The Chemistry of the Early Universe

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Outline

- Pregalactic chemistry
- Chemistry and Pop. III star formation
- Chemistry at low metallicity

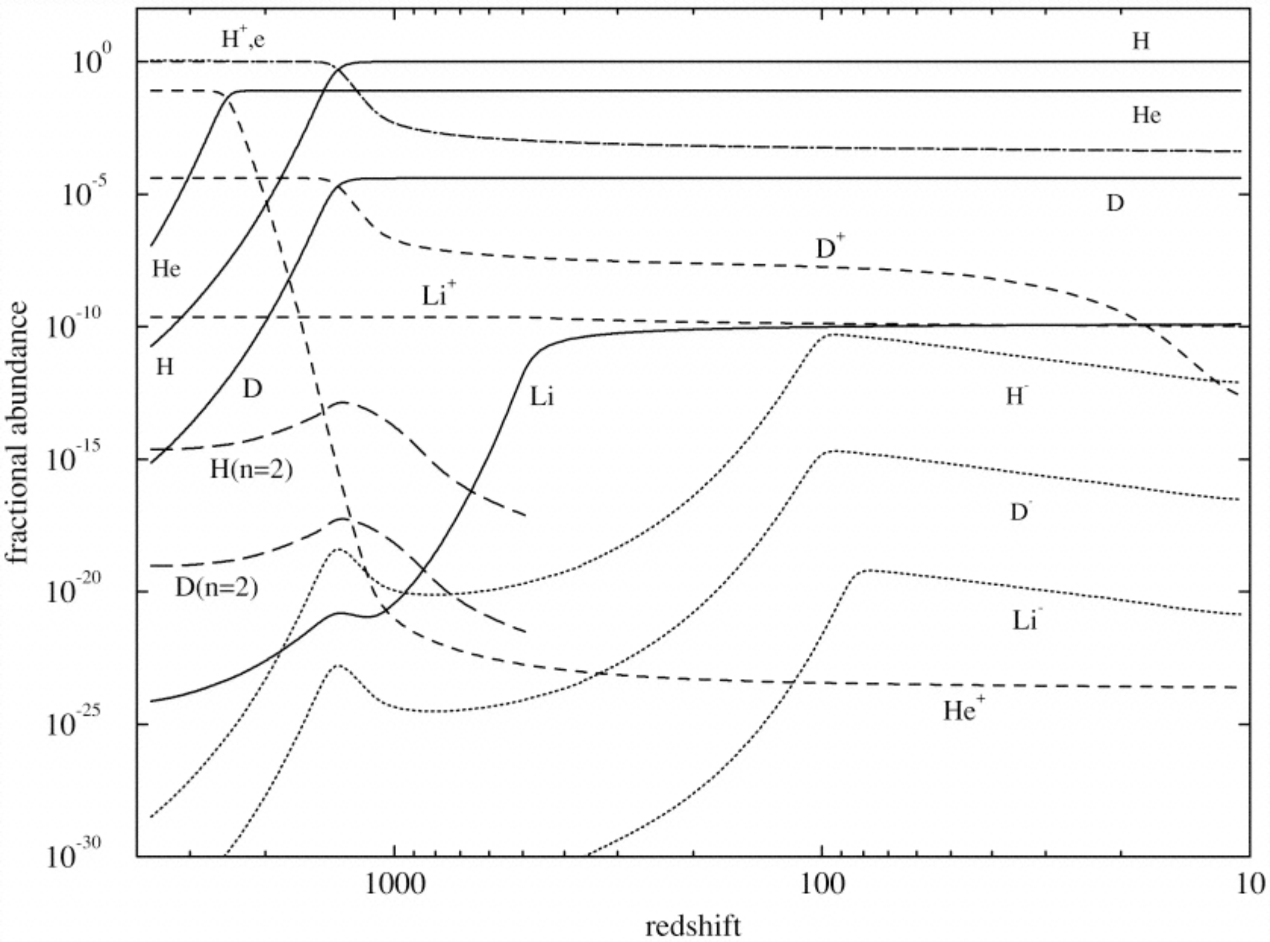
Pregalactic chemistry

- Composition of IGM at end of recombination:
  - Hydrogen: 99.98% atomic, 0.02% ionized
  - Helium: mostly He, minimal He^+
  - Lithium: mostly Li^+, minimal Li
- From this starting point, we can make a lot of ions and molecules: H^-, H_2^+, H_2, HD, D_2, H_3^+, H_2D^+, HeH^+, LiH, LiH^+, etc.

