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Photodissociation of H_2 and HD in a non-thermal radiation background: application to the early Universe chemistry

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OUTLINE:

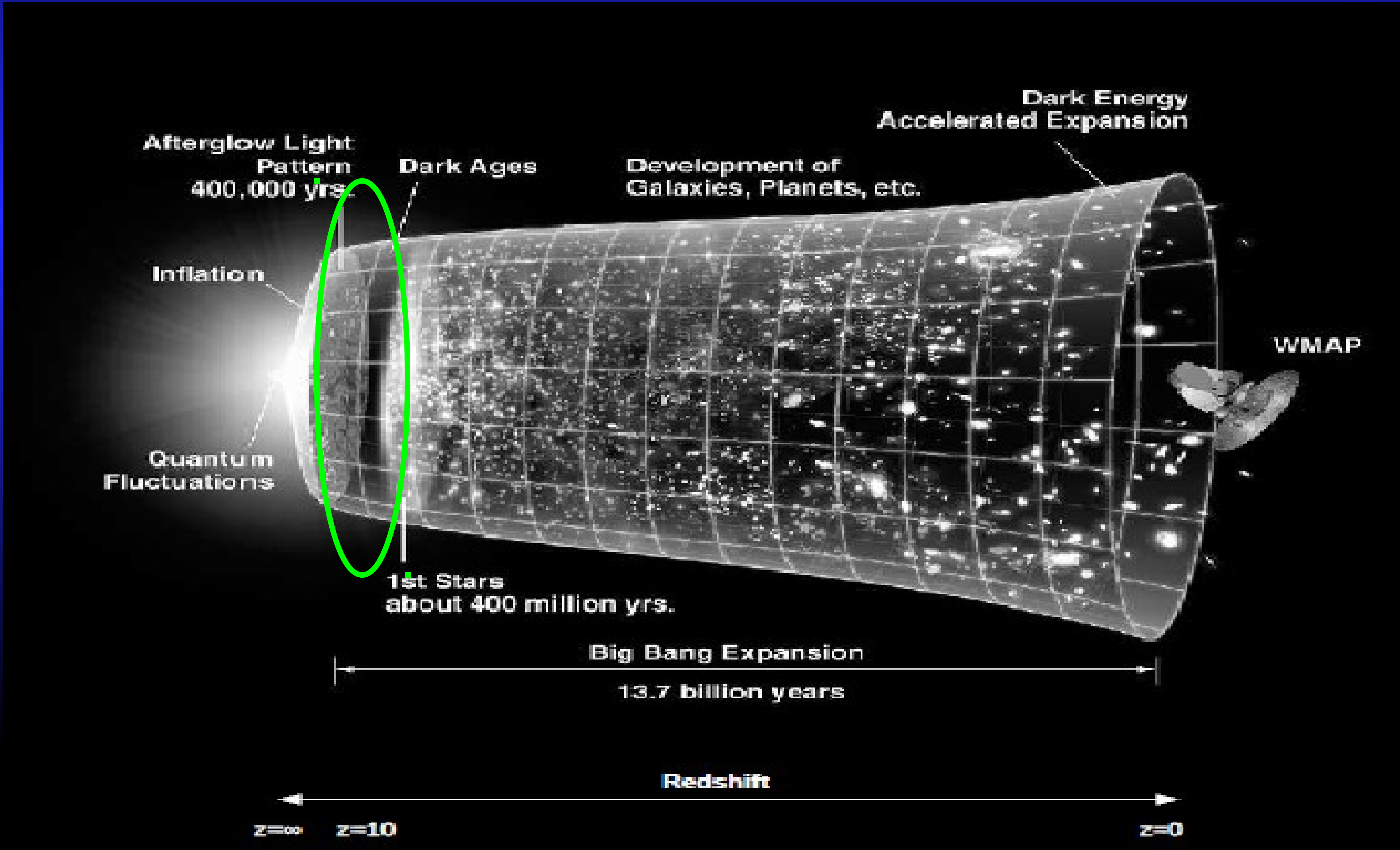
1. early Universe: the “standard” chemistry

2. direct H_2 and HD photodissociation cross-sections: characteristics

3. spectral distortions:
radiation transport in the expanding Universe →
primordial atomic recombination

4. “modified” rate coefficients → chemistry

UNIVERSE HISTORY...



KINETIC MODELS: CHEMICAL SPECIES (I)

H^+ D^+

H D

H^- D^-

He^{++} He^+
He

Li Li^+

Li^-

e^- γ

HD^+

HD

H_3^+ H_2D^+

HeH^+

LiH LiH^+

H_2^+ H_2

KINETIC MODELS: A BRIEF OVERVIEW... (II)

'60s: studies on elementary processes useful in molecular hydrogen formation in the early Universe
(Saslaw & Zipoy (1967), Peebles & Dicke (1968))

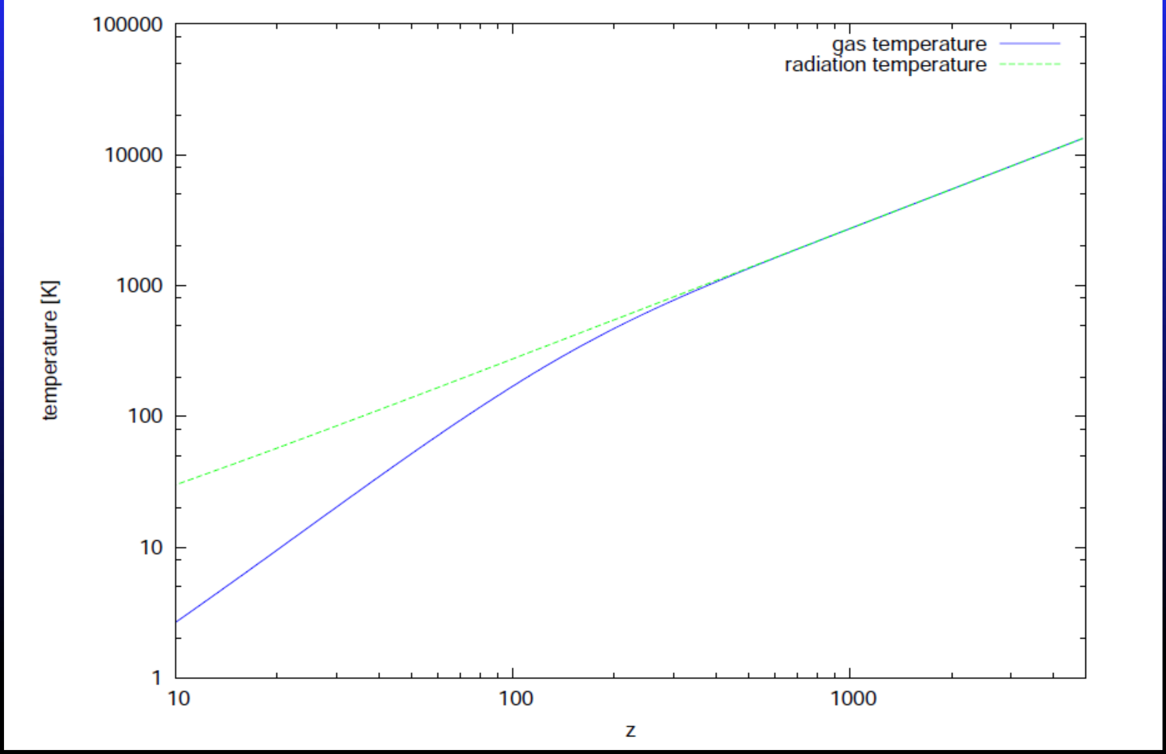
Chemical kinetics in the early Universe:

Dalgarno & Lepp (1987)
Black (1990)
Shapiro (1992)
Puy et al. (1993,1996)
Dalgarno & Fox (1994)
Lepp, Stancil & Dalgarno (1996), Lepp & Stancil (1998)
Bougleux & Galli (1997)
Galli & Palla (1998, 2002)
Schleicher et al. (2008)

KINETIC MODEL: MATTER AND RADIATION TEMPERATURE (III)

$$\frac{dT_m}{dt} = -2H(t)T_m + \frac{8\sigma_t a T_r^4 (T_r - T_m) x_e}{3 m_e c} + (\Gamma - \Lambda)_{\mathrm{mol}}$$

$$T_r = 2.7(1+z)$$



RECFAST

Wong et al.

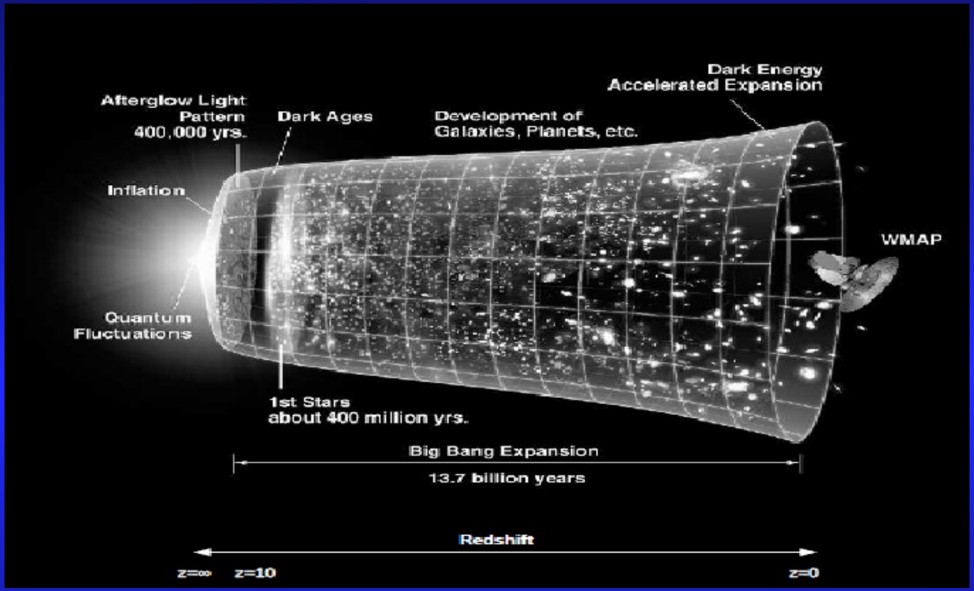
2008, MNRAS, **386**, 1023-1028

CosmoRec

Rubiño Martín et al.

2010, MNRAS, **403**, 439-452

KINETIC MODEL: ODEs SYSTEM (IV)



$$\frac{dn_i}{dt} = k_{form} n_j n_k - k_{dest} n_i + \ldots$$

$$\frac{dn_i}{dz} = \frac{dt}{dz}\frac{dn_i}{dt}$$

$$n(z) = \Omega_b n_{cr} (1+z)^3$$

KINETIC MODEL: CHEMICAL PROCESSES (V)

MASSIVE PARTICLES SCATTERING

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

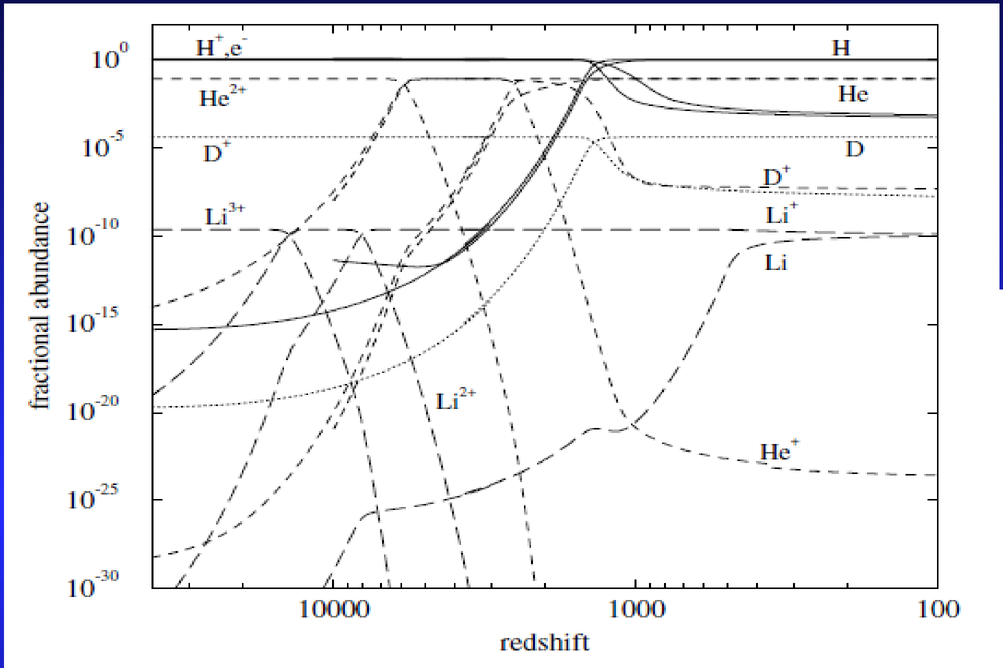
$$n_b = 1.123 \times 10 \cdot (1 - Y_p) \Omega_b h^2 (1 + z)^3 \quad [m^{-3}]$$

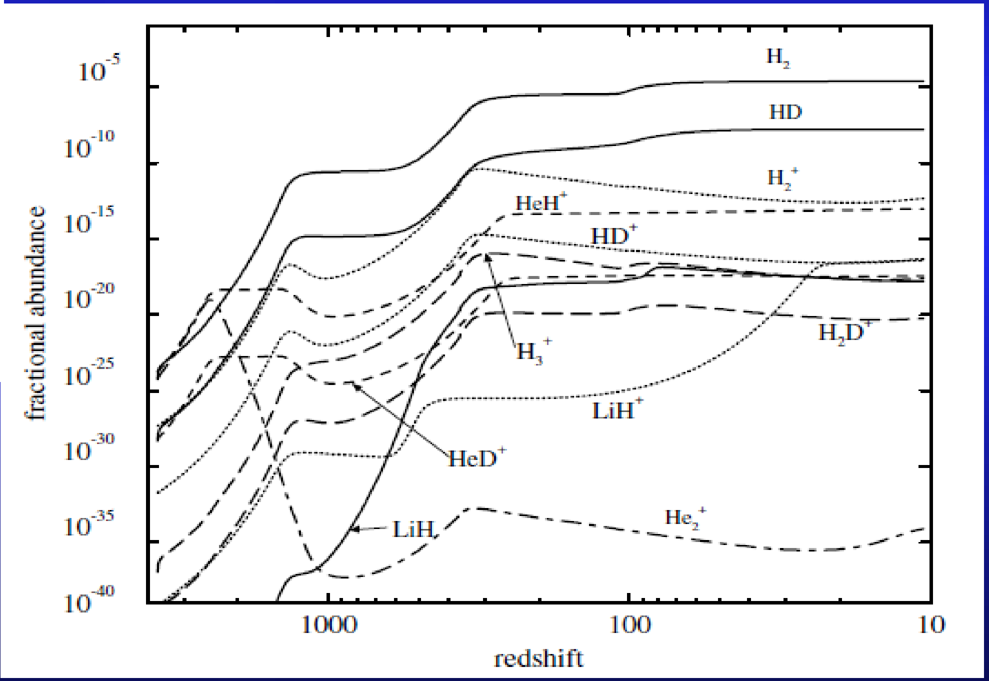
PHOTONIC PROCESSES

$$k_{rad}(\mathrm{T_{rad}}) = 4\pi \int_0^\infty \frac{\sigma(\nu)}{h\nu} J_\nu(\mathrm{T_{rad}}) d\nu$$

$$J_\nu(\mathrm{T_{rad}}) = \frac{2h\nu^3}{c^2} \frac{1}{\mathrm{e}^{\mathrm{h}\nu/\mathrm{kT_{rad}}} - 1}$$

KINETIC MODEL: FRACTIONAL ABUNDANCES (VI)

