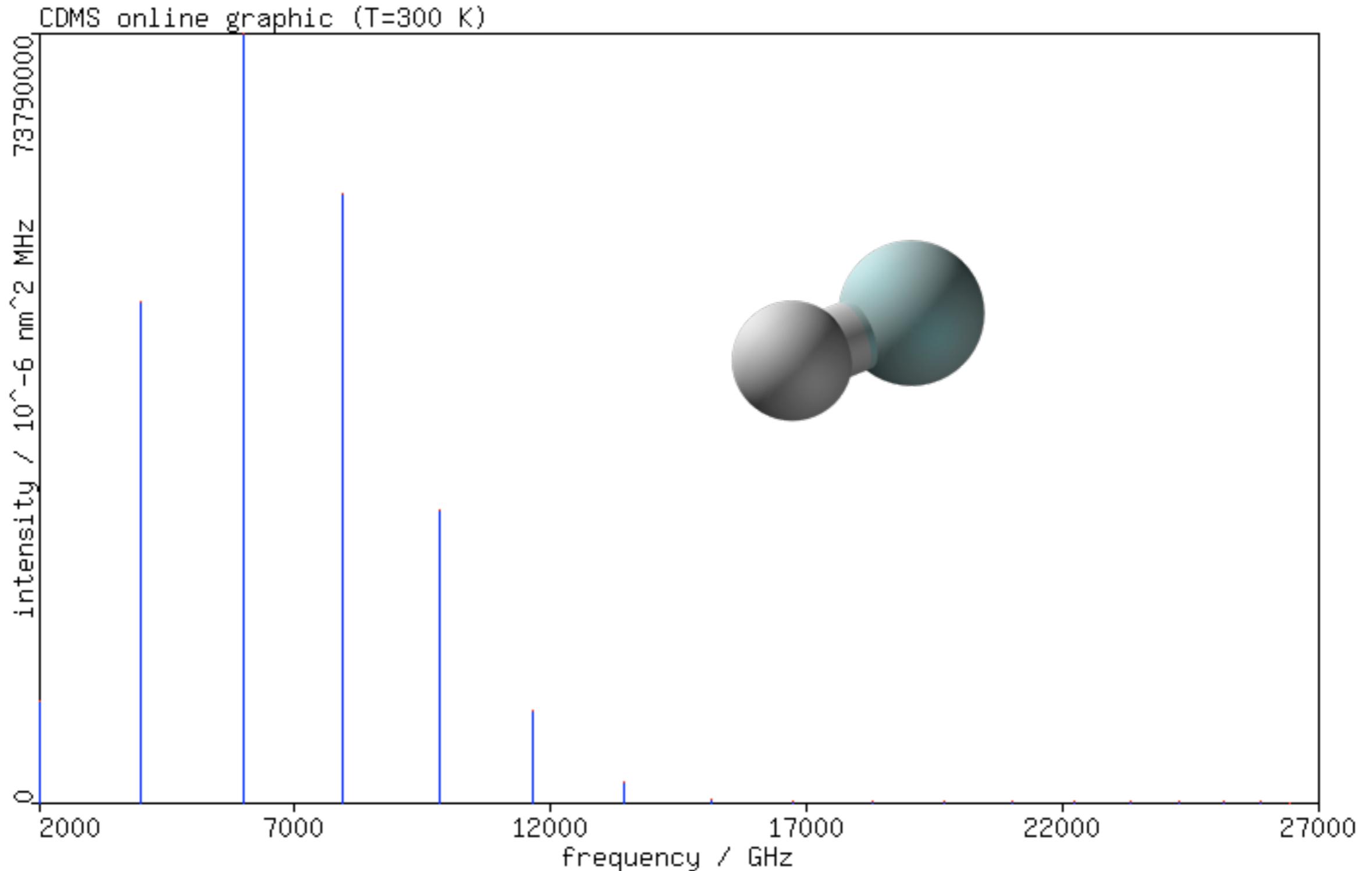


Lecture 5: "Gas-phase Processes and First Molecules"

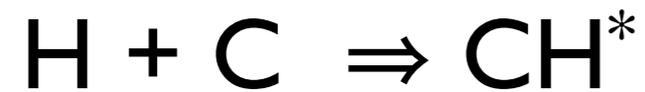


I. Chemical Processes in Space

Name	Representation	Example	Rate*
Radiative association	$A + B \rightarrow AB + \nu$	$C^+ + H_2 \rightarrow CH_2^+$	$\sim 10^{-10} - 10^{-17} \text{ cm}^3 \text{ s}^{-1}$
Ion-molecule	$A^+ + B \rightarrow C^+ + D$	$CO + H_3^+ \rightarrow HCO^+ + H_2$	$\sim 10^{-7} - 10^{-10} \text{ cm}^3 \text{ s}^{-1}$
Neutral-neutral	$A + B \rightarrow C + D$	$O + CH_3 \rightarrow H_2CO + H$	$\sim 10^{-10} - 10^{-16} \text{ cm}^3 \text{ s}^{-1}$
Charge transfer	$A^+ + B \rightarrow B^+ + C$	$C^+ + Mg \rightarrow C + Mg^+$	$\sim 10^{-9} \text{ cm}^3 \text{ s}^{-1}$
Radiative recombination	$A^+ + e^- \rightarrow A + \nu$	$Mg^+ + e^- \rightarrow Mg + \nu$	$\sim 10^{-12} \text{ cm}^3 \text{ s}^{-1}$
Dissociative recombination	$AB^+ + e^- \rightarrow A + B$	$HCO^+ + e^- \rightarrow CO + H$	$\sim 10^{-7} \text{ cm}^3 \text{ s}^{-1}$
Ionization	$A + h\nu \rightarrow A^+ + e^-$	$C + h\nu \rightarrow C^+ + e^-$	$\sim 10^{-10} \times RF^{**} \text{ cm}^3 \text{ s}^{-1}$
Dissociation	$AB + h\nu \rightarrow A + B$	$CO + h\nu \rightarrow C + O$	$\sim 10^{-10} \times RF \text{ cm}^3 \text{ s}^{-1}$

Arrhenius rate: $k = \alpha \left(\frac{T}{300} \right)^\beta \exp(-\gamma/T)$

Radiative Association: bond formation



Formation of an excited collisional complex



Energy conservation \Rightarrow emission of photon

or (more likely)



A key process to form first molecules & chemical bonds (early Universe)

$$k \approx 10^{-17} - 10^{-12} \text{ cm}^3\text{s}^{-1}$$

Radiative Association: bond formation

Timescales:

10^{-2} s - vibrational transition,

10^{-8} s - electronic transition,

10^{-13} s - collisional timescale (or lifetime of collisional complex)

=> molecule formation only after $\sim 10^{11}$ collisions (10^5 if electronic transitions are available)!

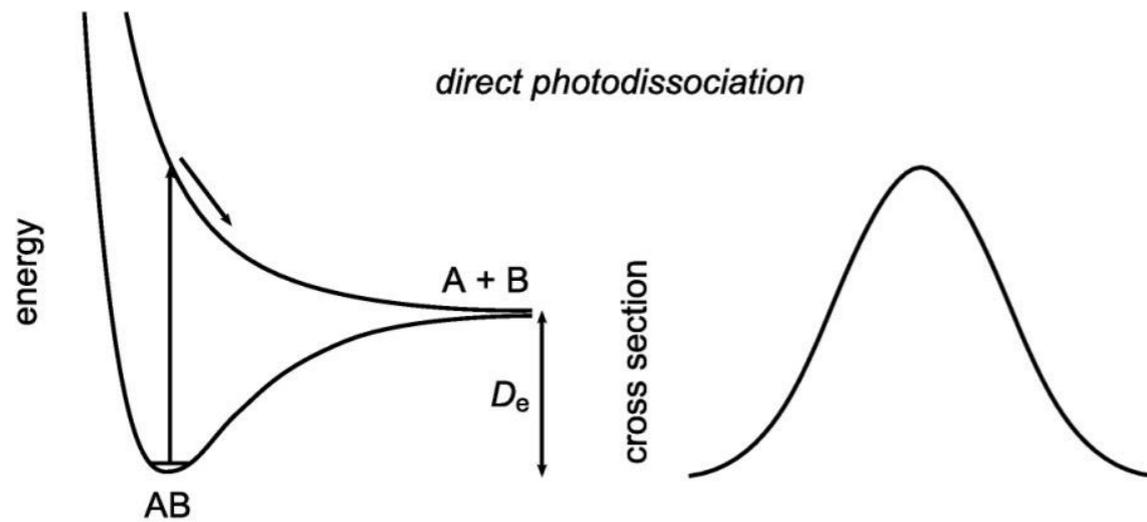
Slow for small reactants, but can be rapid for complex radicals

Hard to measure in laboratory (3-body processes dominate)