- Divide up the possible products into two classes: primary and secondary
- Primary products can be produced directly from our starting material, e.g. H^-, H_2^+, HeH^+
- Secondary products form via reaction chain relying on at least one primary product, e.g. H_2, HD, H_3^+

- Primary products - evolution determined by three important timescales
  - Photodestruction time: $t_{ph} = 1 / R_{ph}$
  - Formation time: $t_{form} = n_x / C_x$
  - Hubble time: $t_H = 1 / H(z)$

- At high redshift, photodissociation dominates:
  - $t_{ph} << t_H$
  - $t_{ph} = t_{form}$ only when n_x very small
- As we move to lower redshift, CMB shifts to lower energies. Eventually, we run out of photons above photodestruction threshold:
  - $t_{ph} >> t_H$
  - n_x increases rapidly until $t_{form} = t_H$
  - $t_{form} \propto (1+z)^{-3}$, $t_H \propto (1+z)^{-3/2}$, so abundance of species X quickly "freezes out"



Stancil, Lepp & Dalgarno (1998)

- Evolution of secondary products more complicated, as depends on primary products
- If multiple formation pathways, then get formation concentrated at several different redshifts
- Important example: H_2

- H_2 forms by two main pathways:

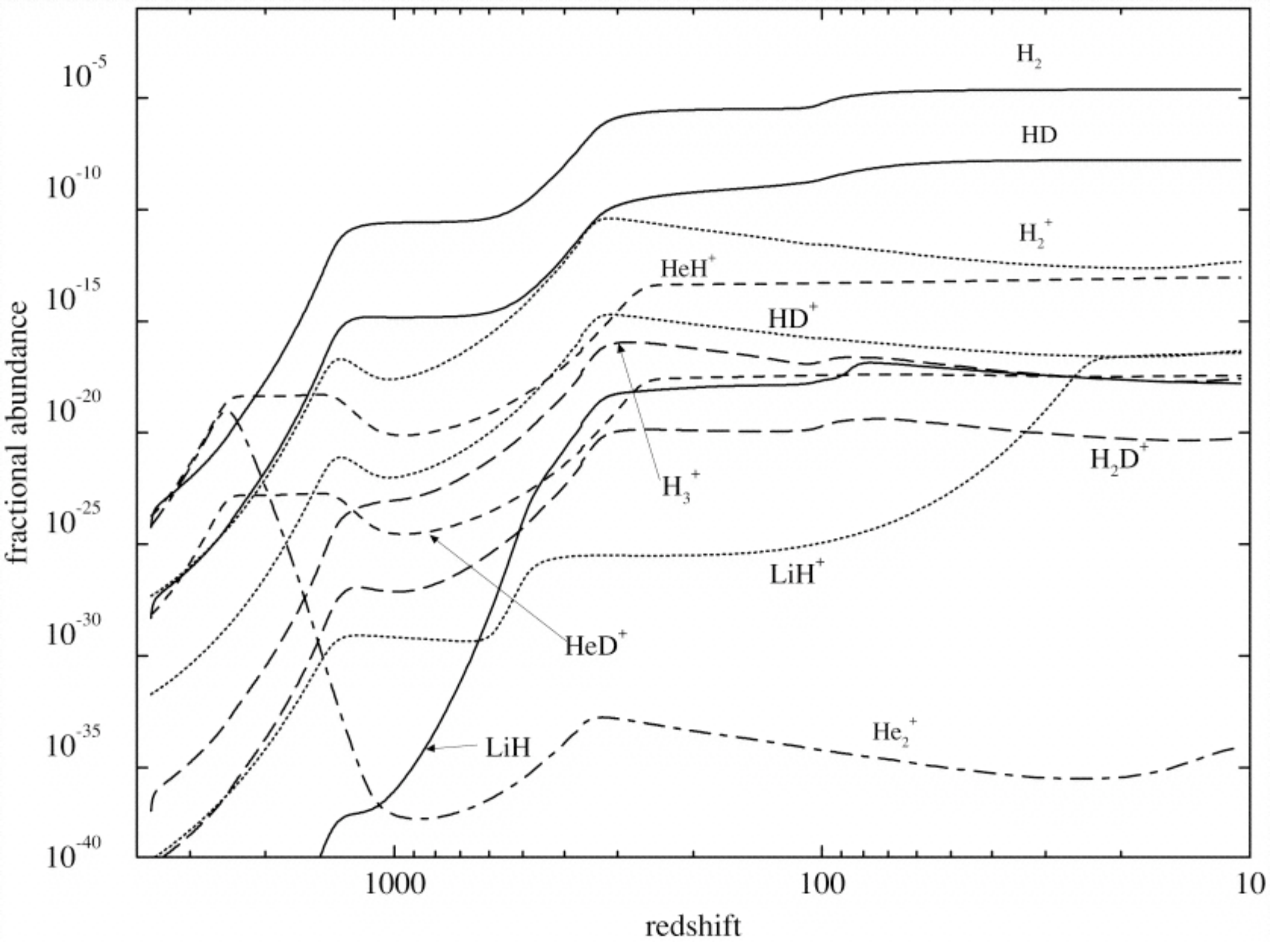
$$H + e^- \rightarrow H^- + \text{photon}$$

$$H^- + H \rightarrow H_2 + e^-$$

$$H + H^+ \rightarrow H_2^+ + \text{photon}$$

$$H_2^+ + H \rightarrow H_2 + H^+$$

- In absence of photodestruction, H^- pathway most effective, but H^- is fragile and electron easy to photodetach