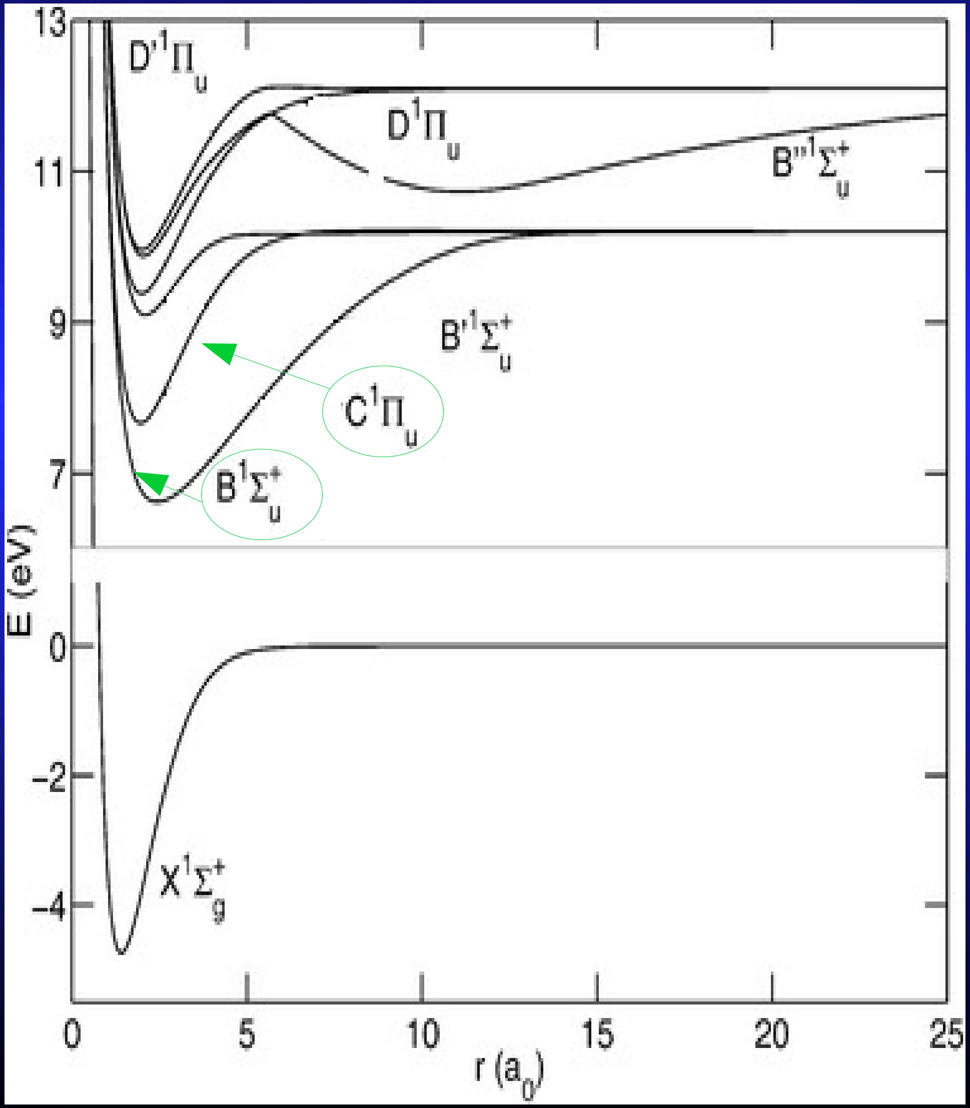




Lepp, Stancil &Dalgarno,

2002, J. Phys. B: At. Mol. Opt. Phys. **35**, R57–R80

THE MECHANISM OF DIRECT PHOTODISSOCIATION



$$H_2 + h\nu \rightarrow H + H$$

Early Universe → No high energy photons available

↓

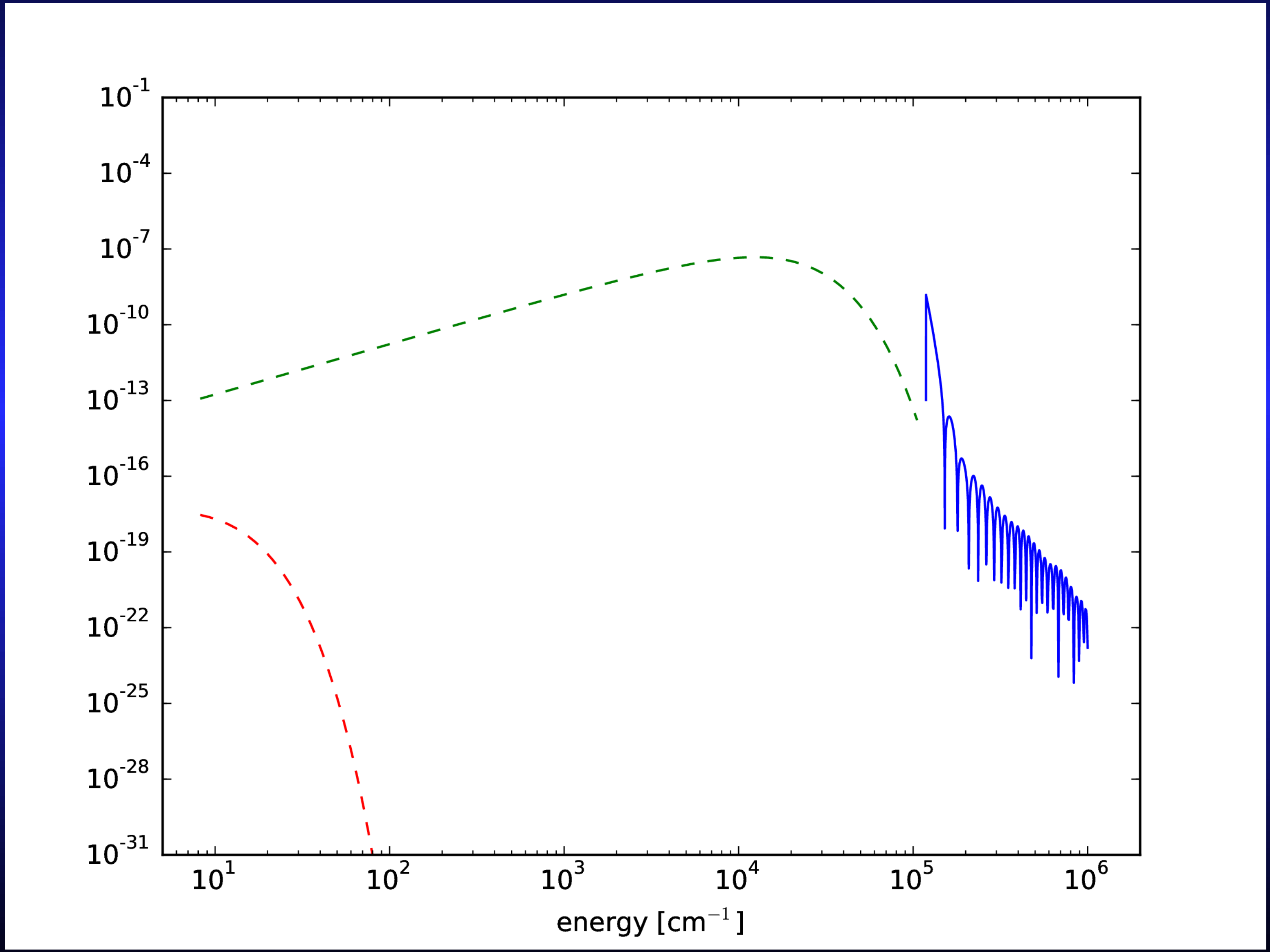
No effect on the chemistry, negligible reaction rates

SEARCH FOR CHEMICAL DATA: DIRECT PHOTODISSOCIATION OF H_2 and HD...

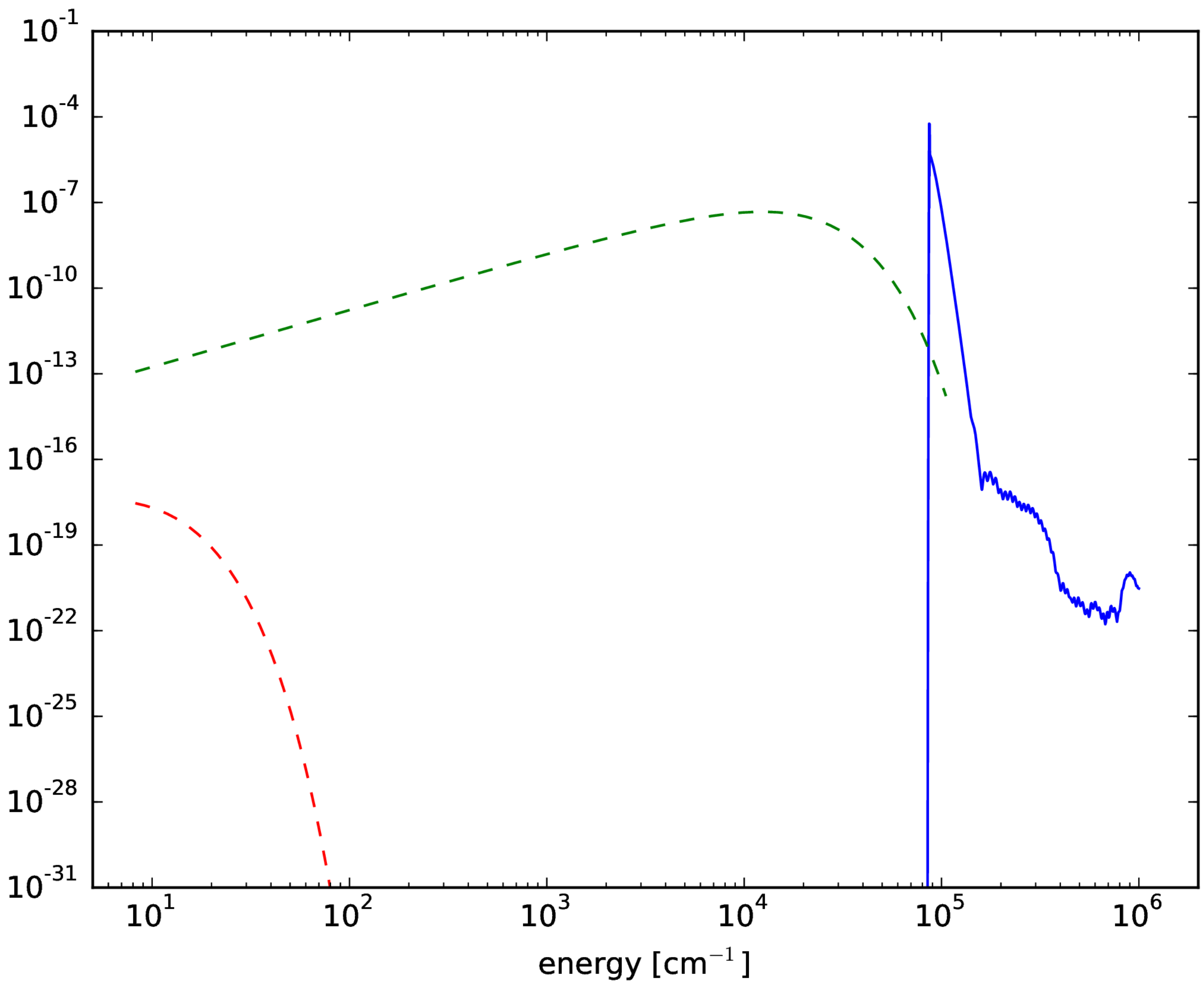
Cross-sections:

Allison & Dalgarno 1969

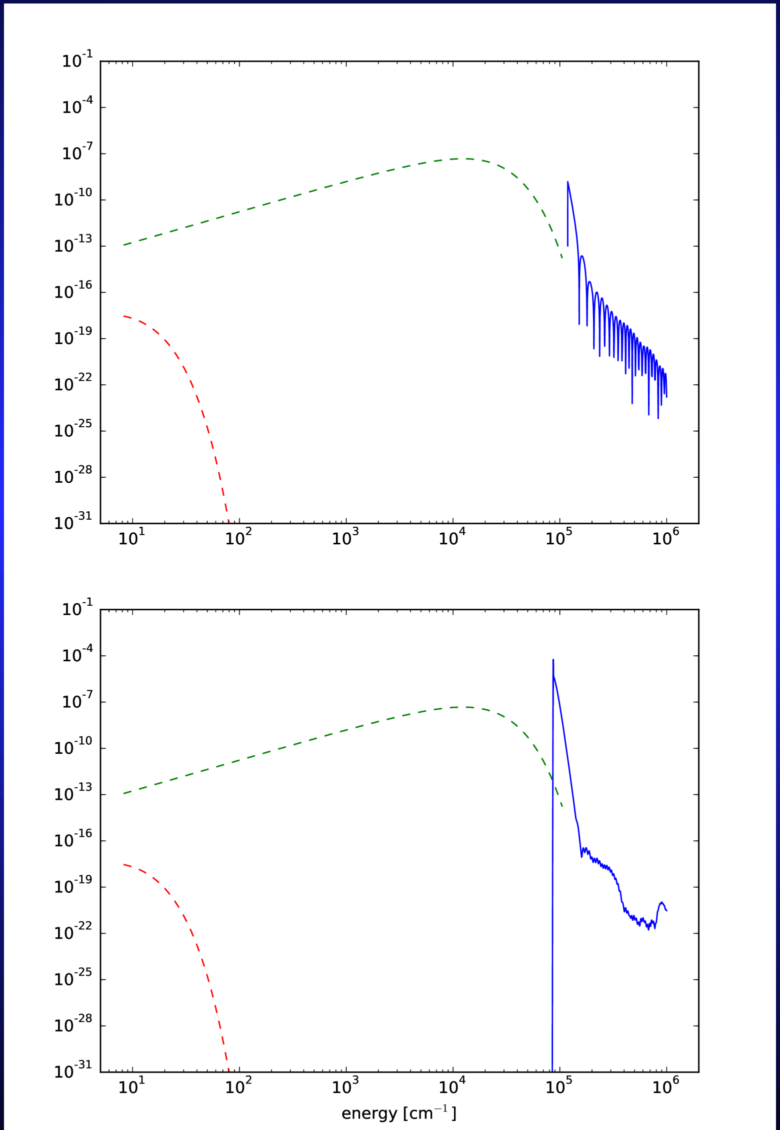
Gay et al. 2012



(Cross-sections by Gay et al. 2012)



(Cross-sections by Gay et al. 2012)



Selectivity of efficiency according to the rovibrational level

No a priori comments...calculations needed...

BEYOND THE "STANDARD" KINETICS...

