Molecular Clouds at the Reionization Epoch

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IAU Symposium 280, Toledo 2011

Question: What were the chemical compositions of the (star-forming) molecular clouds at the reionization epoch?

...or alternatively,
What are the compositions of molecular clouds in the limit of very low (but non-vanishing) heavy-element abundances?

Collaborators on this project:
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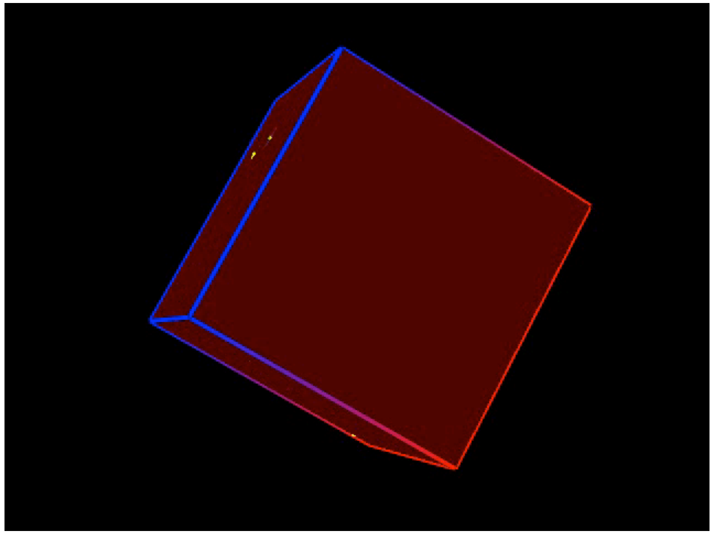


patchy reionization:
first stars and seed black holes.
UV Xrays

Theory and Computational Ingredients:

- “two-body” ion-molecule gas-phase chemistry (except for H_2 formation, which also includes grain-catalysis and negative-ion H^- sequence).

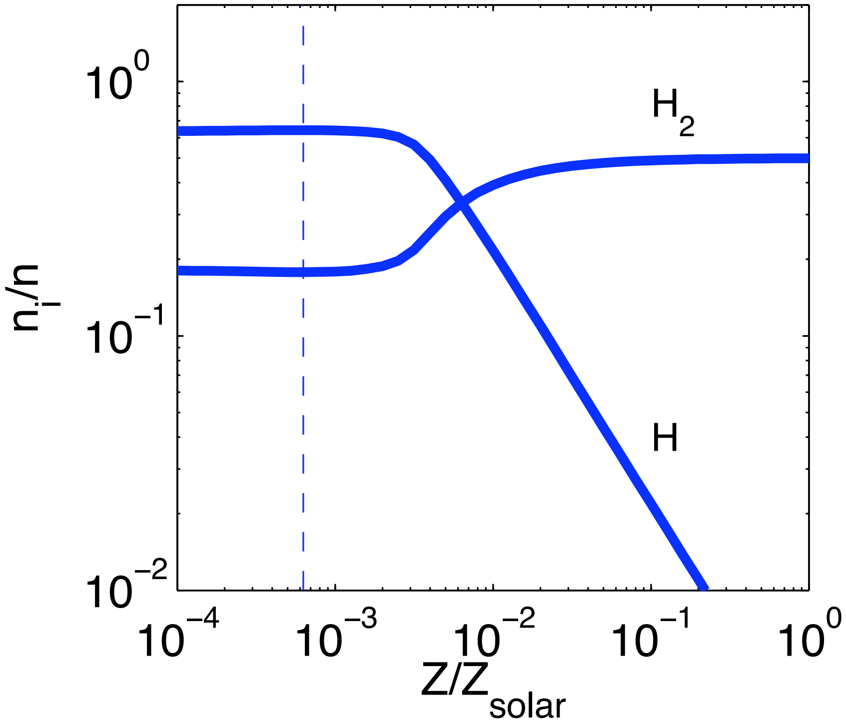
- constant density, isothermal clouds.

- metallicity proportional to a single scaling parameter Z (with Z=1 for solar abundances of the heavy elements).

- dust abundance and photoabsorption cross section per H nucleus assumed to vary linearly with Z.

- ionization driven chemistry (by, e.g., X-rays from accreting seed black holes) moderated by FUV photo-processes (due, e.g., to radiation from massive population III or II stars.)