Stancil, Lepp & Dalgarno (1998)

Complications

- Spectral distortion of CMB: (e.g. Switzer & Hirata, 2005; Hirata & Padmanabhan, 2006)
- Stimulated radiative association: (e.g. Stancil & Dalgarno, 1997, 1998; Zygelman, Stancil & Dalgarno, 1998)
- Non-LTE level populations: (e.g. Coppola et al, 2011; see also posters by Longo and Coppola, this meeting)

Population III

- Gas falls into protogalaxy, shock-heated to protogalactic virial temperature
- H_2 fraction in IGM too small to cool this shock-heated gas => most H_2 forms in situ
- As H_2 forms, cooling time drops, allowing gravitational collapse to begin

How much H2 do we form?

- Consider a toy model of the chemistry that includes only H^+ recombination, plus formation of H_2 via H^- (Tegmark et al, 1997)
- At fixed T, fractional ionization evolves as:

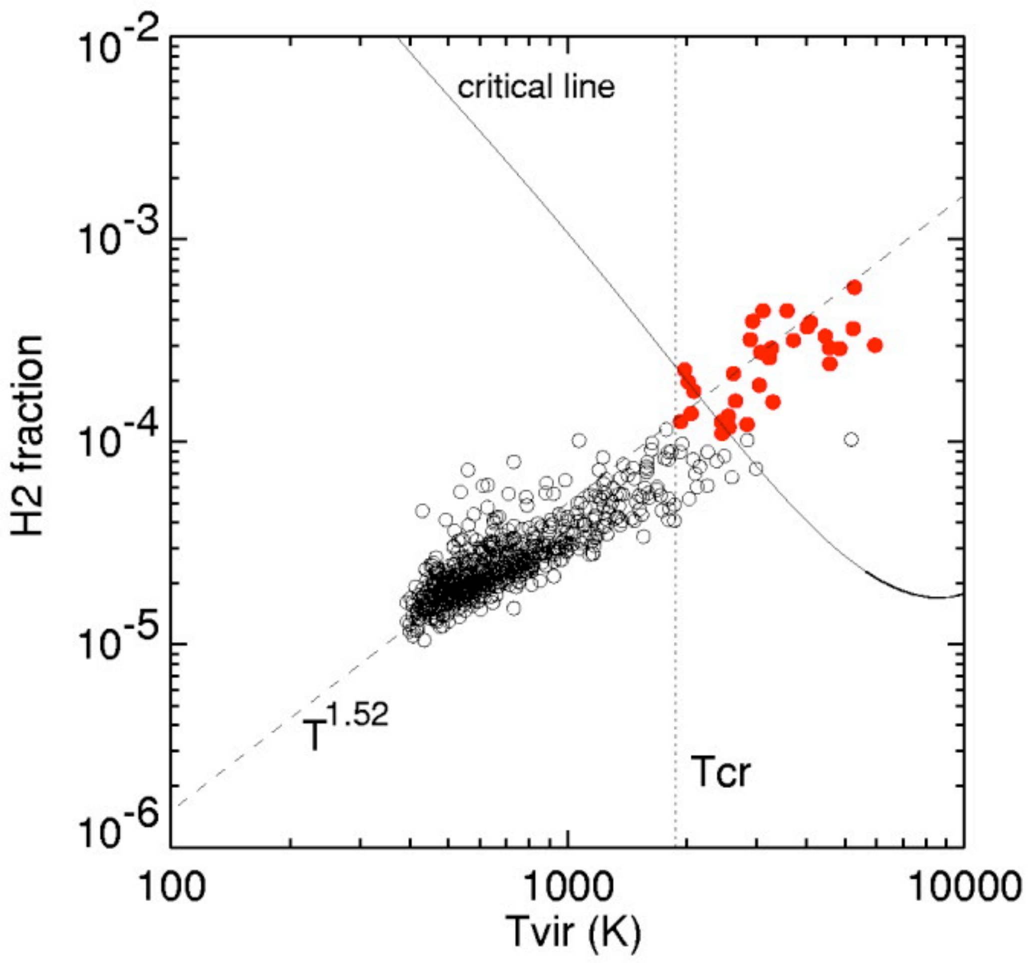
$$x_e = x_0 / (1 + t / t_{rec})$$

- H_2 fraction evolves as:

$$x_{H2} = (k_{ra}/k_{rec}) \ln (1 + t / t_{rec})$$

where k_{ra} is rate coefficient for formation of H^- by radiative association

- Logarithmic dependence on time, most H_2 forms within first few recombination times
- $(k_{ra} / k_{rec}) \propto T^{1.5}$, so form much more H_2 at high T than at low T
- H_2 cooling rate also strongly increasing function of T
- Critical protogalactic virial temperature at which we form enough H_2 to cool within a Hubble time