MASSIVE PARTICLES

SCATTERING

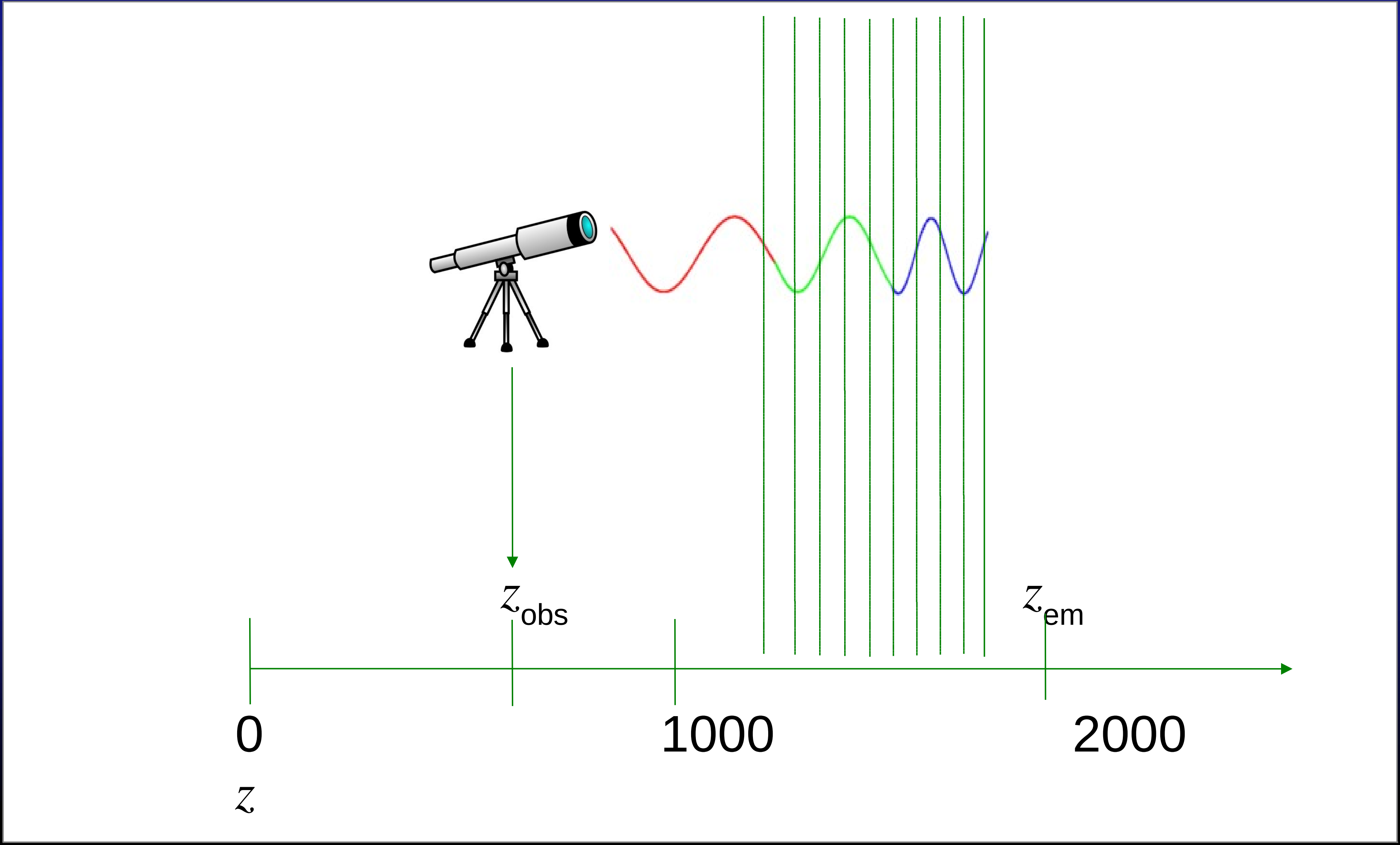
PHOTONIC PROCESSES

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

$$n_b = 1.123 \times 10 \cdot (1 - Y_p)\Omega_b h^2 (1+z)^3 \quad [m^{-3}]$$

$$k_{photo}(z) = 4\pi \int_0^\infty \frac{\sigma(\nu)}{h\nu} \left[B_z(\nu) + \sum_{i \to j} I^z_{ij}(\nu) \right] d\nu.$$

SPECTRAL DISTORTIONS (I)



SPECTRAL DISTORTIONS (II)

- matter/antimatter annihilation
- decaying particles
- interaction with matter

....

- primordial atomic recombination ($z \sim 1100$)

$$A^+ + e^- \longrightarrow A + h\nu$$

He^{++} He^+

H^+

- molecular radiative cascade

$$H_2(v) \longrightarrow H_2(v') + h\nu$$

SPECTRAL DISTORTIONS (III)

$$\frac{1}{c}\frac{\mathrm{d}J_\nu}{\mathrm{d}z} = \frac{\kappa_\nu J_\nu - j_\nu}{H_0(1+z)^2\sqrt{1+\Omega_0 z}} + \frac{3J_\nu}{c(1+z)}$$

$$\kappa_\nu = \frac{c^2}{8\pi\nu^2} n_1 A_{\mathrm{ul}} \frac{g_{\mathrm{u}}}{g_{\mathrm{l}}}\left(1 - \frac{g_{\mathrm{l}} n_{\mathrm{u}}}{g_{\mathrm{u}} n_{\mathrm{l}}}\right)\phi(\nu - \nu_{\mathrm{ul}})$$

$$j_\nu = \frac{h\nu}{4\pi} n_{\mathrm{u}} A_{\mathrm{ul}} \phi(\nu - \nu_{\mathrm{ul}})$$

$$\left.\frac{\Delta J_\nu}{J_\nu}\right|_{z=0} = [R(z_{\mathrm{i}}) - 1][1 - \mathrm{e}^{-\tau(z_{\mathrm{i}})}]$$

$$R(z_{\mathrm{i}}) = \left[\frac{g_{\mathrm{u}} n_{\mathrm{l}}(z_{\mathrm{i}})}{g_{\mathrm{l}} n_{\mathrm{u}}(z_{\mathrm{i}})} - 1\right]^{-1}\left\{\exp\left[\frac{h\nu_{\mathrm{ul}}}{kT_{\mathrm{r}}(z_{\mathrm{i}})}\right] - 1\right\}$$

Bougleux, E. & Galli, D. **1997**
MNRAS, **288**, 638-648

SPECTRAL DISTORTIONS (IV)

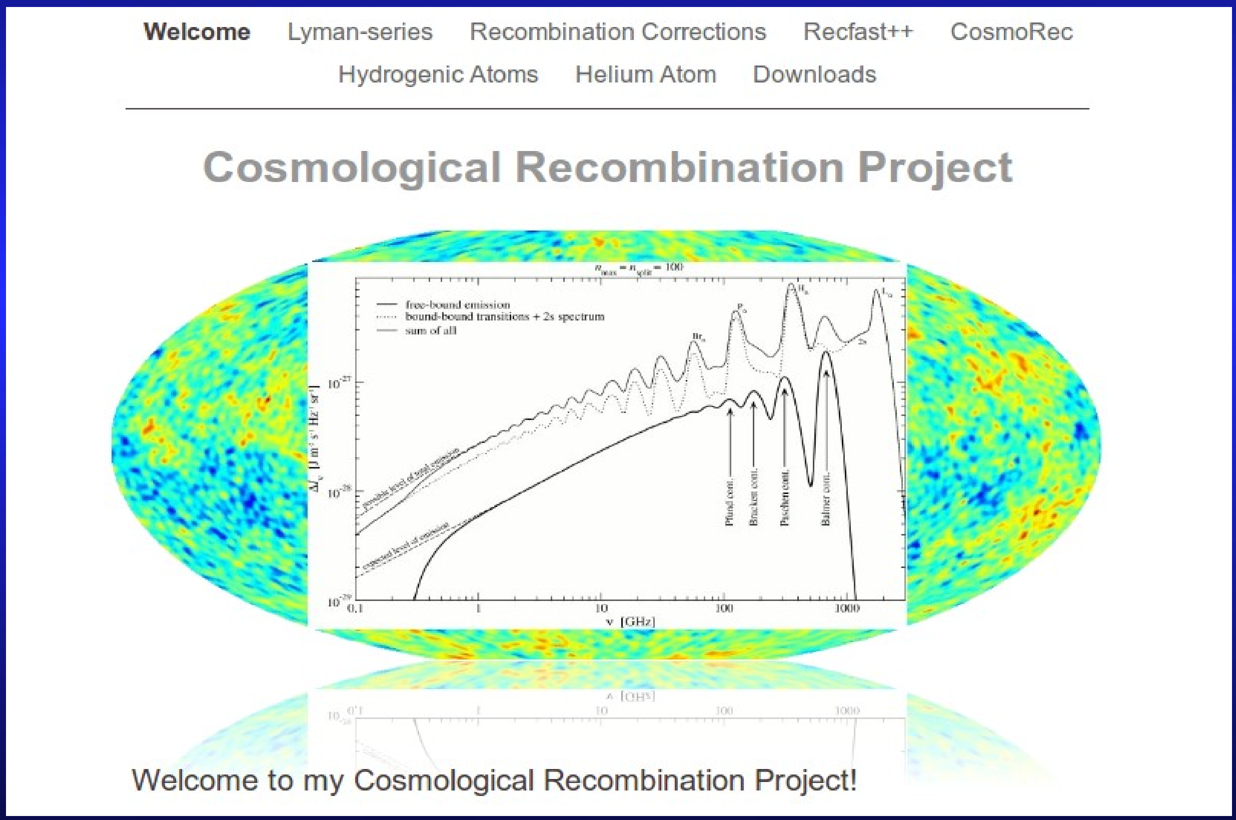
$$j_{\nu_{ij}}(z) = h\nu_{ij}\Delta R_{ij}(z)\phi(\nu(z))$$

$$\Delta R_{ij}(\nu) = A_{ij}N_i \frac{e^{h\nu_{ij}/kT_r}}{e^{h\nu_{ij}/kT_r} - 1}\left[1 - \frac{N_j}{N_i}e^{-h\nu_{ij}/kT_r}\right]$$

$$I_{ij}^{z_{obs}}(\nu) = \frac{c}{4\pi}\int_{z_{em}}^{z_{obs}} \frac{j_{\nu_{ij}}(z)}{(1+z)^3}(1+z_{obs})^3 \left|\frac{dt}{dz}\right| dz$$

$$I_{ij}^{z_{obs}}(\nu) = \frac{ch}{4\pi}\frac{\Delta R_{ij}(z_{em})}{H(z_{em})}\frac{(1+z_{obs})^3}{(1+z_{em})^3}$$

PRIMORDIAL ATOMIC RECOMBINATION



CosmoRec

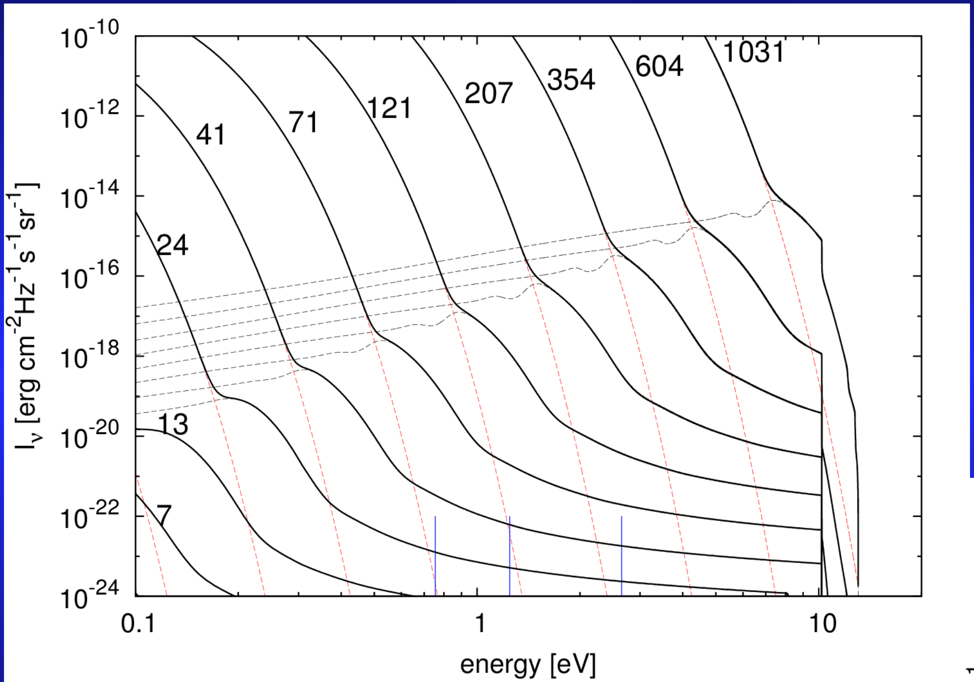
by

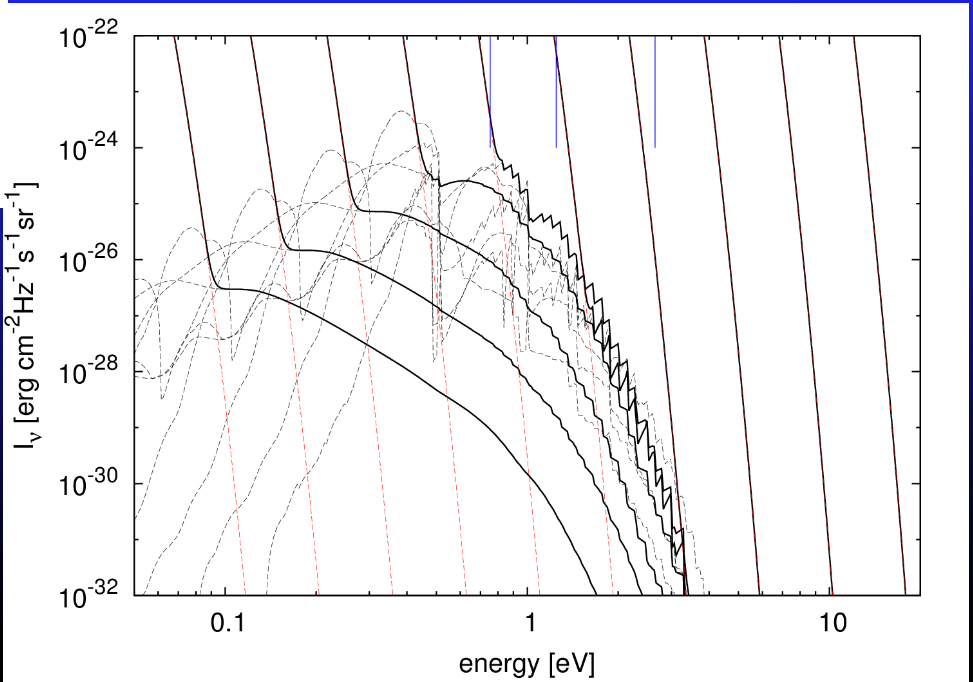
Jens Chluba

- effective multi-level approach;
- fast and accurate (~1.3 sec)
- solves a detailed radiative transfer problem for Ly-n
- available @ www.Chluba.de/CosmoRec

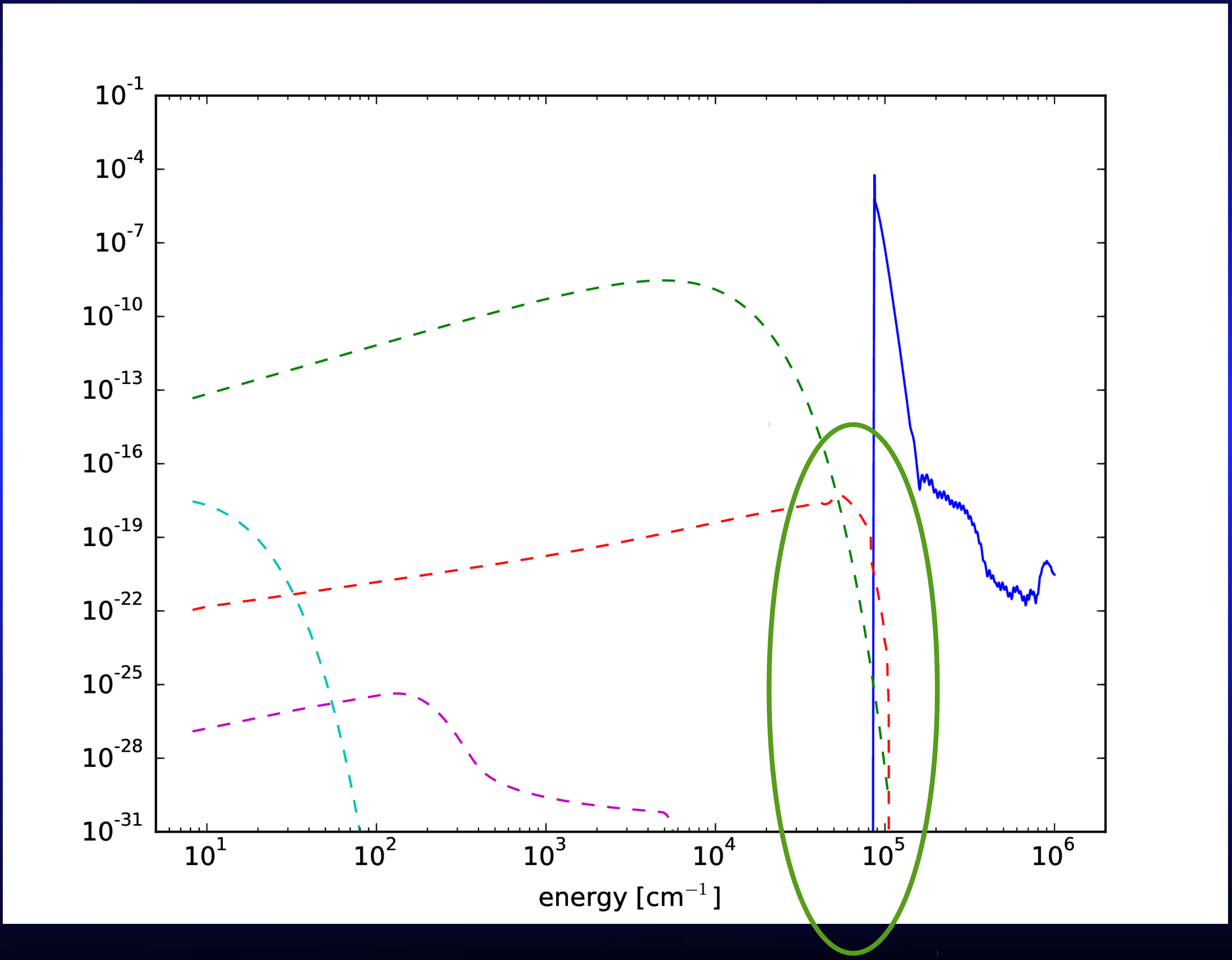
http://www.cita.utoronto.ca/~jchluba/Science_Jens/Recombination/Welcome.htm

