Cosmic-Ray Ionization of Molecular Clouds

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Ionization and Astrochemistry

- Interstellar chemistry is driven by fast ion-molecule reactions
- Requires source of ionization
  - UV photons with $E > 13.6$ eV are absorbed by atomic H in H II regions
  - species with $IP > 13.6$ eV are primarily neutral
  - species with $IP < 13.6$ eV are singly ionized
- In diffuse and dense molecular clouds H and H_2 are ionized by cosmic rays
- $\zeta_2 = 2.3\zeta_p$; $\zeta_H = 1.5\zeta_p$; Glassgold & Langer 1974 ApJ, 193, 73

An aside on ISM properties

- Dense clouds
  - $n > 10^4$ cm^{-3}; T~30 K; $f(H_2)$~1
  - x_e~10^{-7}; carbon in CO
- Diffuse molecular clouds
  - n~10^2 cm^{-3}; T~70 K; $f(H_2)=0.1-1$
  - x_e~10^{-4}; carbon in C^+
- Diffuse atomic clouds
  - n~10 cm^{-3}; T~100 K; $f(H_2) < 0.1$
  - x_e~10^{-4}; carbon in C^+

Exhibit A: Dense Clouds

Exhibit B: Diffuse Clouds

Particle Interactions

- Ionization

$$p + H_2 \rightarrow H_2^+ + e^- + p'$$

- Spallation and Fusion

$$[p, \alpha] + [^{12}C, ^{14}N, ^{16}O] \rightarrow [^6Li, ^7Li, ^9Be, ^{10}B, ^{11}B]$$

- Nuclear Excitation

$$[p, \alpha] + ^{12}C \rightarrow ^{12}C^* \rightarrow ^{12}C + \gamma_{4.44\ \mathrm{MeV}}$$

- Inelastic Collisions

$$p + H \rightarrow p' + H + \pi^0$$

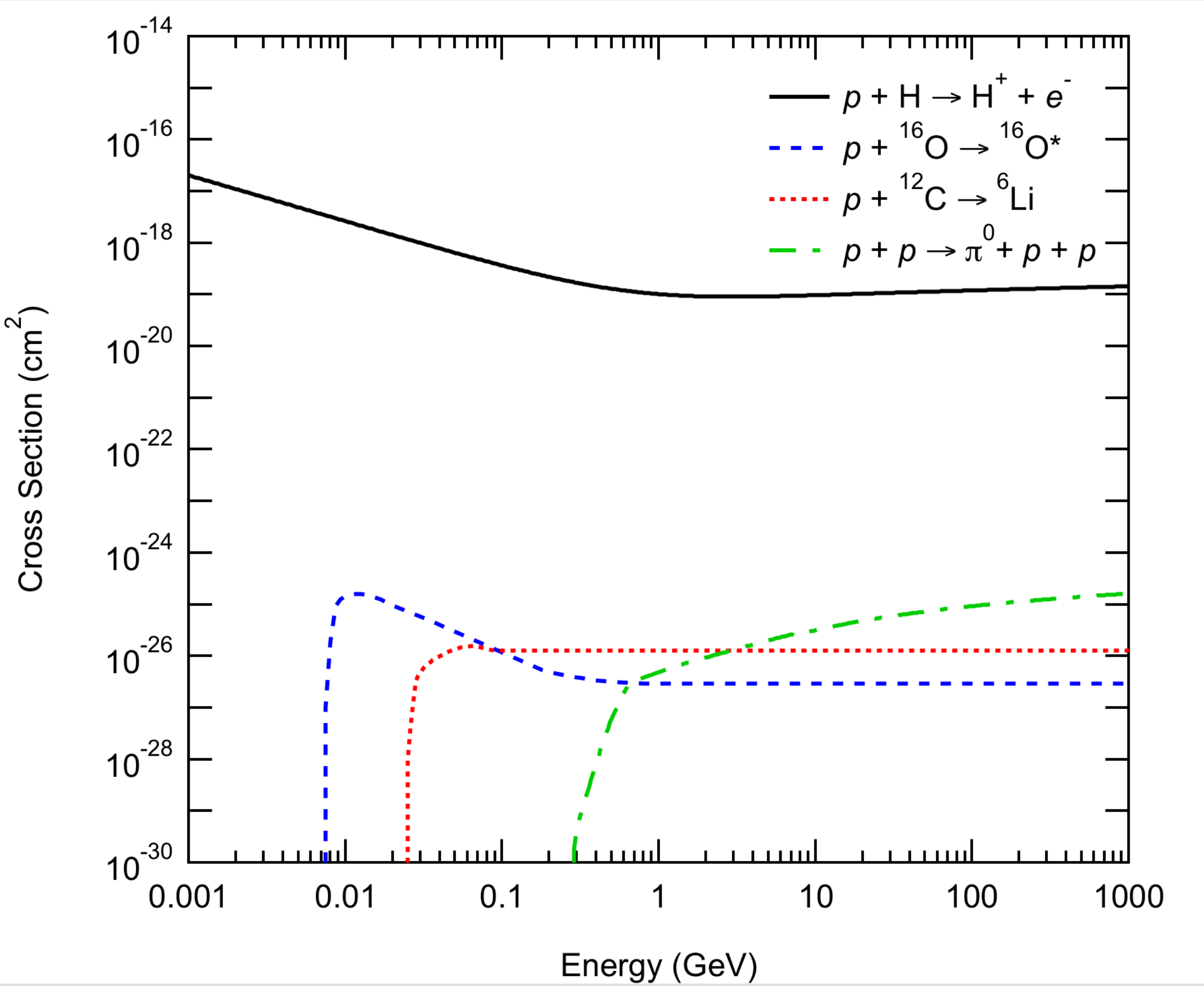
$$\pi^0 \rightarrow \gamma + \gamma$$

Rate of Interactions

$$R_x = 4\pi G_x \int j(E)\sigma_x(E)dE$$

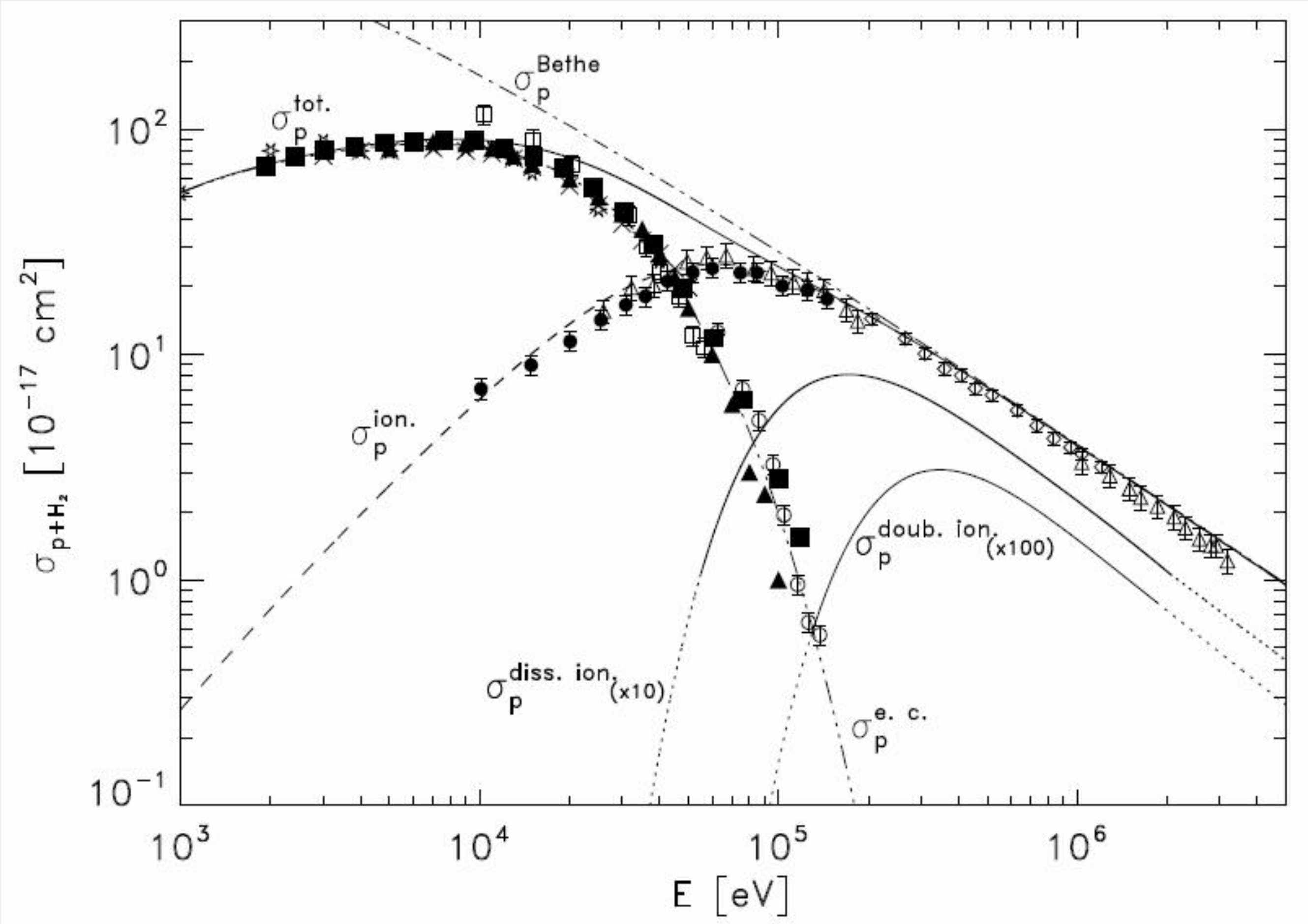
- G_x: Interaction specific coefficient
- σ_x: Interaction cross section
- $j(E)dE$: Differential proton spectrum

