Oxygen Chemistry in Molecular Clouds

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H_2O, O_2, and Water Ice

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Hollenbach, Kaufman, Bergin & Melnick (2009)

OH^+, H_2O^+, and H_3O^+

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I. Introduction: The Story of O

1. Oxygen is the third most abundant element in the universe

   $x_O = O/H \sim 5x10^{-4}$

   $x_C = C/H \sim 3x10^{-4}$

2. Abundant molecules with O (such as CO, O_2, H_2O) can be important in cooling molecular clouds (Goldsmith & Langer 1978), and are therefore important in understanding star formation.

3. To date, there have been mysteries around the basic astrochemistry of O.
   a. Why are observed abundances of O_2 and H_2O so low?
   b. Where is the elemental O?
   c. What are cosmic ray ionization rates?

4. If we cannot understand basic O chemistry, we are in terrible shape for understanding the chemistry of clouds.

II. H_2O, O_2, and Water Ice (Hollenbach et al 2009)

Summary of Observations (SWAS, Odin, and Herschel) in ambient (unshocked) molecular clouds

$x(H_2O) \sim 10^{-8}$ $N(H_2O) \sim 10^{15}$ cm^{-2}

$x(O_2) \leq 3\text{x}10^{-8}$ $N(O_2) \leq 3\text{x}10^{15}$ cm^{-2}

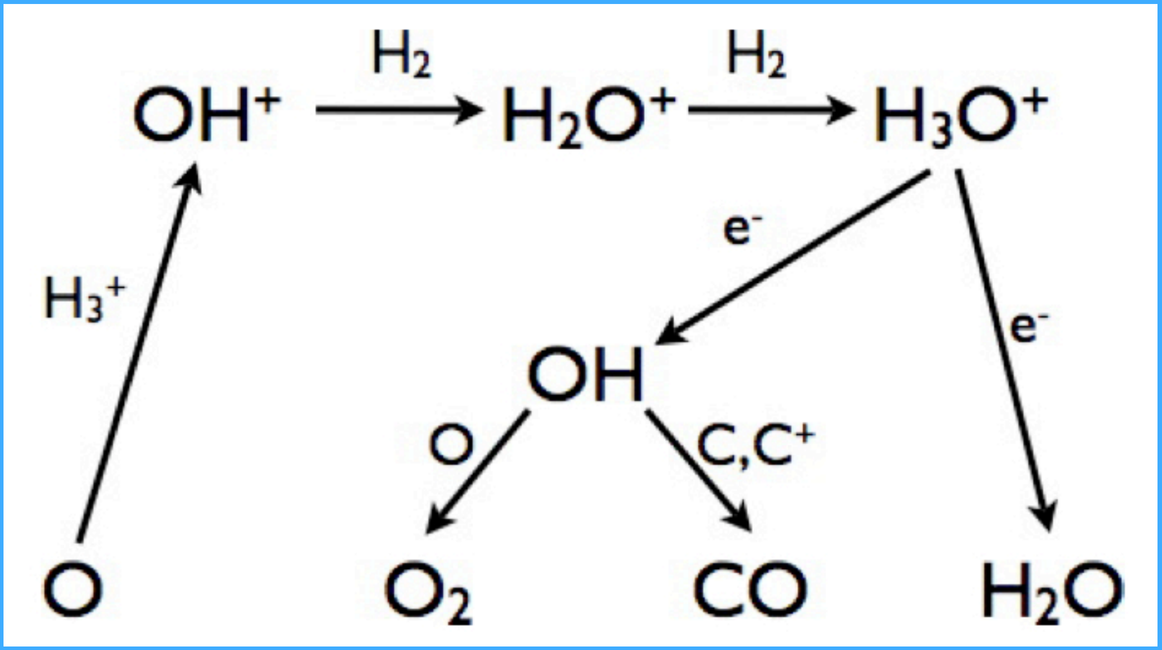
Water Ice threshold at $A_V \sim 3$

Gas phase chemical models of molecular clouds predicted H_2O and O_2 abundances higher by factors of ~100.