SPECTRAL DISTORTIONS (V)



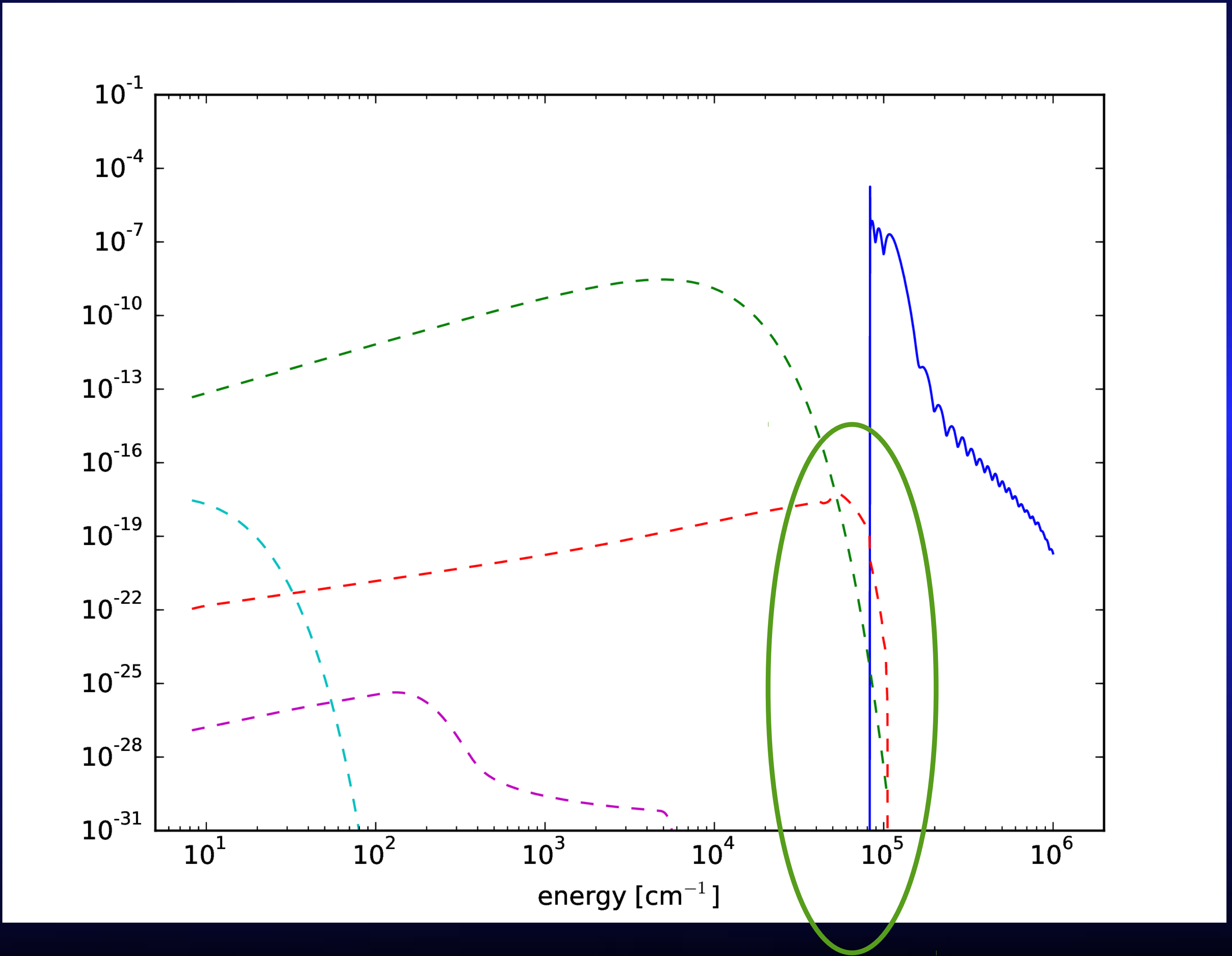


Coppola et al. 2013
MNRAS **434** (1) 114-122



v=0, j=30

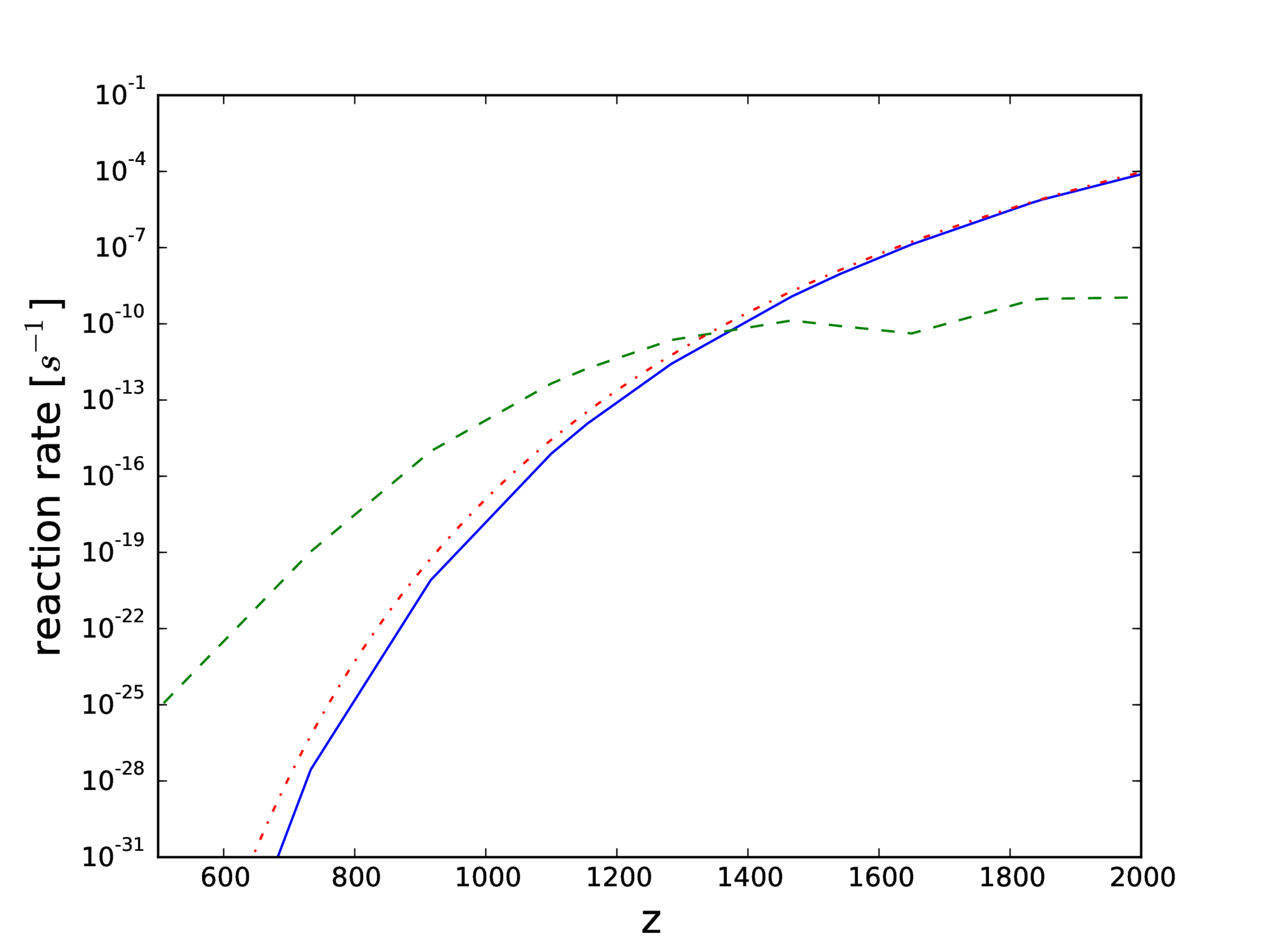
(Cross-sections by Gay et al. 2012)



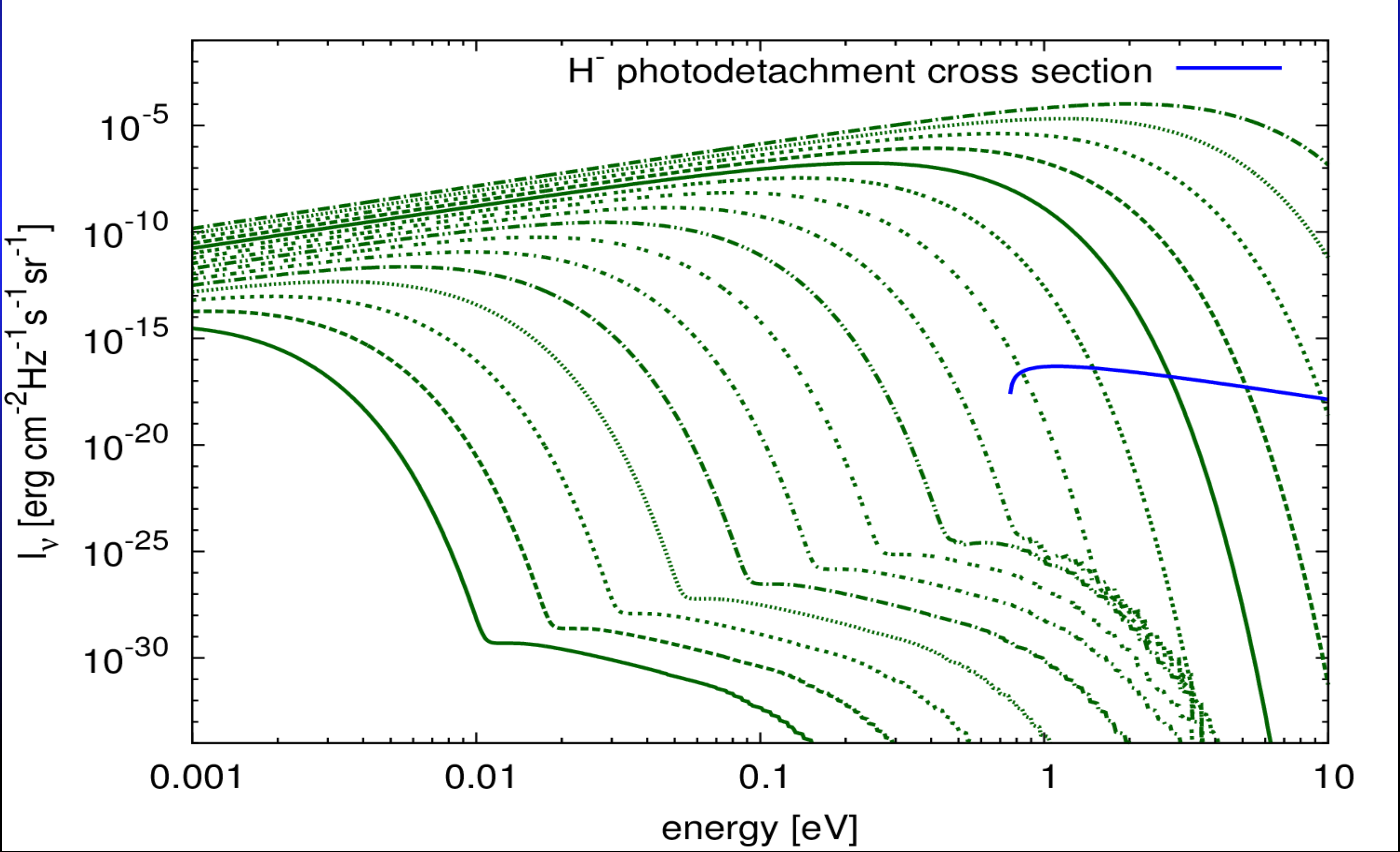
v=9, j=16

(Cross-sections by Gay et al. 2012)

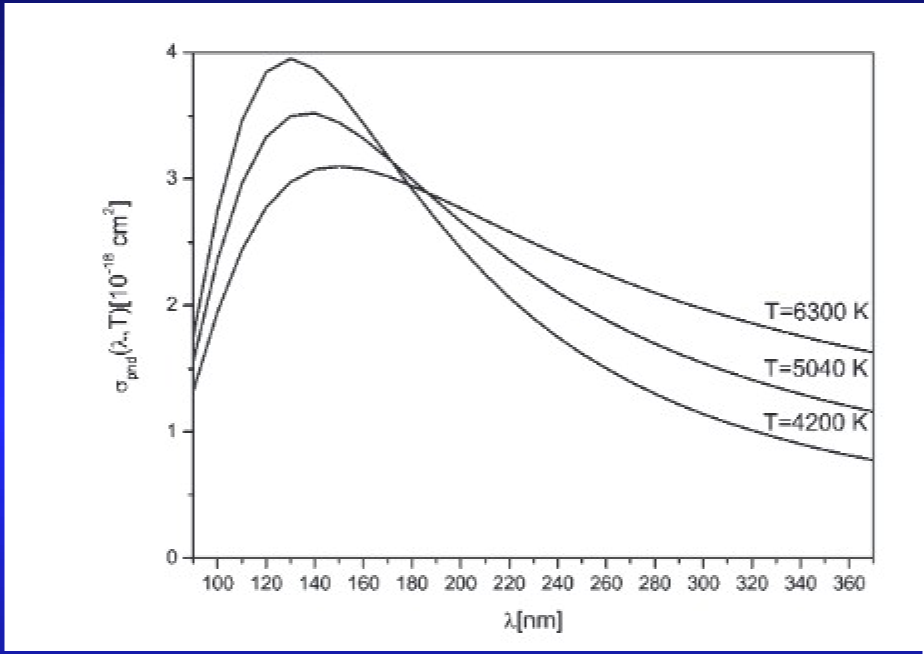
SPECTRAL DISTORTIONS (I)