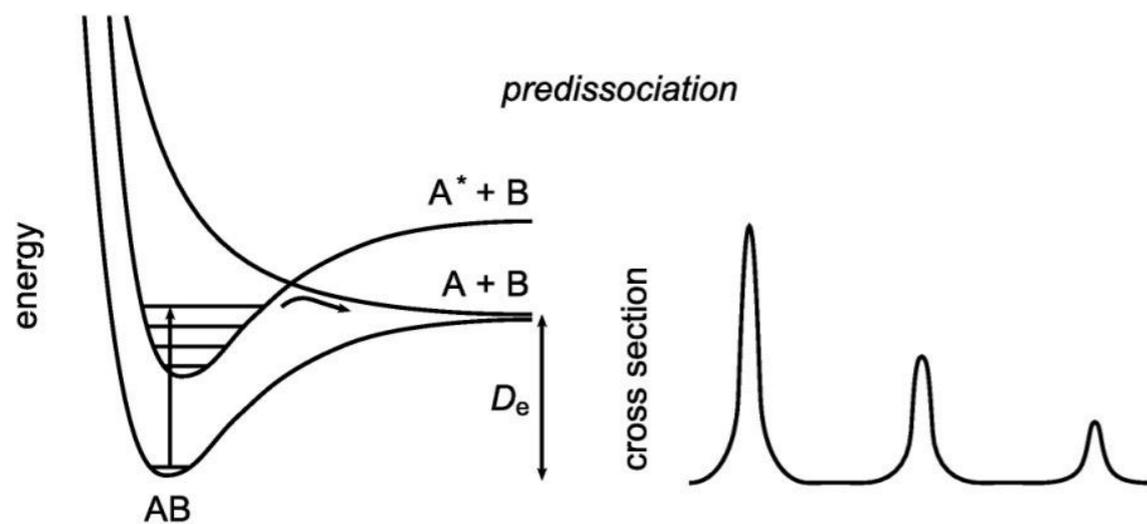
Hard to calculate for complex species

Photodissociation: bond destruction

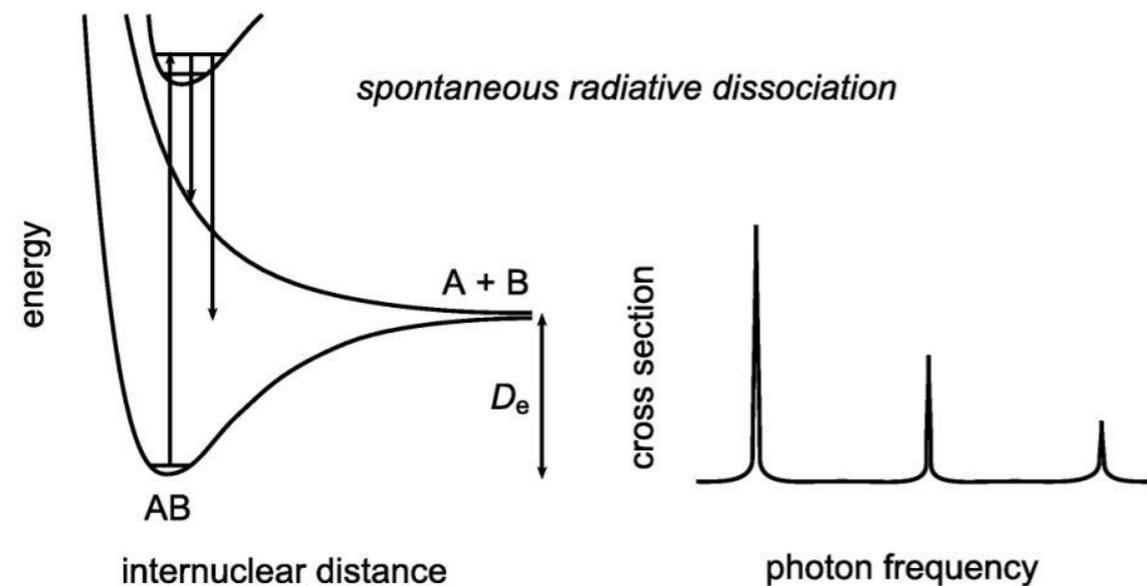
Bonding energies: 5-10 eV => FUV



Direct dissociation: transition to a continuum of excited electronic state

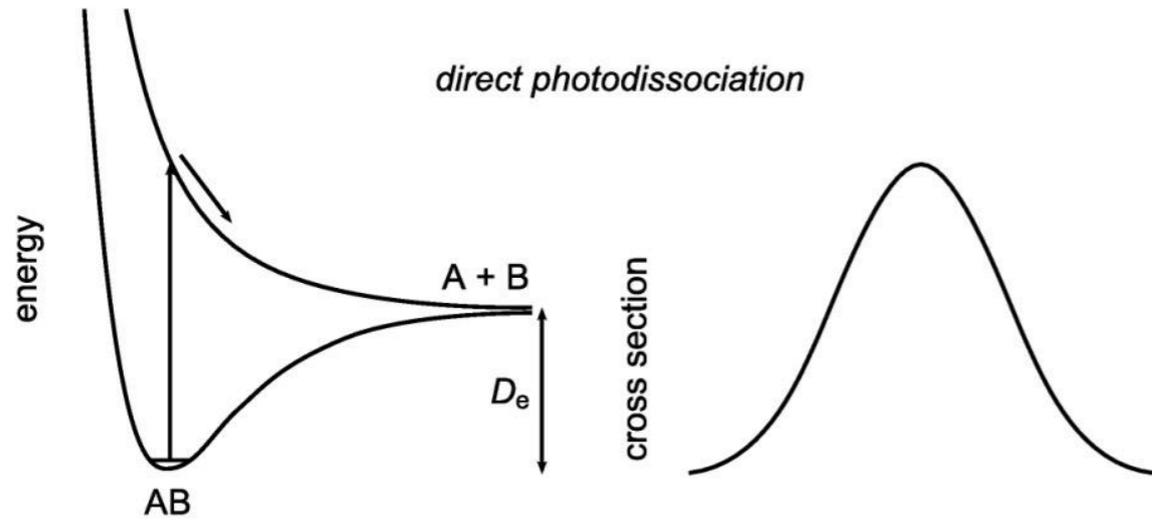


Predissociation: excited electronic state is mixed with dissociative state



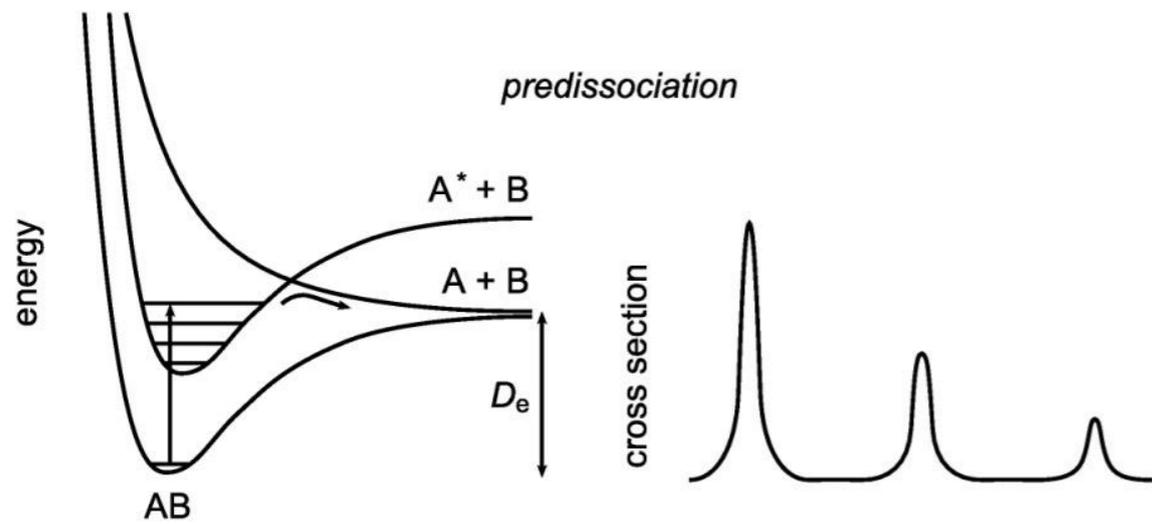
Spontaneous radiative dissociation: sometimes electronic excited states decay into continuum of the ground-state

Photodissociation: bond destruction

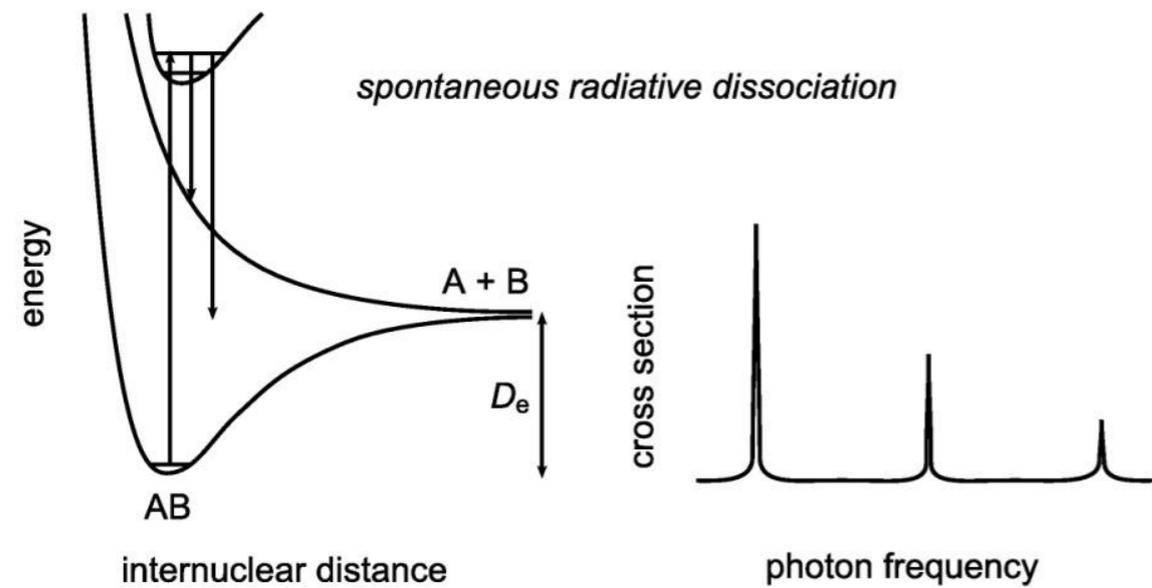


Examples:

H_2O , OH, ...