H/H_2



hydrogen gas density $n = 10^4$ cm^{-3}

ionization rate $\zeta = 10^{-15}$ s^{-1}

[selected so that composition can reach a steady-state within a Hubble time ~ 2.5×10^8 yr at redshift ≈10.]

gas temperature T = 100 K (“warm”)

H_2 formation on dust grains
($R = R_0 Z$ cm^3 s^{-1})

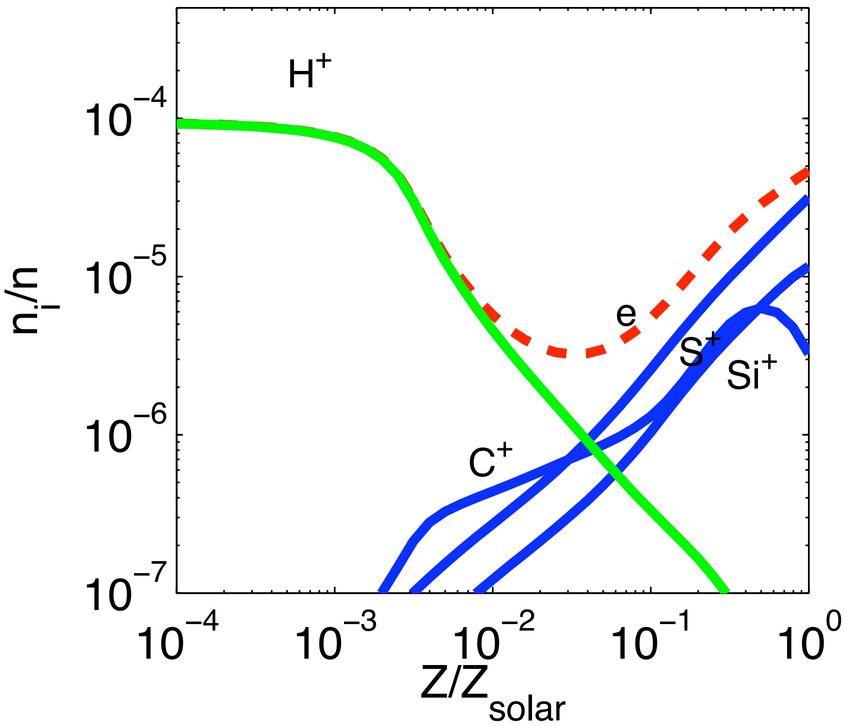
and in the gas−phase

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

Removal:

$H_2 + e^* \rightarrow H_2 + e + e^*$

Fractional Ionization:



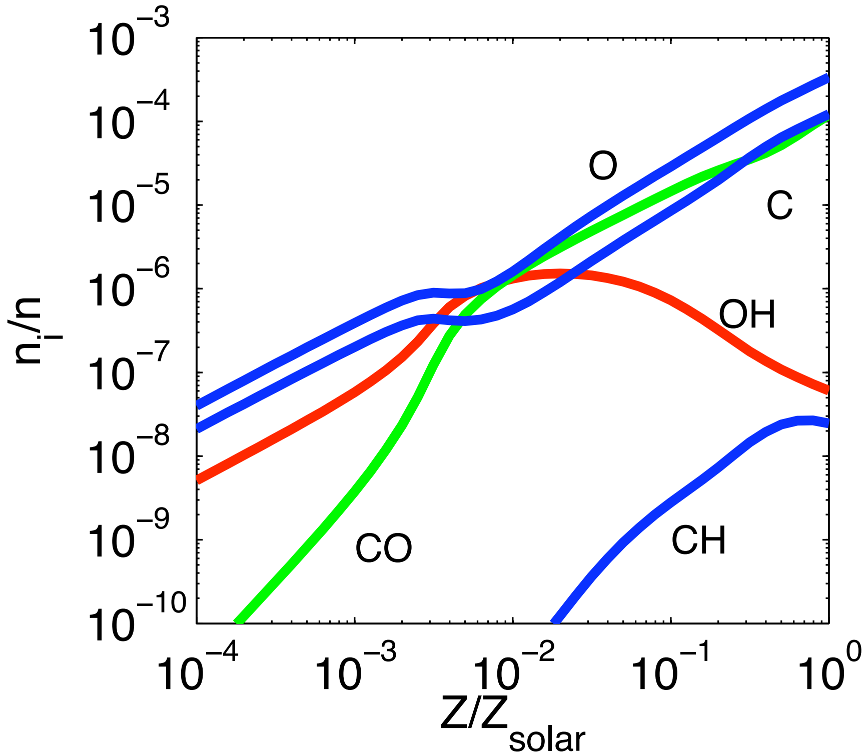
positive charge carried by:

- metal ions and molecular ions at "high Z"
- protons at "low Z"

CO and OH:

OH formation: $H^+ \xrightarrow{O} O^+ \xrightarrow{H_2} OH^+ \xrightarrow{H_2} H_2O^+ \xrightarrow{H_2} H_3O^+ \begin{cases} \xrightarrow{e} OH \\ \xrightarrow{e} H_2O \end{cases}$

Main Point: CO contains two heavy elements, as opposed to a diatomic hydride such as OH that contains just one. So for sufficiently low metallicities the abundances of the diatomic hydrides must become large compared to CO.



OH removal and CO formation:

$OH \xrightarrow{C} CO \xrightarrow{He^+}$

$OH \xrightarrow{C^+} CO^+ \xrightarrow{H_2} HCO^+ \xrightarrow{e} CO \xrightarrow{He^+}$

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.

