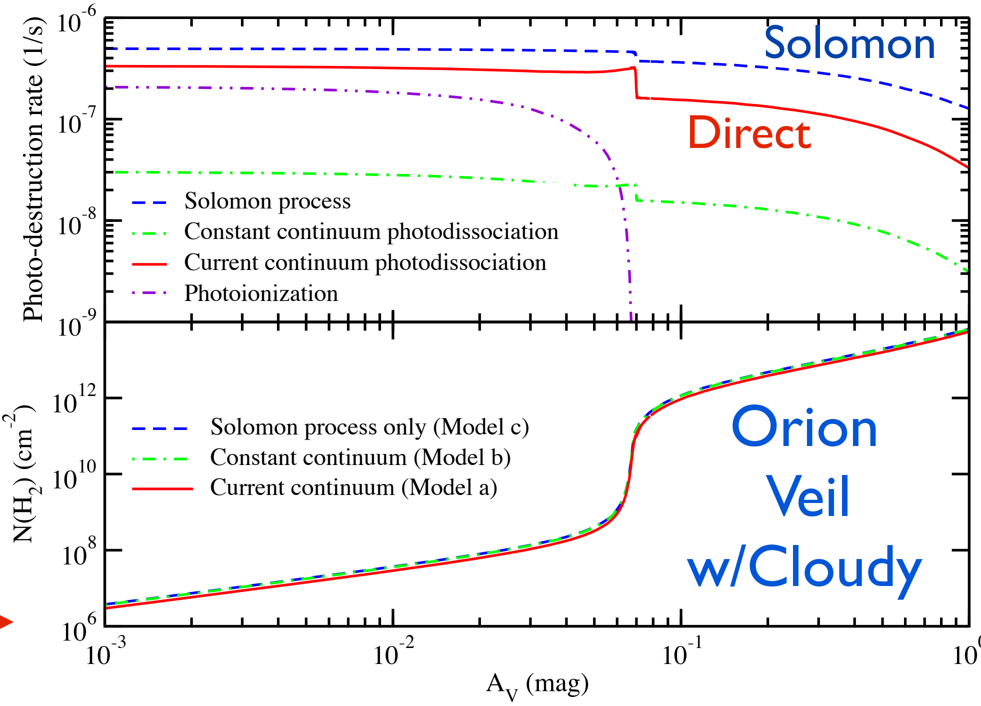
Our Approach

- Compute cross sections from all RV levels, from threshold to high photon energies (10-50 nm)
- Repeat for multiple electronic transitions
- Provide RV-resolved and LTE cross sections
- In some cases, pure rovibrational dissociation transition (within X) is important (HeH^+, LiH, LiH^+)
- Neglect: spin-splitting, Λ-doubling, fine-structure, vibrational coupling, ...

Applications

- Astrochemistry: molecule destruction process in chemical networks
  - Cool gas, low density → photo-rates for v=0,J=0
  - Warm gas, low density (levels not in LTE) → PD from excited v,J - usually *not* treated (e.g. PDRs)
  - Warm gas, high density (levels in LTE) → LTE PD cross sections - usually *not* treated (e.g. PPDs)

H_2 photo-destruction rates



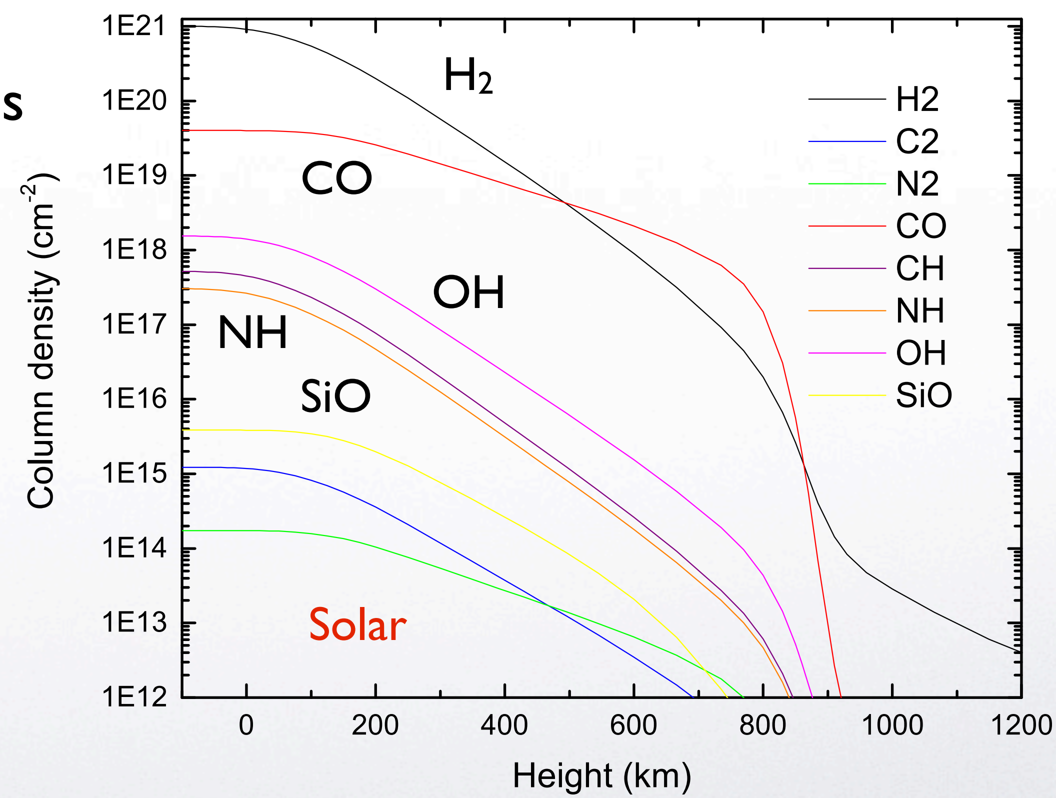
H_2 column density

From Gay et al. 2012, ApJ, 746, 78

Applications

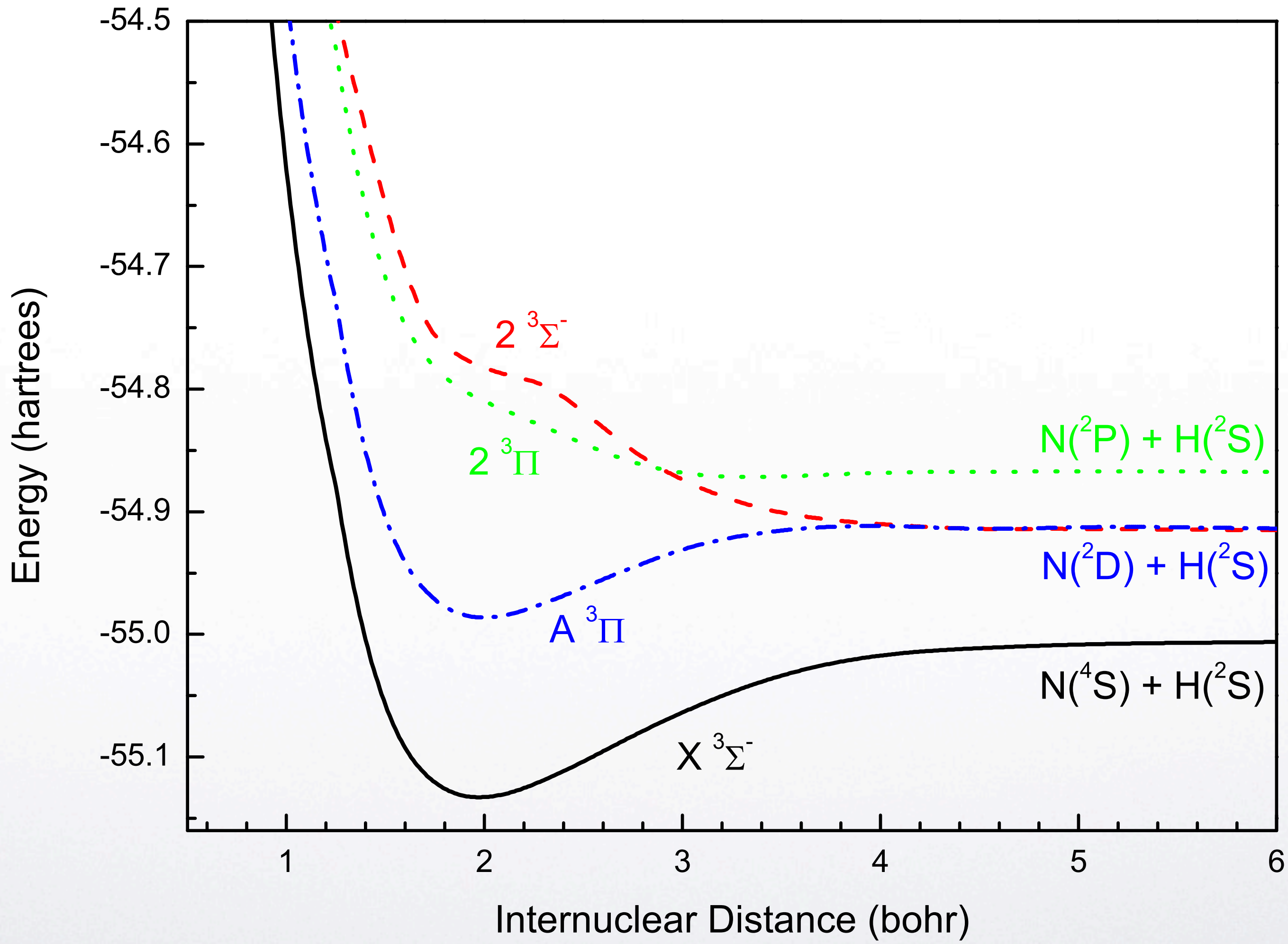
- Continuum opacity (high density): removal of UV photons