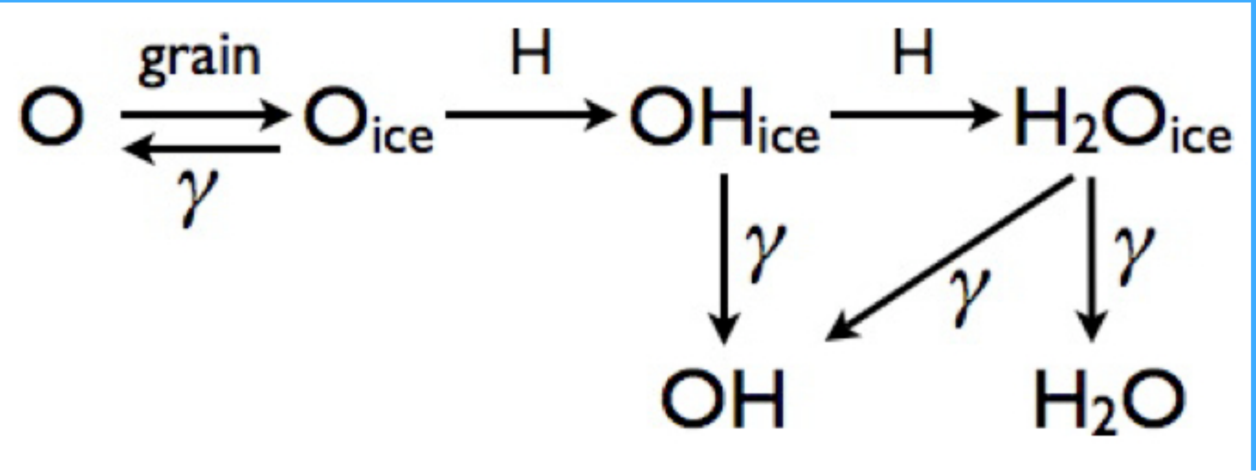
II. H_2O, O_2, and Water Ice (Hollenbach et al 2009)