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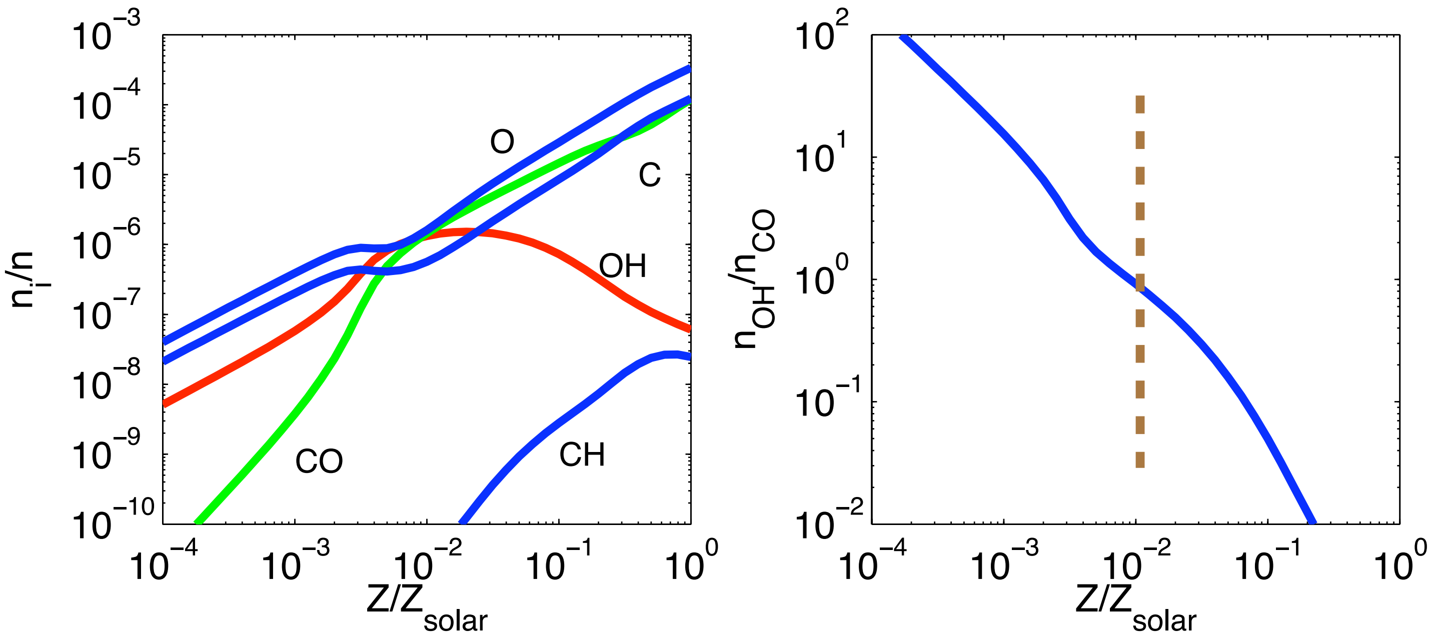
$OH \xrightarrow{H^+} OH^+$ at "low Z"

Two Regimes:



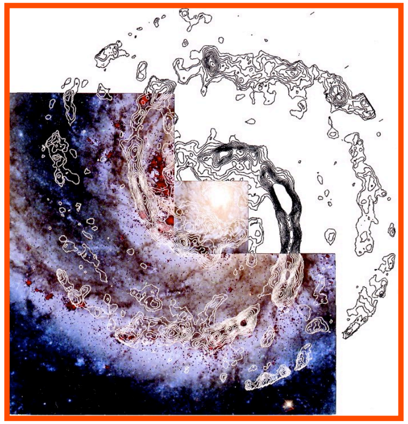
$$\frac{n(OH)}{n(CO)} \propto \frac{n(He^+)}{n(C^+)} \propto$$

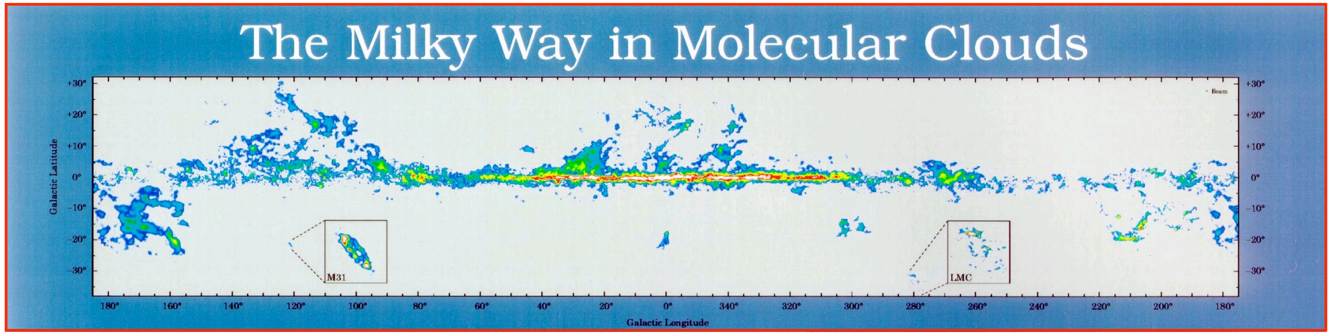
- Z^{-2} in "high Z limit" ....n(OH) / n(CO) << 1
- Z^{-1} in "low Z limit" ....n(OH) / n(CO) >> 1

Note: Other diatomic hydrides, e.g., CH, SiH, SH, HF etc. much less abundant than OH.