  - Cool gas → v=0, J=0 PD cross sections (planetary)
  - Warm gas → LTE PD cross sections (solar, stellar)



Fontenla et al. 2015, ApJ, to be submitted

NH Photodissociation

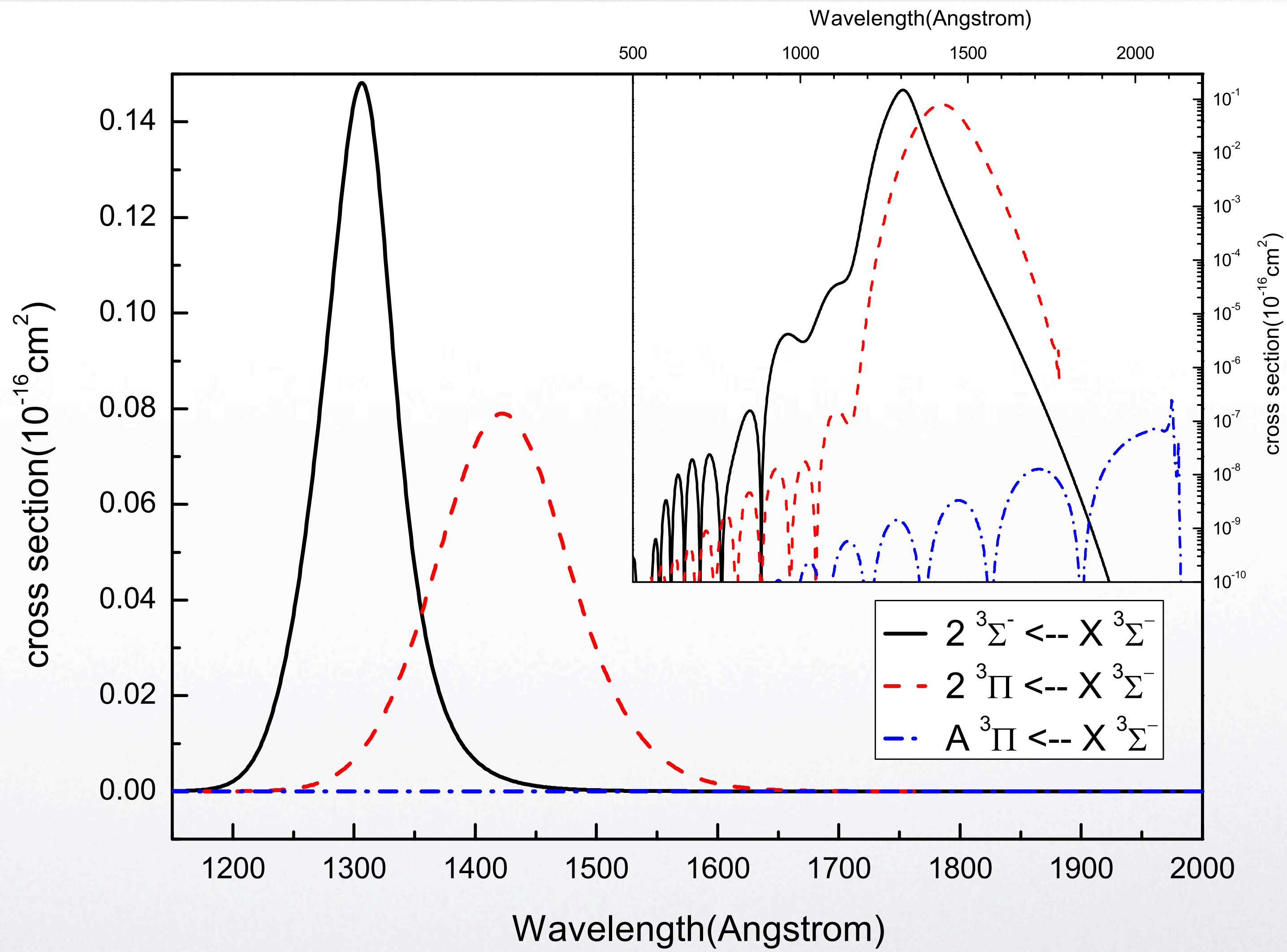


Goldfield & Kirby, 1987, J. Chem. Phys., 94,2

NH Potential Energies

NH Photodissociation

- 3 electronic transitions considered
- Transitions to the A $^3\Pi$ not important
- Good agreement with Kirby & Goldfield (1991, J. Chem. Phys., 87, 7)

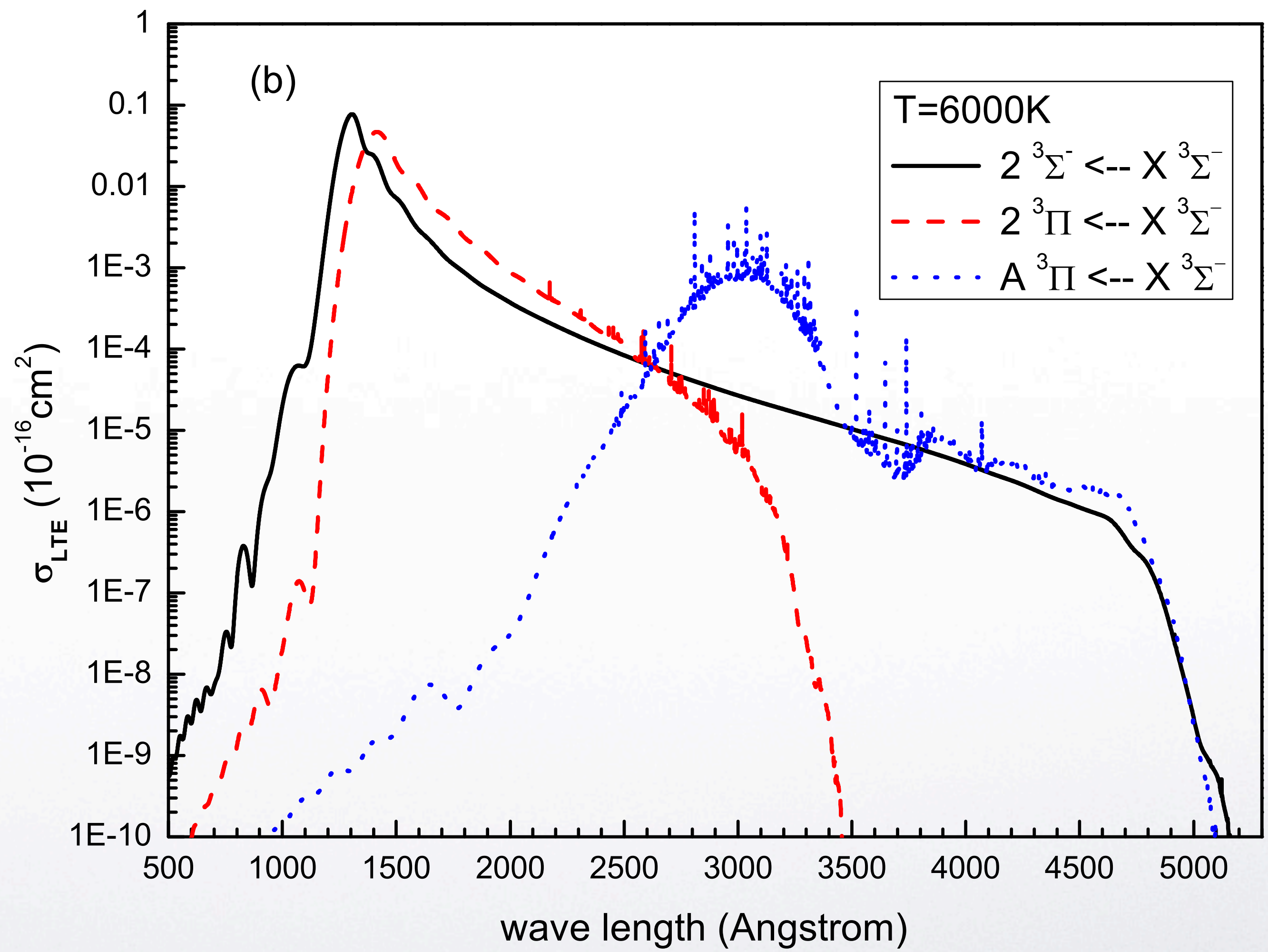


Shen et al., 2015, ApJ, to be submitted

NH(v=0,J=0) Cross Sections

NH Photodissociation

- RV-excited and LTE not previously calculated
- 577 rovibrational levels included
- A $^3\Pi$ gives significant cross section near 3000 angstroms