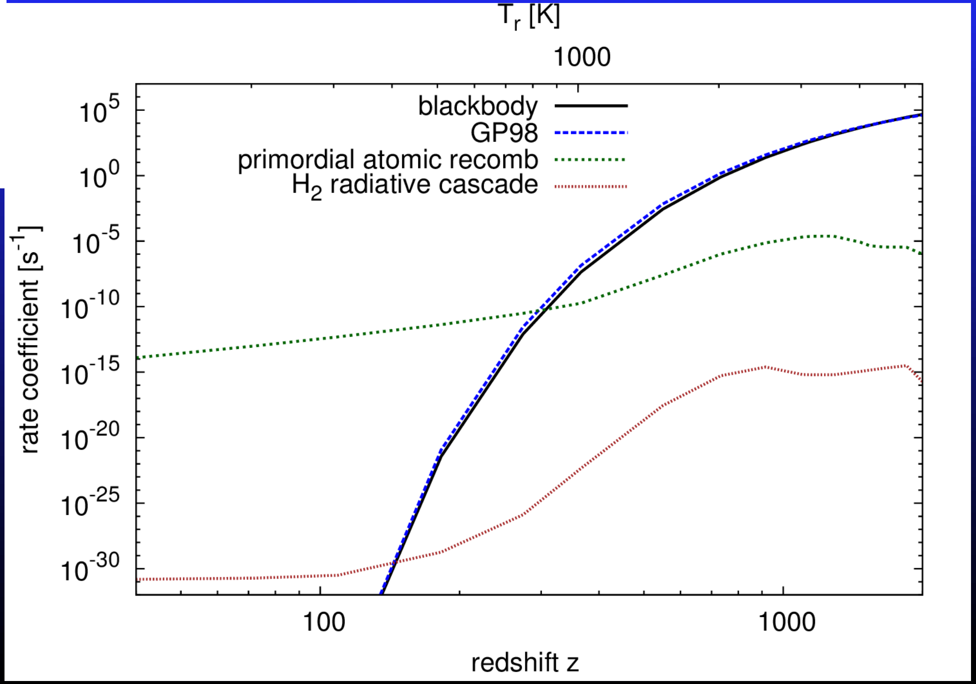


SPECTRAL DISTORTIONS



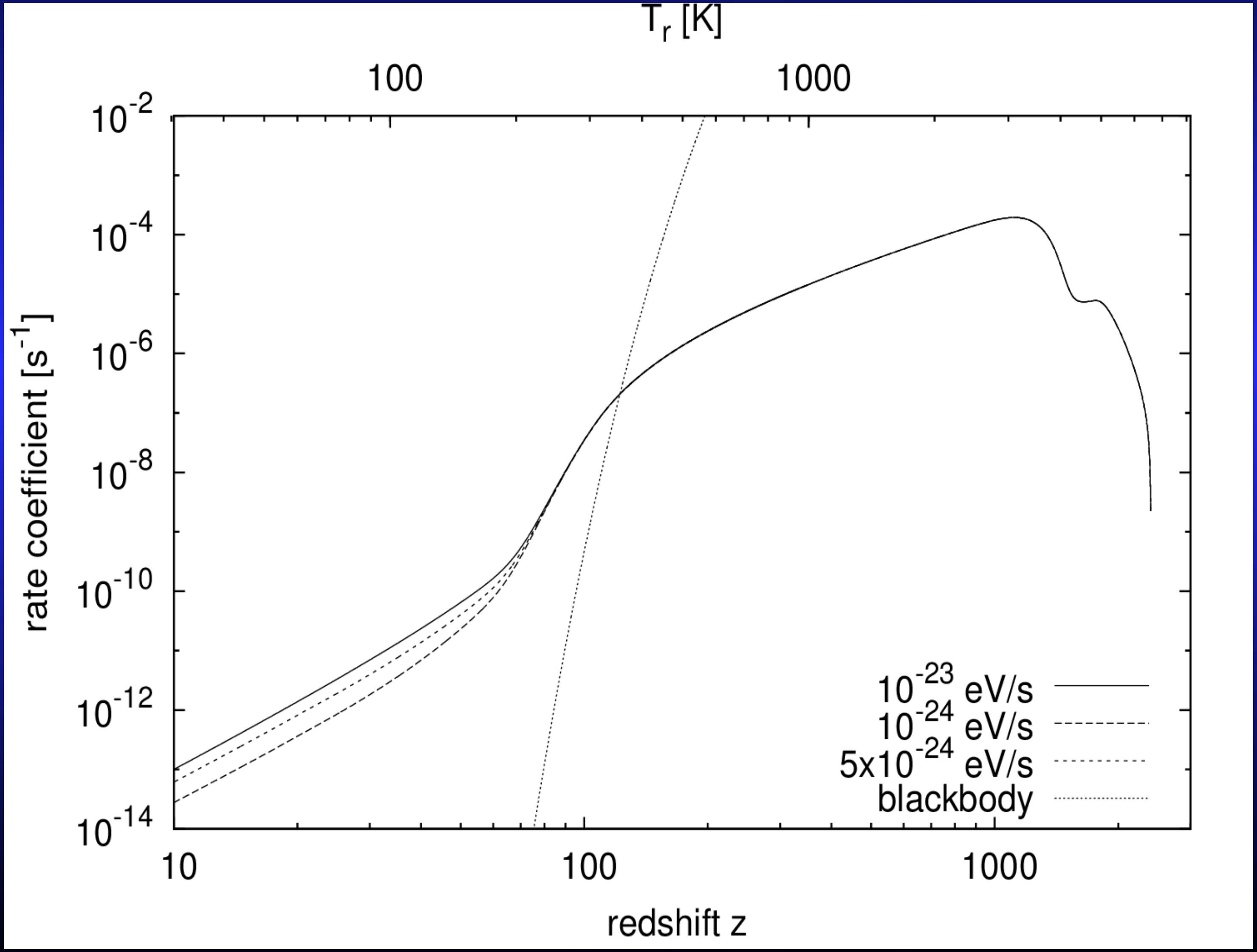
SPECTRAL DISTORTIONS: H_2^+ photodissociation





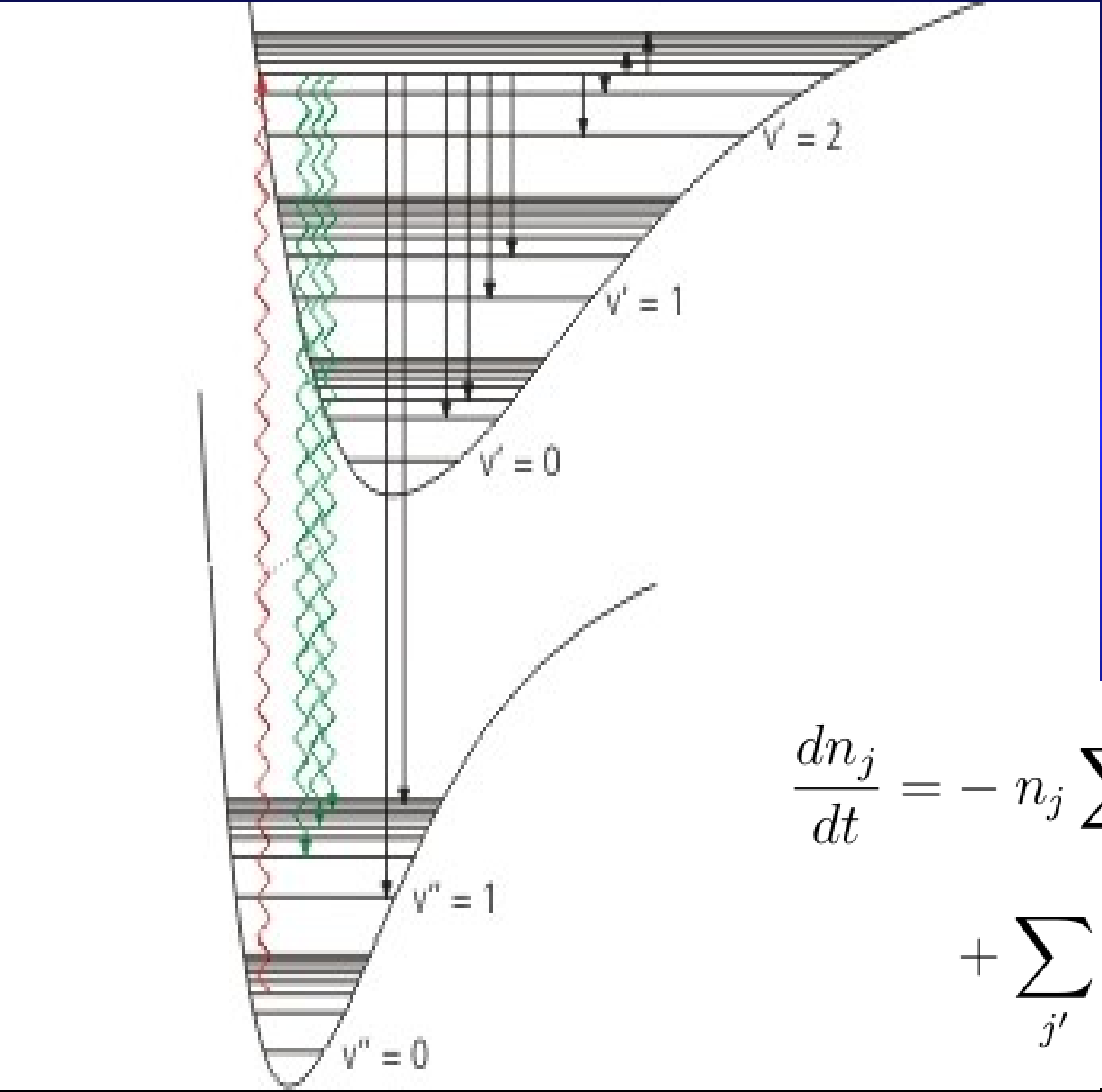
Coppola et al. 2013
MNRAS **434** (1) 114-122

SPECTRAL DISTORTIONS: DARK MATTER ANNIHILATION



Coppola et al. 2013
MNRAS **434** (1) 114-122

STATE-TO-STATE APPROACH

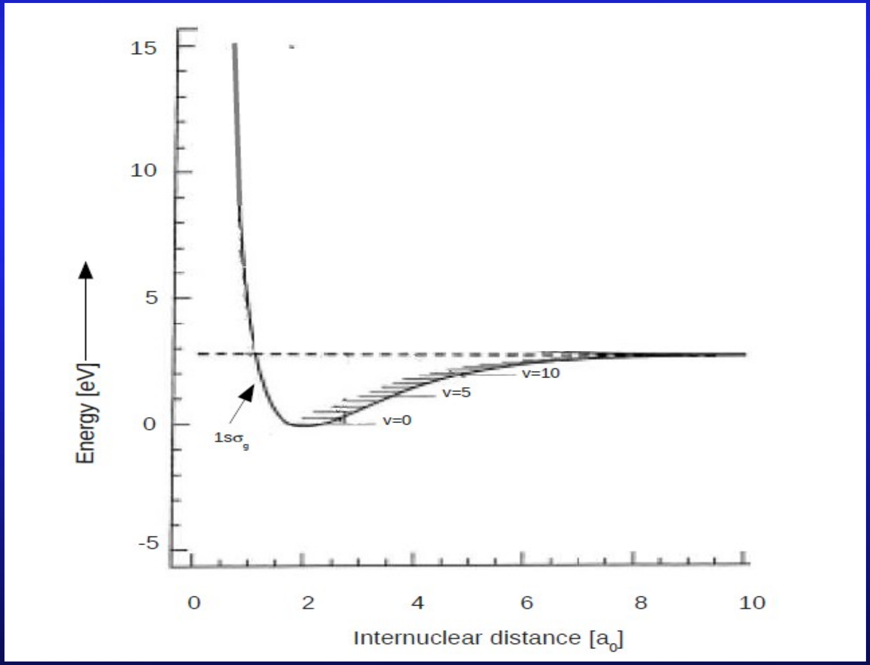


- Electronic
- Vibrational
- Rotational

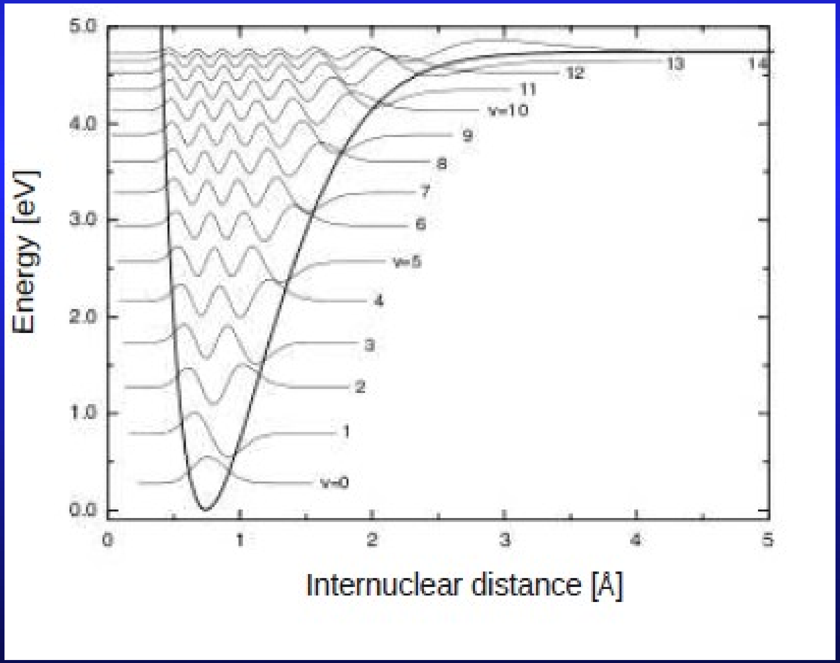
$$\frac{dn_j}{dt} = -n_j \sum_{j'} (R_{jj'} + P_{jj'} + C_{jj'} n_{j'}) + \\ + \sum_{j'} R_{jj'} n_{j'} + \sum_{j'} \sum_{j''} \mathbf{C}_j^{j'j''} n_{j'} n_{j''}$$

KINETIC MODEL: CHEMICAL SPECIES

H_2^+ → 18 levels



H_2 → 15 levels

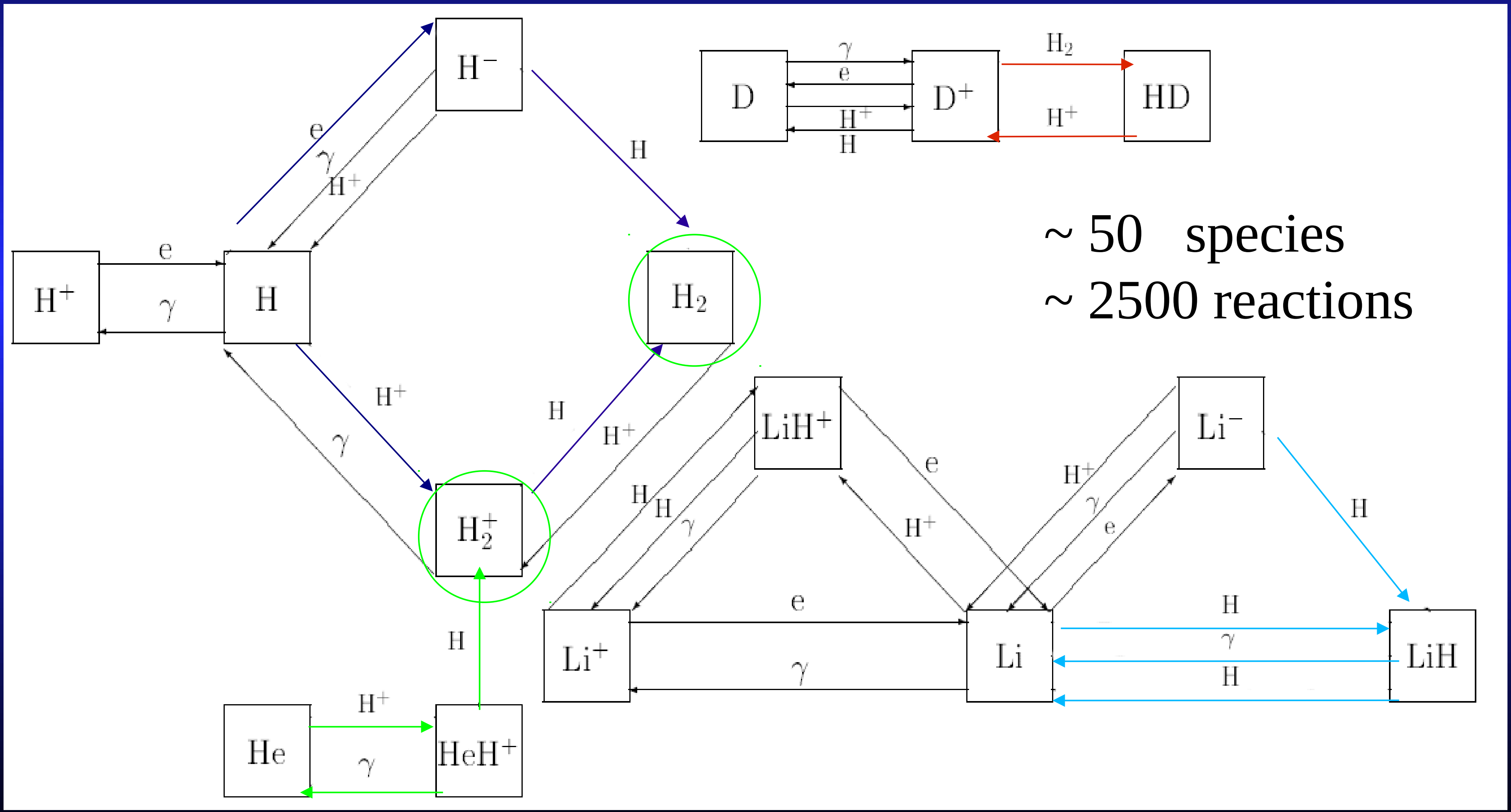


KINETIC MODEL: CHEMICAL PROCESSES

1] $H + H_2(v) \longrightarrow H + H_2(v)$
2] $H + H^- \longrightarrow H_2(v) + e^-$
3] $H + H^+ \longrightarrow H_2^+(v) + h\nu$
4] $H_2^+(v) + H \longrightarrow H_2(v') + H^+$
5] $H_2(v) + H \longrightarrow H_2^+(v') + H^+$
6] $H + H_2^+(v) \longrightarrow H + H_2^+(v)$
7] $H^+ + H_2(v) \longrightarrow H^+ + H_2(v)$
8] $H_2^+(v) + H \longrightarrow H + H + H^+$
9] $H_2(v) + H^+ \longrightarrow H + H + H^+$
10] $H_2(v) + h\nu \longrightarrow H_2^+(v') + e^-$
11] $H_2^+(v) + h\nu \longrightarrow H + H^+$
12] $H_2(v) + h\nu \longrightarrow H + H$
13] $H_2^+(v) + e^- \longrightarrow H + H$
14] $H_2(v) + e^- \longrightarrow H + H^-$
15] $H_2(v) + e^- \longrightarrow H_2(v) + e^- + h\nu$
16] $H_2(v) \longrightarrow H_2(v') + h\nu$
17] $H_2^+(v) \longrightarrow H_2^+(v') + h\nu$
18] $H + H_2(v) \longrightarrow H + H + H$
19] $HeH^+ + H \longrightarrow H_2^+(v) + He$

Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

KINETIC MODEL: STATE-TO-STATE KINETICS

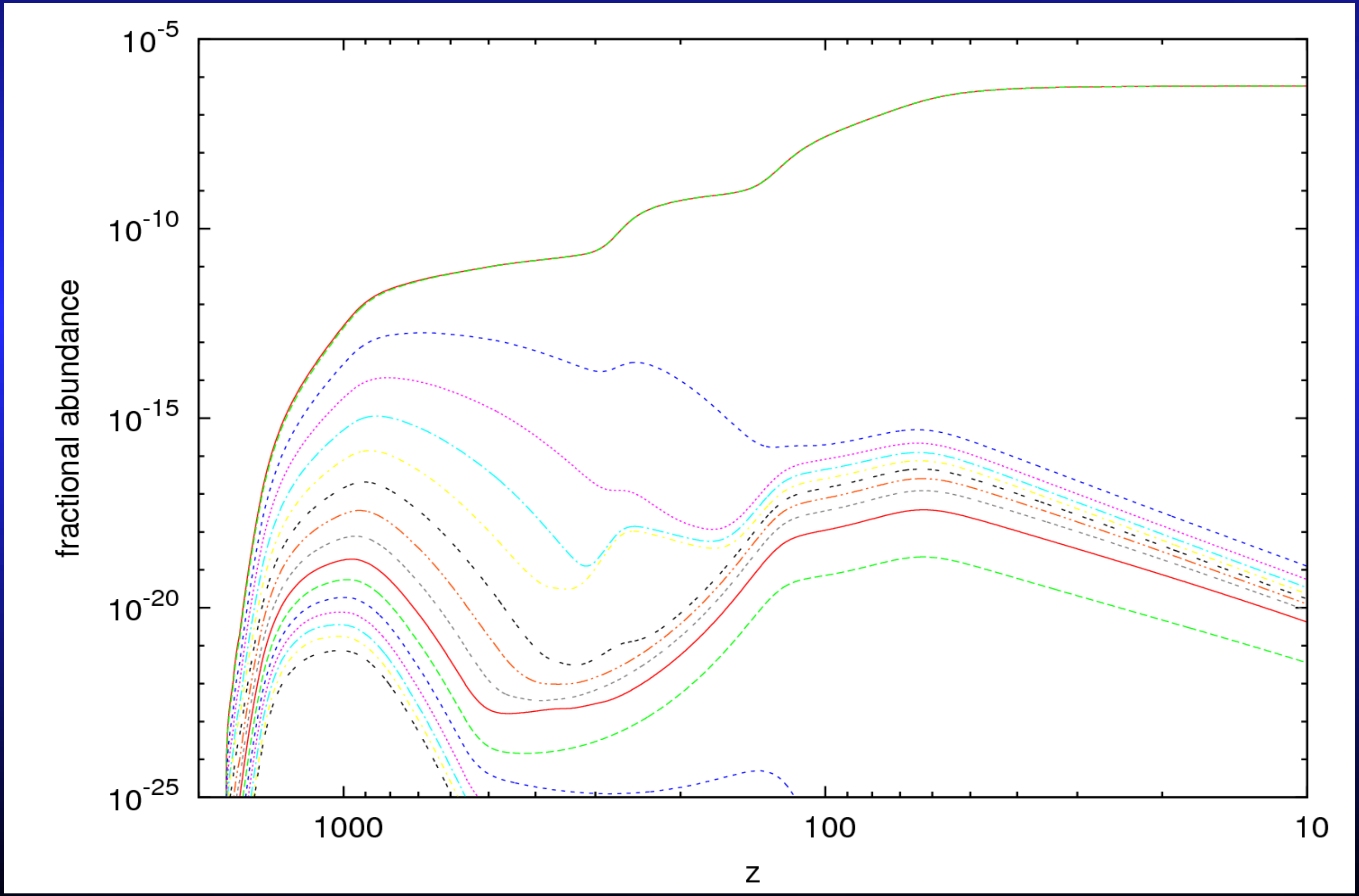


~ 50 species

~ 2500 reactions

Galli & Palla, 1998, A&A, **335**, 403–420

RESULTS: VDF H_2 (I)

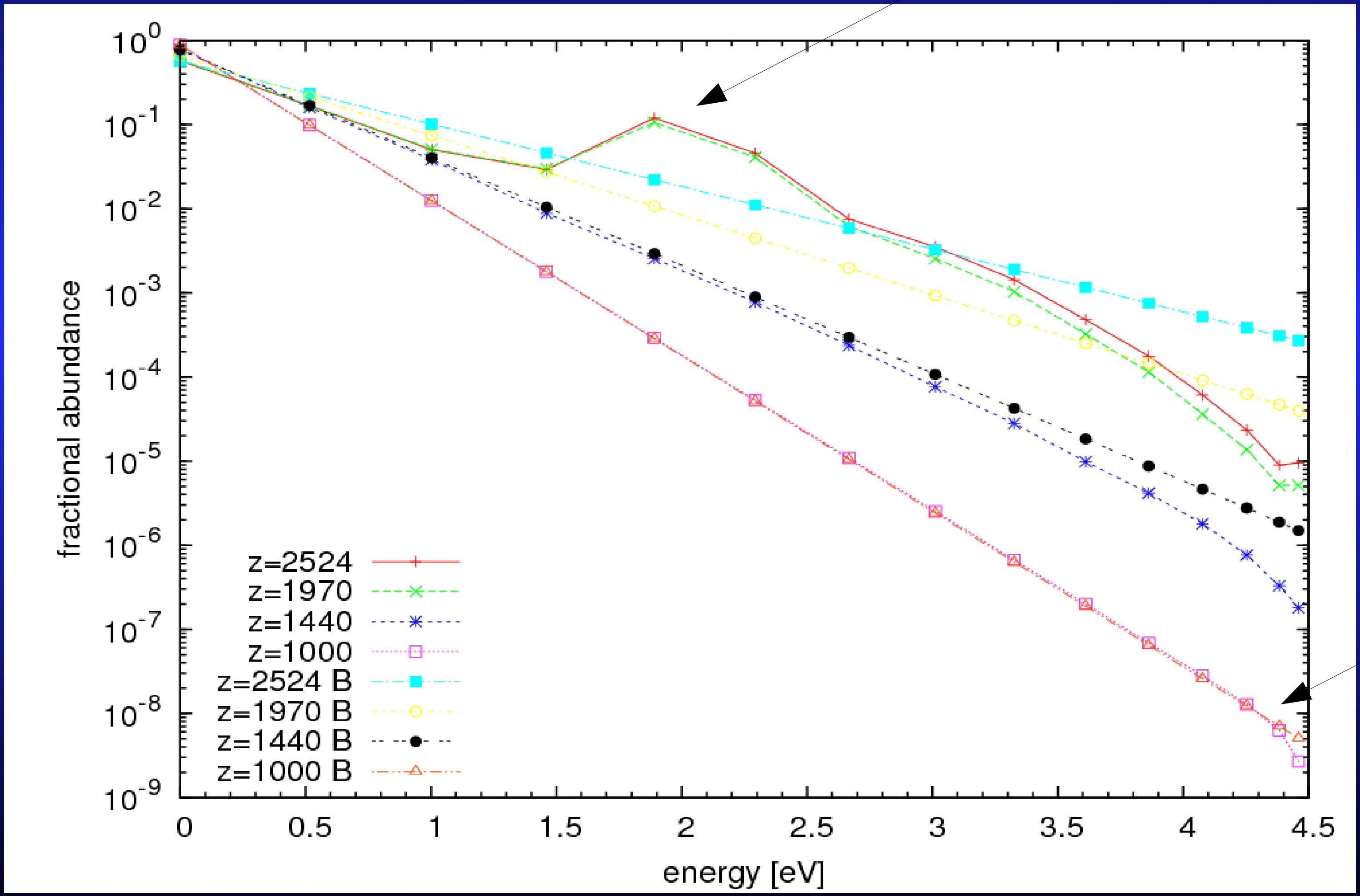


Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2 (II)

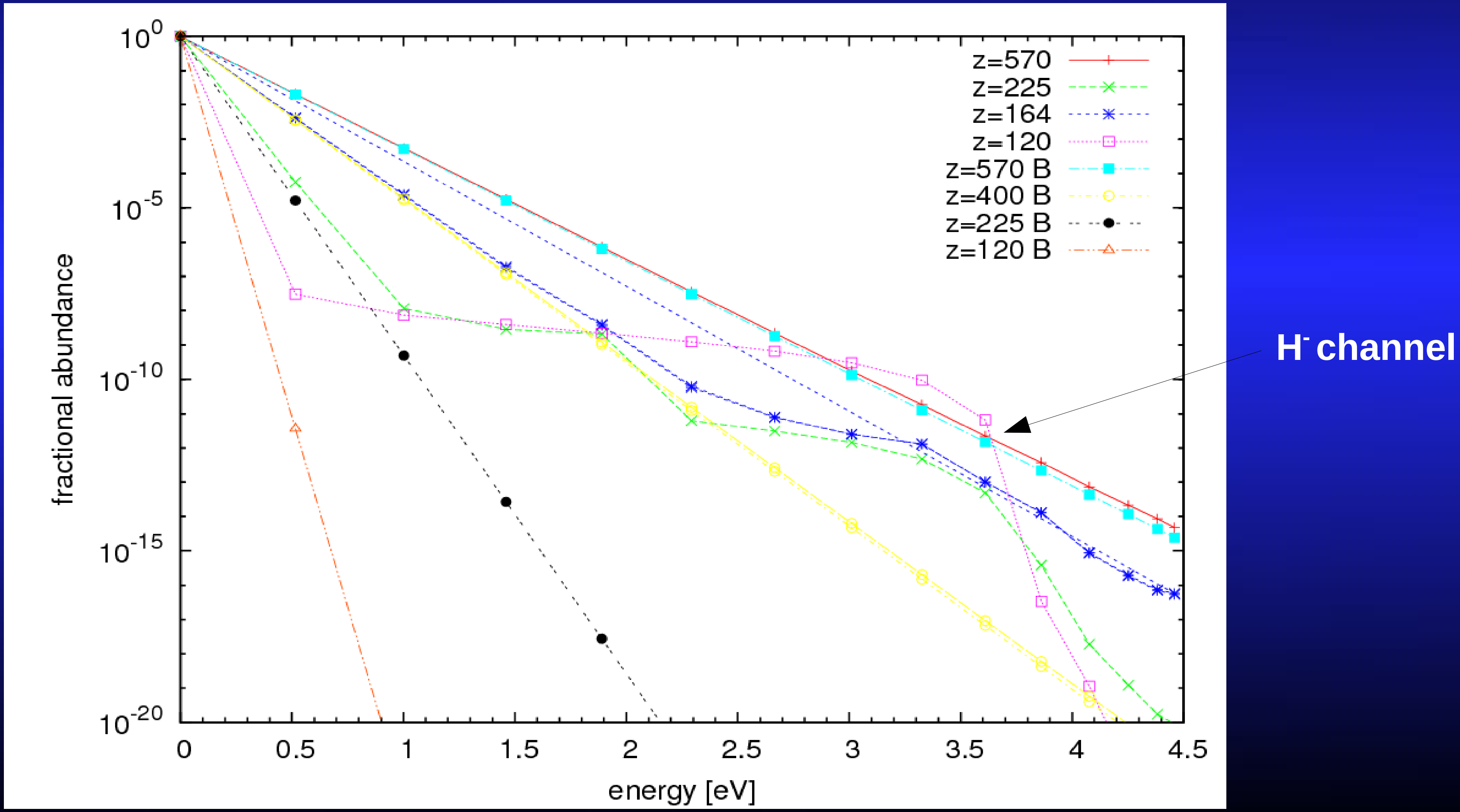
H_2^+ channel

Equilibrium!!!



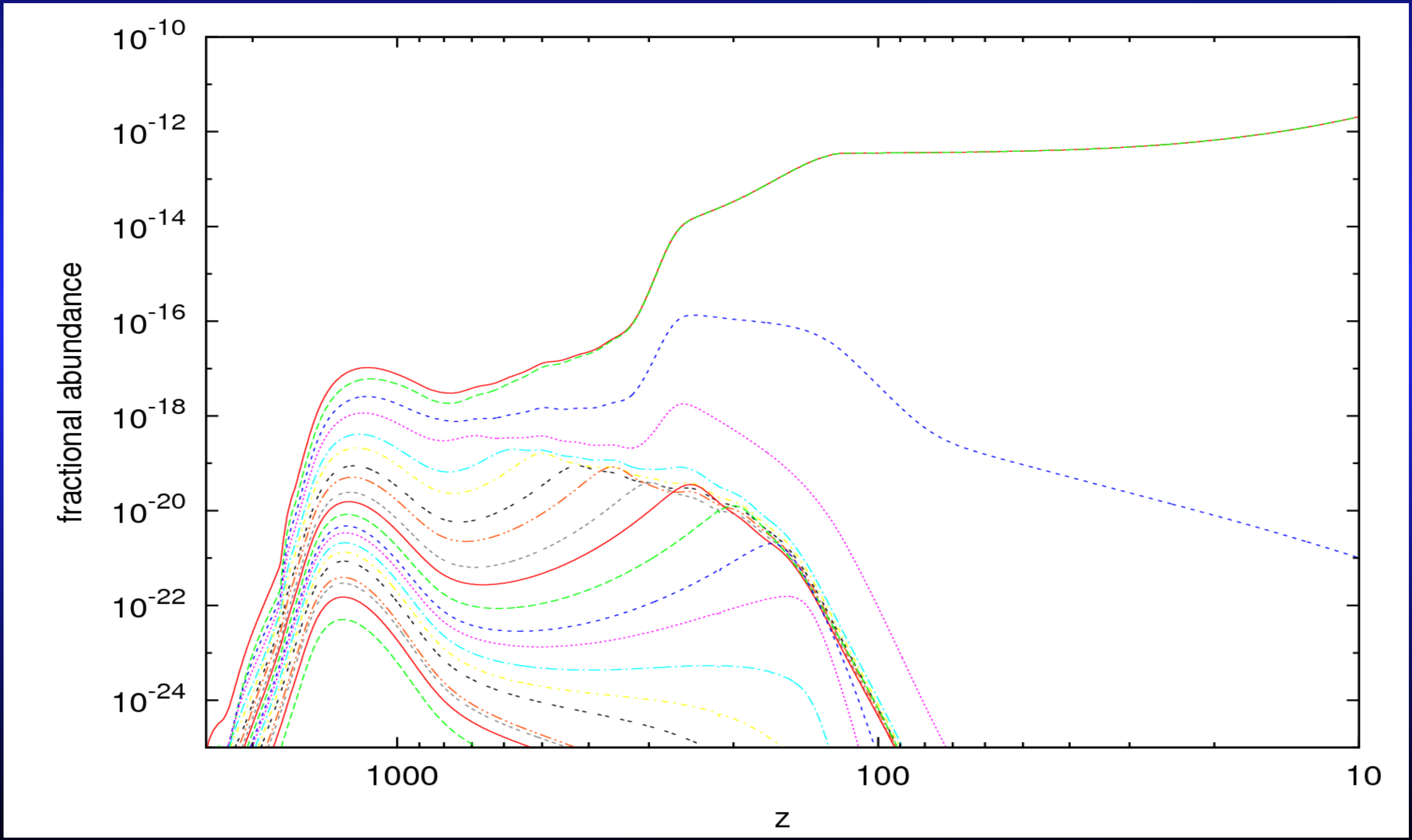
Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2 (III)