Z^{-2} in “high Z limit” ....$n(OH) / n(CO) \ll 1$ ...familiar galaxies

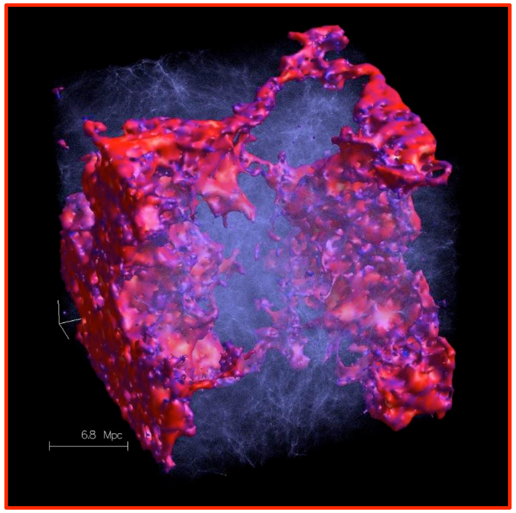
“CO dominated”



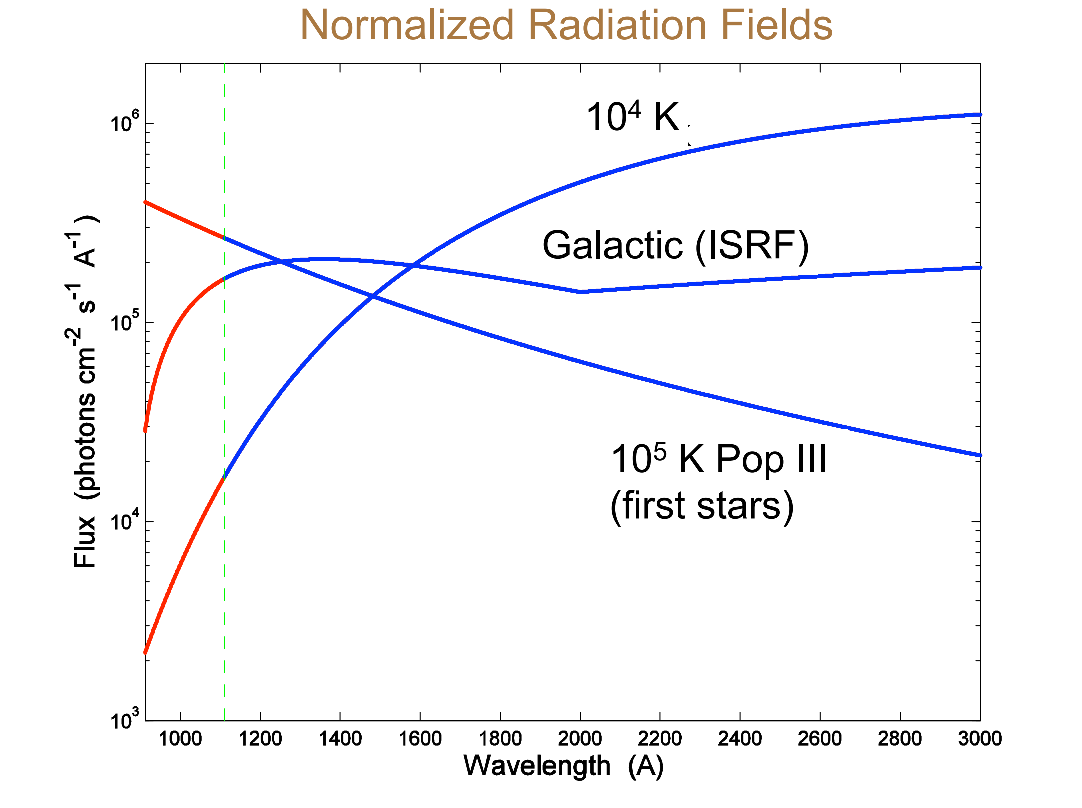


Z^{-1} in “low Z limit” ....$n(OH) / n(CO) \gg 1$ ...molecular clouds at reionization?