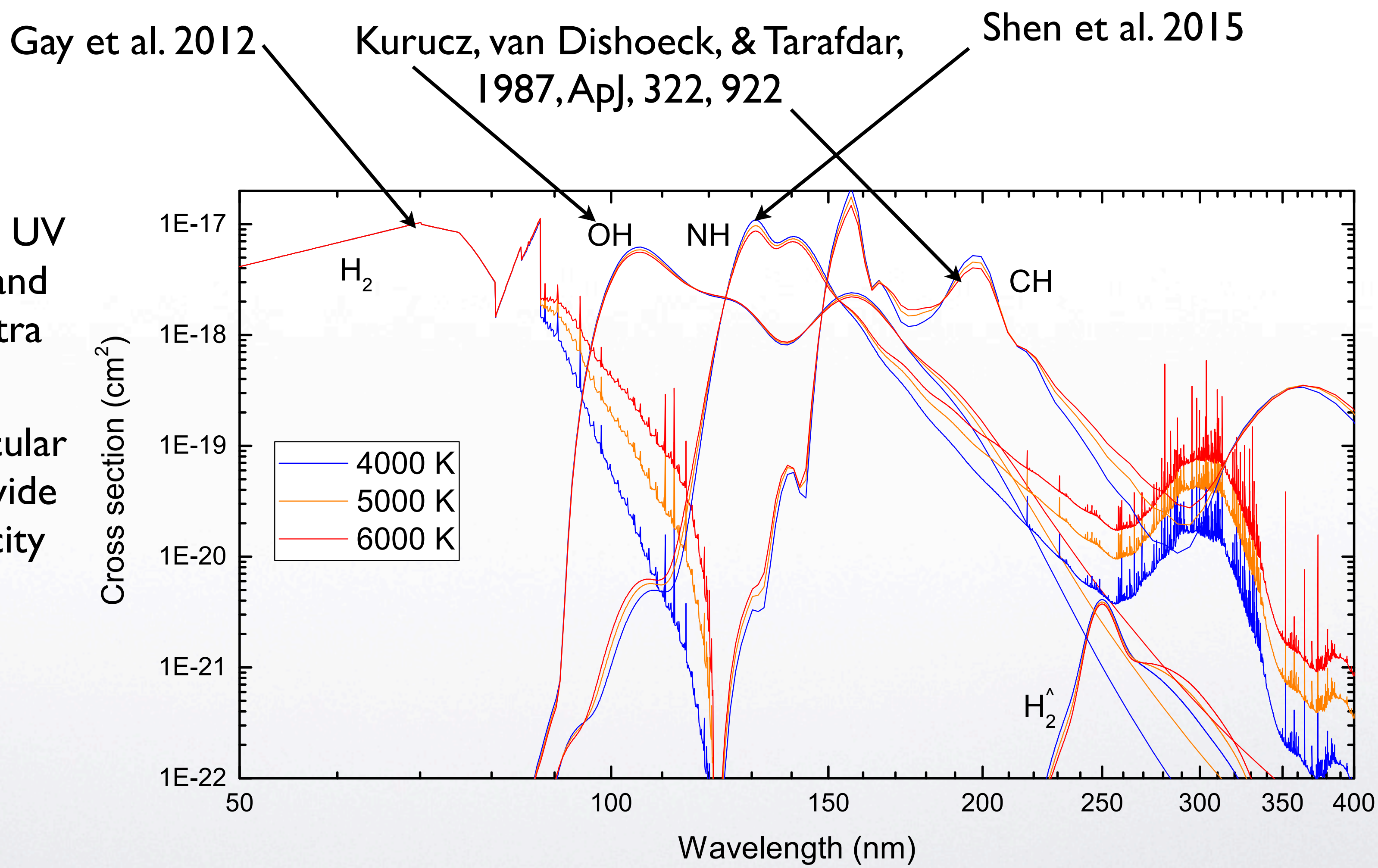


Shen et al., 2015, ApJ, to be submitted

NH LTE Cross Sections

NH Photodissociation

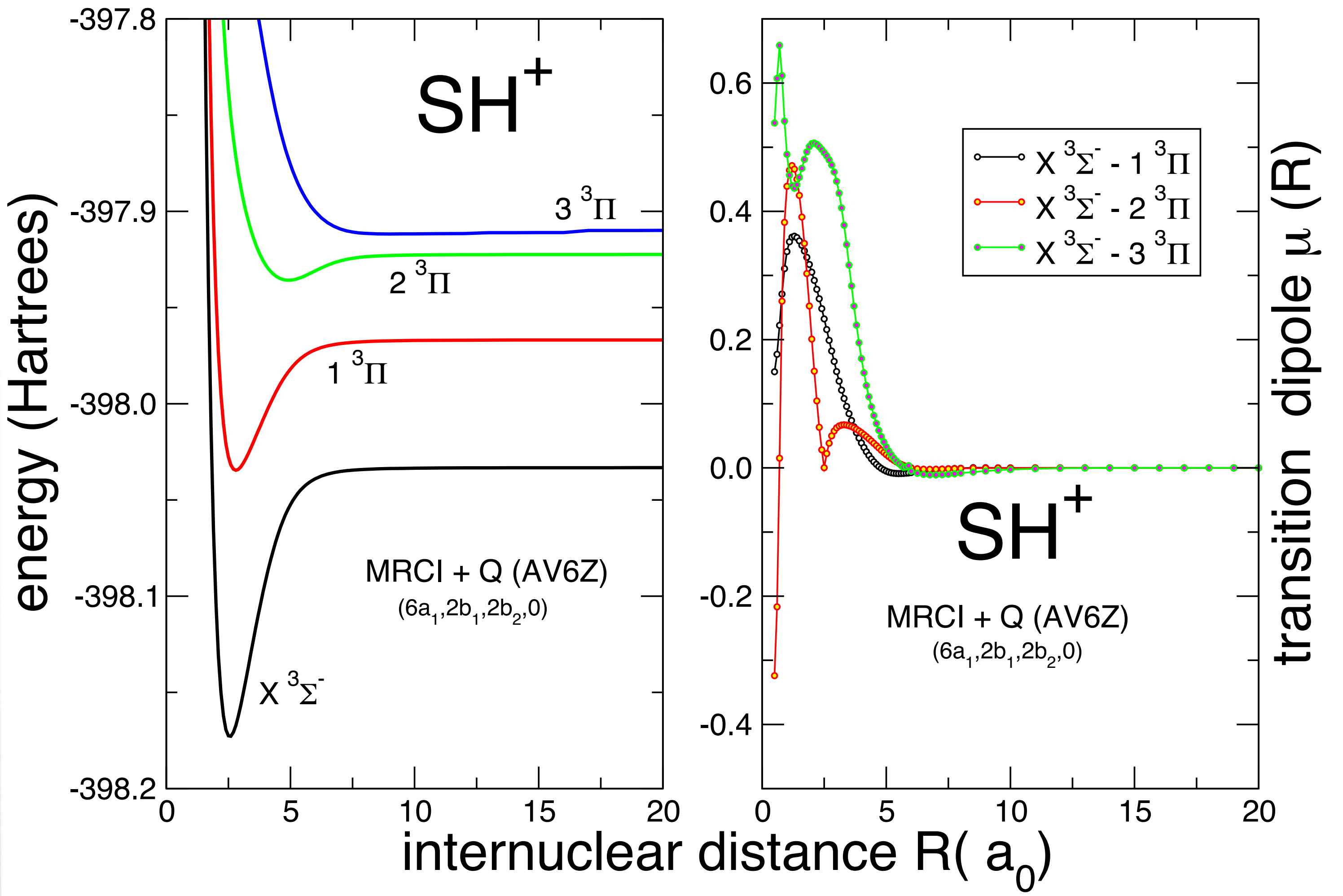
- Problem: missing UV opacity in solar and cool stellar spectra
- Dominant molecular species may provide this missing opacity