Chemistry

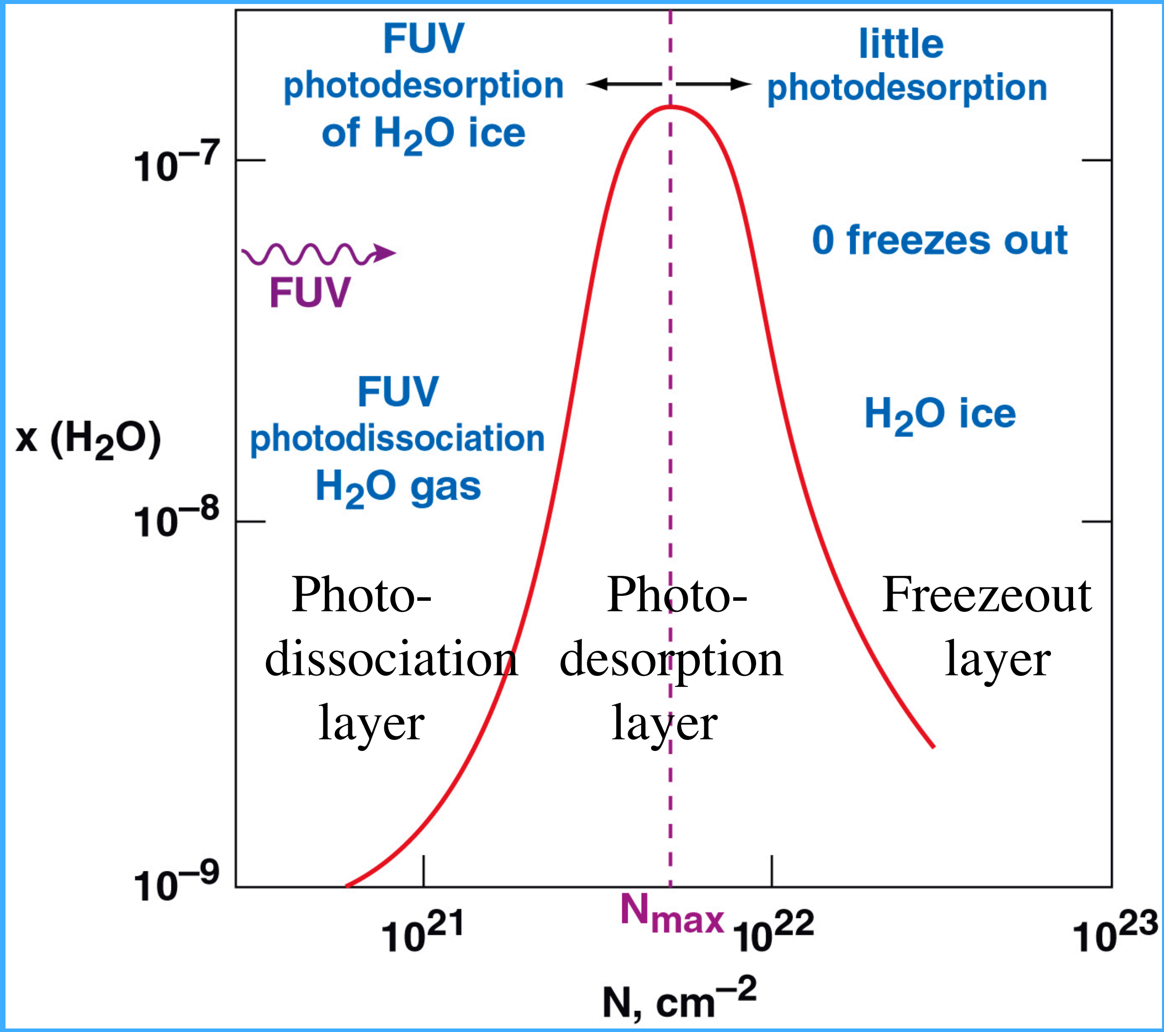
Gas phase chemistry



Freezing, grain surface chemistry and desorption



II.



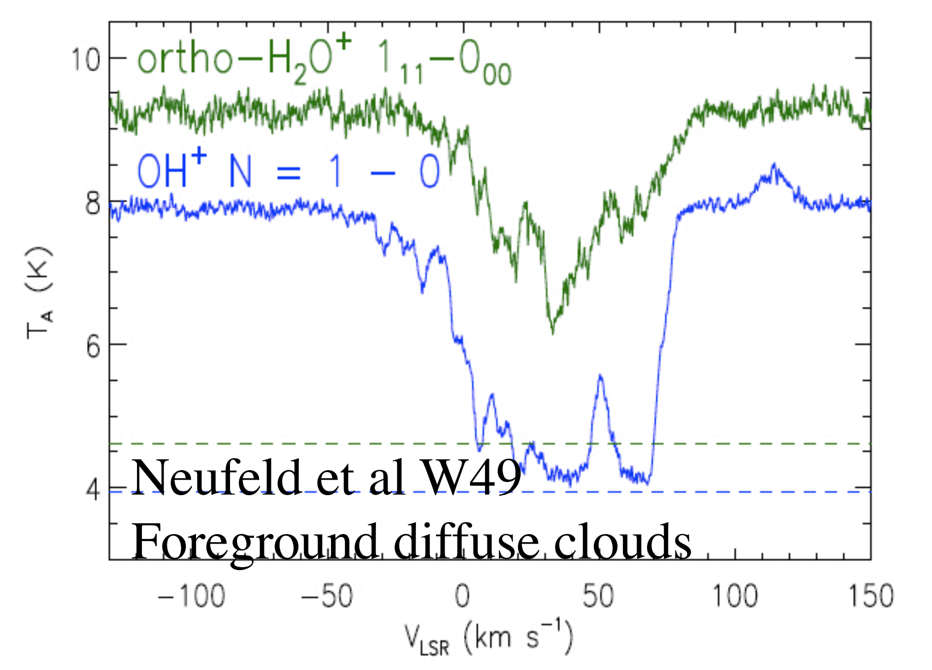
Bottom Lines: 1. $N(H_2O) \sim N(O_2) \sim 10^{15}$ cm^{-2} independent of FUV and n