Interaction Cross Sections



Indriolo & McCall 2013, Chem. Soc. Rev., 42, 7763 (and references therein)

H_2 Ionization Cross Section

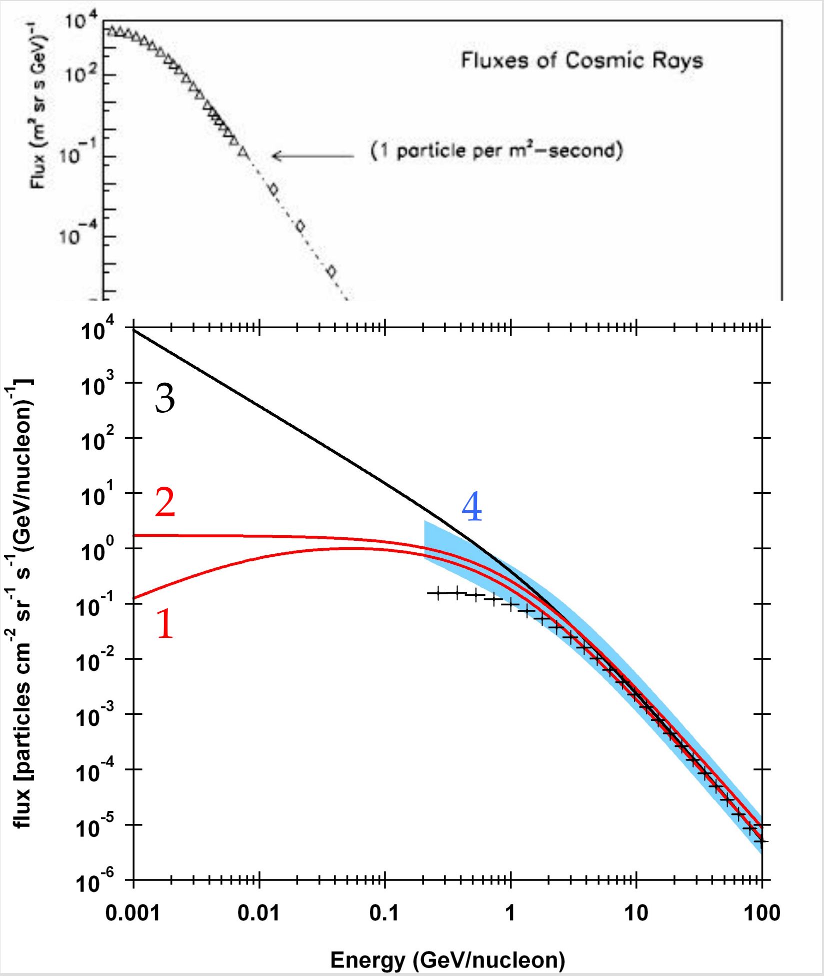


Padovani et al. 2009, A&A, 501, 619 (and references therein)

Cosmic Ray Energy Distribution

- Power law in energy ($\phi \sim E^{-2.7}$) spanning 12 decades in E, and 30 decades in flux
- Poorly constrained below 1 GeV

(1): Spitzer & Tomasko (1968)
(2): Gloeckler & Jokipii (1969)
(3): Nath & Biermann (1994)
(4): Mori 1997



Swordy 2001

What Ionization Rate Tells Us

- Cosmic-ray ionization of H and H_2 is most efficient at keV to MeV energies
- Particle spectrum is measured above about 1 GeV, but poorly constrained in energy range most important for ionization
- Determination of ionization rate from molecular observations can add constraints to low-energy particle flux

Ionization Rate From Molecules

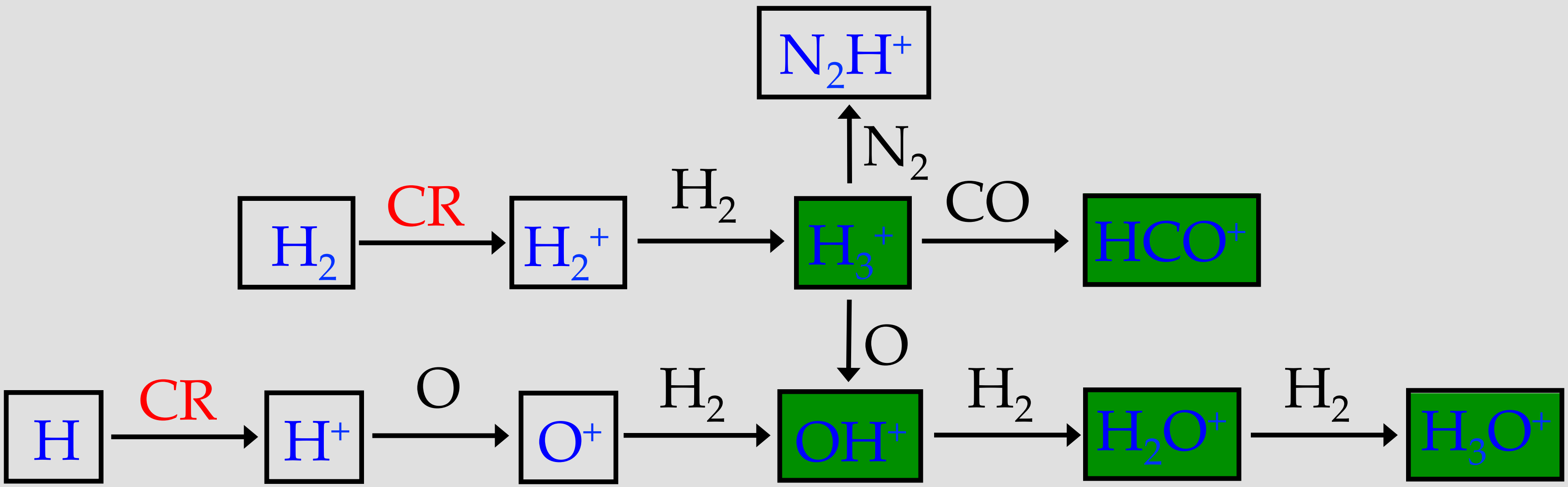
- Rate of change for abundance of any species can be written as a differential equation accounting for formation and destruction mechanisms, e.g.,

$$\frac{d}{dt}n(H_3^+) = n(H_2)n(H_2^+)k(H_2|H_2^+) - n(H_3^+)n(e)k(H_3^+|e) - n(H_3^+)n(CO)k(H_3^+|CO)$$

formation destruction

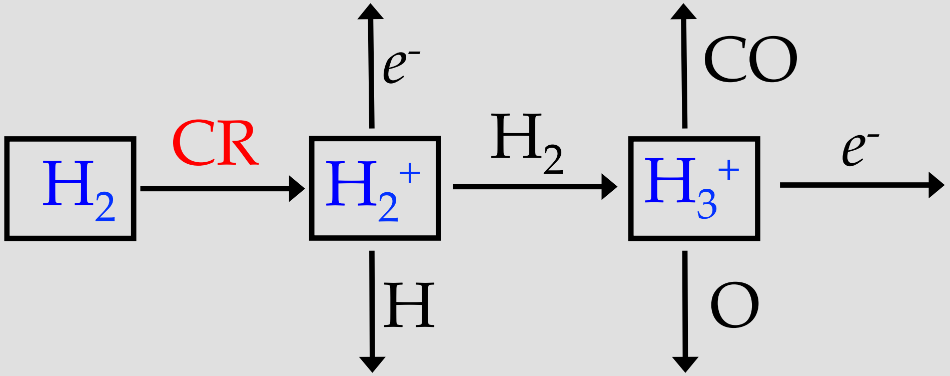
- More terms can be added to account for alternate formation and destruction pathways
- Formation rates of species closely linked to cosmic-ray ionization will be influenced by ionization rate

Ion-Molecule Reactions



- H_3^+ acts as a "universal proton donor"
- Molecular ions linked to CR ionization

Hydrogen Chemistry



- Formation
  - $CR + H_2 \rightarrow H_2^+ + e^- + CR'$
  - $H_2^+ + H_2 \rightarrow H_3^+ + H$
- Destruction
  - $H_3^+ + e^- \rightarrow H + H + H$
- Dense Clouds
  - $H_3^+ + CO \rightarrow HCO^+ + H_2$
  - $H_3^+ + O \rightarrow OH^+ + H_2$
- Atomic Clouds
  - $H_2^+ + H \rightarrow H_2 + H^+$
  - $H_2^+ + e^- \rightarrow H + H$