Yoshida et al (2003)

- $n \sim 10^4$ cm^{-3}: temperature reaches minimum value, $T \sim 200$ K; H_2 level populations approach LTE
- $n \sim 10^8 - 10^{10}$ cm^{-3}: onset of three-body H_2 formation:

$$H + H + H \rightarrow H_2 + H$$

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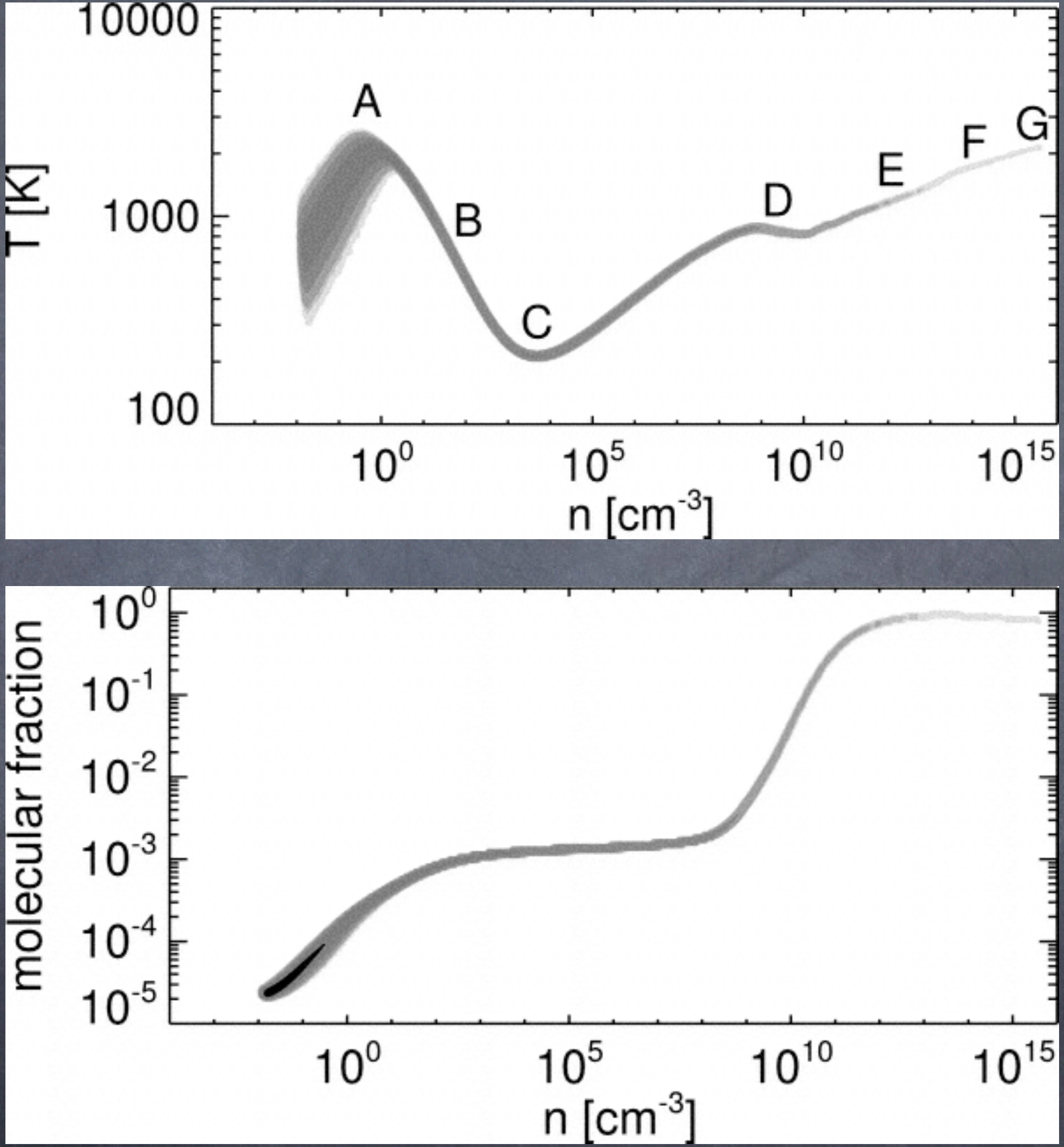