Fontenla et al. 2015, ApJ, to be submitted

Diatomic LTE Opacities

SH^+ Photodissociation

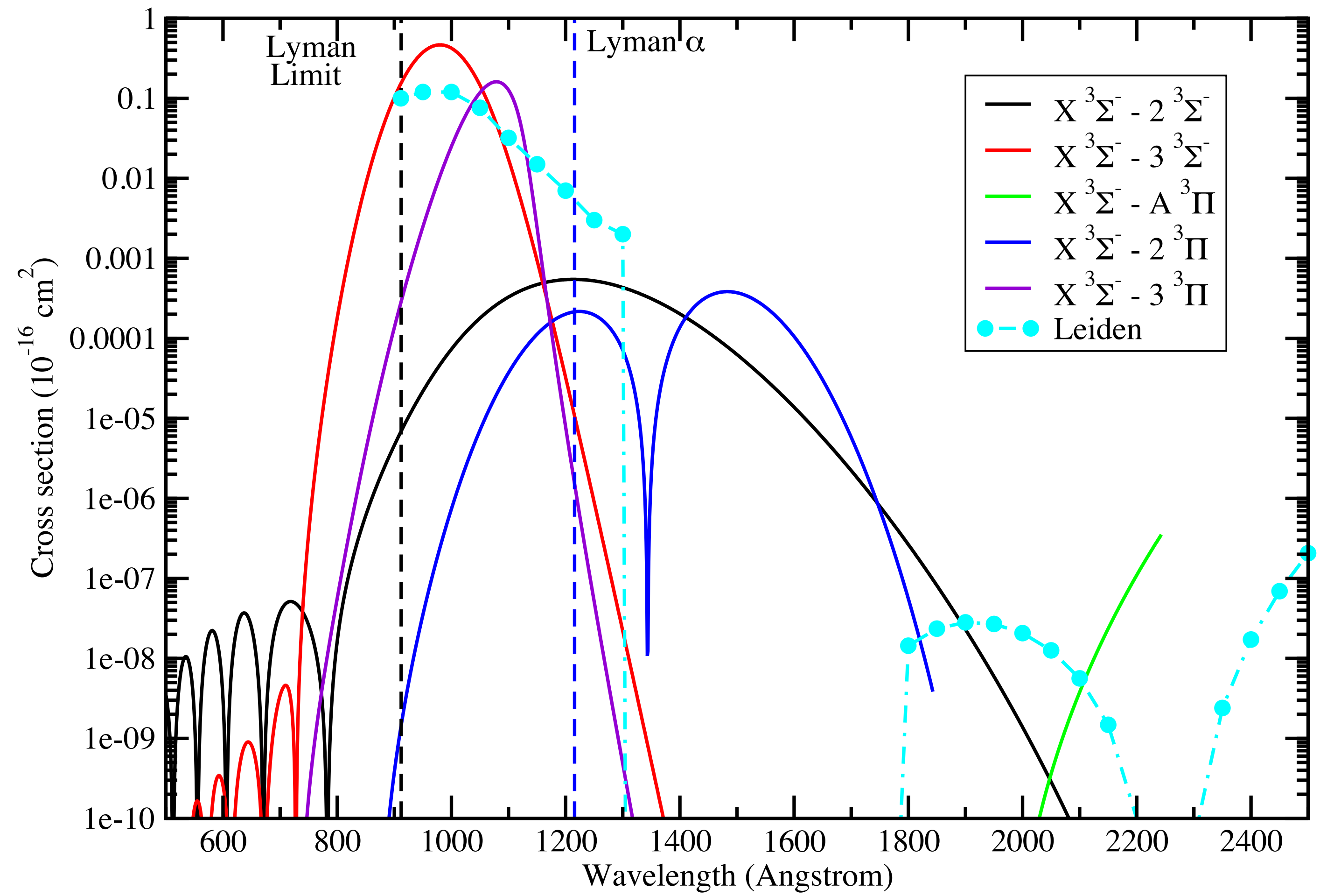


McMillan et al., 2015 ApJ, in prep.

SH^+ Potentials and TDMs

SH$^+$ Photodissociation

- 5 electronic transitions considered
- Transitions to the 3 $^3\Sigma^-$ and 3 $^3\Pi$ dominate
- RV-excited and LTE cross sections in progress
- SH$^+$ observed in Orion Bar (Nagy et al. 2013, A&A, 550, A96)

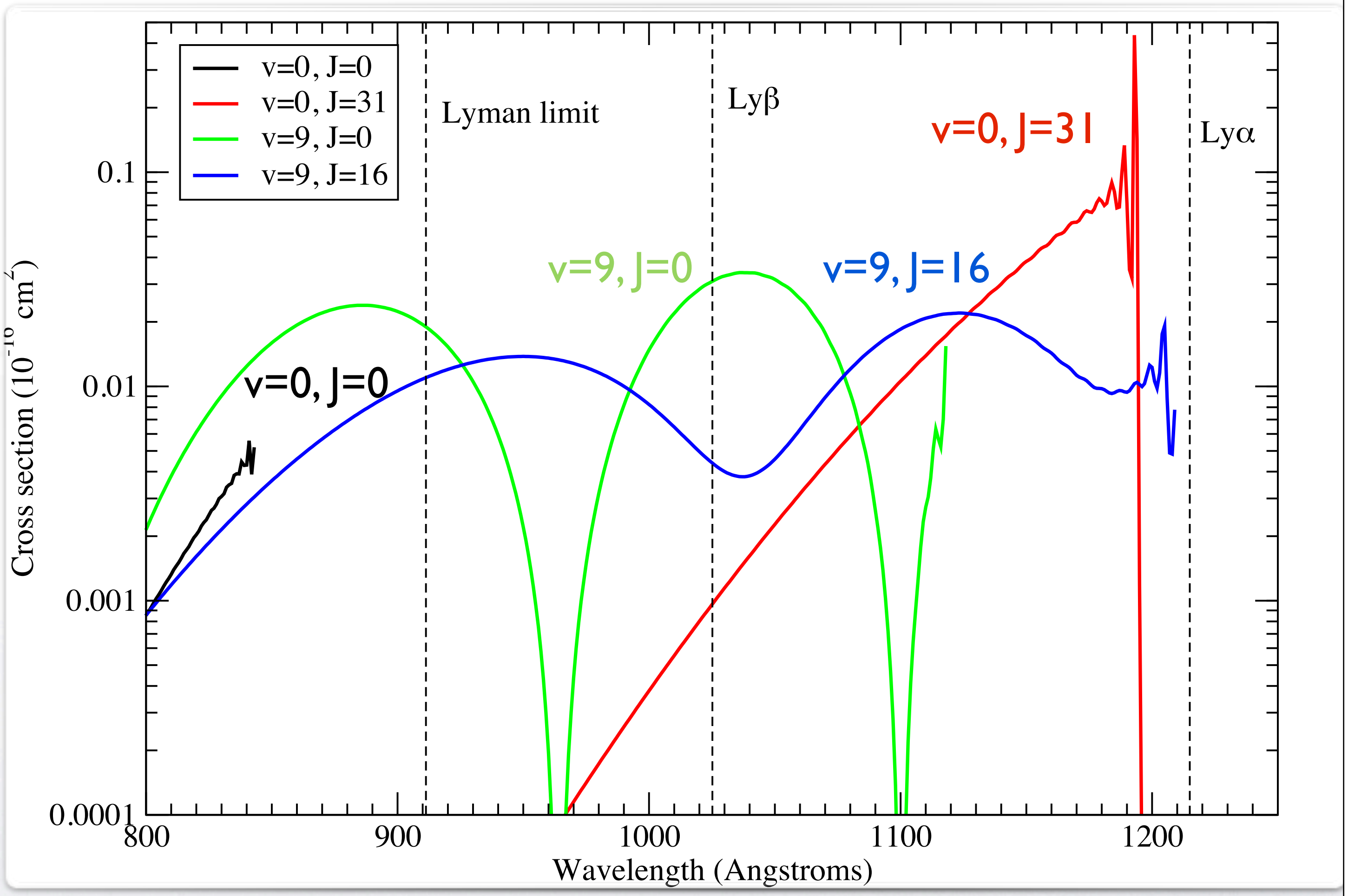


McMillan et al., 2015 ApJ, in prep.