2. Matches observations of diffuse clouds, molecular clouds, ice thresholds

3. Predicts in certain cases interior regions with gas phase C greater than O

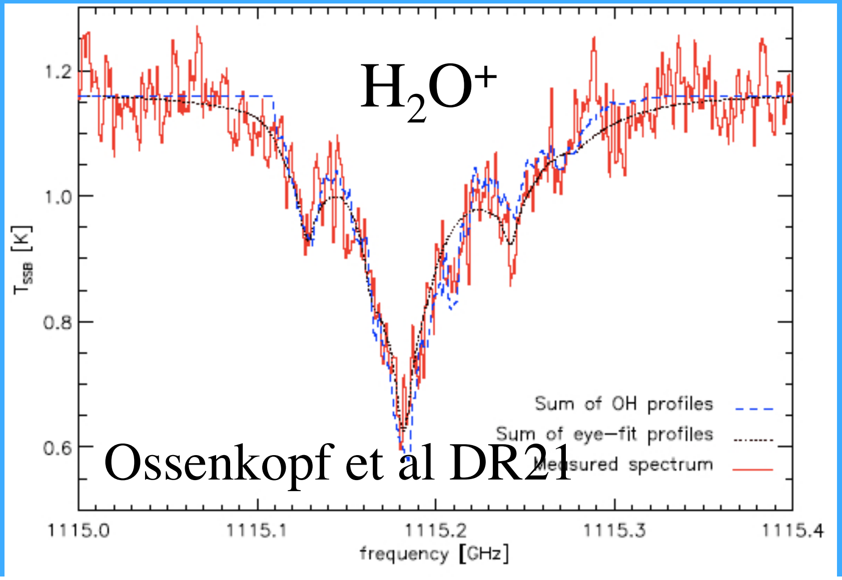
III. OH^+, H_2O^+, and H_3O^+ (in progress)

Summary of observations by Herschel



Diffuse Clouds (cm^{-2})

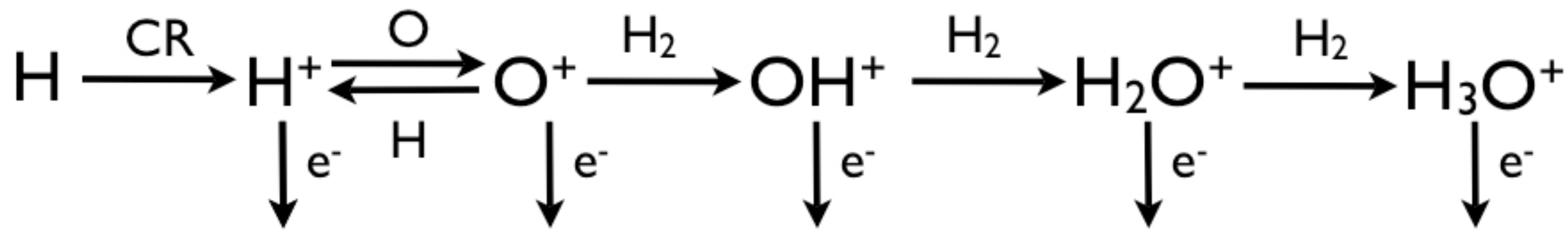
- $N(OH^+) \sim 3\times10^{12}-10^{14}$
- $N(H_2O^+) \sim 10^{12}-10^{13}$
- $N(H_3O^+) \sim 10^{12}-10^{13}$



Molecular Clouds/PDRs

- $N(OH^+) \sim 10^{13}$ (cm^{-2})
- $N(H_2O^+) \sim 10^{13}$
- $N(H_3O^+) \leq 10^{13}$

III. OH^+, H_2O^+, and H_3O^+ (in progress)



OH^+ and H_2O^+ abundances peak in atomic region of PDR.
In this region, $x(e) \sim x(C^+) \sim 10^{-4}$.