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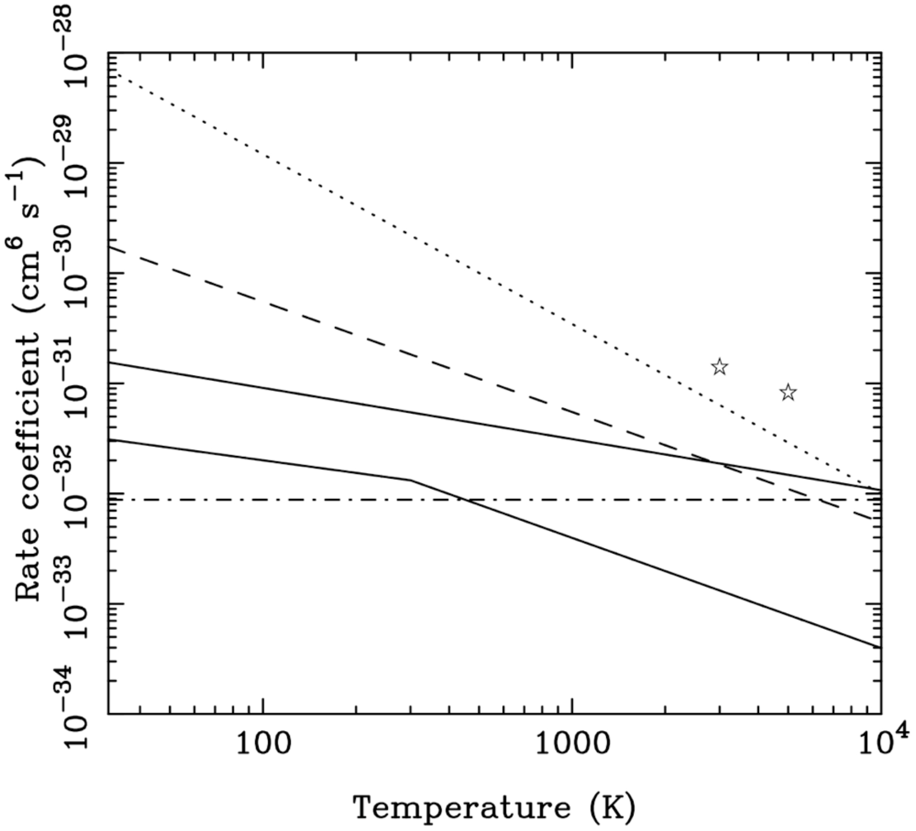