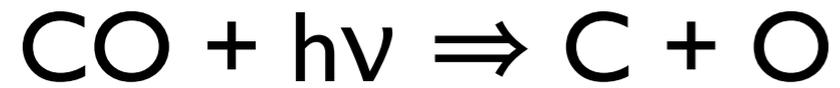


CO



Only H_2

Photodissociation: bond destruction



Line dissociation: H_2 , CO



Lyman $_{\alpha}$ dissociation: OH , CN , NH_3

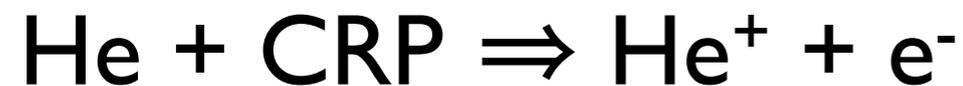
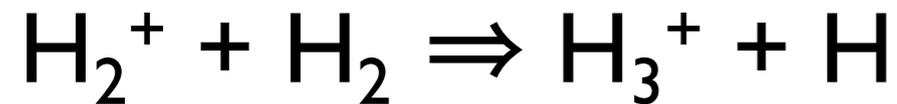
Continuum dissociation: CH_4

Calculated only for a few tens species

Strongly depends on radiation energy distribution



Cosmic Ray & UV Ionization



From observations:

$$k_{\text{CRP}} \approx 10^{-17} \text{ s}^{-1}$$

Relativistic energy particles (89% protons, 10% ^4He , 1% heavy elements)
 \Rightarrow penetrate a large gas columns \Rightarrow energy source even in “dark” regions

Key process to form H_3^+
 \Rightarrow enables proton transfer reactions
 \Rightarrow rich molecular chemistry

I.P. of He is 24.6 eV \Rightarrow

He^+ breaks chemical bonds \Rightarrow destruction of molecules (CO!)

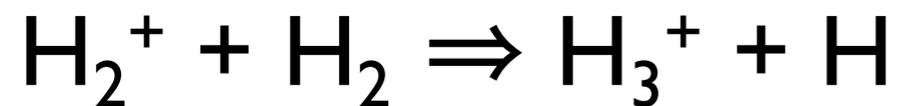
Ion-Molecule Reactions: bond rearrangement



Ion induces dipole moment => long-range strong attraction => no activation barriers



Rates increase at low T if a molecule is polar due to a long-distance Coloumb attraction



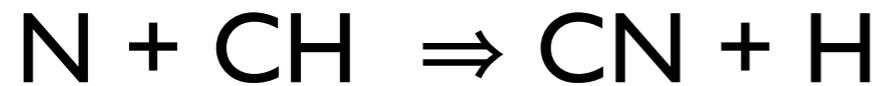
Langevin rate: $k_L = 2\pi e \left(\frac{\alpha}{\mu}\right)^{1/2}$

(μ - reduced mass, α - polarizability)

$$k \approx 10^{-9} - 10^{-7} \text{ cm}^3 \text{ s}^{-1}$$

A key process to form complex ions and complex neutrals (after DR)
=> ~50% of all processes in astrochemical models

Neutral-Neutral Reactions: bond rearrangement



Long-range attraction is weak



Usually have barriers due to bond breaking for molecular rearrangement

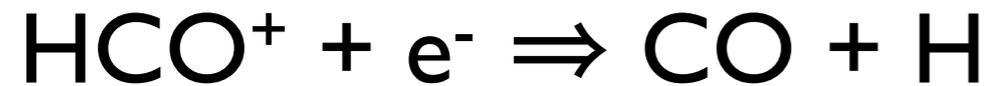
Some are rapid reactions even at ~ 10 K (radical-radical, radical-neutral)

Particularly competitive at high temperatures, > 100 K

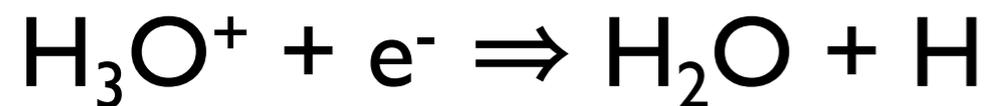
$$k \approx < 10^{-11} - 10^{-9} \text{ cm}^3\text{s}^{-1}$$

Many barriers are 'guessed' values, ~ 100 - 1000 K

Dissociative Recombination: bond destruction



Capture of e- by an ion => formation of neutral in excited electronic state => dissociation



Rapid processes, increased rates at low T



If radiative (no break-up), then usually slow

A final step in formation of neutral species

$$k \approx 10^{-7} \text{ cm}^3\text{s}^{-1}$$

Branching ratios and products are not well known

Radiative Attachment



$$k \approx < 10^{-7} \text{ cm}^3\text{s}^{-1}$$



Effective for molecules with large e-affinities

Excess of energy is re-radiated => less efficient for small molecules

<10% of anion/neutral for hydrocarbons
(predicted by Herbst 1981)

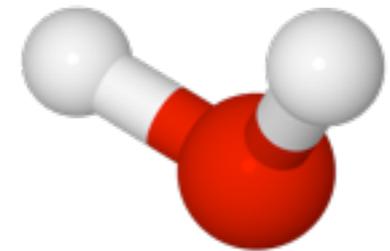
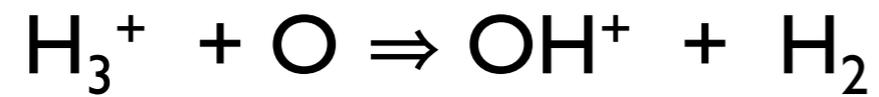
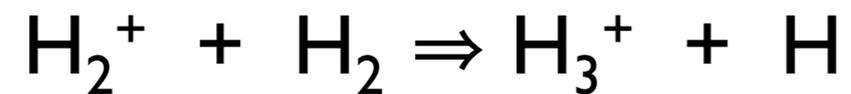
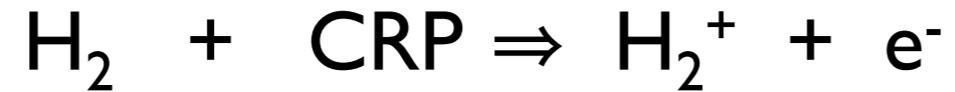
Discovered in ISM with predicted abundances (McCarthy et al. 2006, Bruencken et al. 2007, etc.)

Important in chemistry of the early Universe

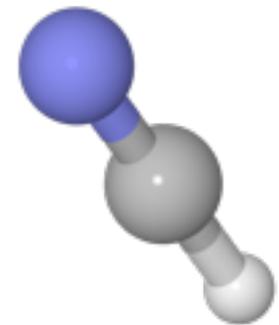
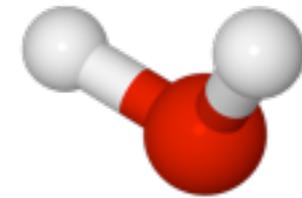
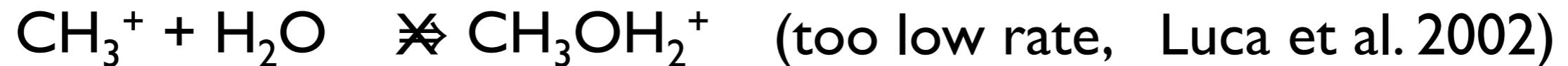
Chemical Reaction Databases

- Ohio State University (OSU), now Kinetic Database for Astrochemistry (KIDA):
5000 reactions, 500 species, 12 elements
- Manchester University (UMIST):
Rate06: 4600 reactions, 420 species, 12 elements
- NIST Chemical Kinetics Database: ~30,000 neutral-neutral reactions (T>300K)
- JPL (Anicich): Compilation of all ion-molecule reactions with references
- Only ~10-20% of accurate rates!

Gas-phase Formation of Water



Gas-phase formation of complex molecules



Chemical Kinetics

$$\frac{\partial n_i}{\partial t} = \sum_{j,k \neq i} k_{jk} n_j n_k - n_i \sum_l k_l n_l + \nabla D n \nabla n_i / n - \nabla U n_i$$

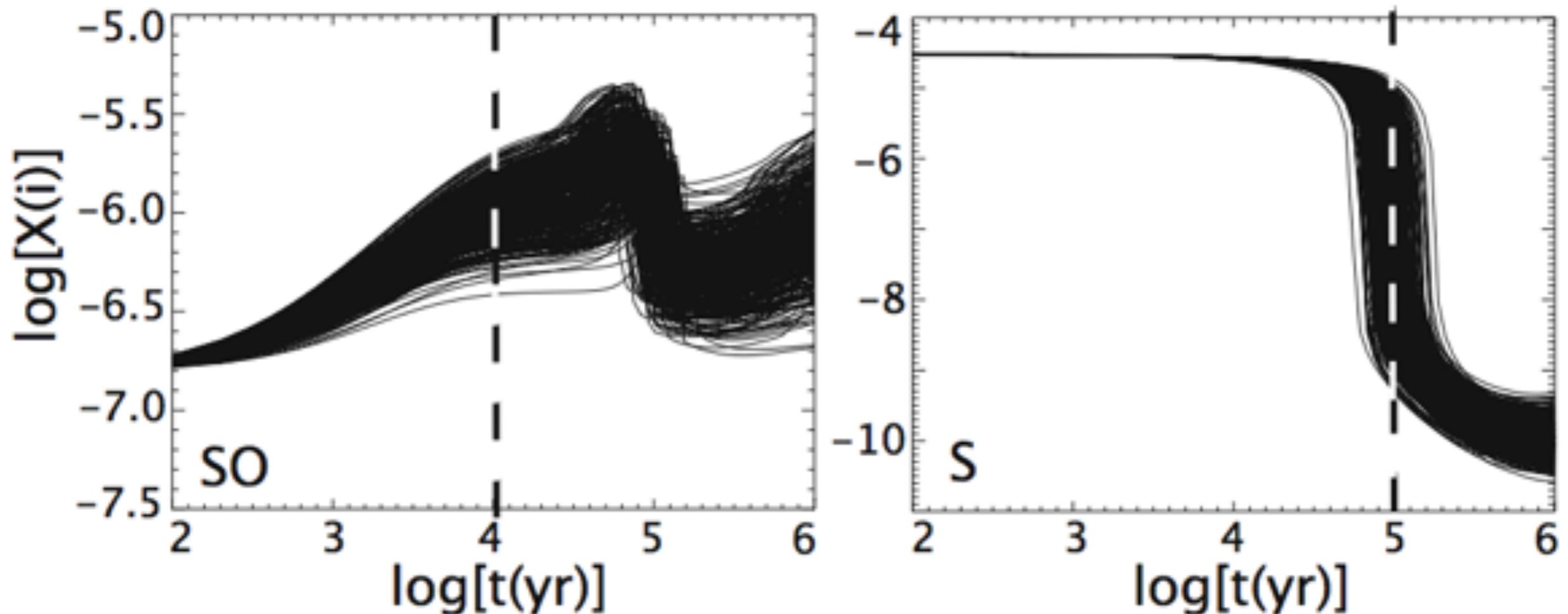
- Physical conditions
 - (For last 2 terms): dynamical parameters (wind, turbulence, advection)
 - Initial abundances
 - A chemical network
 - A numerical solver
-
- Steady-state: $n_i(t) = \text{const}$ (derivative is 0) \Rightarrow algebraic equations