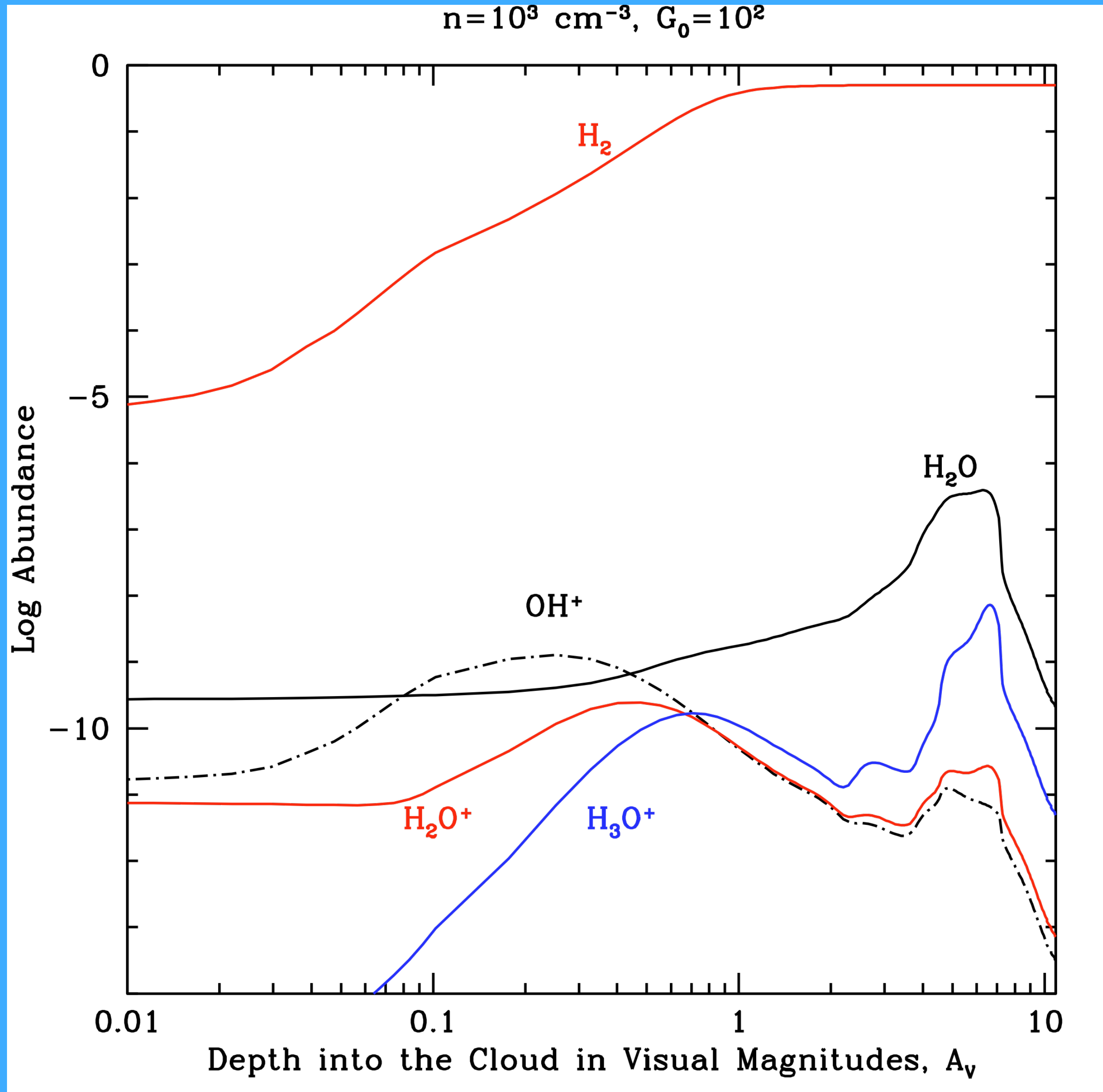
If $x(H_2) \leq 0.01$, $x(OH^+) \quad \alpha \quad (\zeta_{cr}/n)x(H_2)$

If $x(H_2) \geq 0.01$, $x(OH^+) \quad \alpha \quad (\zeta_{cr}/n)[x(H_2)]^{-1}$

See also Neufeld et al 2010 (found $\zeta_{cr} \sim 10^{-16}\ s^{-1}$ for diffuse clouds toward W49).