SH$^+$(v=0,J=0) Cross Sections

H_2 Lyman and Werner Continua

- v=0-14 PD cross sections computed by Allison & Dalgarno (1969, At. Data, 1, 92), only J=0
- We did all 301 RV levels
- Get good agreement with Allison & Dalgarno
- Resolve resonances

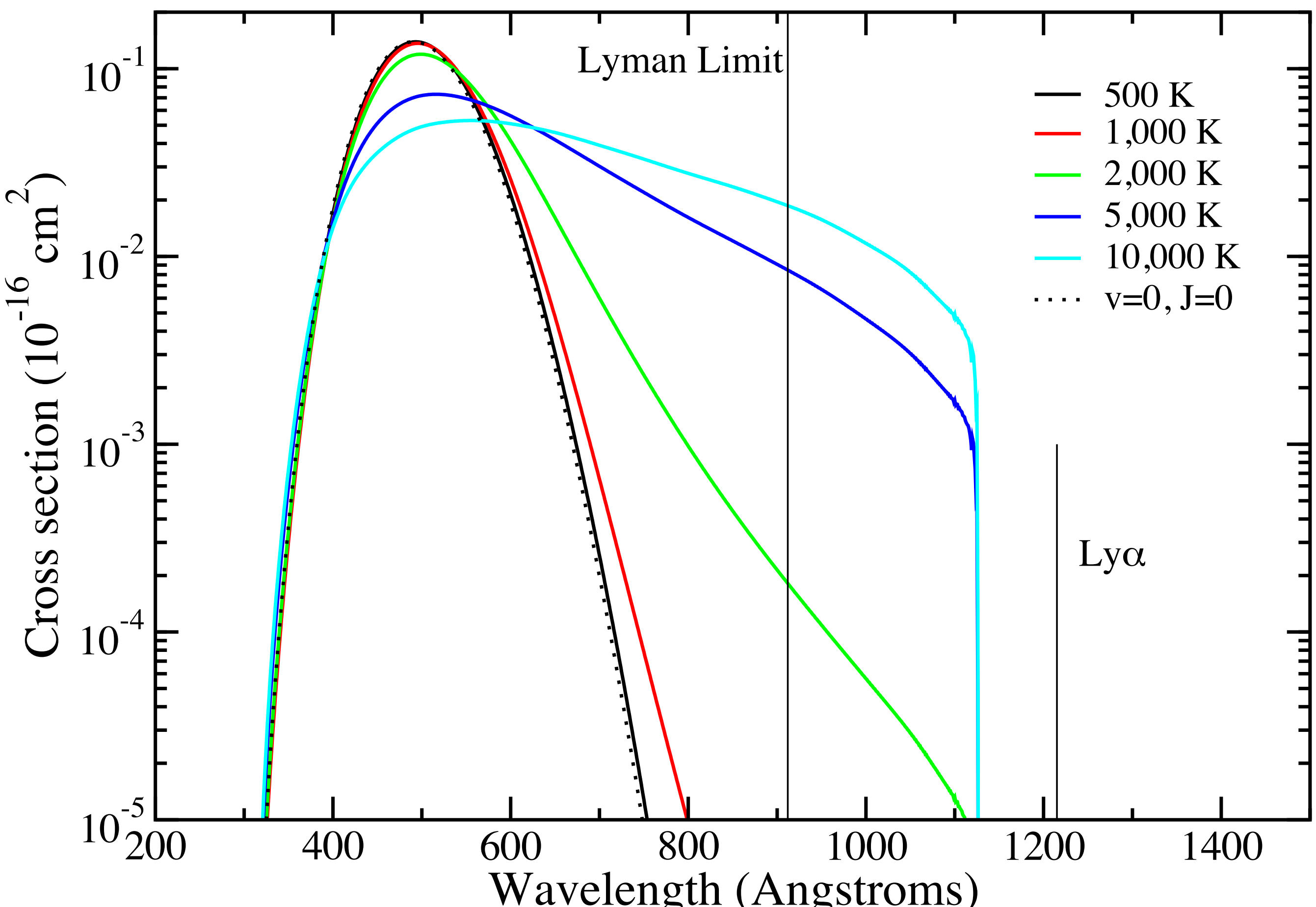


Gay et al. 2012, ApJ, 746, 78

H_2 Photodissociation Cross Sections

HeH^+ Photodissociation