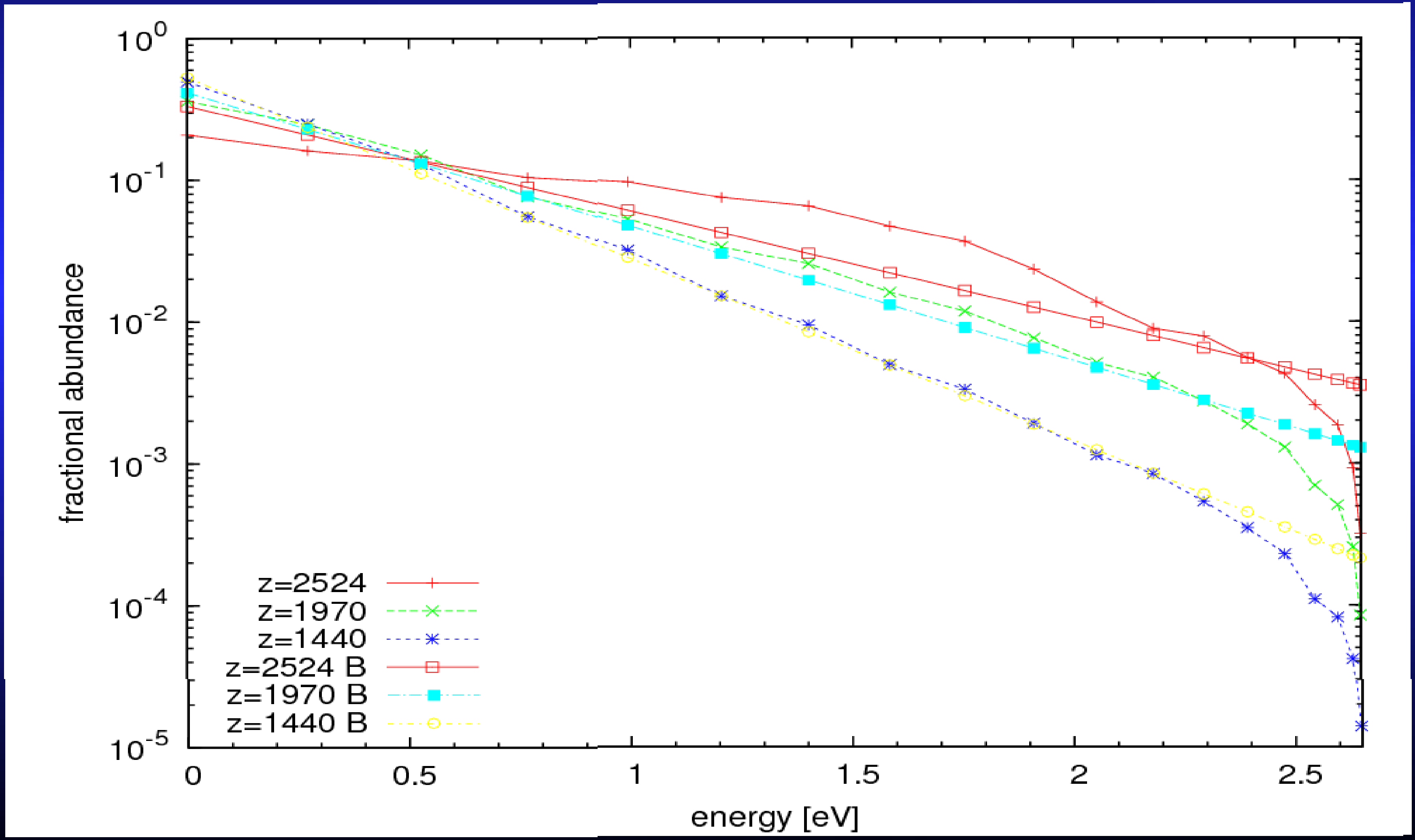
Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2^+ (I)



Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

RESULTS: VDF H_2^+ (II)



Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

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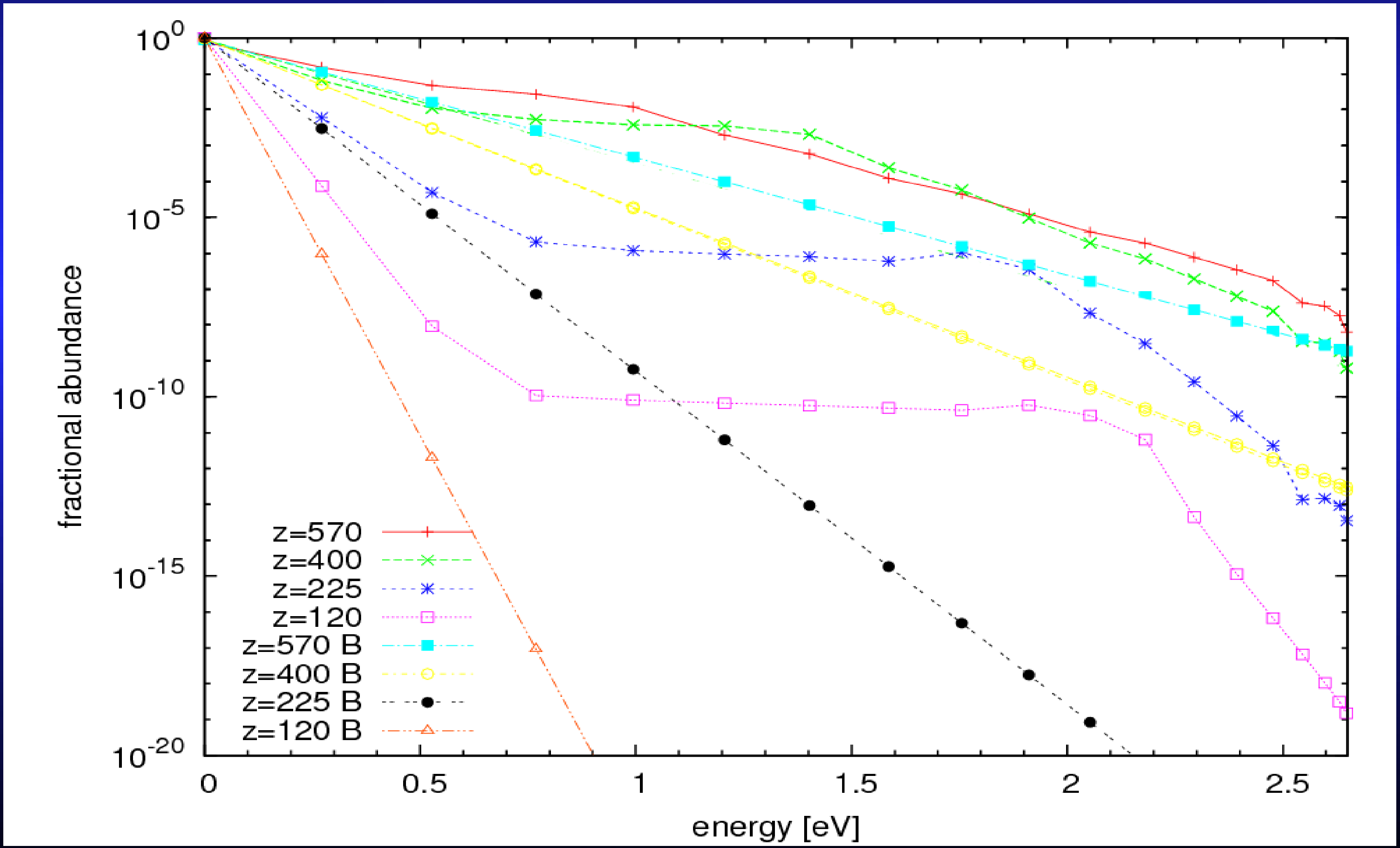
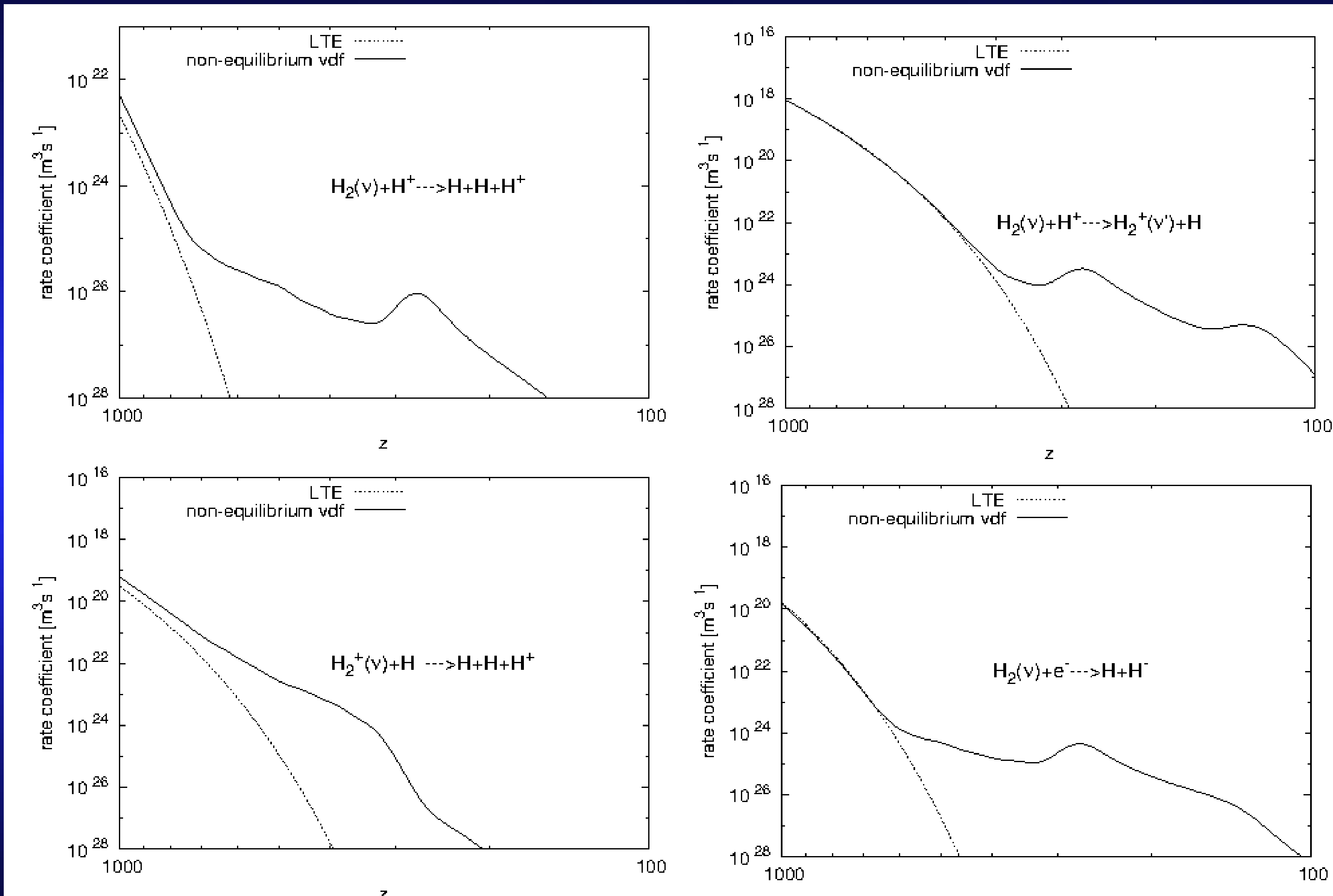
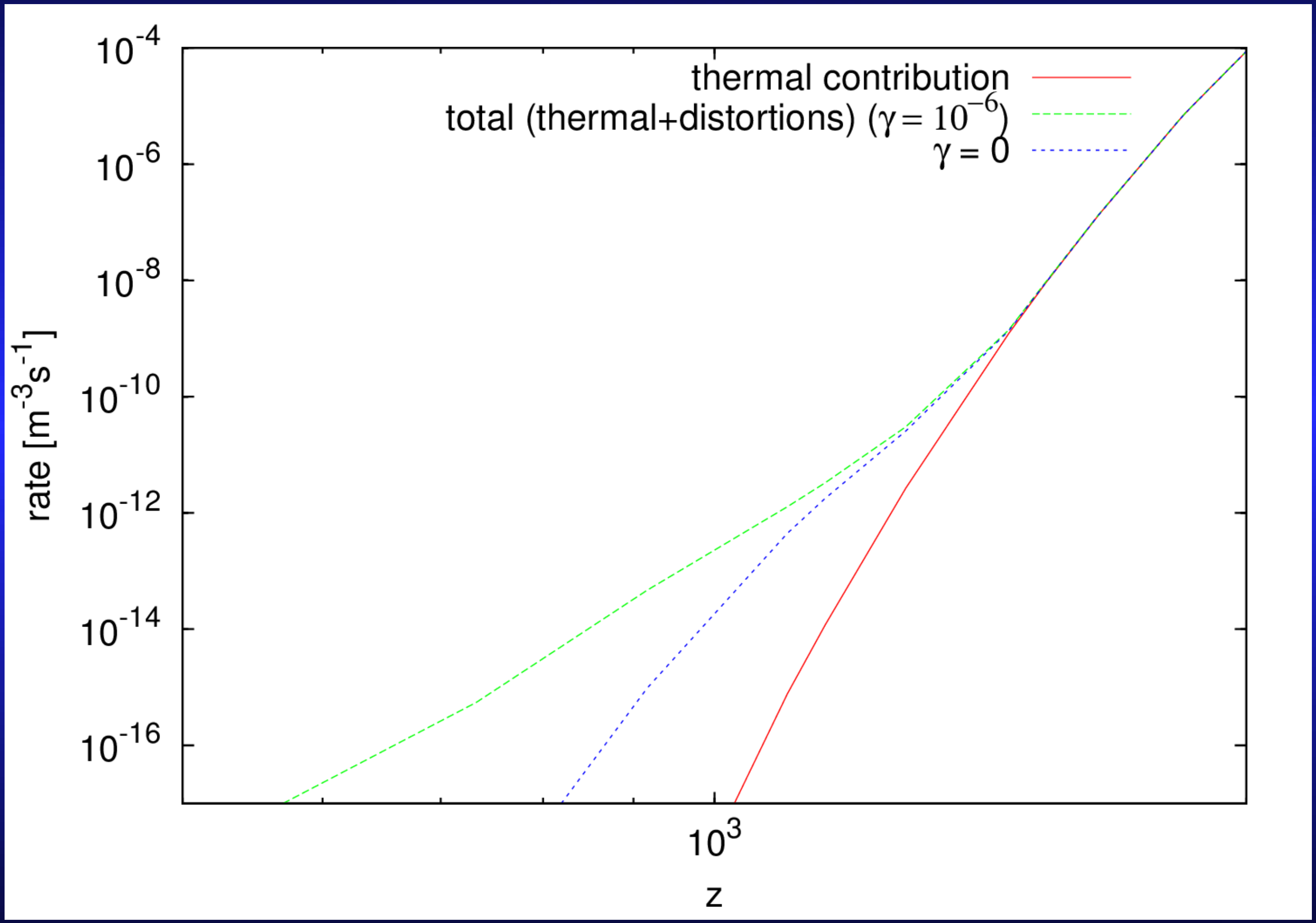