III. OH^+, H_2O^+, and H_3O^+ (in progress)

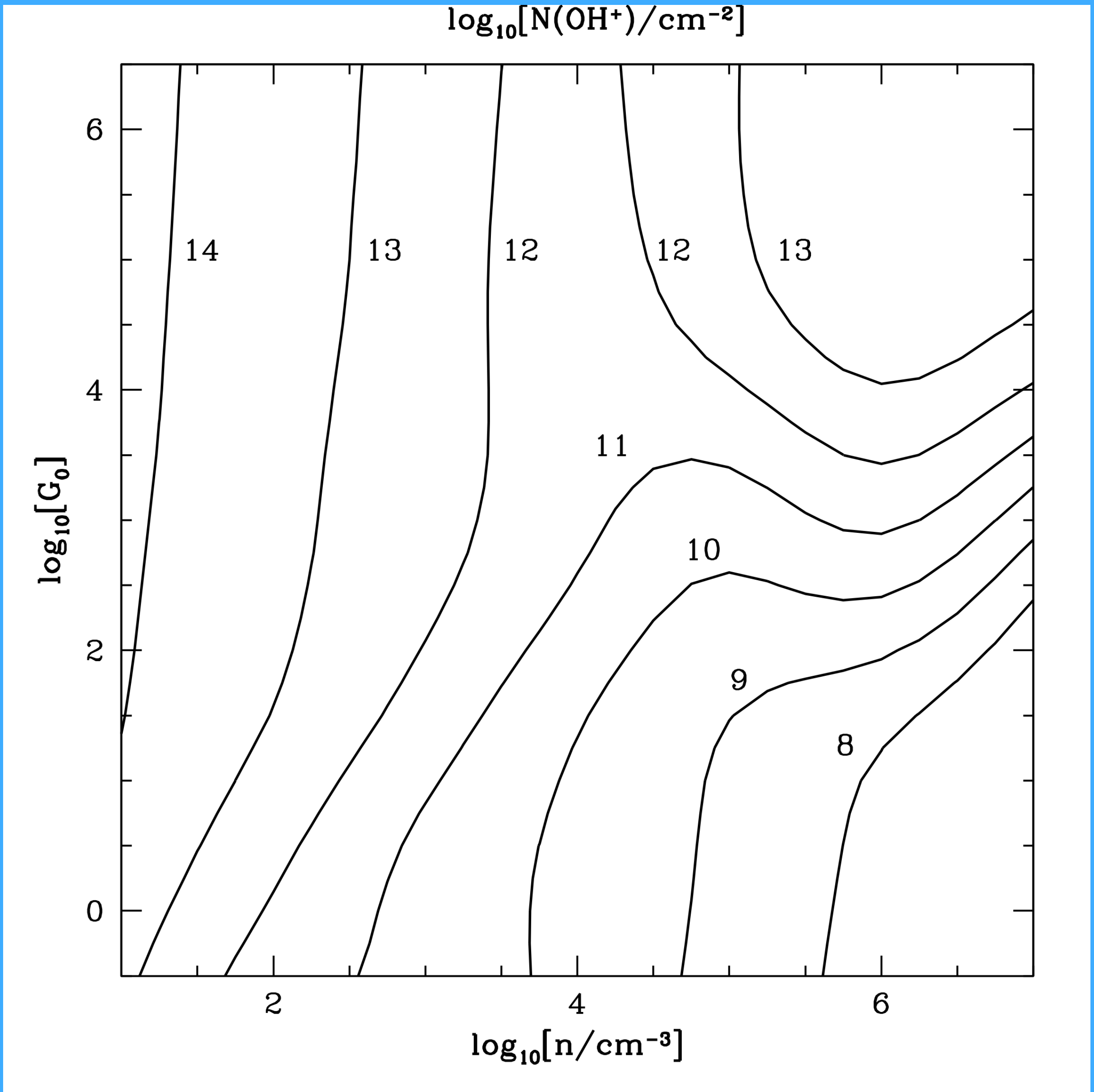
$\zeta_{cr} = 10^{-16}\ s^{-1}$



III. OH^+, H_2O^+, and H_3O^+ (in progress)

$\zeta_{cr} = 10^{-16}\ s^{-1}$

Upper right hand corner distorted by chemical production of H^+



III. OH^+, H_2O^+, and H_3O^+ (in progress)

Chemical Production of H^+

1. Via OH

$H_2 + O \rightarrow OH + H$ (requires high T and n)