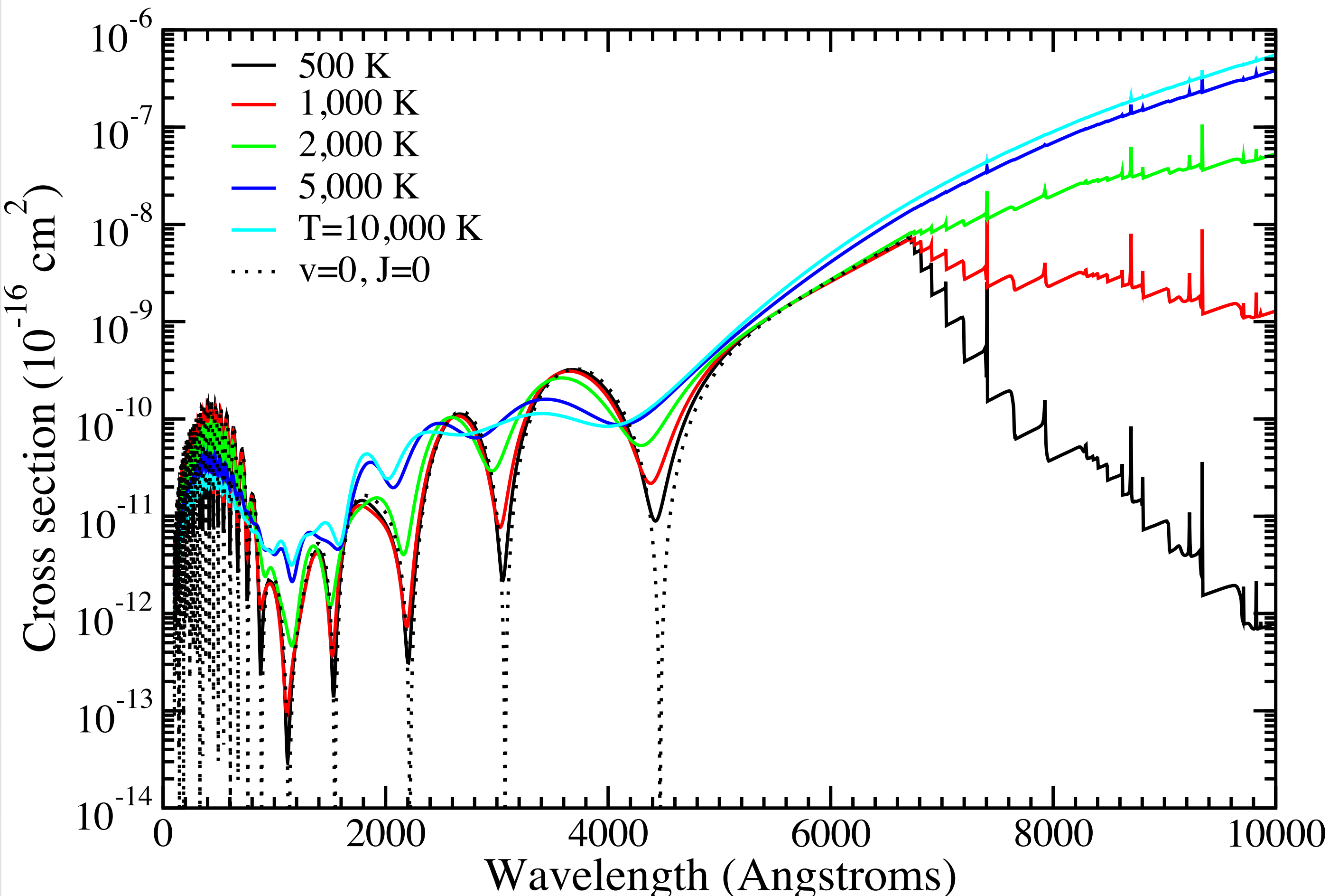
$$A^1\Sigma^+ \leftarrow X^1\Sigma^+$$



Miyake et al. 2011, ApJ, 735, 21

HeH^+ LTE Cross Sections

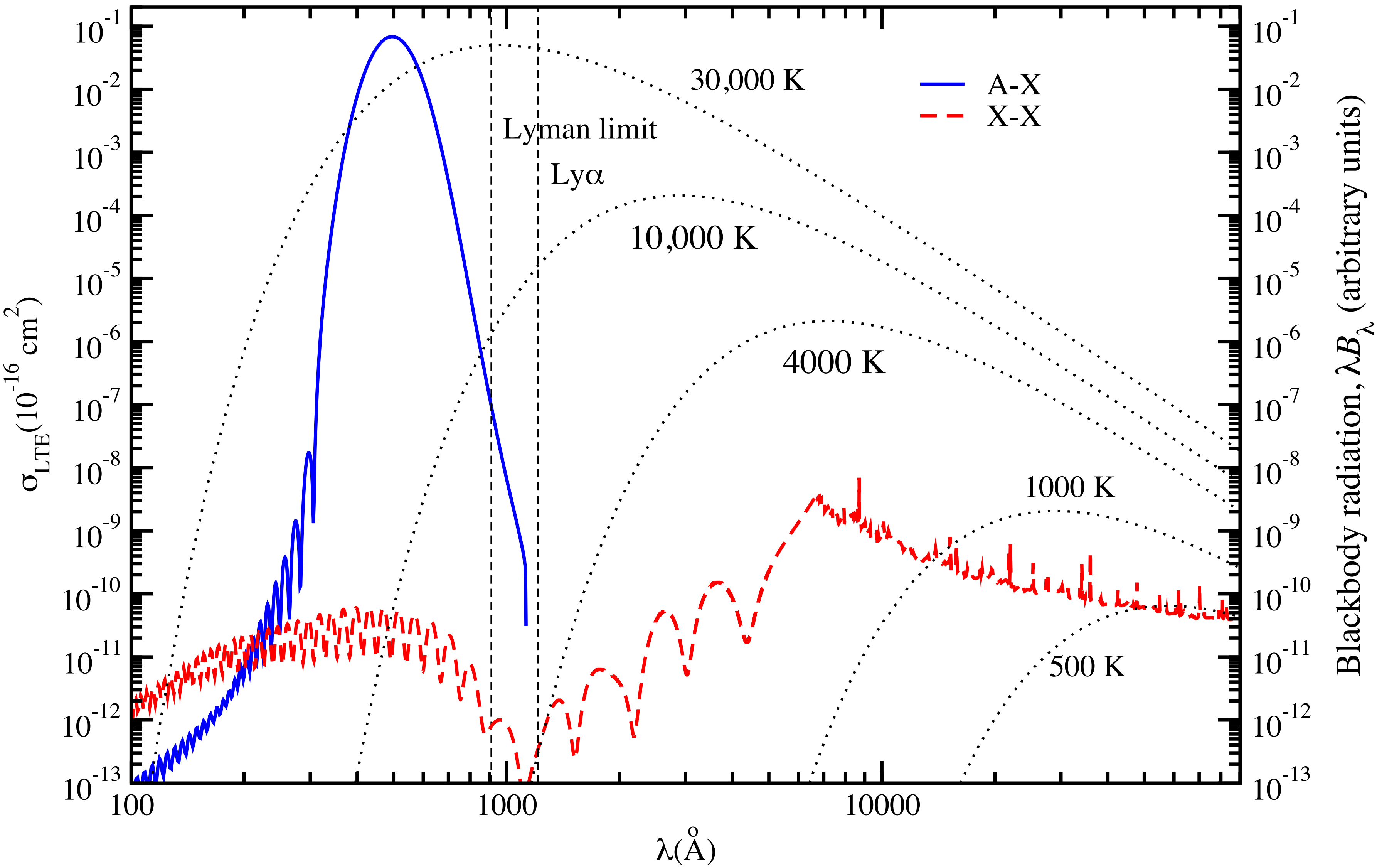
HeH^+ Photodissociation



Miyake et al. 2011, ApJ, 735, 21

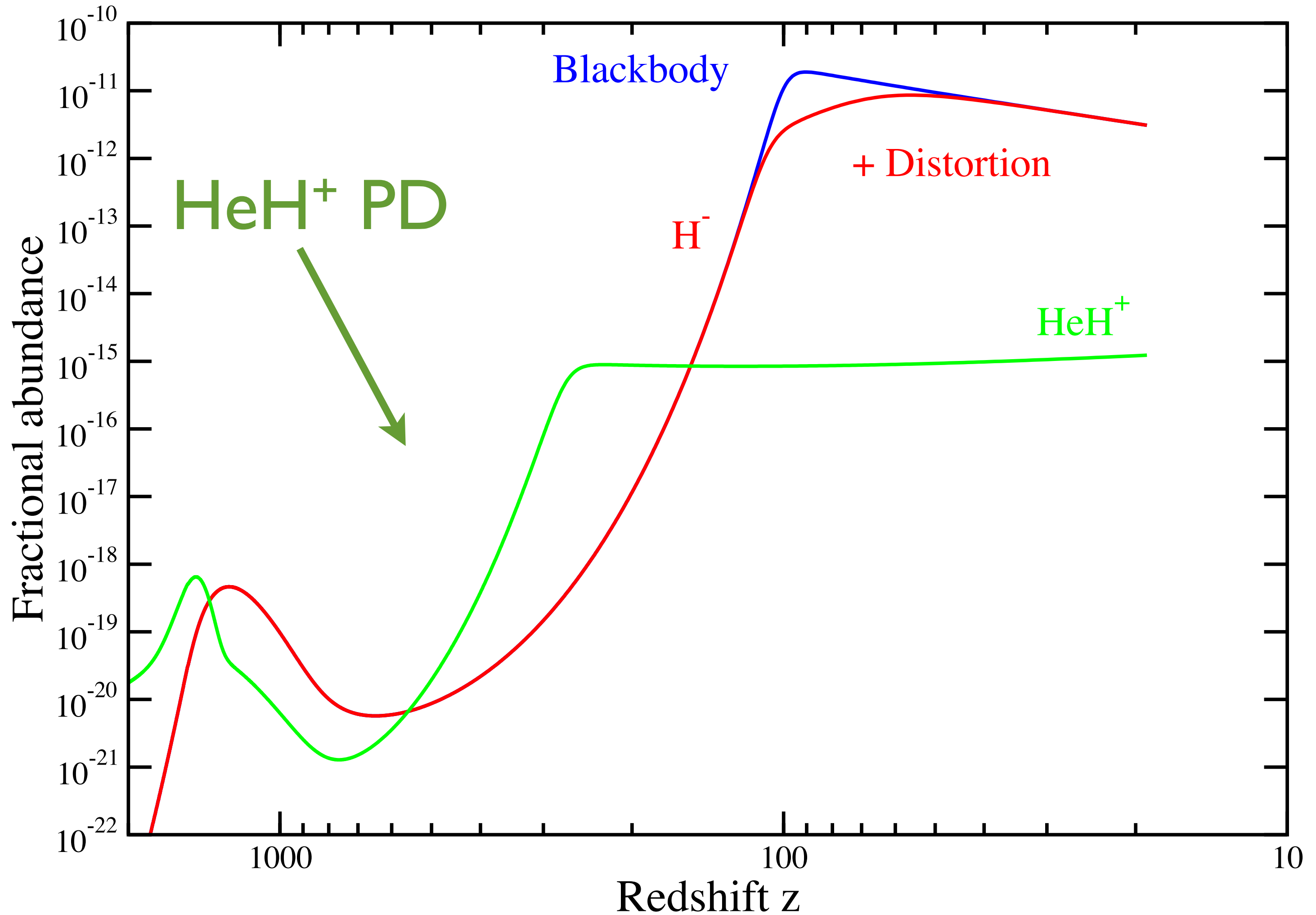
HeH^+ LTE Rovibrational in X

Early Universe



HeH^+ LTE Rovibrational (1000 K)