Chemical codes

- **ALCHEMIC** (MPIA Heidelberg): gas-grain
- **GADGET** (ITA Heidelberg): gas-phase, early Universe
- **NAHOON** (Bordeaux Obs.): gas-grain, uncertainties
- **MONACO** (Univ. of Virginia): gas-grain, Monte Carlo stochastic chemistry
- **ASTROCHEM** (Grenoble): gas-grain
- **OSU codes** (now at Univ. of Virginia): gas-grain, warm-up
- Many codes for photon-dominated chemistry (**CLOUDY**, Meudon, Leiden, etc., see Roellig et al. 2007)

Computed abundances have error bars

- Chemistry of planetary atmospheres: Dobrijevic et al. (1998, 2001)
- Molecular clouds, protoplanetary disks: Vasyunin et al. (2004, 2007), Wakelam et al. (2005, 2006)



Modeled abundances are uncertain by factor of >3

Pause

II. Chemistry in the Early Universe

- Simple chemistry, only light elements: H, D, He, Li
- Almost isotropic physical conditions (no structures)
- First molecules: cooling of gas \Rightarrow formation of first stars (Pop III)
- High- z molecules are detected ($z \sim 7$)!

The Universe after Big Bang

Epoch	Time, s	T_R, K	n_H, cm^{-3}
Lepton	10^{-4}	10^{12}	–
Radiation-dominated	2	10^{10}	–
Matter-dominated	$10^{11}-10^{12}$	4000	500
Present	10^{18}	2.73	$2 \cdot 10^{-7}$

Radiative temperature: $T_R = 2.73\text{K} (1 + z)$

Density: $n_H = 200 \left(\frac{1+z}{1000}\right)^3 \left(\frac{\Omega}{0.1}\right)^4 \left(\frac{H}{50}\right)^8 \text{cm}^{-3}$

Standard Cosmological Model

Composition at the beginning of the matter-dominated era:

H : D : ^4He : ^3He : ^7Li
1 : $4 \cdot 10^{-5}$: $8 \cdot 10^{-2}$: 10^{-5} : $2 \cdot 10^{-10}$
(all atoms fully ionized)

(1) $\text{H} + h\nu \rightarrow \text{H}^+ + e$, rate \sim ambient radiation field

(2) $\text{H}^+ + e \rightarrow \text{H}$, rate $\sim T^{-0.61}$

Temperature of matter $T_M = T_R$ due to Thompson scattering of photons on electrons

As Universe cools, recombination becomes more important:
 $n(\text{H}^+) = n(\text{H})$ at $z = 1340$, $T_R = T_M = 3630$ K

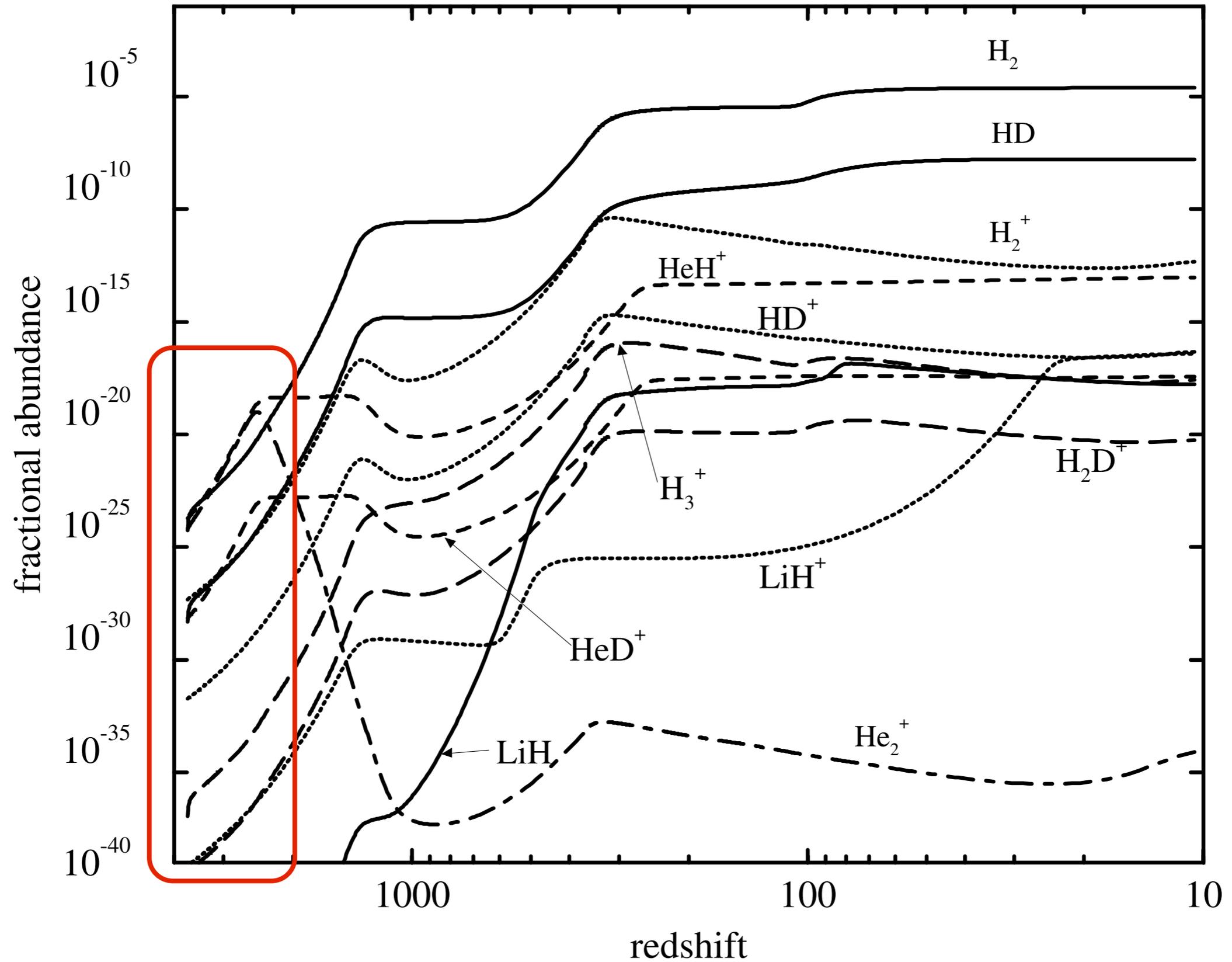
After that no thermodynamical equilibrium \Rightarrow chemical kinetics has to be considered to predict molecular abundances

First neutral & molecule: He and He₂⁺

ionization potentials [in eV]

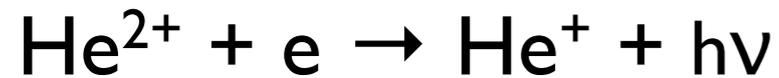
	1 st	2 nd	3 rd
H	13.6		
He	24.6	54.4	
Li	5.4	75.6	122.5

First Molecules



Chemistry of He

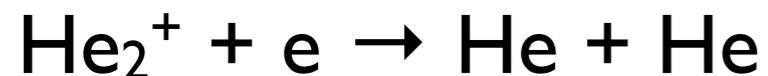
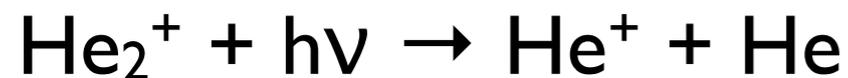
He⁺ recombines earlier than H⁺:



First molecules were He₂⁺ and HeH⁺:



They were removed by photodissociation & dissociative recombination:



Reaction rates of He-chemistry

Table 3. Reaction rates for Helium species

reaction	rate (cm ³ s ⁻¹ or s ⁻¹)
He1) He ⁺⁺ + e → He ⁺ + γ	$1.891 \times 10^{-10} \left[\sqrt{\frac{T_g}{9.37}} \left(1 + \sqrt{\frac{T_g}{9.37}} \right)^{0.2476} \times \left(1 + \sqrt{\frac{T_g}{2.774 \times 10^6}} \right)^{1.7524} \right]^{-1}$
He2) He ⁺ + γ → He ⁺⁺ + e	$5.0 \times 10^1 T_r^{1.63} \exp\left(-\frac{590000}{T_r}\right)$
He3) He ⁺ + e → He + γ	$3.294 \times 10^{-11} \left[\sqrt{\frac{T_g}{15.54}} \left(1 + \sqrt{\frac{T_g}{15.54}} \right)^{0.309} \times \left(1 + \sqrt{\frac{T_g}{3.676 \times 10^7}} \right)^{1.691} \right]^{-1}$
He4) He + γ → He ⁺ + e	$1.0 \times 10^4 T_r^{1.23} \exp\left(-\frac{280000}{T_r}\right)$
He5) He + H ⁺ → He ⁺ + H	$4.0 \times 10^{-37} T_g^{4.74}$
He6) He ⁺ + H → He + H ⁺	$3.7 \times 10^{-25} T_g^{2.06} \times \left[1 + 9.9 \exp\left(-\frac{T_g}{2570}\right) \right]$
He7) He + H ⁺ → HeH ⁺ + γ	5.0×10^{-21}
He8) He + H ⁺ → HeH ⁺ + γ	$7.6 \times 10^{-18} T_g^{-0.5}$ $3.45 \times 10^{-16} T_g^{-1.06}$
He9) He + H ₂ ⁺ → HeH ⁺ + H	$3.0 \times 10^{-10} \exp\left(-\frac{6717}{T_g}\right)$
He10) He ⁺ + H → HeH ⁺ + γ	$1.6 \times 10^{-14} T_g^{-0.33}$ 1.0×10^{-15}
He11) HeH ⁺ + H → He + H ₂ ⁺	9.1×10^{-10}
He12) HeH ⁺ + e → He + H	$1.7 \times 10^{-7} T_g^{-0.5}$
He13) HeH ⁺ + H ₂ → H ₃ ⁺ + He	1.3×10^{-9}
He14) HeH ⁺ + γ → He + H ⁺	$6.8 \times 10^{-1} T_r^{1.5} \exp\left(-\frac{22750}{T_r}\right)$
He15) HeH ⁺ + γ → He ⁺ + H	$7.8 \times 10^3 T_r^{1.2} \exp\left(-\frac{240000}{T_r}\right)$

Chemistry of H

Molecular hydrogen cannot form on dust grains as at present time => slow gas-phase reactions

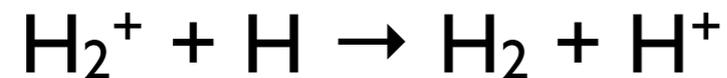
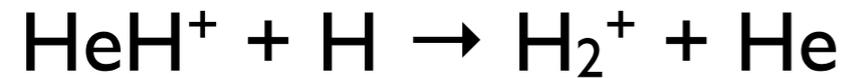
Direct formation by radiative association:



(H₂ does not have a dipole moment => difficult to get rid of excess of energy via radiation)

Formation of H₂ from HeH⁺

First H₂ were formed via ion-molecule reactions with HeH⁺:

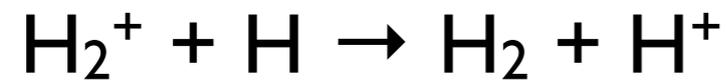


(here He and H are catalysts!)

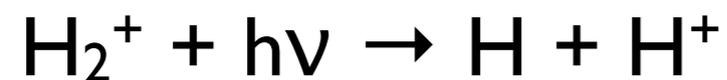
At that time, H₂ is quickly destroyed by background radiation (photodissociation)

Formation of H₂ from H⁺

Later, formation H₂ involves RA & ion-molecule reaction:



H₂⁺ is destroyed by photodissociation and DR:



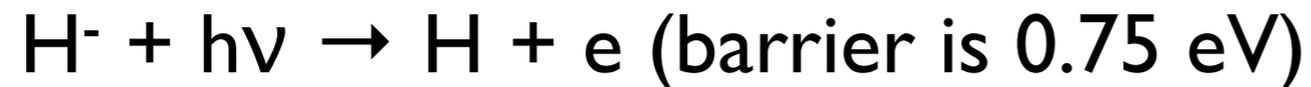
Photodissociation of H₂⁺ is efficient when T_R > 4000 K =>
no H₂ at earlier times!

Formation of H₂ from H⁻

At $z \sim 100$, H₂ can be formed through H⁻:

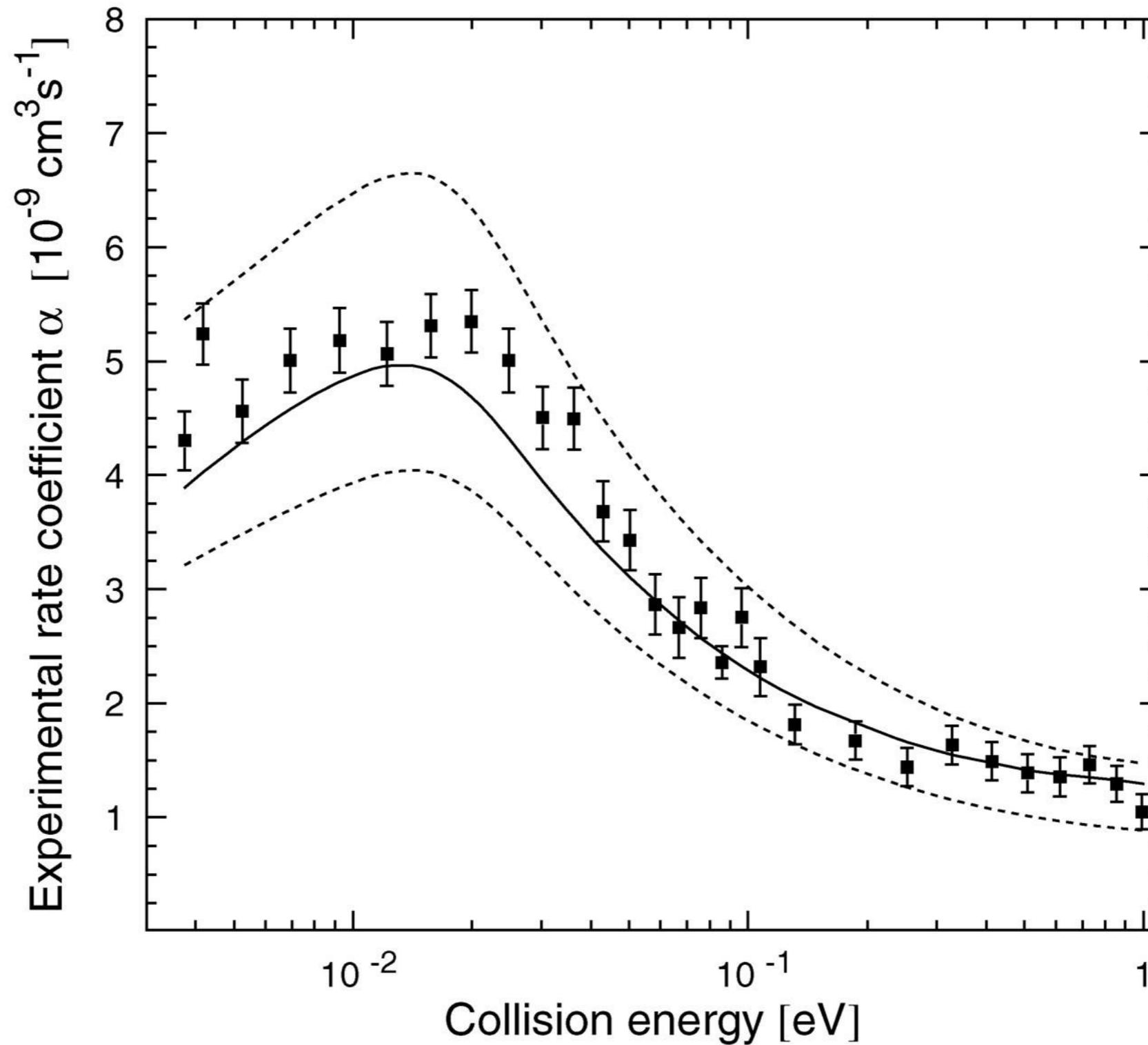


H⁻ is destroyed by photodetachment reaction:



$\Rightarrow T_R < 1000 \text{ K}$ are needed to slow down this process

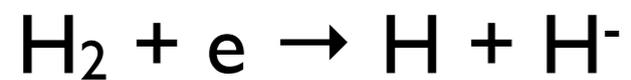
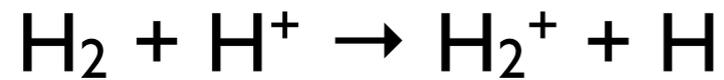
New experiments on $\text{H}^- + \text{H}$