Ionization Rate from H_3^+

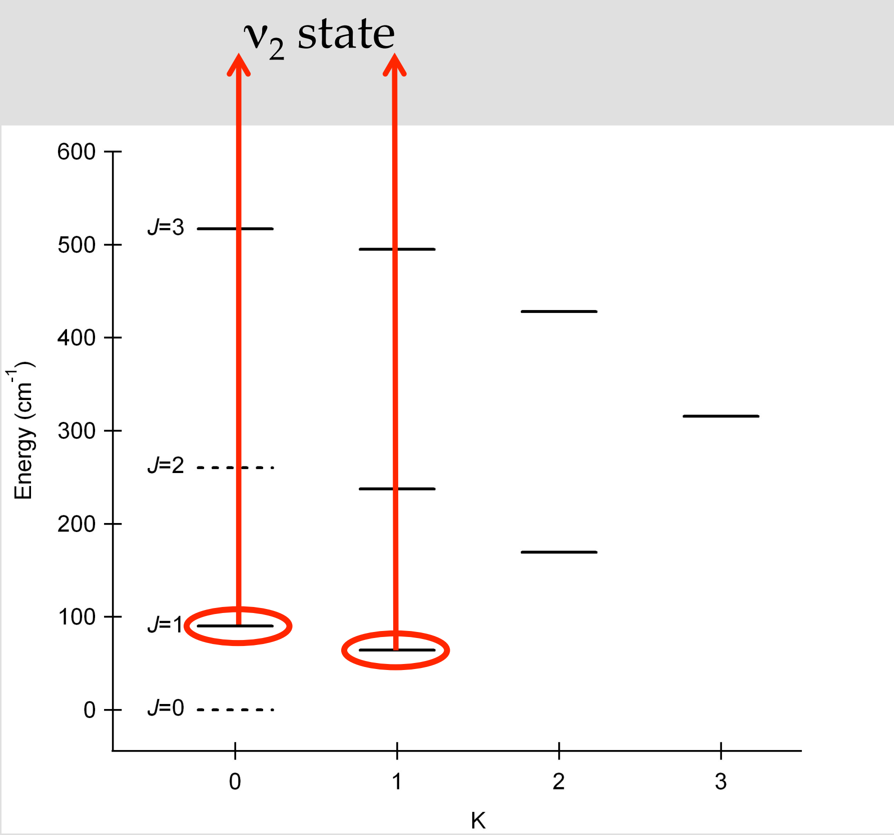
CR + H_2 $\quad$ $H_3^+ + e^-$

$$\zeta_2 n(\mathrm{H}_2) = k(\mathrm{H}_3^+|e^-)n(\mathrm{H}_3^+)n_e$$

$$\zeta_2 = k(\mathrm{H}_3^+|e^-)x_e n_{\mathrm{H}} \frac{N(\mathrm{H}_3^+)}{N(\mathrm{H}_2)}$$

- $k(\mathrm{H}_3^+|e^-)$ measured in laboratory (2×10^{-7} cm^3 s^{-1})
- x_e approximated by $x(\mathrm{C}^+)$ (1.5×10^{-4})
- n_H estimated from molecular observations (100 cm^{-3})
- $N(\mathrm{H}_2)$ measured or estimated (10^{20}-10^{21} cm^{-2})
- $N(\mathrm{H}_3^+)$ determined from NIR observations

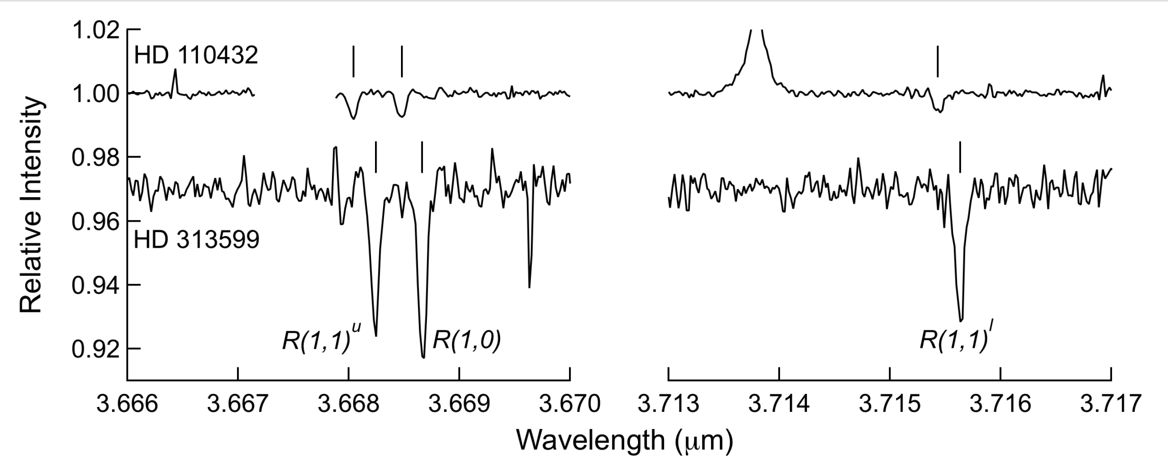
Targeted Transitions



Energy level diagram for the ground vibrational state of H_3^+

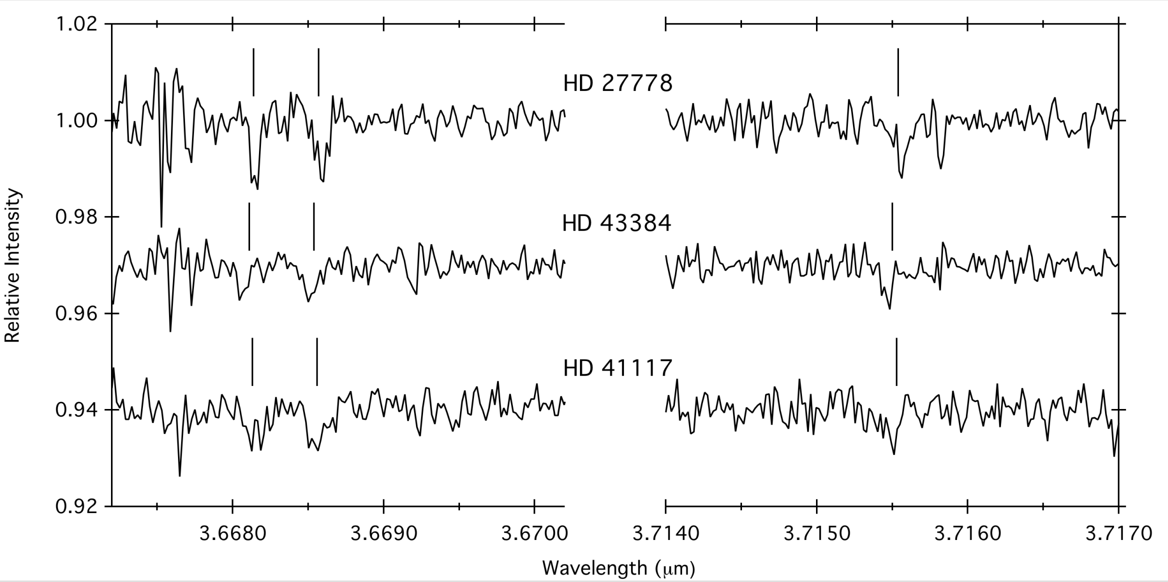
- Transitions of the $\nu_2 \leftarrow 0$ band of H_3^+ are available in the infrared
- Given average diffuse cloud temperatures (70 K) only the (J,K)=(1,0) & (1,1) levels are significantly populated
- Observable transitions are:
  - $R(1,1)^u$: 3.668083 μm
  - *R(1,0)*: 3.668516 μm
  - $R(1,1)^l$: 3.715479 μm
  - *Q(1,1)*: 3.928625 μm
  - *Q(1,0)*: 3.953000 μm