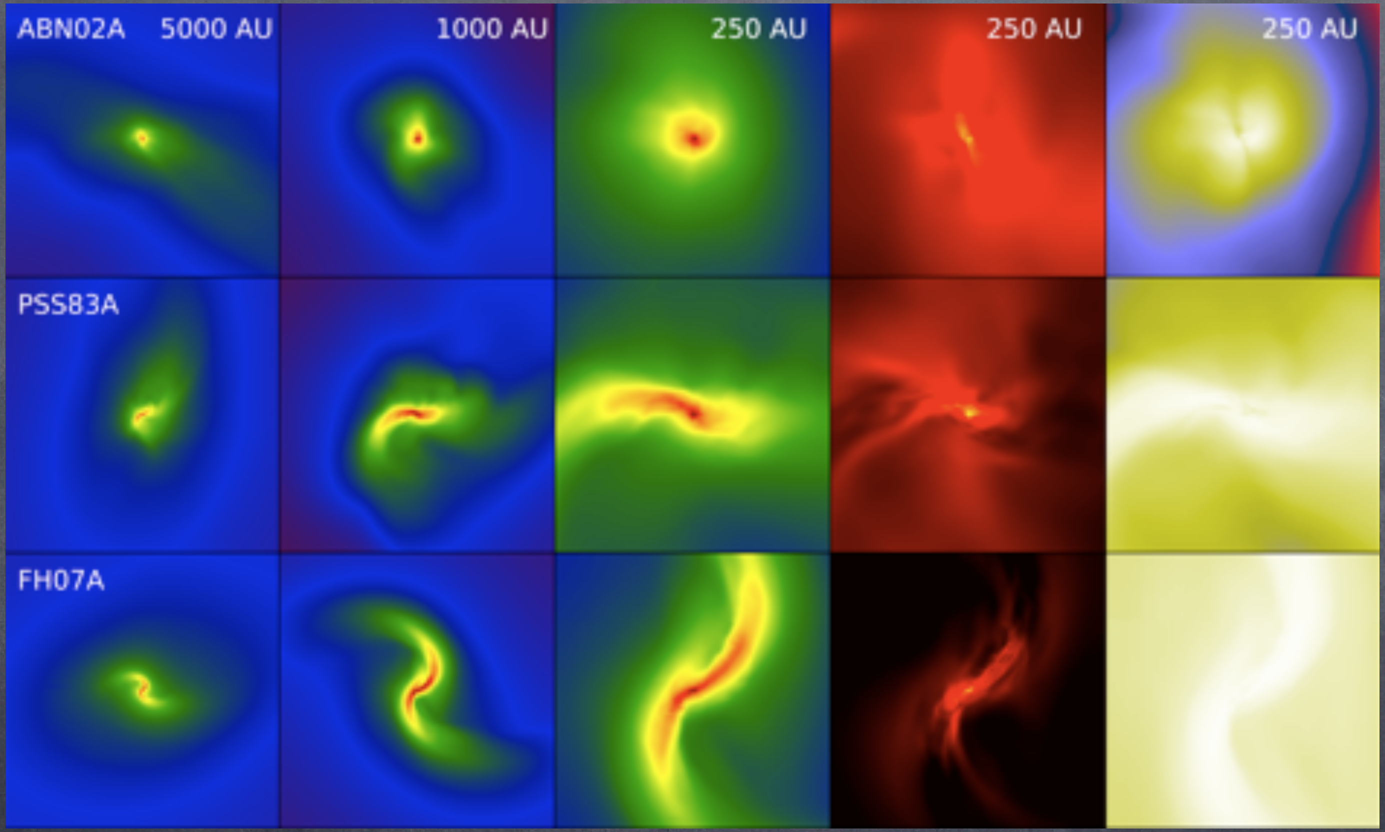
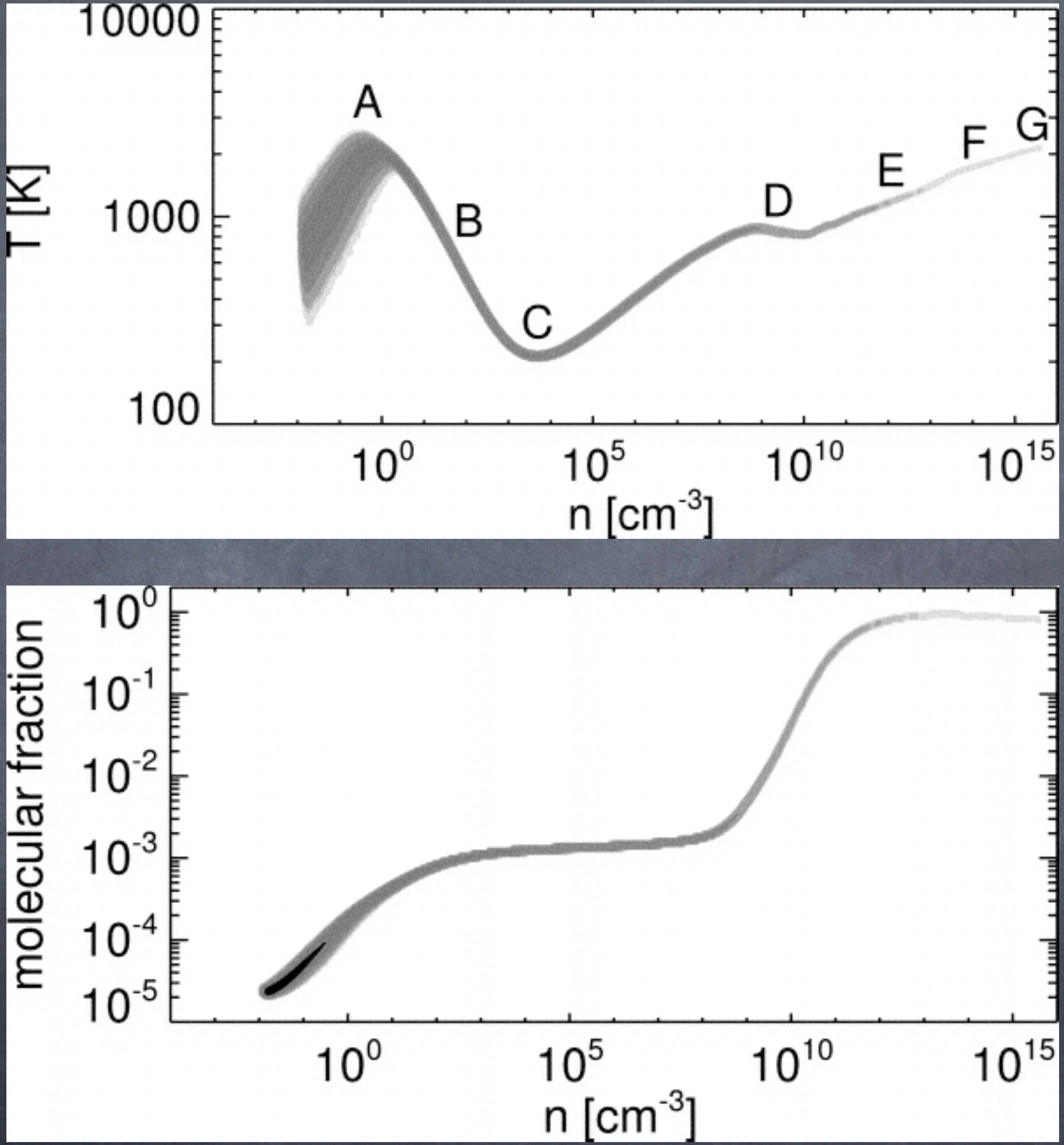