Early Universe

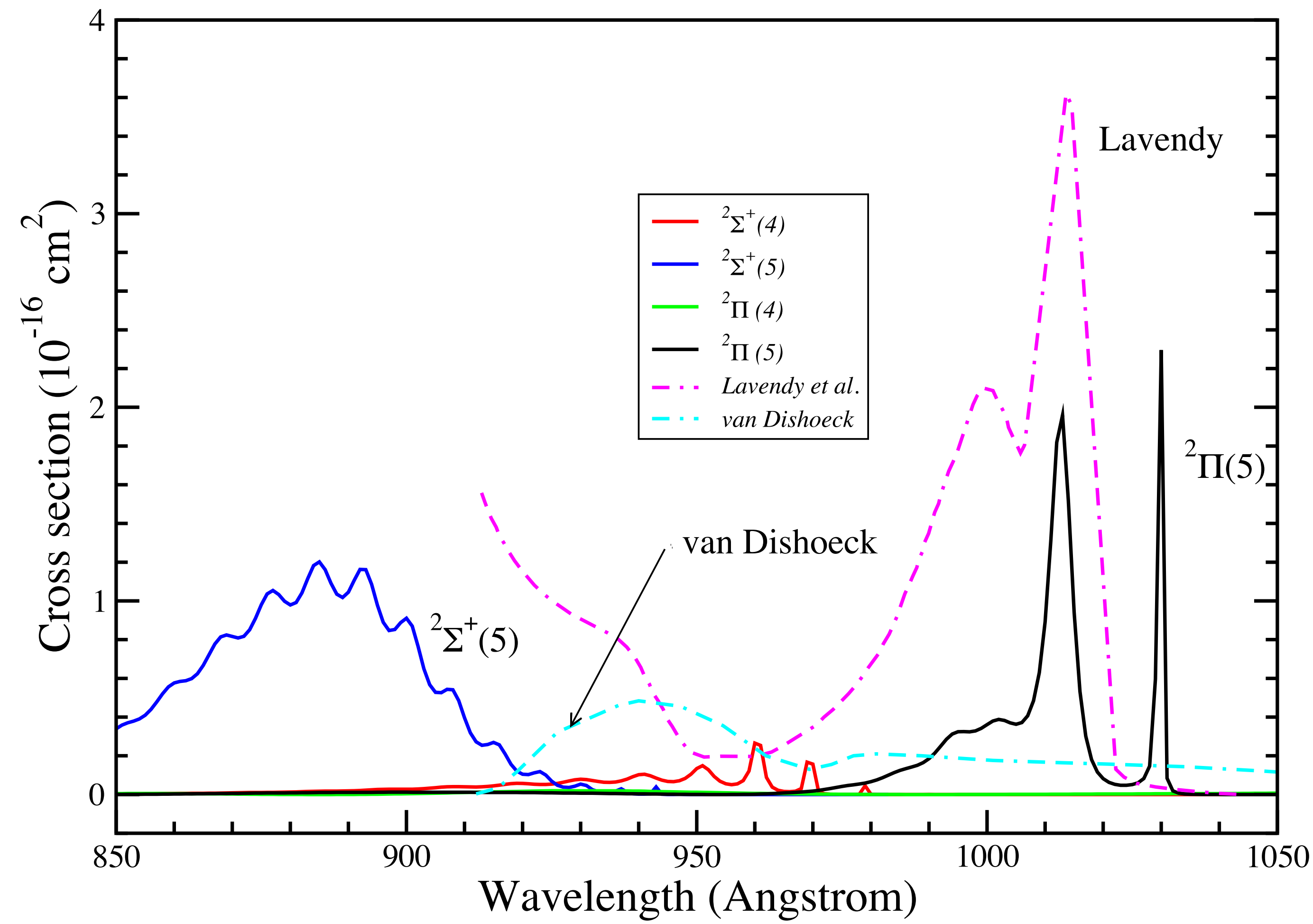


HeH^+ Abundance

CN Photodissociation

- Four electronic transitions considered

- About a factor of 2 smaller than early work of Lavendy et al. (1987, J. Phys. B, 30, 3067)