Example H_3^+ Observations



Indriolo 2012,
Phil. Trans. R. Soc. A 370, 5142

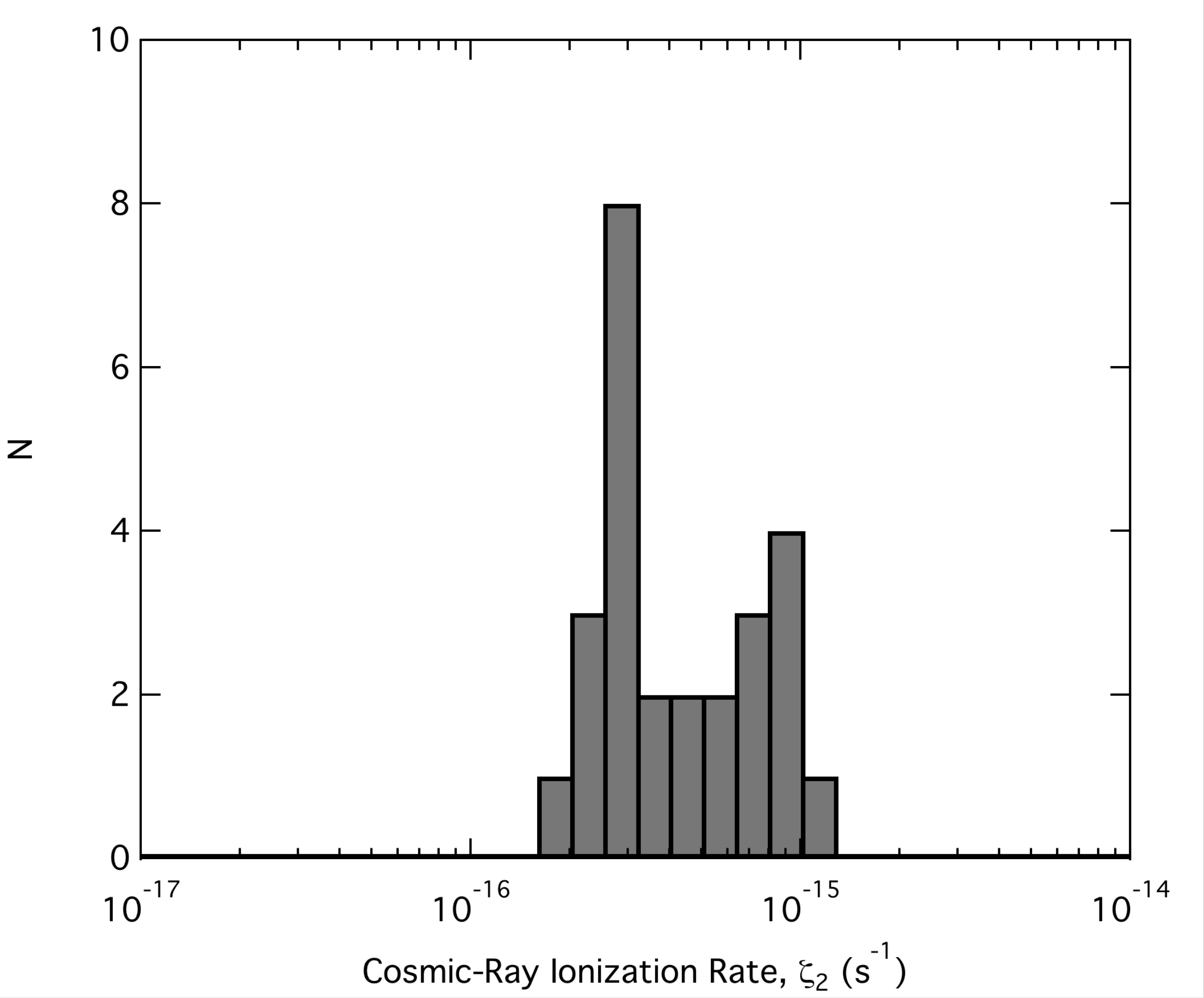
	$N(H_3^+)$ (10^{14} cm^{-2})	ζ_2 (10^{-16} s^{-1})
HD 110432	0.52	3.9±2.1
HD 313599	3.16	6.8±5.1



Albertsson et al. 2014, ApJ, 787, 44

	$N(H_3^+)$ (10^{14} cm^{-2})	ζ_2 (10^{-16} s^{-1})
HD 27778	0.65	7.5±4.3
HD 43384	0.41	2.5±1.6
HD 41117	0.53	4.9±3.2

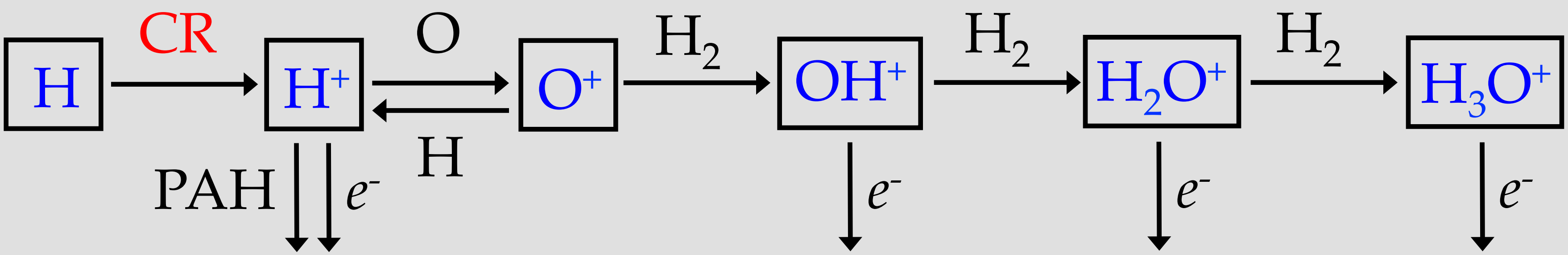
Distribution of ζ_2



Limitations of H_3^+

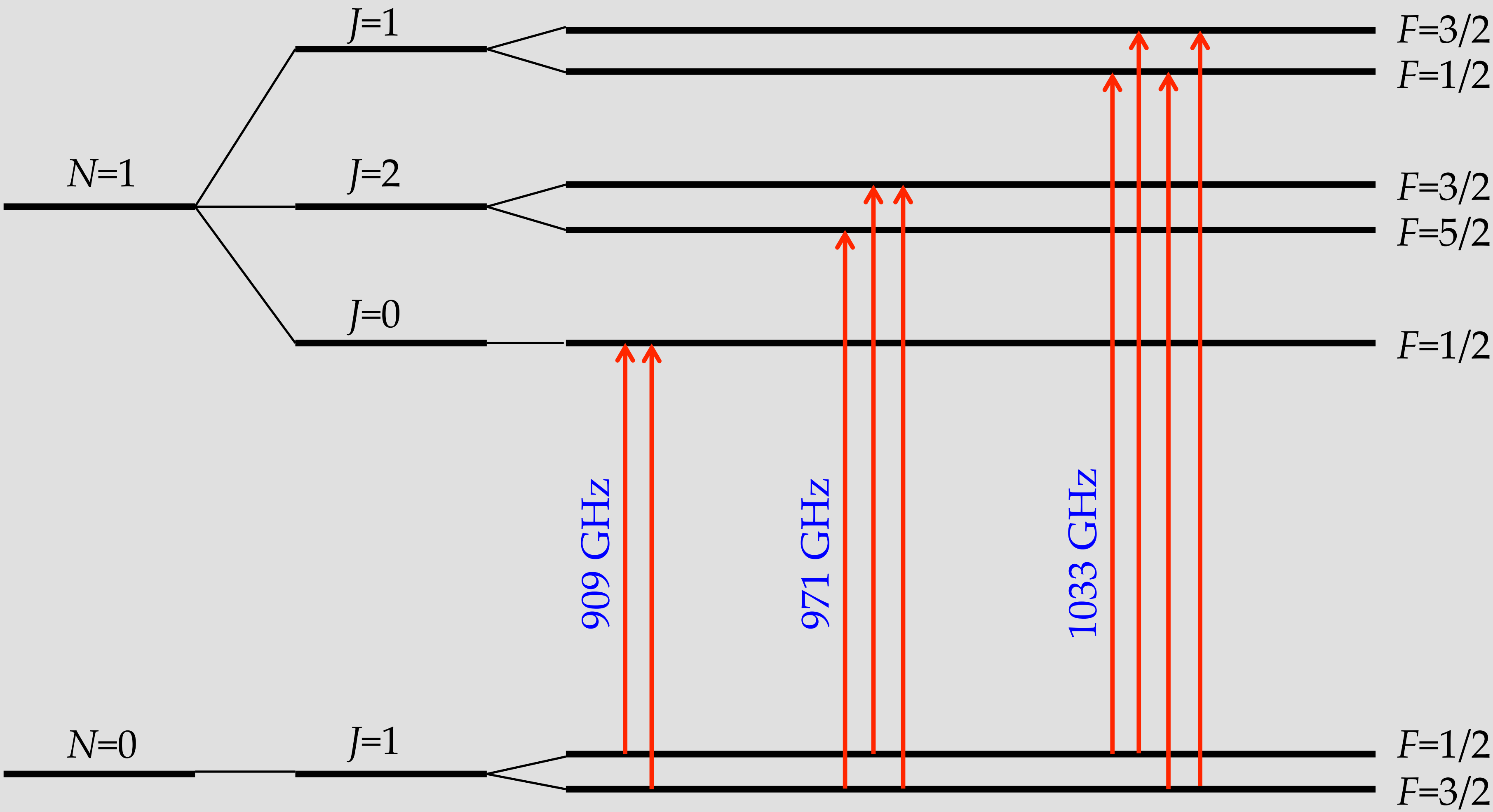
- Absorption lines are weak, requiring high S/N and long observations
- More than half of all observations have resulted in non-detections
- Even with high S/N non-detections, most upper limits are near 10^{-16} s^{-1}
- Most suitable background sources (OB stars) are within about 2 kpc