Rate coefficient (cm^6 s^{-1})
10^{-28}
10^{-29}
10^{-30}
10^{-31}
10^{-32}
10^{-33}
10^{-34}
100
1000
10^4
Temperature (K)

Glover (2008)



Turk et al (2011)

- n ~ 10^{10} cm^{-3}: H_2 lines become optically thick at line centers, but cooling continues through line wings (Omukai et al, 1999)
- n ~ 10^{14} cm^{-3}: H_2 CIE cooling (Ripamonti & Abel, 2004)
- n ~ 10^{16} cm^{-3}: continuum becomes optically thick, H_2 dissociates (Yoshida et al, 2008)



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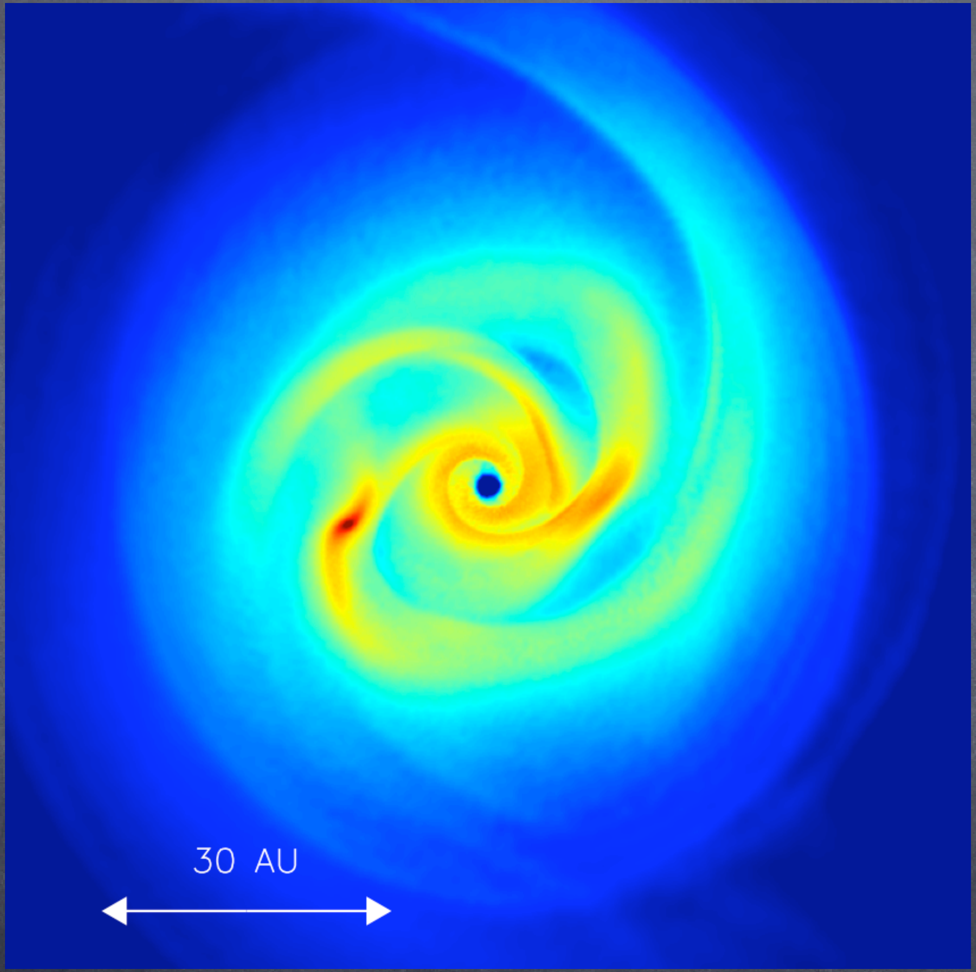
- Protostellar mass at formation ~ 0.01 $M_\odot$
- Surrounded by envelope with 100+ $M_\odot$
- Until recently, it was assumed that protostar accreted most of this mass (e.g. Abel et al, 2002)
- Recent studies indicate that H_2 cooling of protostellar accretion disk allows it to fragment (e.g. Clark et al, 2011; Greif et al, 2011)
- IMF resulting from this still not known - solar mass Pop. III stars possible???