“OH dominated”



FUV Photoprocesses in Low-Metallicity Clouds:



H_2 bands
optically thick

dust free
optically thin

FUV Photoprocesses:

photodissociation

	ISRF	PopIII/H_2
H2	4.970e-11	0.000e+00
H2+	5.731e-10	4.312e-10
CH	9.025e-10	4.750e-10
CH+	3.280e-10	7.366e-12
CH2	5.743e-10	3.361e-10
CH2+	1.357e-10	4.991e-11
CH3	2.733e-10	2.344e-10
CH4	1.219e-09	9.496e-10
CH4+	2.754e-10	1.105e-10
C2	2.345e-10	1.136e-10
C2H	5.169e-10	2.877e-10
C2H2	3.255e-09	2.708e-09
C2H4	3.055e-09	1.982e-09
C3	3.812e-09	2.372e-09
c-C3H2	1.863e-09	1.223e-09
OH	3.776e-10	2.528e-10
OH+	1.258e-11	9.219e-16
H2O	7.461e-10	4.805e-10
H2O	4.926e-11	3.223e-11
O2	7.905e-10	5.128e-10
O2+	3.465e-11	2.632e-11
HO2	6.587e-10	3.205e-10
H2O2	9.475e-10	7.312e-10
O3	1.842e-09	9.336e-10
CO	2.043e-10	0.000e+00
CO+	1.015e-10	1.087e-10
CO2	8.904e-10	3.855e-10
HCO	1.084e-09	4.466e-10
HCO+	5.393e-12	0.000e+00
H2CO	1.020e-09	6.384e-10

	ISRF	PopIII/H_2
CH3OH	1.678e-09	1.045e-09
NH	4.888e-10	3.353e-10
NH+	5.280e-11	9.777e-12
NH2	7.451e-10	3.412e-10
NH3	6.825e-10	4.531e-10
NH3	4.836e-10	4.193e-10
N2	2.286e-10	0.000e+00
NO	4.745e-10	2.444e-10
NO2	1.389e-09	9.651e-10
N2O	1.878e-09	1.407e-09
CN	2.926e-10	4.885e-12
HCN	1.556e-09	1.287e-09
HC3N	5.618e-09	4.606e-09
CH3CN	2.455e-09	1.947e-09
SH	9.715e-10	6.153e-10
SH+	2.570e-10	4.679e-11
H2S	3.095e-09	2.276e-09
CS	9.753e-10	9.468e-10
CS2	6.079e-09	3.554e-09
COS	3.737e-09	2.653e-09
SO	4.187e-09	3.683e-09
SO2	1.908e-09	1.690e-09
SIH	2.667e-09	7.269e-10
SIH+	2.555e-09	9.623e-10
SIO	1.584e-09	9.615e-10
HF	1.176e-10	1.209e-10
MgH	4.928e-10	2.896e-10
ALH	3.081e-09	3.425e-10
PH	5.658e-10	4.622e-10
PH+	1.398e-10	6.201e-11