Oxygen Chemistry

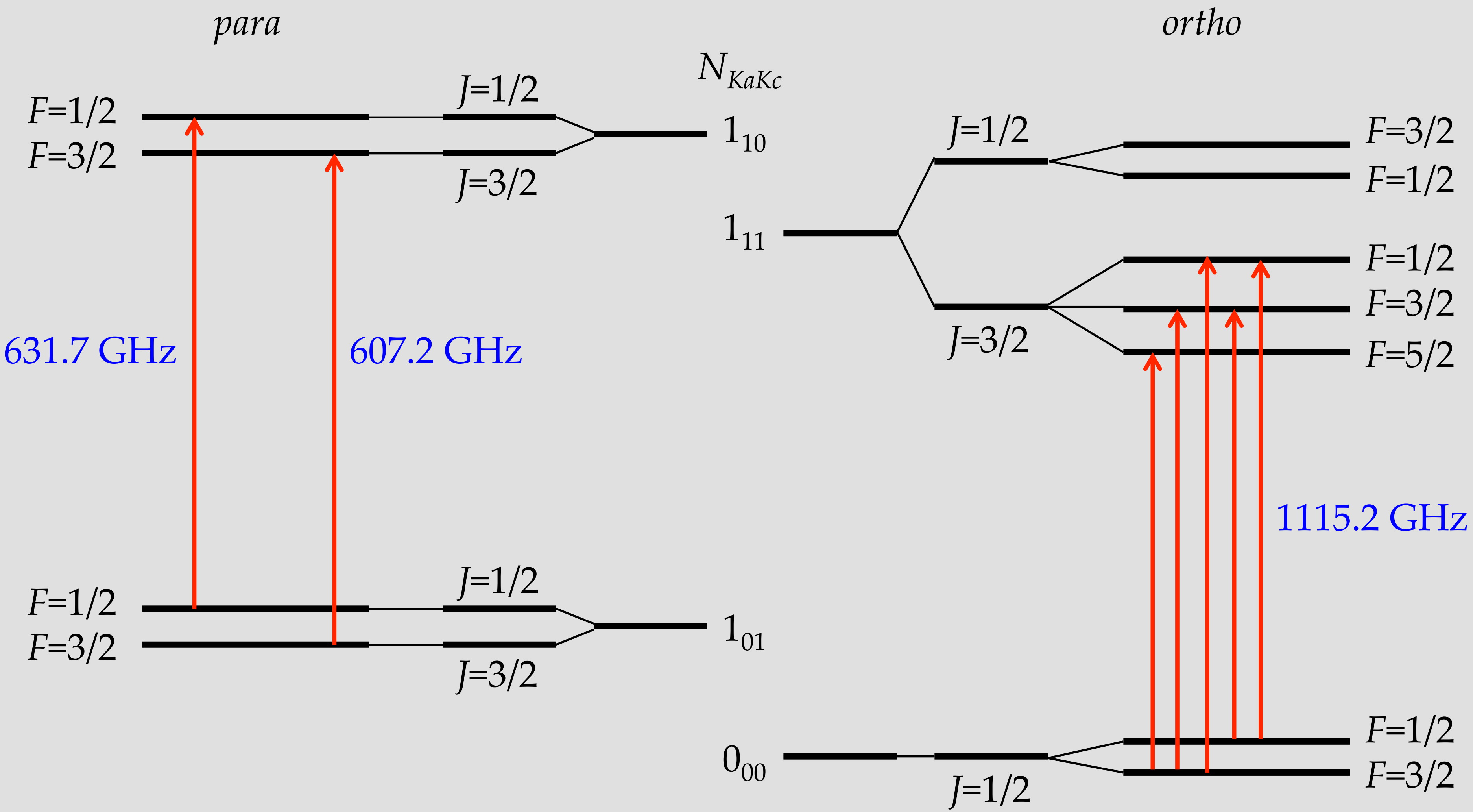


- $CR + H \rightarrow H^+ + e^- + CR'$
- $H^+ + O \rightarrow O^+ + H$
- $O^+ + H_2 \rightarrow OH^+ + H$
- $OH^+ + H_2 \rightarrow H_2O^+ + H$
- $H_2O^+ + H_2 \rightarrow H_3O^+ + H$
- $OH^+ + e^- \rightarrow$ products
- $H_2O^+ + e^- \rightarrow$ products
- $H_3O^+ + e^- \rightarrow$ products
- $O^+ + H \rightarrow H^+ + O$
- $H^+ + e^- \rightarrow H + h\nu$
- $H^+ + PAH \rightarrow PAH^+$