Clark et al (2011)

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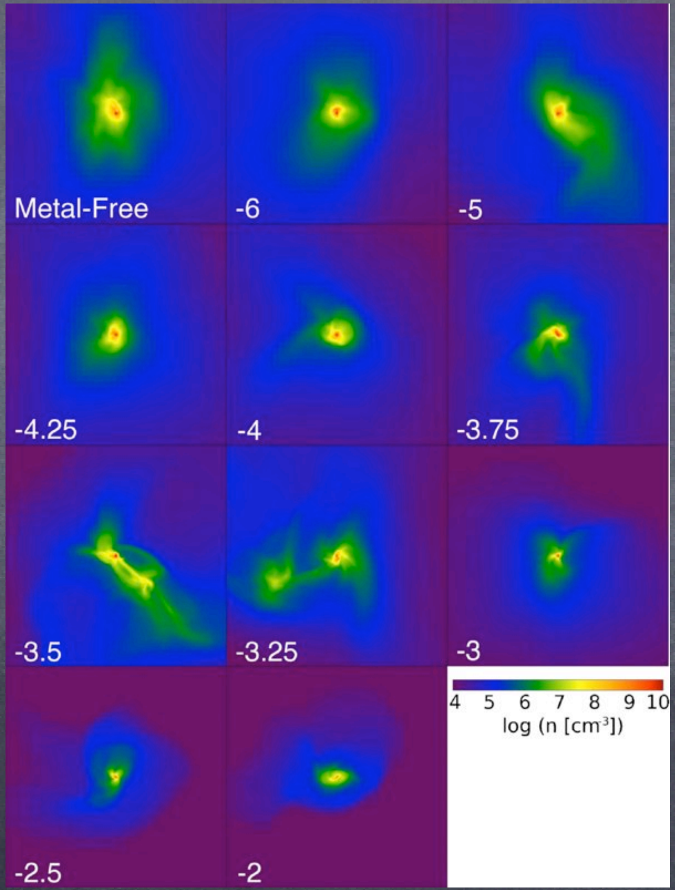
Chemistry at low Z

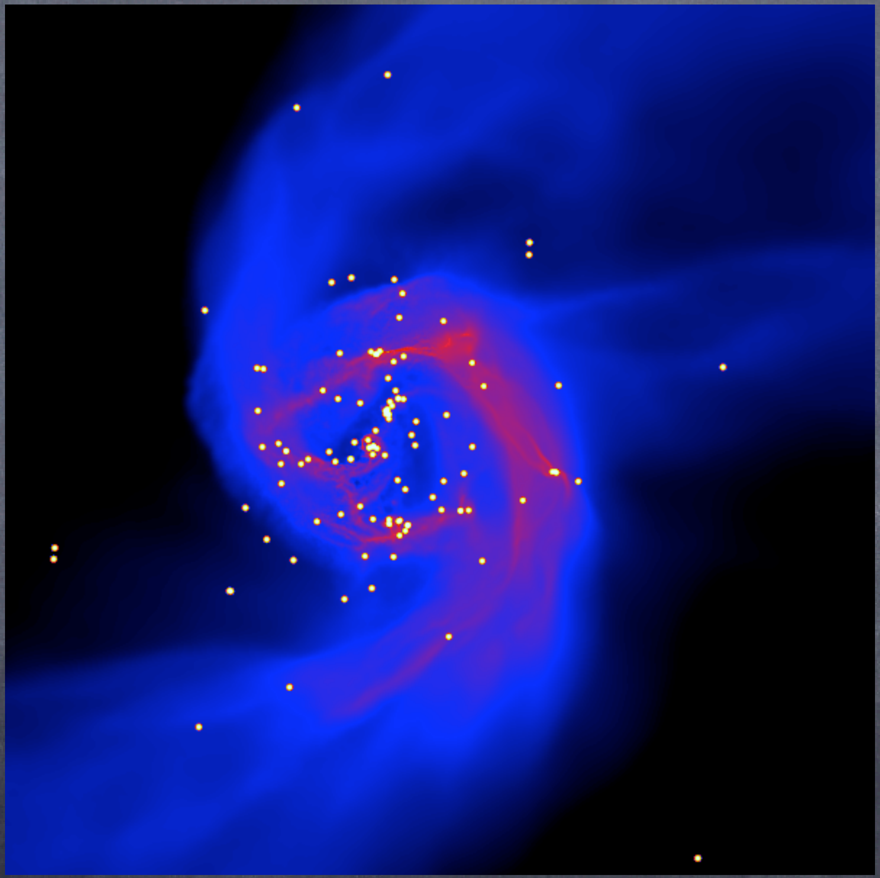
- Introduction of metals => more coolants
- Most work to date has focussed one of two regimes:
  - Low density, low H_2 fraction, most metals in atomic form, CII and OI f.s. dominate
  - High density, high H_2 fraction, dust cooling dominates
- Unclear how important molecular chemistry is for determining thermal balance

Atomic regime



Smith et al (2009)

Dust-cooled regime



Clark et al (2008); see also Dopcke et al (2011)

Open questions

- What's the ratio of dust to gas-phase metals?
- What are the dust properties (composition, size distribution, etc.)?
- Can atomic fine structure cooling alone lead to formation of low mass stars, or do we need the dust?
- How important are the molecular coolants?