$OH + C^+ \rightarrow CO^+ + H$

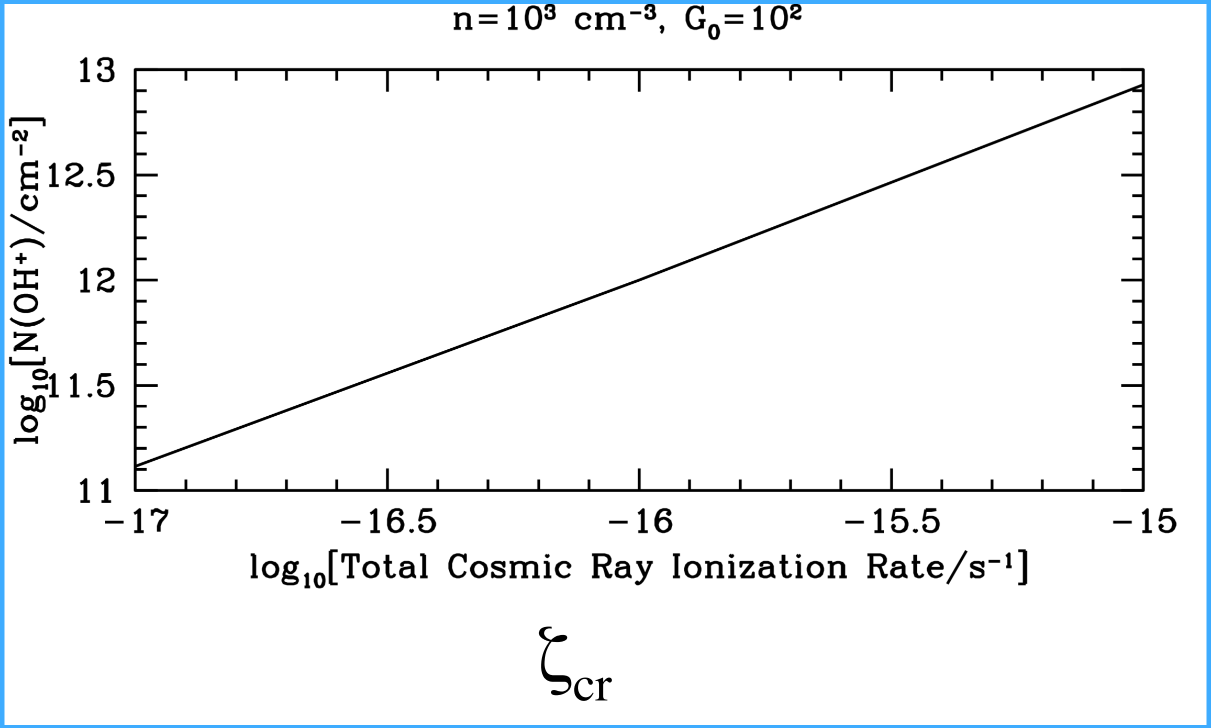
$CO^+ + H \rightarrow CO + H^+$

2. Via CH^+

$C^+ + H_2 \rightarrow CH^+ + H$ (requires high T and n)

$CH^+ + FUV \rightarrow C + H^+$

III. OH^+, H_2O^+, and H_3O^+ (in progress)



Note that $N(OH^+)$ and $N(H_2O^+)$ are proportional to ζ_{cr} .

IV. Summary

1. Steady state models with freezing, desorption give low columns ~10^{15} cm^{-2} of H_2O and O_2 in ambient molecular clouds (not the shocked regions or regions of exceptionally high H ionization or regions of high $T_{dust} > 100$ K!).

2. Observed columns of OH^+ and H_2O+ constrain the cosmic ray ionization rate ($N \alpha \ \zeta_{cr}/n$) in diffuse clouds and on the surfaces of molecular clouds. Abundances peak at x(H_2 ~ 0.01). Caveats are:
   a. Geometry (both sides? Edge on?)
   b. Need to know density ([CII] and [OI]?)
   c. Not true for high FUV field and density
   d. Time dependent effects

3. H_3O^+ is more complicated because of possible second peak deep in cloud where O is still abundant, but e not.