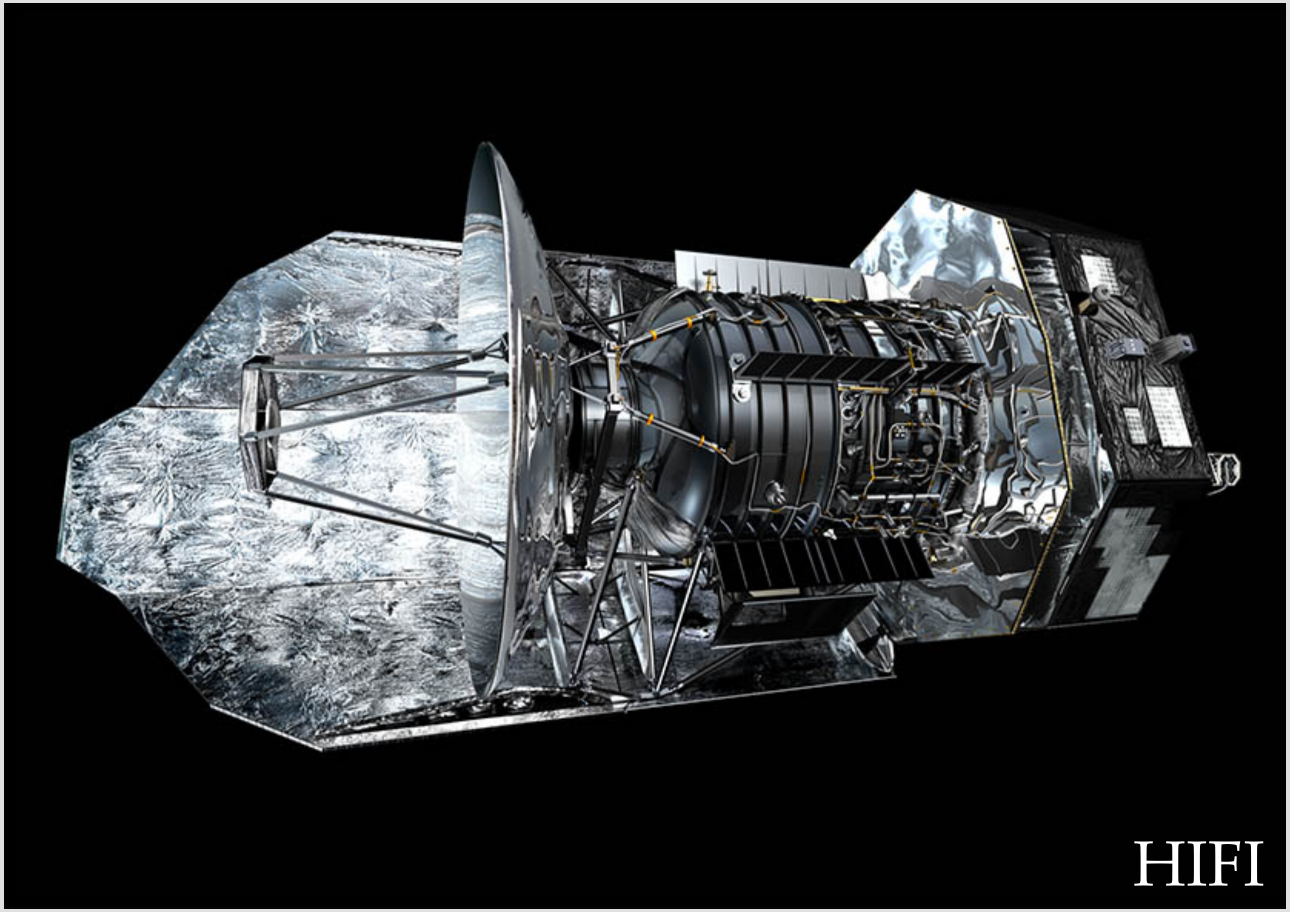
OH^+ Transitions



H_2O^+ Transitions



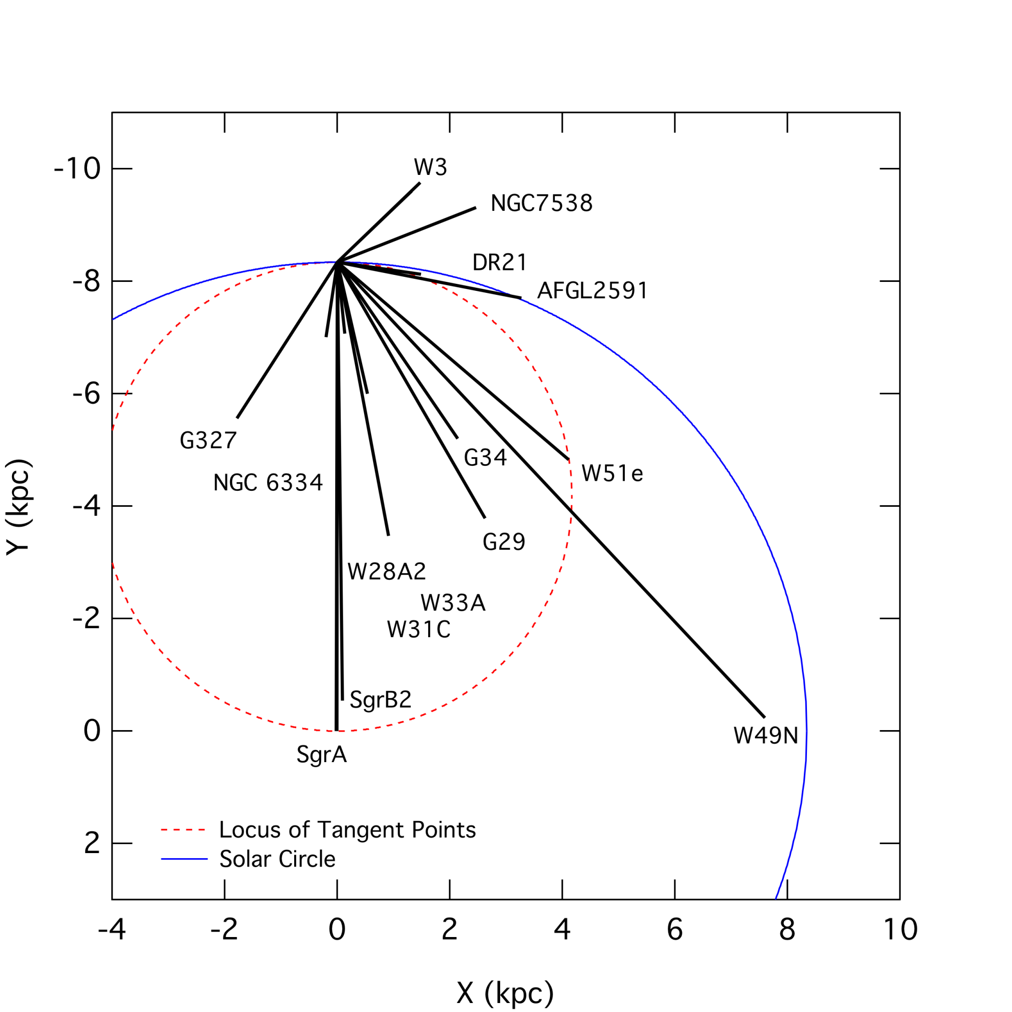
Instrument & Telescope



Herschel Space Observatory

Herschel Observations

- 20 Galactic sight lines surveyed in multiple *Herschel* programs in both OH^+ and H_2O^+
- Observations probe gas up to 11 kpc distant
- Roughly 100 separate components where ionization rate can be determined



H_2 Fraction & Ionization Rate

$OH^+ + H_2$ | $H_2O^+ + H_2$ | $H_2O^+ + e^-$

$$n(\mathrm{OH}^+)n(\mathrm{H}_2)k(\mathrm{OH}^+|\mathrm{H}_2) = n(\mathrm{H}_2\mathrm{O}^+)[n(\mathrm{H}_2)k(\mathrm{H}_2\mathrm{O}^+|\mathrm{H}_2) + n_e k(\mathrm{H}_2\mathrm{O}^+|e^-)]$$

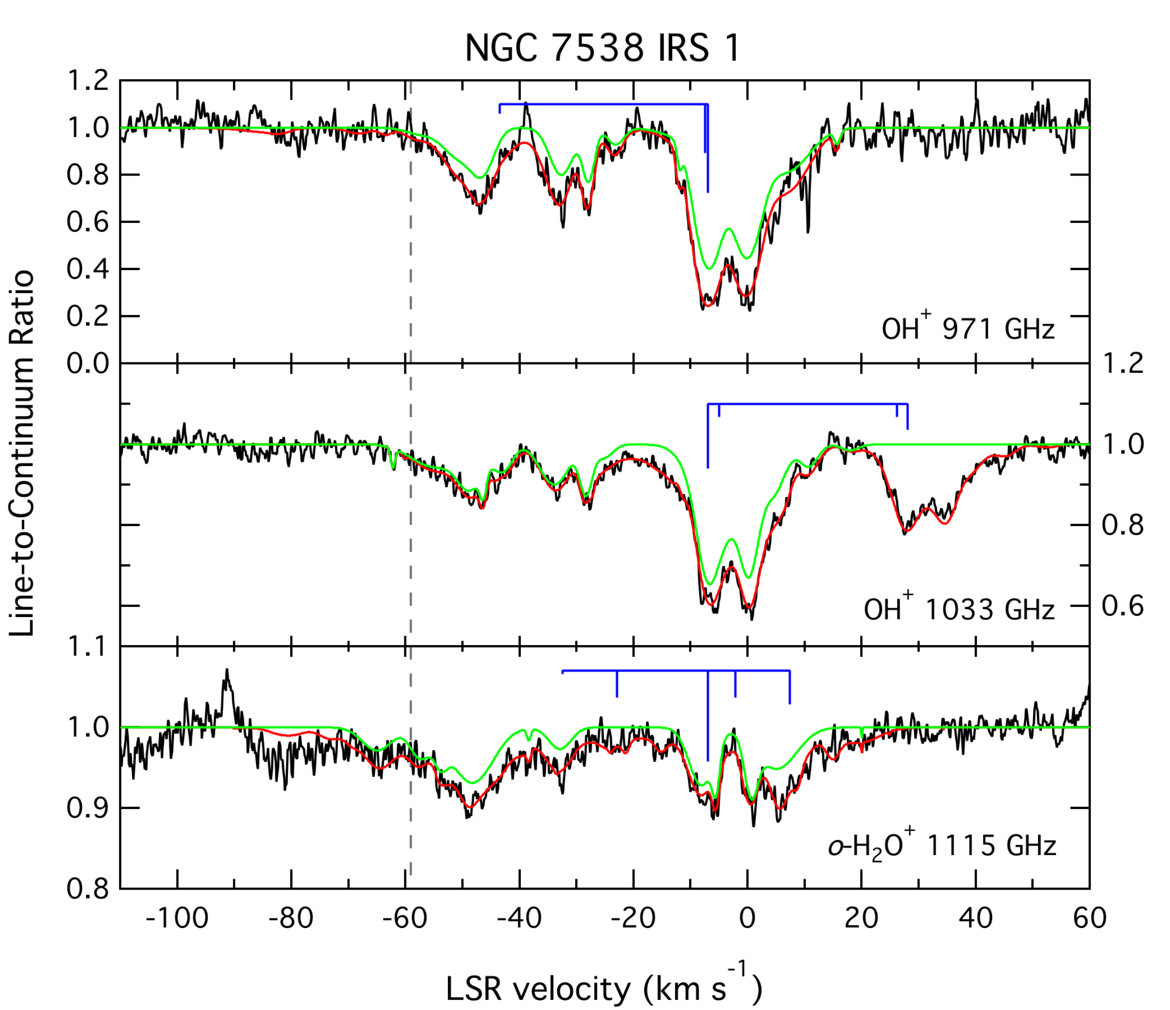
$$f_{\mathrm{H}_2} = \frac{2x_e k(\mathrm{H}_2\mathrm{O}^+|e^-)/k(\mathrm{OH}^+|\mathrm{H}_2)}{N(\mathrm{OH}^+)/N(\mathrm{H}_2\mathrm{O}^+) - k(\mathrm{H}_2\mathrm{O}^+|\mathrm{H}_2)/k(\mathrm{OH}^+|\mathrm{H}_2)}$$

CR + H | $OH^+ + H_2$ | $OH^+ + e^-$

$$\epsilon\zeta_\mathrm{H} n(\mathrm{H}) = n(\mathrm{OH}^+)[n(\mathrm{H}_2)k(\mathrm{OH}^+|\mathrm{H}_2) + n_e k(\mathrm{OH}^+|e^-)]$$

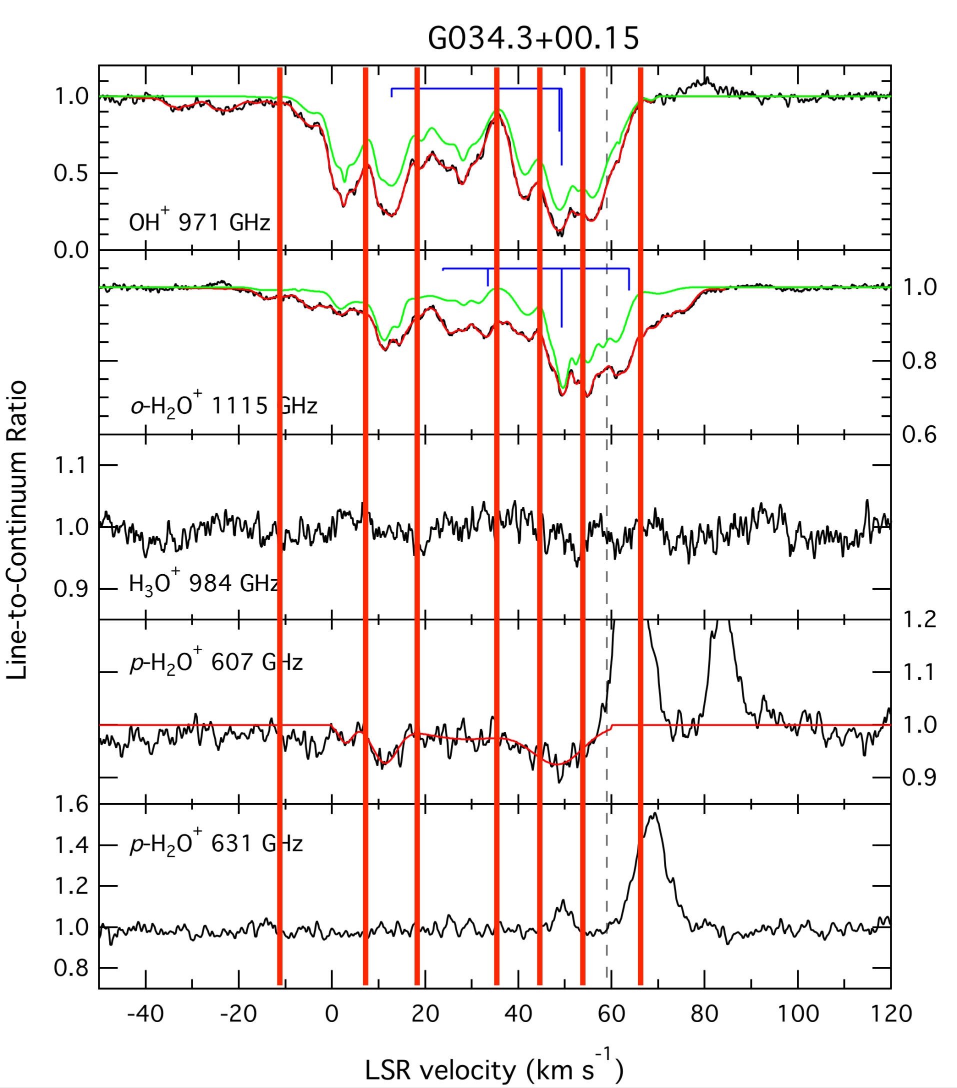
$$\epsilon\zeta_\mathrm{H} = \frac{N(\mathrm{OH}^+)}{N(\mathrm{H})} n_\mathrm{H} \left[\frac{f_{\mathrm{H}_2}}{2} k(\mathrm{OH}^+|\mathrm{H}_2) + x_e k(\mathrm{OH}^+|e^-)\right]$$