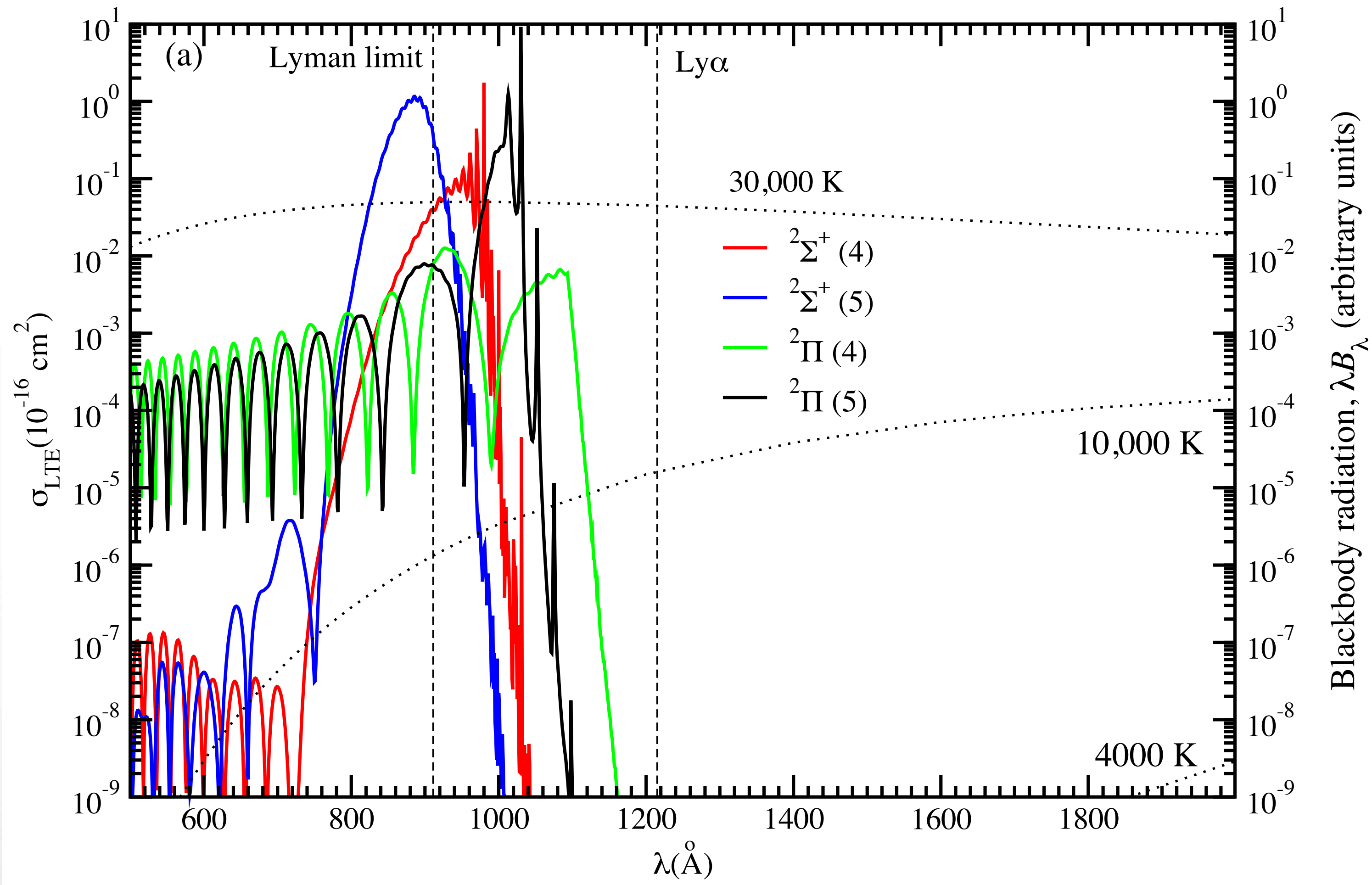


El-Qadi & Stancil, 2013, ApJ, 779, 970

CN(v=0,J=0) Cross Sections

CN Photodissociation

- Dominant transitions shortward of Lyman α

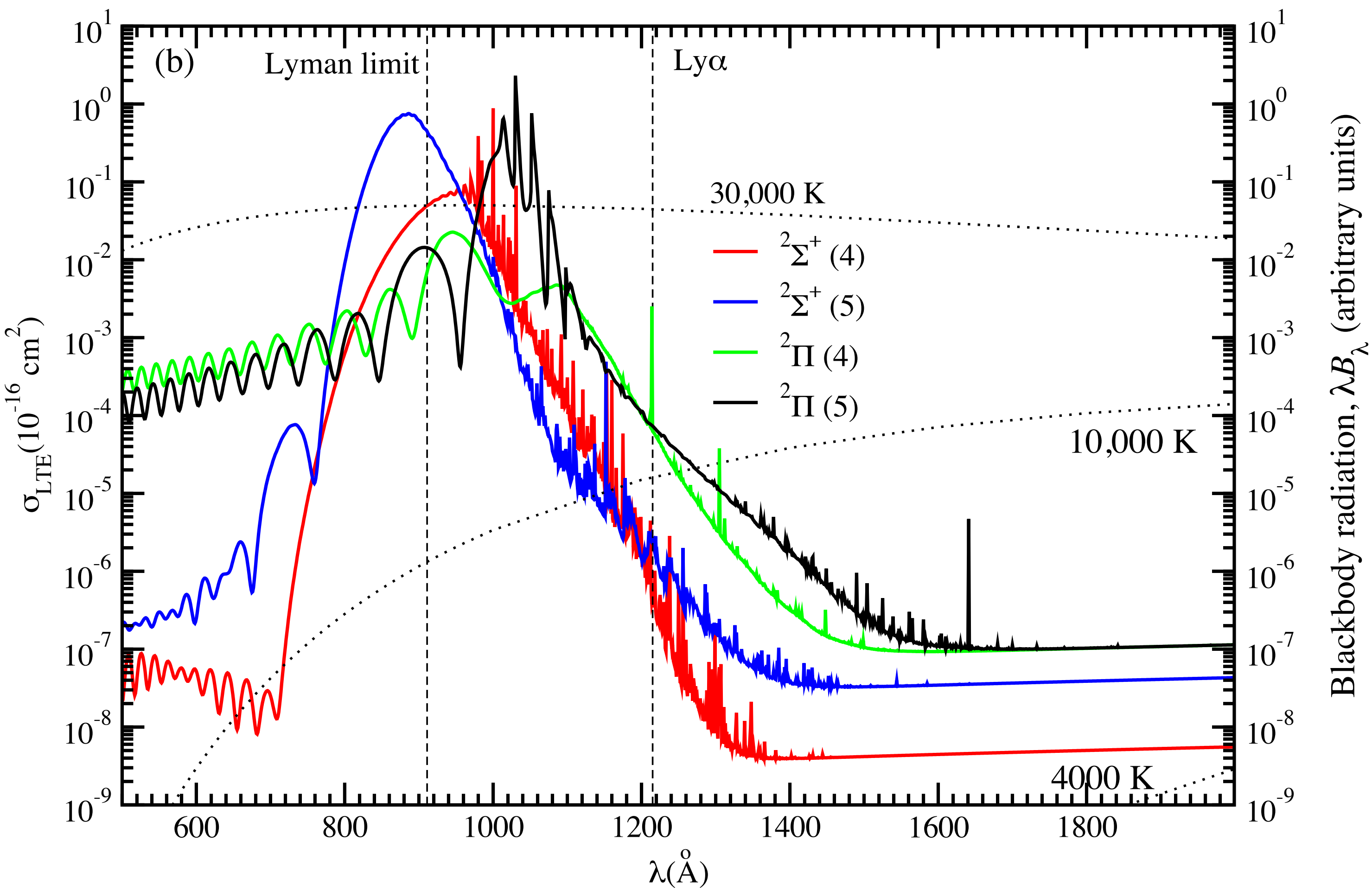


El-Qadi & Stancil, 2013, ApJ, 779, 970

CN(v=0,J=0) Cross Sections

CN Photodissociation

- 5068 rovibrational levels considered
- Cross sections shifted to longer wavelengths

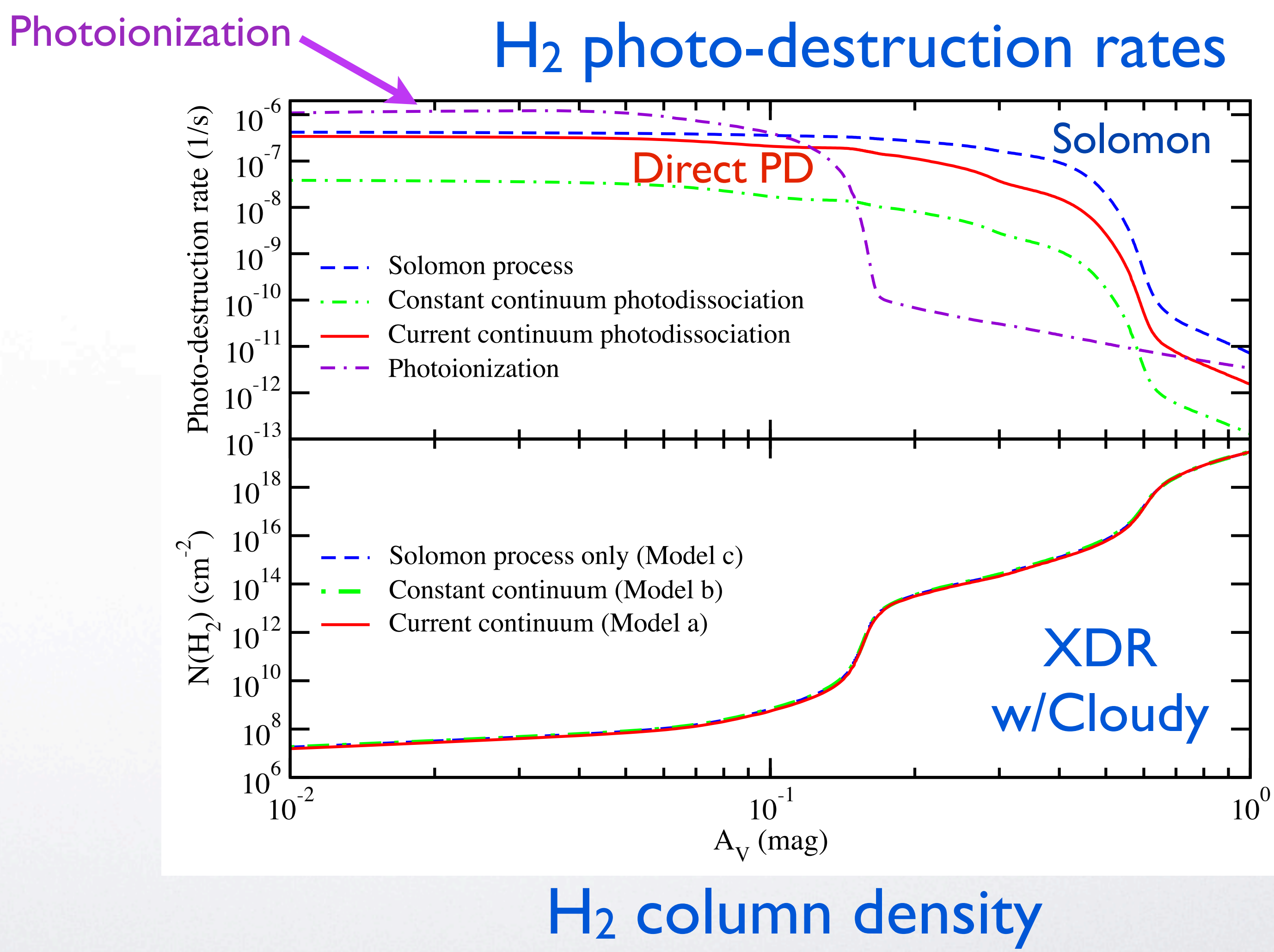


El-Qadi & Stancil, 2013, ApJ, 779, 970

CN LTE Cross Sections (3000 K)

Effect of Photoionization

- H_2(v=0,J=0) photoionization cross section from Yan, Sadeghpour, & Dalgarno (1998, ApJ, 496, 1044)
- Dominates photo-destruction for A_V<0.1
- PI from excited v,J levels should be considered
- v,J=0 PI cross sections calculated by Tsai & Flannery (1977, PRA, 16, 1124)



H_2 Photo-destruction rates

Database Websites

UGA Molecular Opacity Project Database

Molecular Opacity Project Database at The University of Georgia

- Home
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List of Molecules and Atoms						
H_2^+	H_2	HD	HeH^+	LiH	HF	NaH
MgH	HCl	CaH	LiCl	CN	CO	
H_2O						H

Last modified: *Jan. 16, 2015.*

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Charge Exchange Database for Astrophysics

Data Index

Targets	Cross Sections				Rate Coefficients			
	Total		State-Selective		Total		State-Selective	
	Data	*Fit*	*Data*	*Fit*	*Data*	*Fit*	*Data*	*Fit*
H	Select	Select	Select	Select		Select		Select
He	Select		Select		Select	Select	Select	Select
H_2	Select	Select	Select	Select		Select		
CO	Select							
H_2O	Select							
CO_2	Select							
N_2	Select							
CH		Select						
CH_2		Select						
CH_3		Select						
CH_4		Select						
C_2H		Select						
C_2H_2		Select						

Last modified: *November 25, 2014*.

Summary and Future Work

- 2-state Fermi Golden Rule approach can give reliable cross sections relatively ``fast”
- Photodissociation (v,J; LTE) cross sections completed for H_2, HeH^+, NH, SH^+, and CN (also H_2^+, SiH^+, HD, MgH, LiCl)
- Currently working on : CH, SiO, CS, TiO, CaH, C_2
- Important to consider triatomics and larger

Summary and Future Work

- Other photodissociation databases:
  - SWRI: http://amop.space.swri.edu/
  - Leiden: http://www.strw.leidenuniv.nl/~ewine/photo/
- Data formats for continuum processes
- We also do charge exchange and collisional excitation calculations (DBs available soon!)