Coppola, Longo, Capitelli, Palla, Galli, 2011, ApJS, **193**, 7-18

“ MODIFIED” RATE COEFFICIENTS

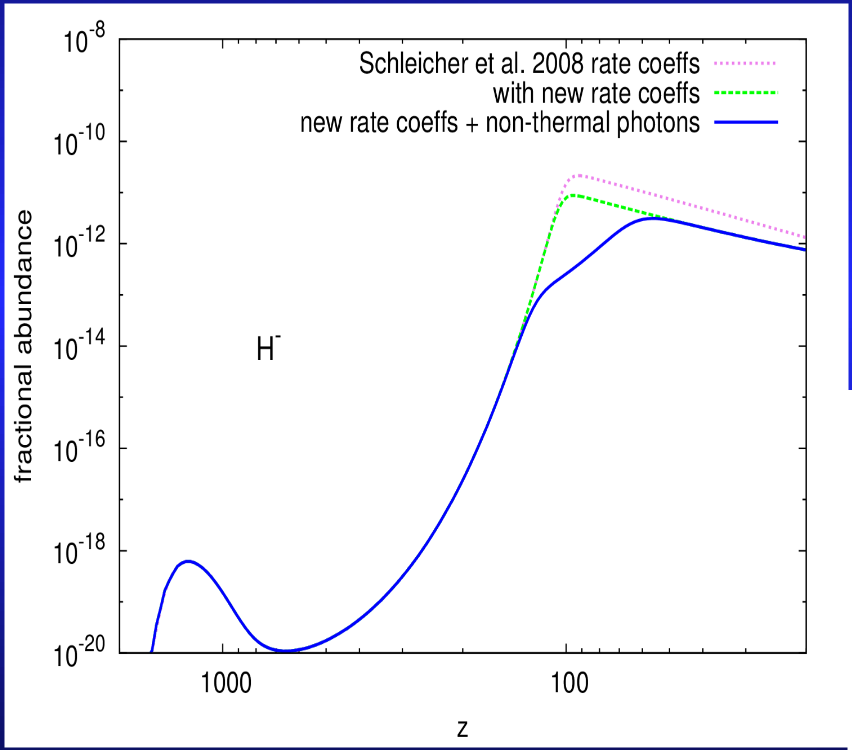


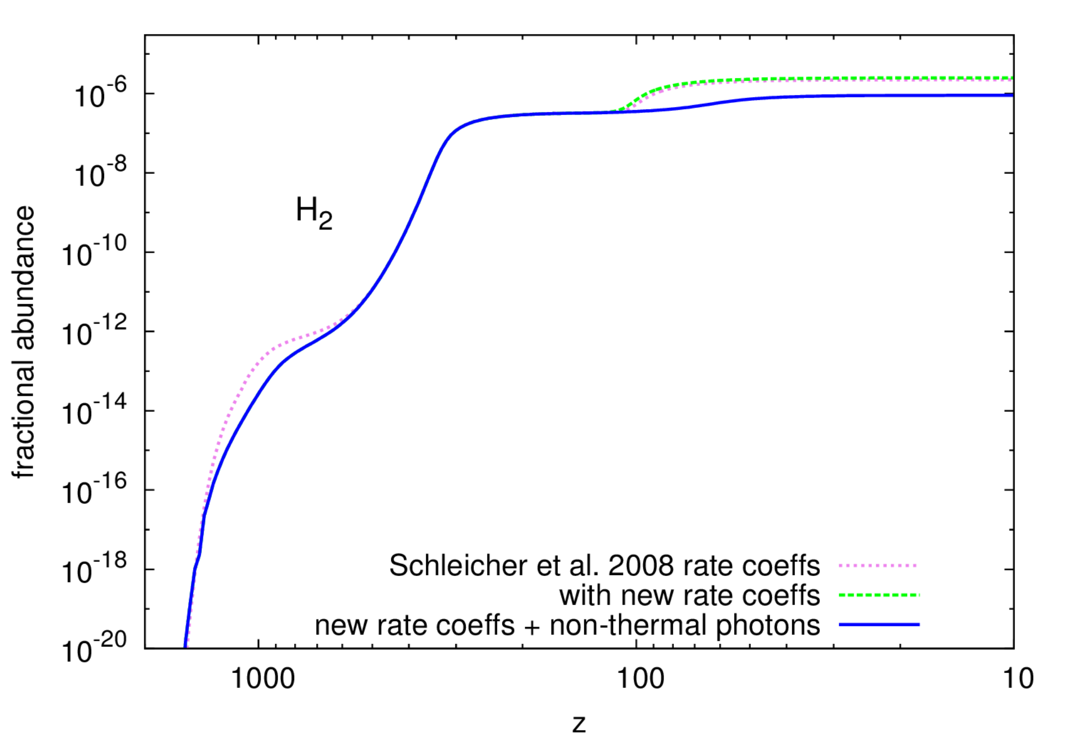
Coppola, C. M.; D'Introno, R.; Galli, D.; Tennyson, J.; Longo, S., 2012, ApJS, **199**, 16



$$\chi_v \propto \mathrm{Boltzmann} + \gamma \cdot \frac{1}{(1+v)}$$

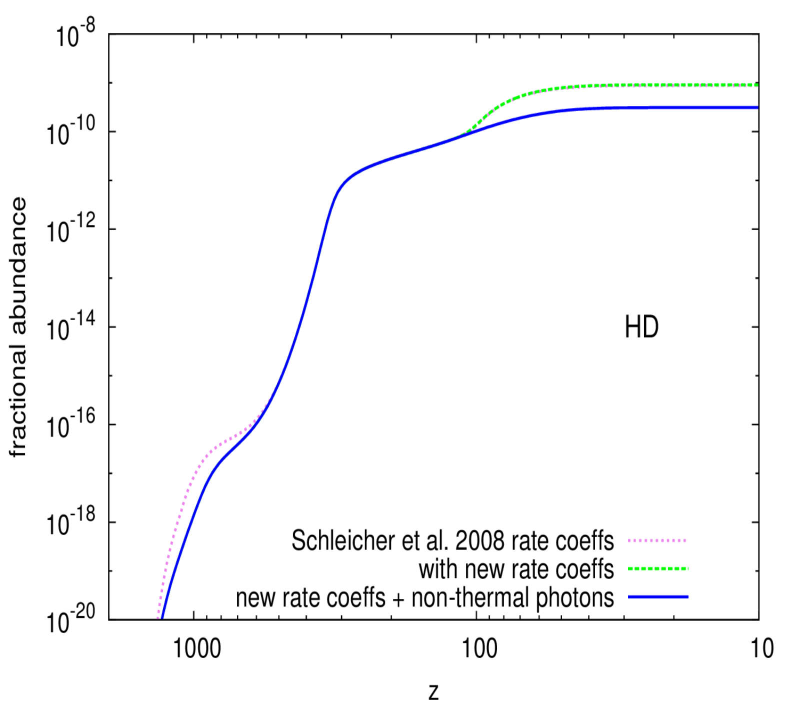
SPECTRAL DISTORTIONS (VIII)

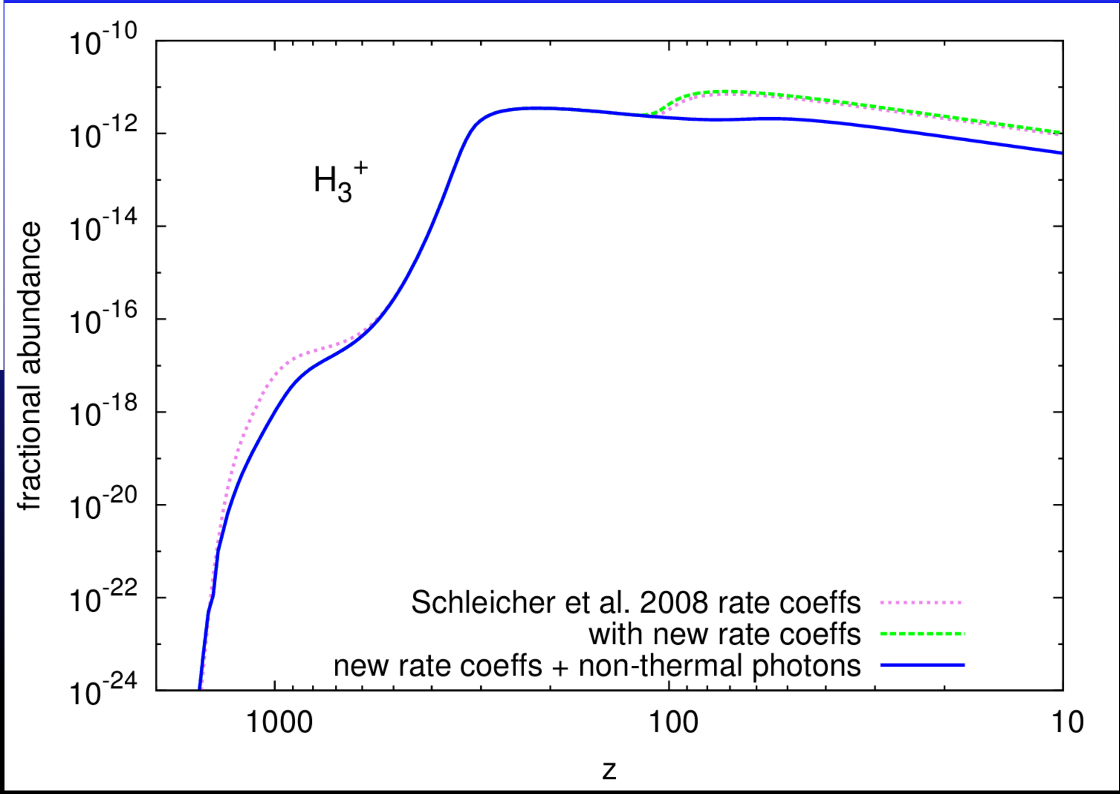




Coppola et al. 2013
MNRAS **434** (1) 114-122

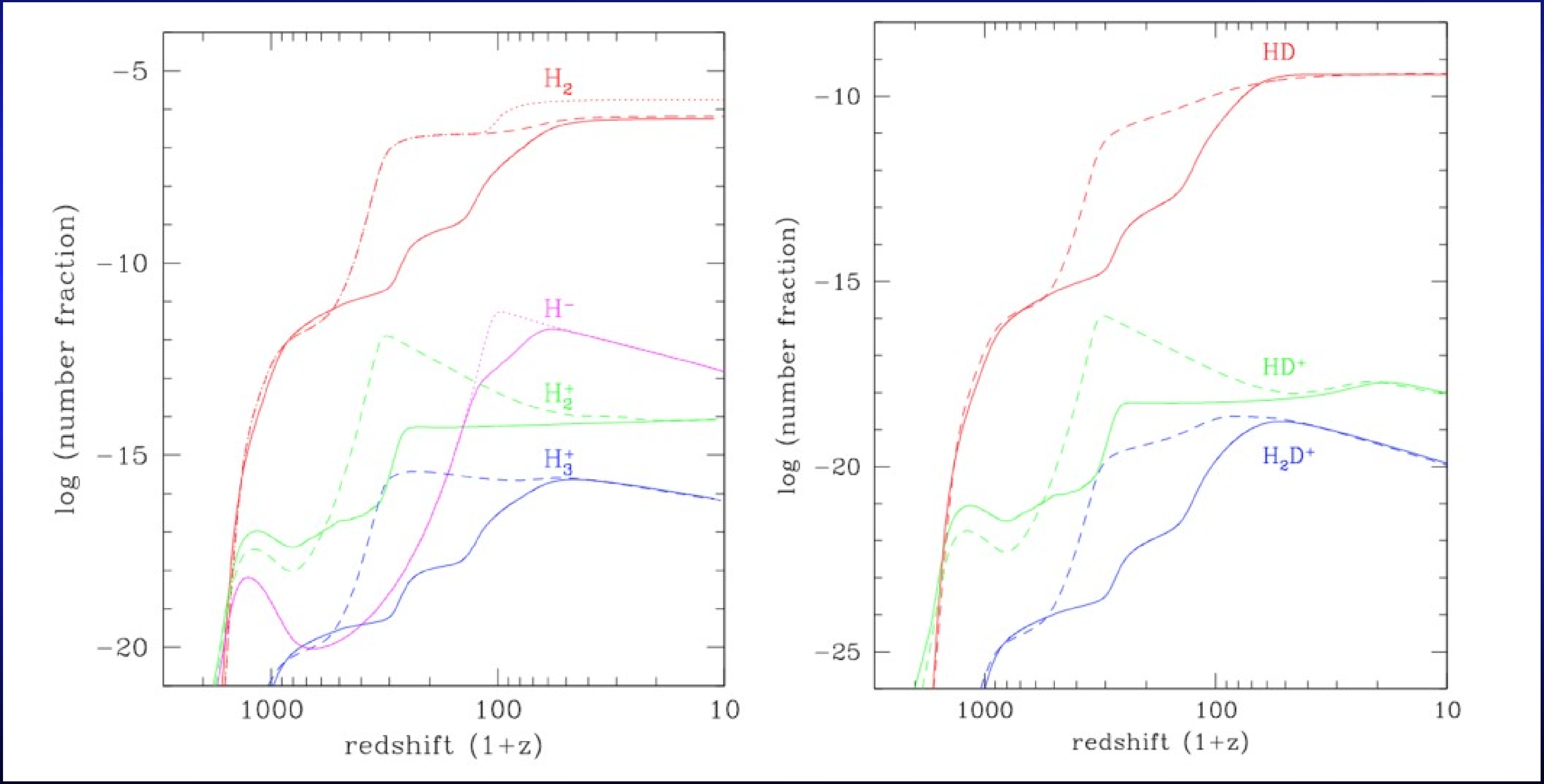
SPECTRAL DISTORTIONS (IX)





Coppola et al. 2013
MNRAS **434** (1) 114-122

" MODIFIED" FRACTIONAL ABUNDANCES



Galli & Palla, Annual Review of Astronomy and Astrophysics, **51,** 163-206, 2013

...CONCLUSIONS...

- rovibrational selectivity
- non equilibrium distributions
- non-thermal photons

→ more realistic description for the early Universe

(same approach for other molecules,
rotational levels etc
→ better description
for the cooling mechanisms)

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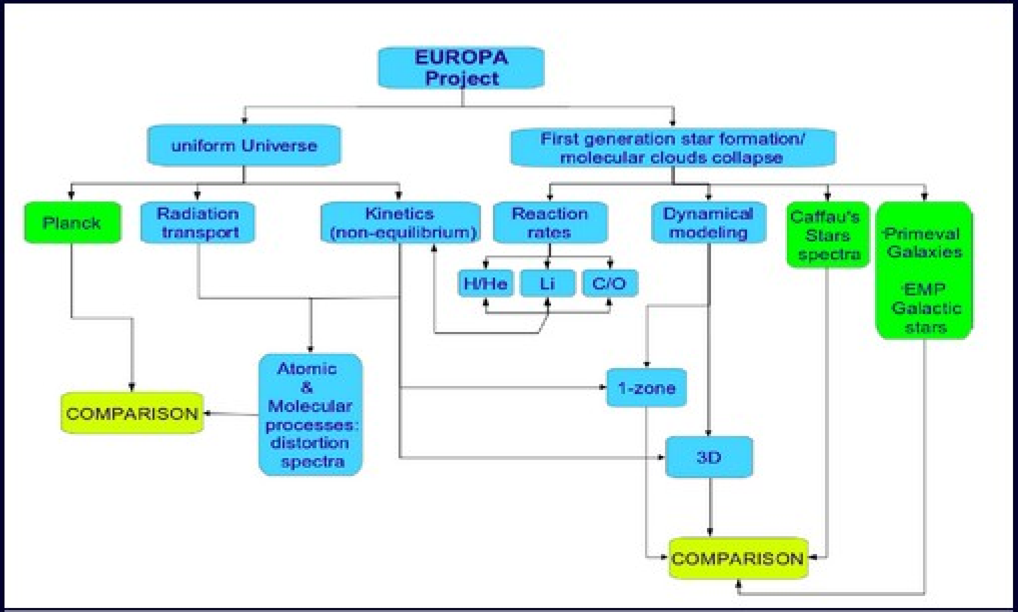
Jonathan Tennyson
Physics & Astronomy Department - UCL

...workshop organizers...

…ONGOING PROJECTS...
EUROPA: Early Universe: Research on Plasma Astrochemistry
International Space Science Institute (Bern)

Home Overview Team Meetings Reports/References Blog

Europa
Early Universe: Research On Plasma Astrochemistry
ISSI International Team



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Francesco Gianturco
Raffaella Schneider

The present era of high precision cosmology requires a proper treatment of the physical and chemical phenomena occuring in the primordial plasma. For this reason, it is crucial to obtain a description as detailed as possible of the environment of the early universe and to discuss feasible strategies to test theoretical models with present and future observational instrumentation. The basic goals of the project that will be divided into two main areas of interests are

http://www.issibern.ch/teams/europa/EUROPA Overview.html


THANKS...