Example OH^+ & H_2O^+ Observations



Indriolo et al. 2014 (in preparation)

Example OH^+ & H_2O^+ Observations



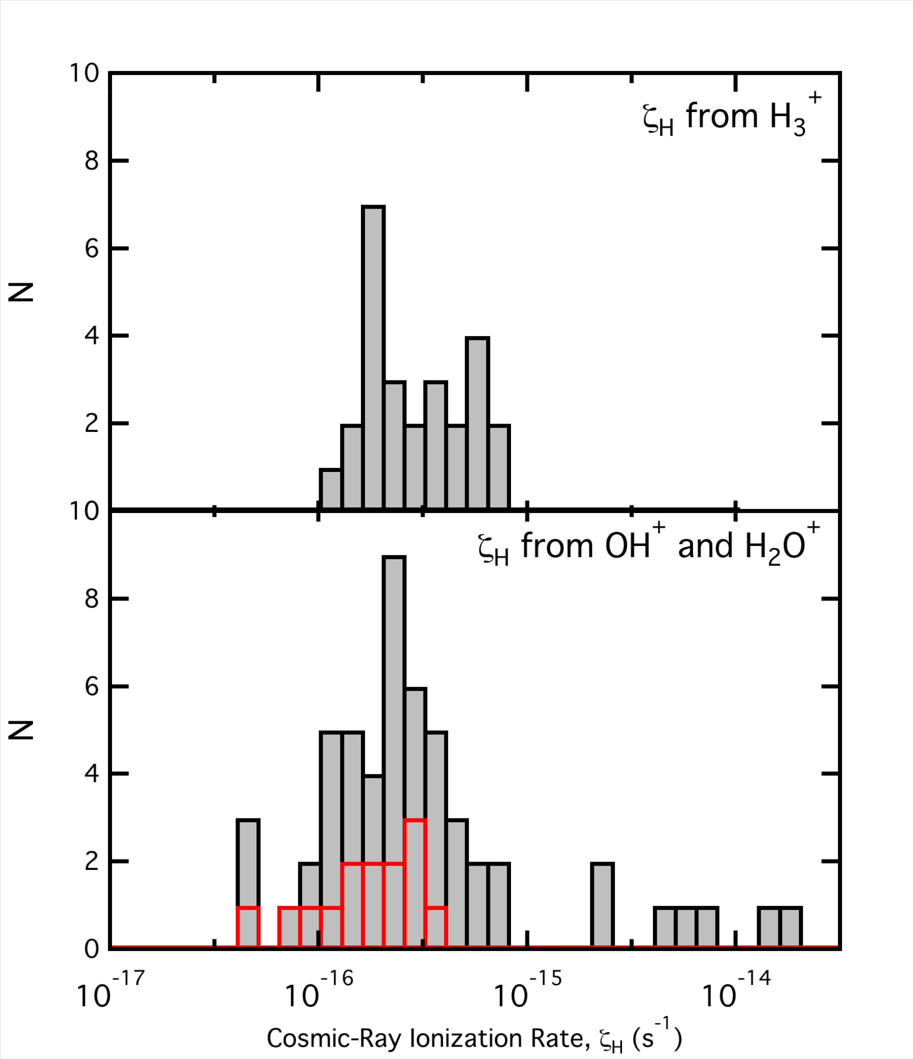
Example OH^+ & H_2O^+ Analysis

G034.3+00.15

v_{LSR} (km/s)	$N(OH^+)$ (10^{13} cm^{-2})	$N(H_2O^+)$ (10^{13} cm^{-2})	N(H) (10^{21} cm^{-2})	$f(H_2)$	ζ_H (10^{-16} s^{-1})
[-12, 7]	2.5	0.26	1.3	0.03	2.1
[7, 18]	3.0	0.67	2.1	0.06	2.8
[18, 36]	2.7	0.31	>3.6	0.03	<0.9
[36, 44]	1.7	0.21	2.4	0.03	0.9
[44, 52]	3.7	0.93	3.6	0.07	2.2
[52, 70]	4.2	1.2	>5.2	0.08	<2.0

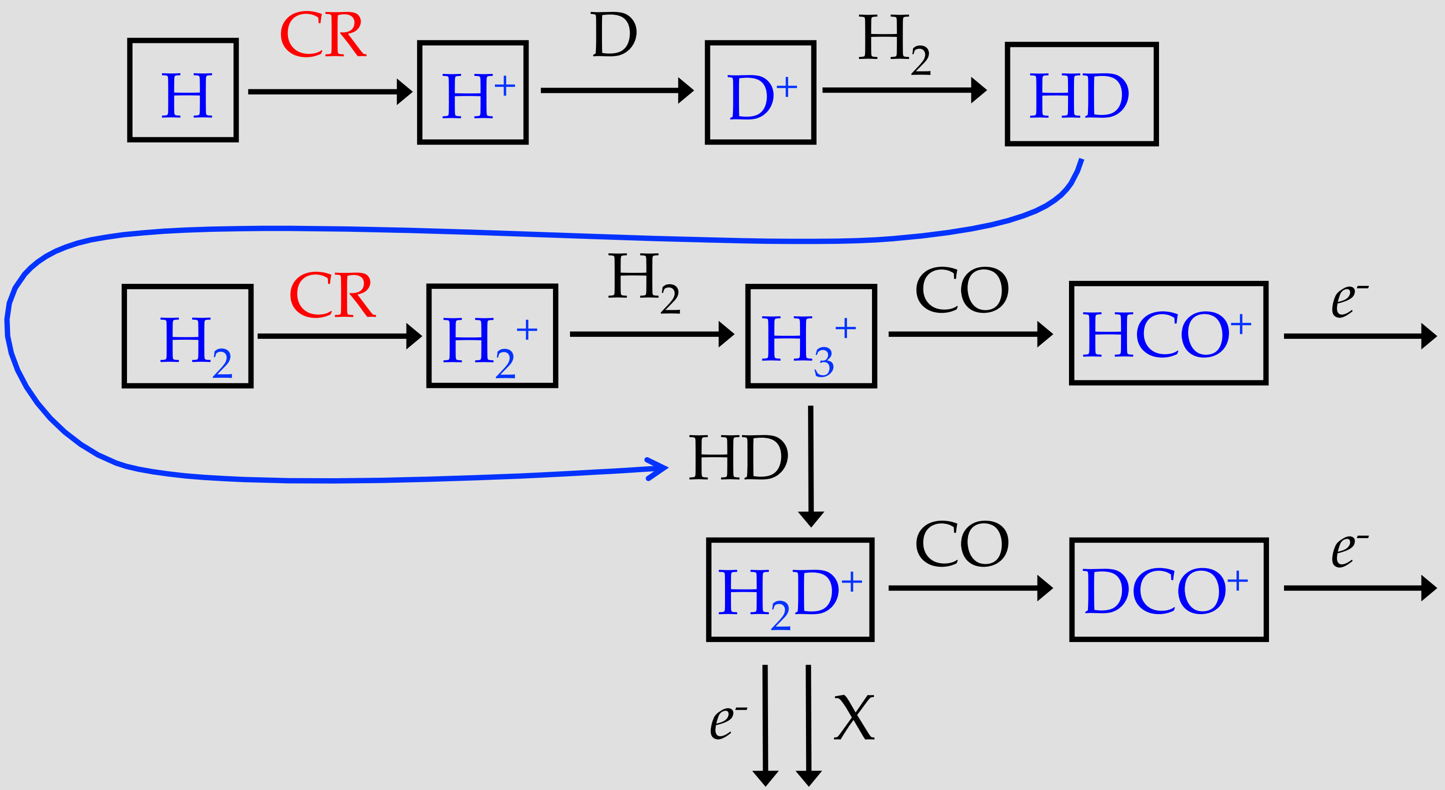
Indriolo et al. 2014 (in preparation)

Distribution of ζ_H



- Gas associated with background sources is shown in red
- $\zeta_H > 10^{-15}$ s^{-1} is from gas in Galactic center region
- Mean ionization rate of atomic H is about 2×10^{-16} s^{-1}
- Good agreement between analysis using OH^+ & H_2O^+ and that using H_3^+