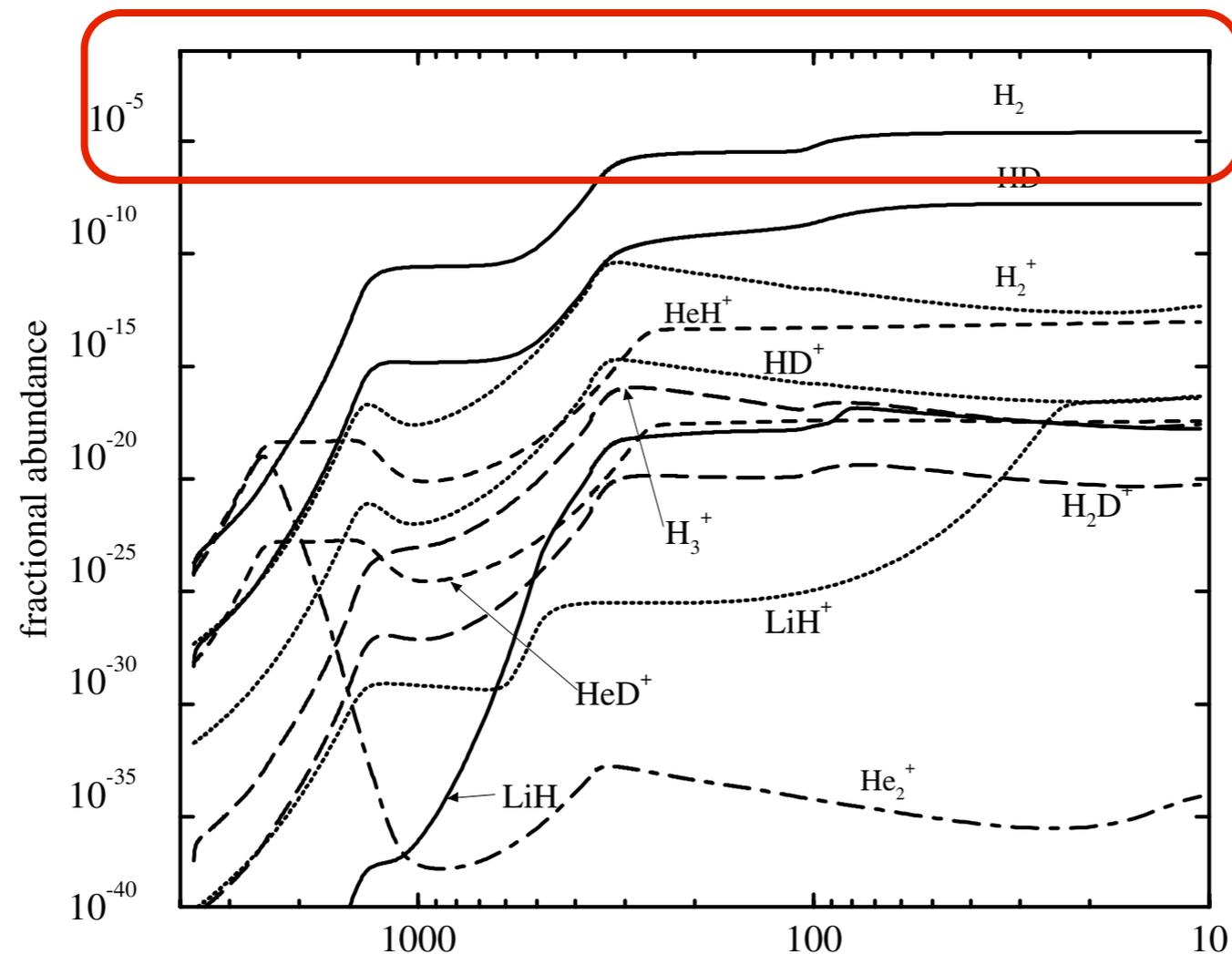
Kreckel et al. (2010), Science

Destruction of H₂

H₂ is efficiently destroyed by photodissociation, ion-molecule reactions with H⁺, and collisional dissociation:



=> small molecular fraction in the early Universe: $X(\text{H}_2) \sim 10^{-6}$



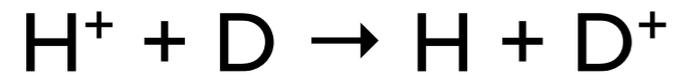
Reaction rates of H-chemistry

Table 1. Reaction rates for Hydrogen species

	reaction	rate (cm ³ s ⁻¹ or s ⁻¹)
H1)	$\mathbf{H}^+ + \mathbf{e} \rightarrow \mathbf{H} + \gamma$	R_{c2}
H2)	$\mathbf{H} + \gamma \rightarrow \mathbf{H}^+ + \mathbf{e}$	R_{2c}
H3)	$\mathbf{H} + \mathbf{e} \rightarrow \mathbf{H}^- + \gamma$	$1.4 \times 10^{-18} T_g^{0.928} \exp\left(-\frac{T_g}{16200}\right)$
H4)	$\mathbf{H}^- + \gamma \rightarrow \mathbf{H} + \mathbf{e}$	$1.1 \times 10^{-1} T_r^{2.13} \exp\left(-\frac{8823}{T_r}\right)$
H5)	$\mathbf{H}^- + \mathbf{H} \rightarrow \mathbf{H}_2 + \mathbf{e}$	1.5×10^{-9} $4.0 \times 10^{-9} T_g^{-0.17}$
H6)	$\mathbf{H}^- + \mathbf{H}^+ \rightarrow \mathbf{H}_2^+ + \mathbf{e}$	$6.9 \times 10^{-9} T_g^{-0.35}$ $9.6 \times 10^{-7} T_g^{-0.9}$
H7)	$\mathbf{H}^- + \mathbf{H}^+ \rightarrow 2\mathbf{H}$	$5.7 \times 10^{-6} T_g^{-0.5} + 6.3 \times 10^{-8} -$ $9.2 \times 10^{-11} T_g^{0.5} + 4.4 \times 10^{-13} T_g$
H8)	$\mathbf{H} + \mathbf{H}^+ \rightarrow \mathbf{H}_2^+ + \gamma$	$\text{dex}[-19.38 - 1.523 \log T_g +$ $1.118(\log T_g)^2 - 0.1269(\log T_g)^3]$
H9)	$\mathbf{H}_2^+ + \gamma \rightarrow \mathbf{H} + \mathbf{H}^+$	$2.0 \times 10^1 T_r^{1.59} \exp\left(-\frac{82000}{T_r}\right)$ $1.63 \times 10^7 \exp\left(-\frac{32400}{T_r}\right)$
H10)	$\mathbf{H}_2^+ + \mathbf{H} \rightarrow \mathbf{H}_2 + \mathbf{H}^+$	6.4×10^{-10}
H11)	$\mathbf{H}_2^+ + \mathbf{e} \rightarrow 2\mathbf{H}$	$2.0 \times 10^{-7} T_g^{-0.5}$
H12)	$\mathbf{H}_2^+ + \gamma \rightarrow 2\mathbf{H}^+ + \mathbf{e}$	$9.0 \times 10^1 T_r^{1.48} \exp\left(-\frac{335000}{T_r}\right)$
H13)	$\mathbf{H}_2^+ + \mathbf{H}_2 \rightarrow \mathbf{H}_3^+ + \mathbf{H}$	2.0×10^{-9}
H14)	$\mathbf{H}_2^+ + \mathbf{H} \rightarrow \mathbf{H}_3^+ + \gamma$	irrelevant
H15)	$\mathbf{H}_2 + \mathbf{H}^+ \rightarrow \mathbf{H}_2^+ + \mathbf{H}$	$3.0 \times 10^{-10} \exp\left(-\frac{21050}{T_g}\right)$ $1.5 \times 10^{-10} \exp\left(-\frac{14000}{T_g}\right)$
H16)	$\mathbf{H}_2 + \mathbf{e} \rightarrow \mathbf{H} + \mathbf{H}^-$	$2.7 \times 10^{-8} T_g^{-1.27} \exp\left(-\frac{43000}{T_g}\right)$
H17)	$\mathbf{H}_2 + \mathbf{e} \rightarrow 2\mathbf{H} + \mathbf{e}$	$4.4 \times 10^{-10} T_g^{0.35} \exp\left(-\frac{102000}{T_g}\right)$
H18)	$\mathbf{H}_2 + \gamma \rightarrow \mathbf{H}_2^+ + \mathbf{e}$	$2.9 \times 10^2 T_r^{1.56} \exp\left(-\frac{178500}{T_r}\right)$
H19)	$\mathbf{H}_3^+ + \mathbf{H} \rightarrow \mathbf{H}_2^+ + \mathbf{H}_2$	$7.7 \times 10^{-9} \exp\left(-\frac{17560}{T_g}\right)$
H20)	$\mathbf{H}_3^+ + \mathbf{e} \rightarrow \mathbf{H}_2 + \mathbf{H}$	$4.6 \times 10^{-6} T_g^{-0.65}$
H21)	$\mathbf{H}_2 + \mathbf{H}^+ \rightarrow \mathbf{H}_3^+ + \gamma$	1.0×10^{-16}
H22)	$\mathbf{H}_3^+ + \gamma \rightarrow \mathbf{H}_2^+ + \mathbf{H}$	irrelevant

Chemistry of D

Formation of HD is dominated by ion-molecule and charge transfer processes:



and minor processes:



HD is destroyed by similar processes as H_2

$$\Rightarrow X(\text{HD}) \sim (\text{D}/\text{H}) * X(\text{H}_2) \sim 10^{-10} - 10^{-9}$$