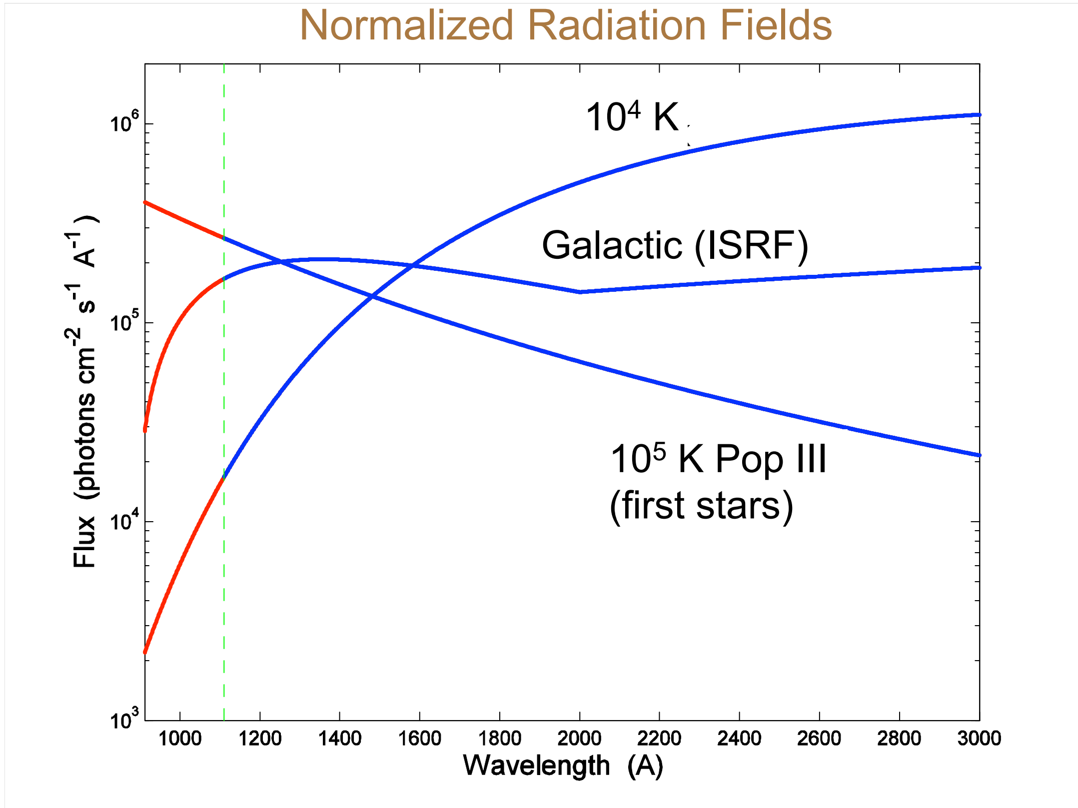
photoionization

	ISRF	PopIII/H_2
LI	3.475e-10	2.049e-10
C	3.150e-10	0.000e+00
CA+	2.453e-12	0.000e+00
NA	1.528e-11	9.715e-12
Mg	7.864e-11	5.840e-11
Al	4.658e-09	2.474e-09
Si	3.144e-09	2.491e-09
P	1.032e-09	6.343e-10
S	6.056e-10	2.598e-10
CL	4.409e-11	0.000e+00
K	2.977e-11	1.845e-11
CA	3.397e-10	1.958e-10
Ti	2.376e-10	1.741e-10
Cr	1.578e-09	9.838e-10
Mn	3.249e-11	2.092e-11
FE	2.847e-10	2.276e-10
Co	5.306e-11	3.847e-11
Ni	9.687e-11	6.859e-11
Zn	4.429e-10	1.849e-11
Rb	2.744e-11	1.635e-11
CH	7.659e-10	1.390e-10
CH4	6.821e-12	0.000e+00
C2	4.106e-10	0.000e+00
C2H2	3.343e-10	0.000e+00
C2H4	4.136e-10	1.287e-10
C2H6	2.409e-10	0.000e+00
O2	7.602e-11	0.000e+00
H2O	3.145e-11	0.000e+00
NH3	2.820e-10	1.017e-10
NO	2.621e-10	9.649e-11
NO2	1.572e-10	2.023e-11
N2O	1.753e-10	0.000e+00
H2S	7.348e-10	3.125e-10
HCL	3.887e-11	0.000e+00
CS2	1.764e-09	5.179e-10
COS	7.021e-10	0.000e+00
H2CO	4.791e-10	1.278e-10

photodetachment

	ISRF	PopIII/H_2
H-	1.452e-07	2.071e-09

FUV Photoprocesses in Low-Metallicity Clouds:



H_2 bands
optically thick

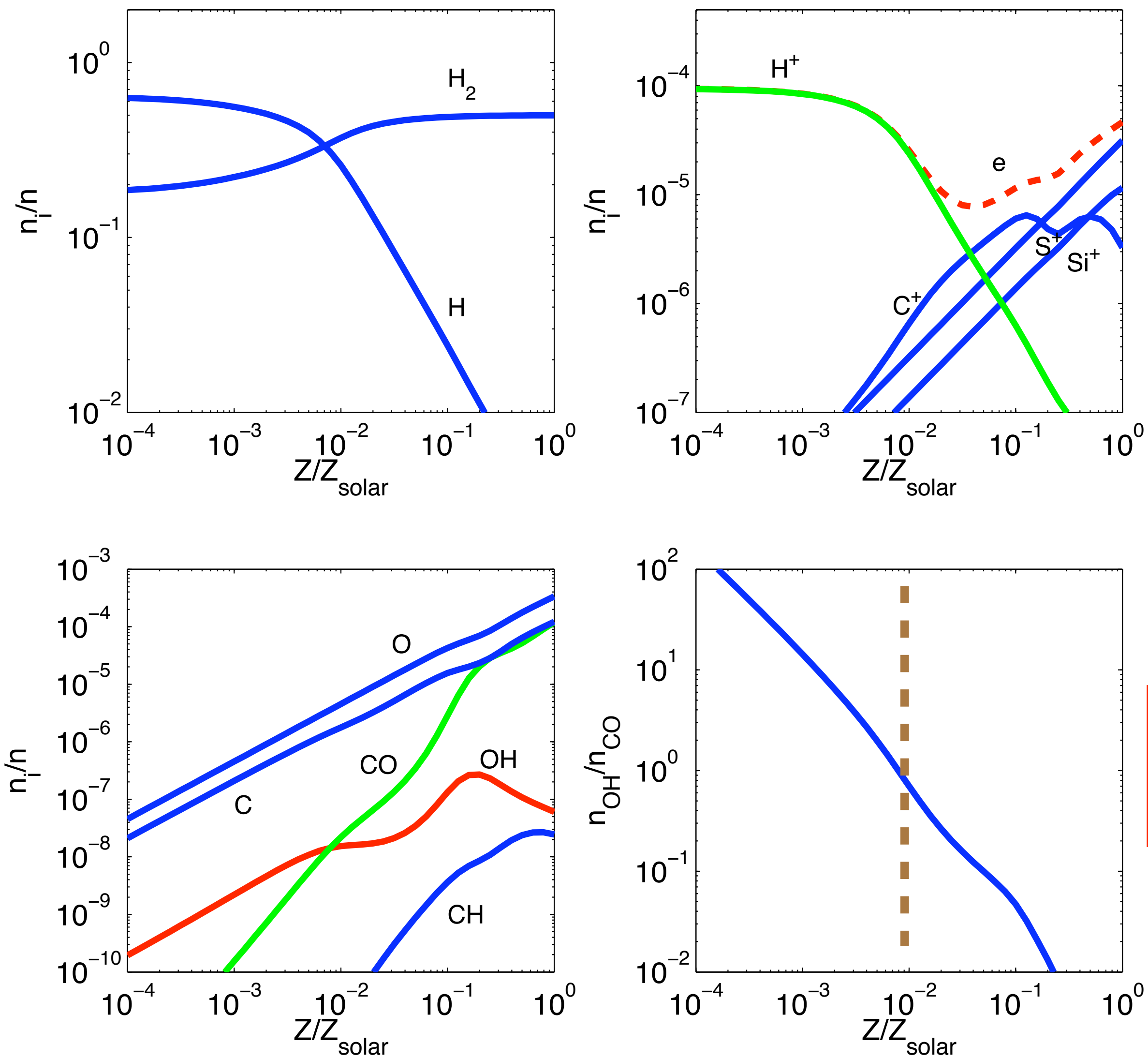
dust free
optically thin

$\Gamma_{CO} = 0$

$\Gamma_{OH} = 2.5 \times 10^{-10}\ s^{-1}$

With FUV radiation (Pop III stars):

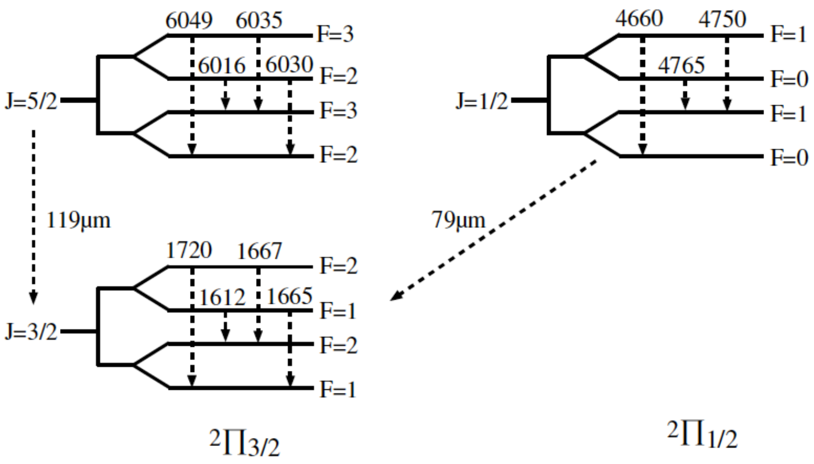
$G_{FUV} = 10^2$

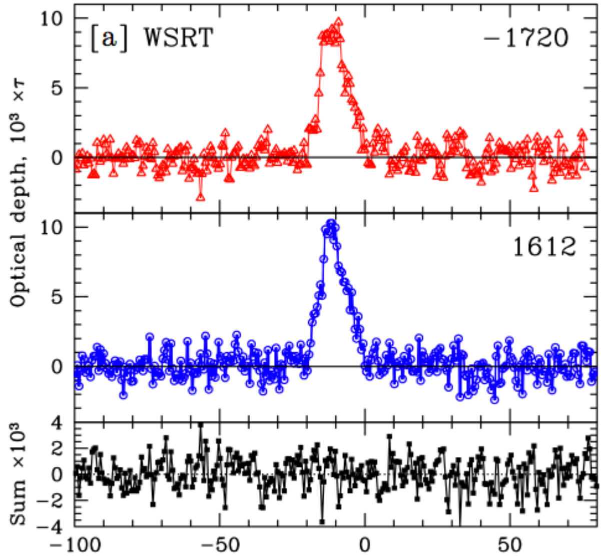


Transition from high- to low-Z regime not affected by photodissociation of OH.

Brief Remark: OH as a probe of time-variable fundamental constants.

[fine-structure constant; proton-electron mass ratio; proton gyromagnetic ratio]





OH maser "conjugate satellite lines";
...reduced systematics.

van Langevelde et al. 1995
Darling 2004
Kanekar et al. 2005; 2010; 2011

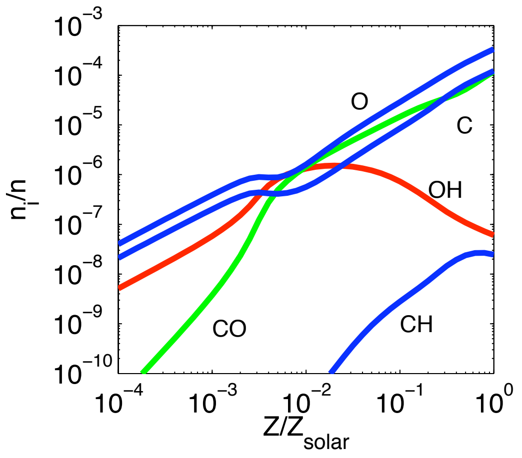
thus far to redshift $z \approx 0.8$

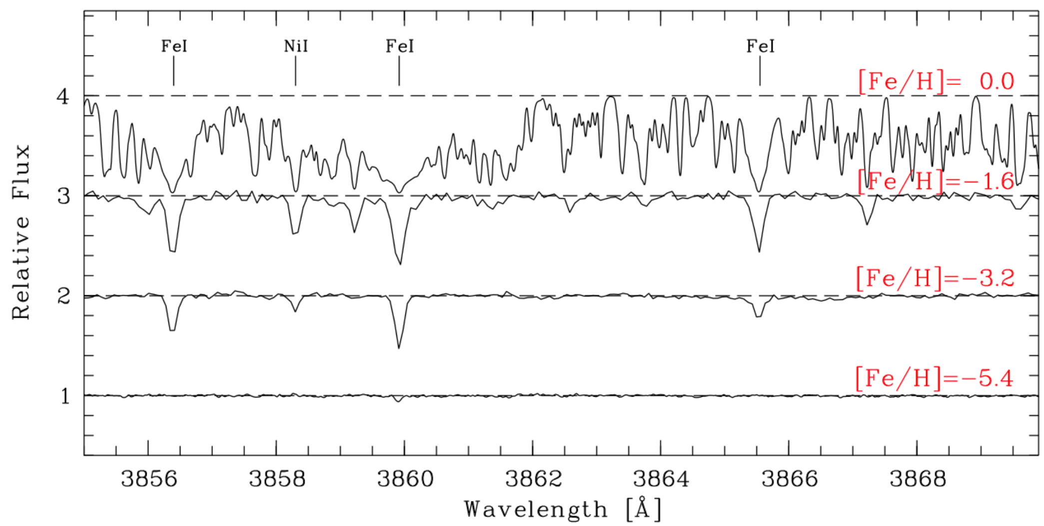
Summary:

- The existence of very low metallicity Pop II stars, with observed [C/H] and [O/H] as low as ~ -3.5 dex, is evidence that at the reionization epoch star-formation occurred in clouds with very low (but non-vanishing) heavy element abundances.

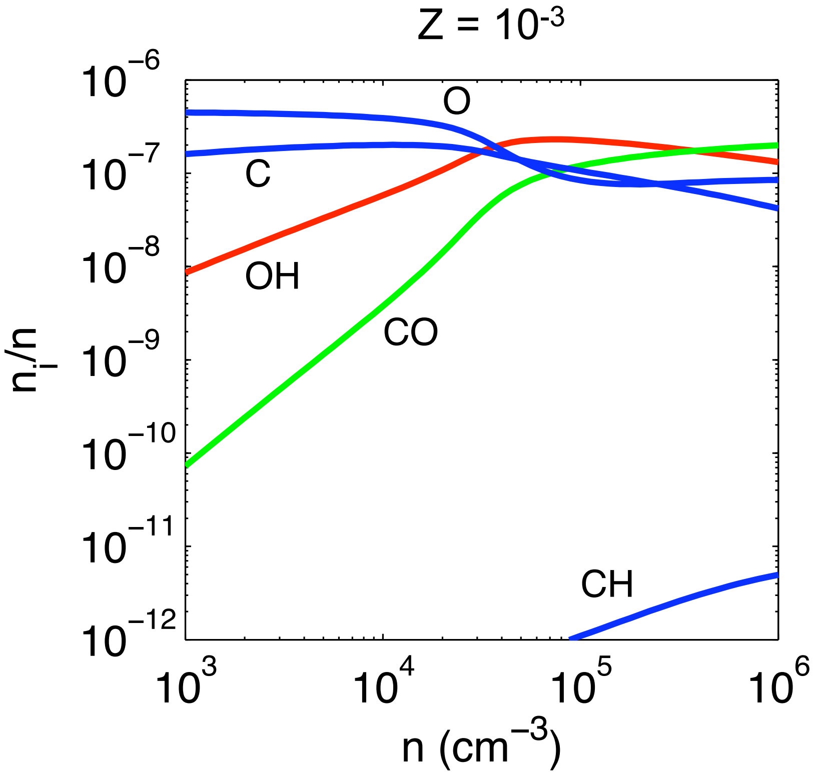
- The most abundant molecule containing a heavy element would have been a diatomic hydride, as opposed to CO as in today's molecular clouds.

- This molecule was OH





Density:



Z = 10-3
10−6
10−7
10−8
10−9
10−10
10−11
10−12
O
C
OH
CO
CH
n_i/n
10^3
10^4
10^5
10^6
n (cm−3)