Reaction rates of D-chemistry

Table 2. Reaction rates for Deuterium species

reaction	rate (cm ³ s ⁻¹ or s ⁻¹)
D1) $\mathbf{D^+ + e \rightarrow D + \gamma}$	
D2) $\mathbf{D + \gamma \rightarrow D^+ + e}$	
D3) $\mathbf{D + H^+ \rightarrow D^+ + H}$	$3.7 \times 10^{-10} T_g^{0.28} \exp\left(-\frac{43}{T_g}\right)$
D4) $\mathbf{D^+ + H \rightarrow D + H^+}$	$3.7 \times 10^{-10} T_g^{0.28}$
D5) $\mathbf{D + H \rightarrow HD + \gamma}$	1.0×10^{-25}
D6) $\mathbf{D + H_2 \rightarrow H + HD}$	$9.0 \times 10^{-11} \exp\left(-\frac{3876}{T_g}\right)$
D7) $\mathbf{HD^+ + H \rightarrow H^+ + HD}$	
D8) $\mathbf{D^+ + H_2 \rightarrow H^+ + HD}$	2.1×10^{-9}
D9) $\mathbf{HD + H \rightarrow H_2 + D}$	$3.2 \times 10^{-11} \exp\left(-\frac{3624}{T_g}\right)$
D10) $\mathbf{HD + H^+ \rightarrow H_2 + D^+}$	$1.0 \times 10^{-9} \exp\left(-\frac{464}{T_g}\right)$
D11) $\mathbf{HD + H_3^+ \rightarrow H_2 + H_2D^+}$	$(2.1 - 0.4 \log T_g) \times 10^{-9}$
D12) $\mathbf{D + H^+ \rightarrow HD^+ + \gamma}$	
D13) $\mathbf{D^+ + H \rightarrow HD^+ + \gamma}$	
D14) $\mathbf{HD^+ + \gamma \rightarrow H + D^+}$	
D15) $\mathbf{HD^+ + \gamma \rightarrow H^+ + D}$	
D16) $\mathbf{HD^+ + e \rightarrow H + D}$	$7.2 \times 10^{-8} T_g^{-1/2}$
D17) $\mathbf{HD^+ + H_2 \rightarrow H_2D^+ + H}$	
D18) $\mathbf{HD^+ + H_2 \rightarrow H_3^+ + D}$	
D19) $\mathbf{D + H_3^+ \rightarrow H_2D^+ + H}$	$2.0 \times 10^{-8} T_g^{-1}$
D20) $\mathbf{H_2D^+ + e \rightarrow H + H + D}$	$1.0 \times 10^{-6} T_g^{-1/2} \times 0.73$
D21) $\mathbf{H_2D^+ + e \rightarrow H_2 + D}$	$1.0 \times 10^{-6} T_g^{-1/2} \times 0.07$
D22) $\mathbf{H_2D^+ + e \rightarrow HD + H}$	$1.0 \times 10^{-6} T_g^{-1/2} \times 0.20$
D23) $\mathbf{H_2D^+ + H_2 \rightarrow H_3^+ + HD}$	$4.7 \times 10^{-9} \exp\left(-\frac{215}{T_g}\right)$ 5.5×10^{-10}
D24) $\mathbf{H_2D^+ + H \rightarrow H_3^+ + D}$	$2.0 \times 10^{-8} T_g^{-1} \exp\left(-\frac{632}{T_g}\right)$

Chemistry of Li

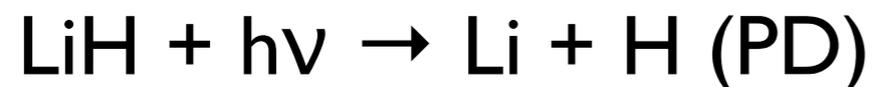
I.P. of Li is 5.4 eV => relevant chemistry begins at $z < 450$:

Major species are LiH and LiH⁺:

LiH⁺ chemistry:

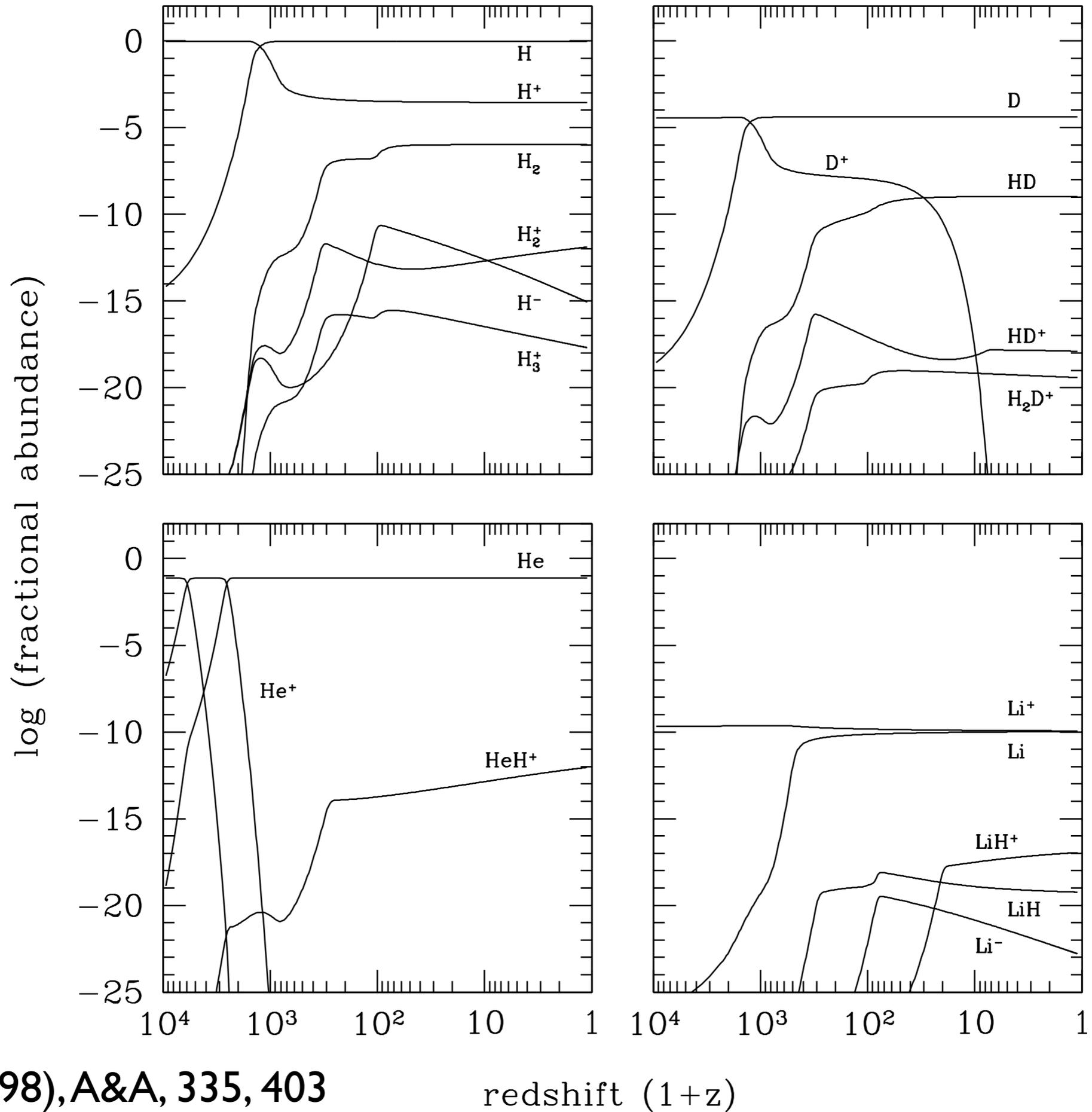


LiH chemistry:

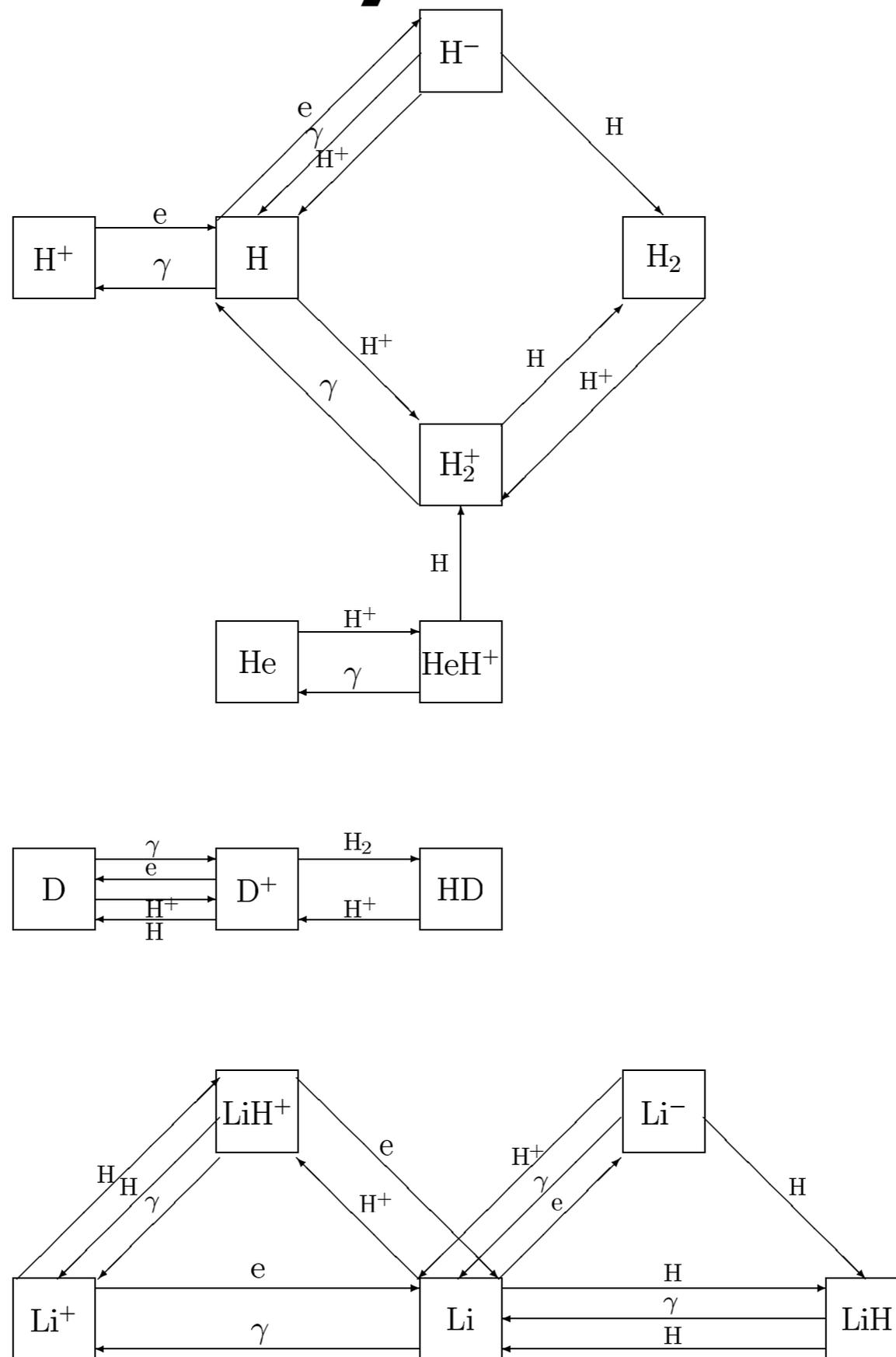


Minor species: $X(\text{LiH}) \sim 1\%$ of $X(\text{LiH}^+) \sim 10^{-18}$

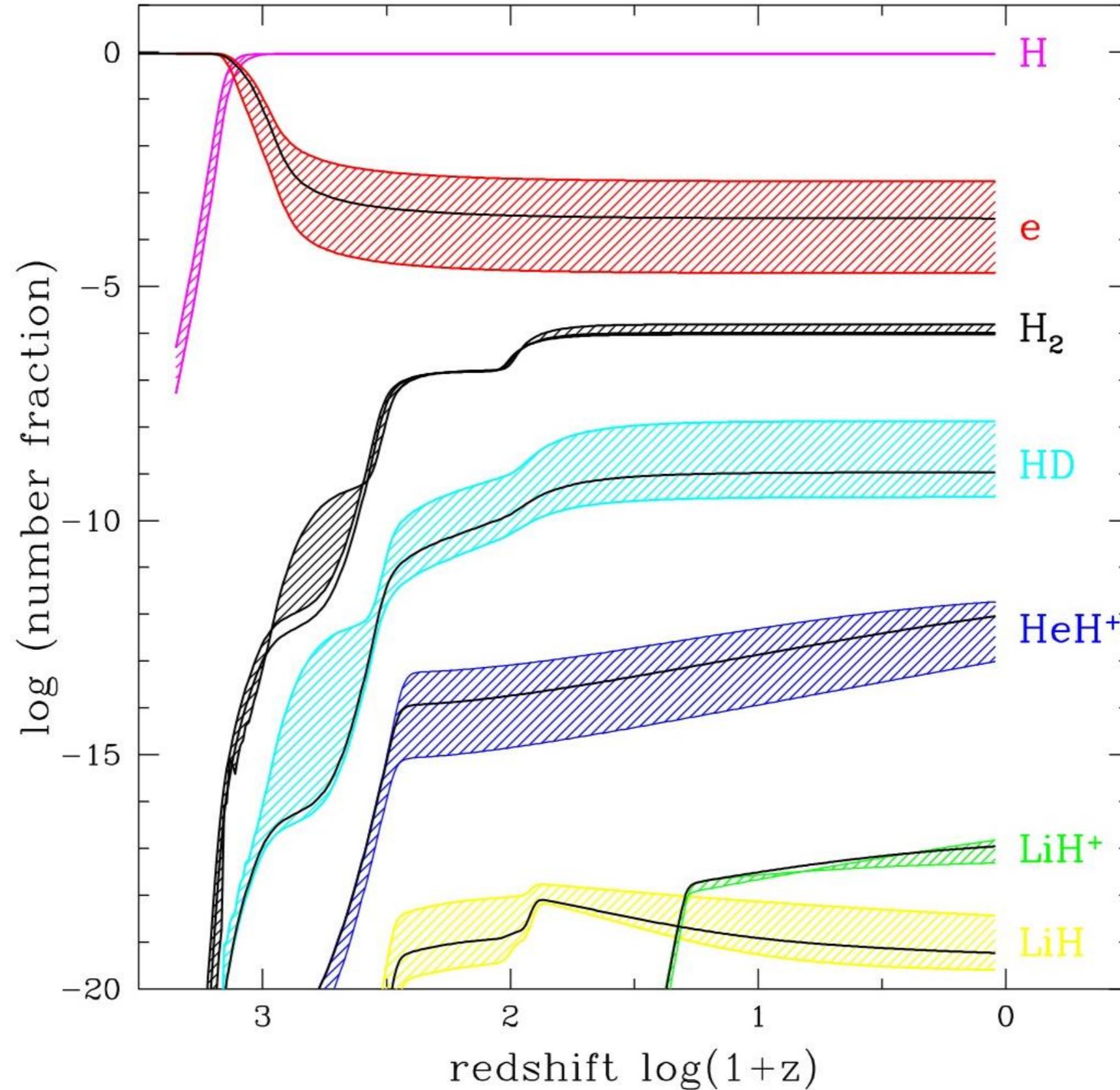
Summary: abundances of early molecules



Scheme: chemistry in the early Universe



Sensitivity to cosmological parameters



Homework

1) Calculate the value of T_R and average density in the Universe, assuming the standard cosmological model with $\Omega = 0.1$ and Hubble constant $H_0 = 50 \text{ km/s Mpc}^{-1}$:

a) At $z = 6.4$

b) At $z = 0$

2) Get the frequencies of HeH^+ transitions in the CDMS (<http://www.astro.uni-koeln.de/cdms/>) and find out if there are transitions detectable at (sub-)mm wavelength region from a high- z redshift objects ($z \sim 10-100$)

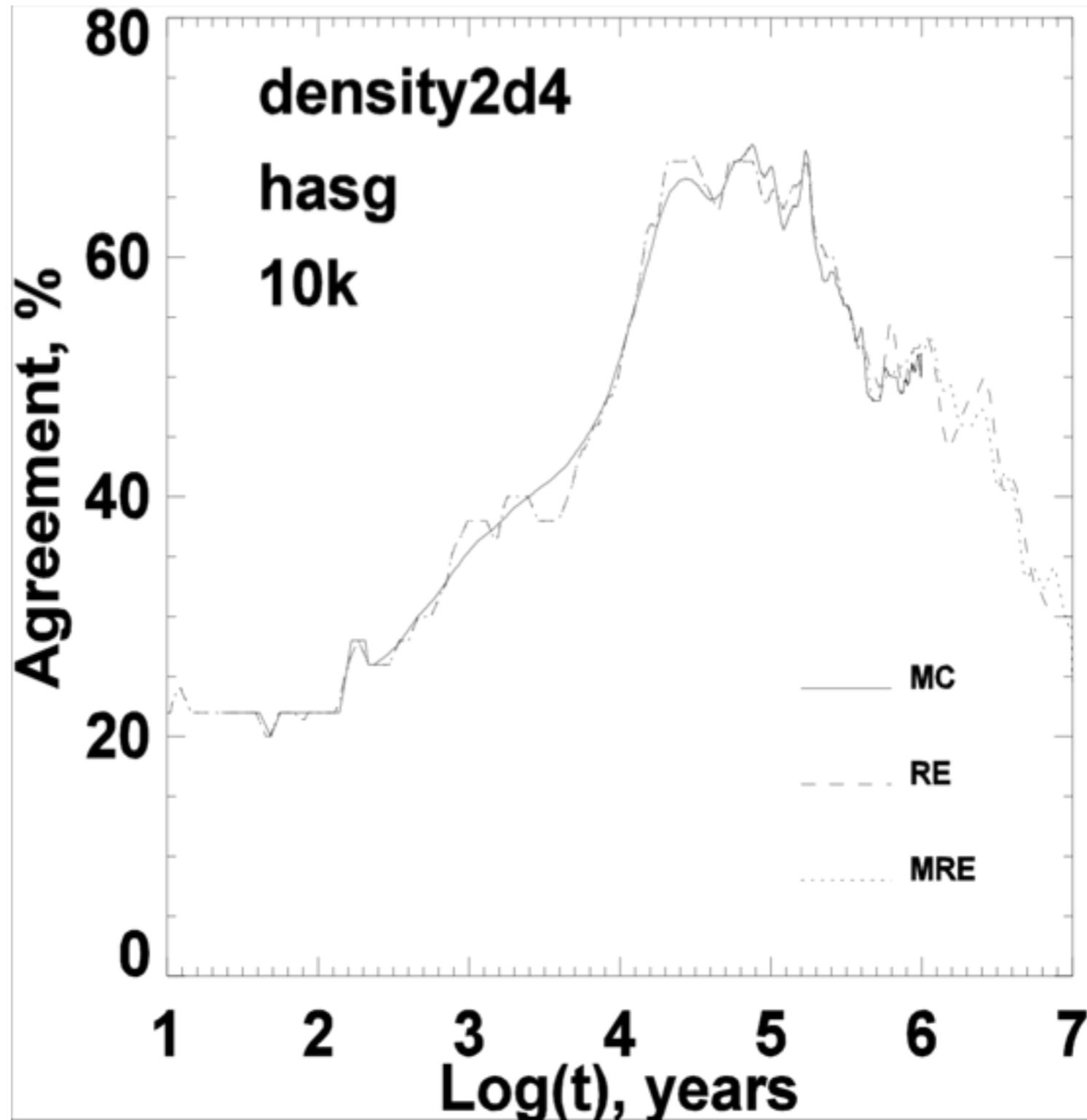
3) How large could be the fraction of HeD^+ molecule compared to HeH^+ in the early Universe?

Suggested literature

- Galli, Palla (1998), A&A, 335, 403
- Lepp, Stancil, Dalgarno (2002), J. Phys. B., At. Mol. Opt. Phys 35, 80
- A. G.G.M. Tielens, "The Physics and Chemistry of the ISM" (2007), Cambridge Uni. Press
- Master course in Astrochemistry, Ewine van Dishoek (2011): <http://www.strw.leidenuniv.nl/~sanjose/astrochem>
- D. Semenov "Chemistry in protoplanetary disks" in "Encyclopedia of Astrobiology" (2010), Springer

The End

Observations vs Theory



About 75% agreement for 50 observed molecules in TMCI