Deuterium Chemistry



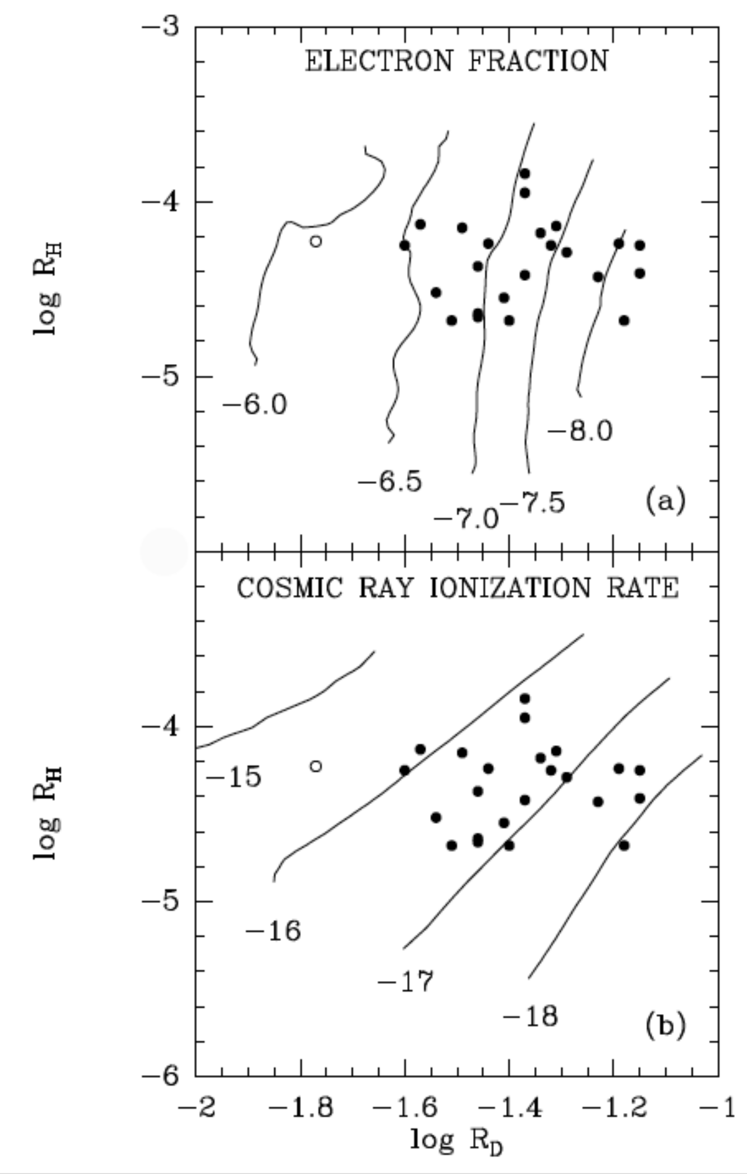
- Limits of analytical expressions become apparent as chemical complexity increases

Chemical Models

- Chemical diversity in dense molecular clouds requires the use of complex reaction networks
  - UDfA: 6173 reactions; 467 species
  - OSU: 6046 reactions; 468 species
- Specific applications call for inclusion of more effects/parameters
  - Grain/surface chemistry; time dependence; radiative transfer; density/temperature profile; shocks/turbulence

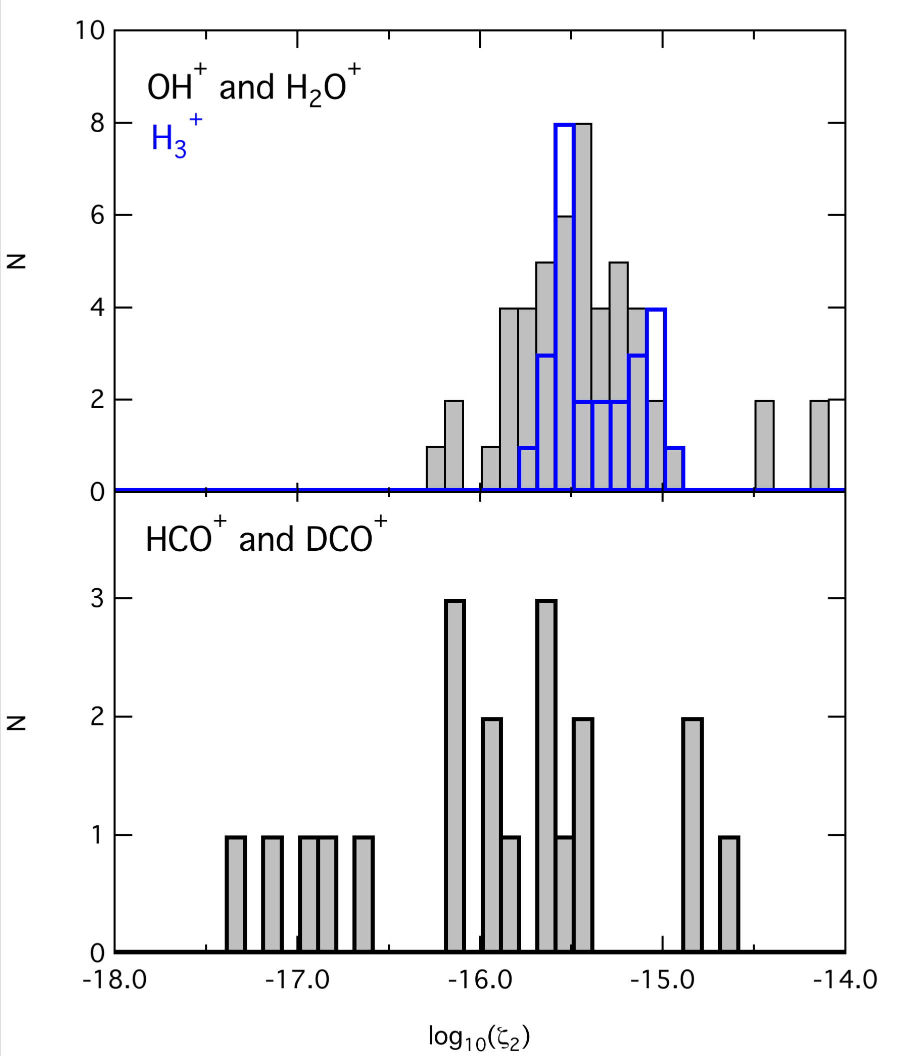
Deuterium Analysis

- Species observed in dense cores
  - DCO^+ J=1-0 at 72.04 GHz
  - $H^{13}CO^+$ J=1-0 at 86.75 GHz
  - $C^{18}O$ J=1-0 at 109.78 GHz
- Caselli et al. 1998 ApJ, 499, 234
  - $R_H = n(HCO^+)/n(CO)$
  - $R_D = n(DCO^+)/n(HCO^+)$
- Observed ratios are used in tandem with model results to constrain electron abundance and cosmic-ray ionization rate
- Similar analysis used in gas near W51C; Ceccarelli et al. 2011 ApJL, 740, L4

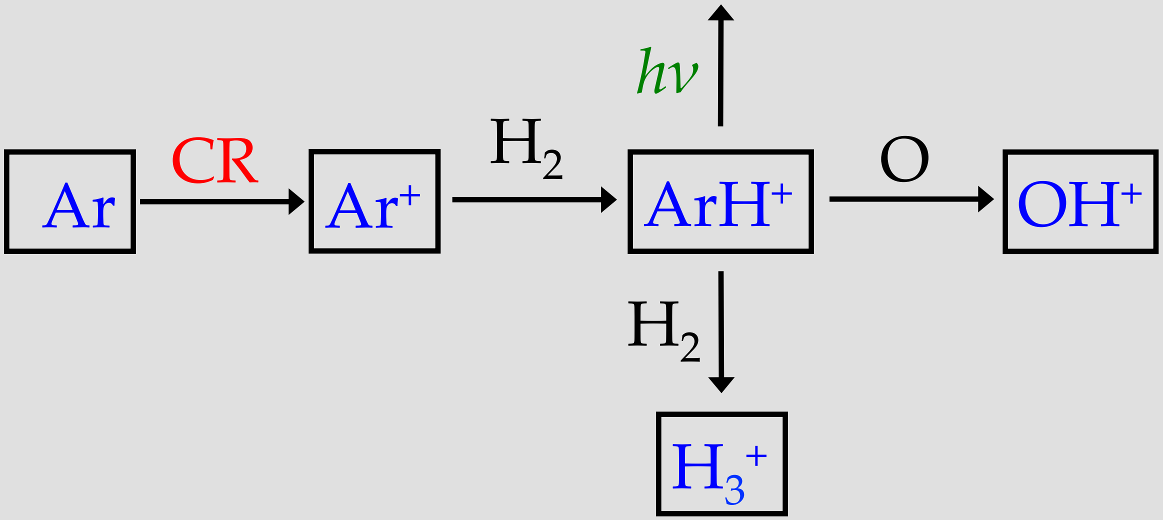


Dense Cloud Ionization Rates

- Wide spread of dense cloud ionization rates
- Tend to be lower than found in diffuse molecular and atomic clouds
- Low-energy particles are lost in outer layers of cloud, and do not penetrate the dense interiors



Argon Chemistry

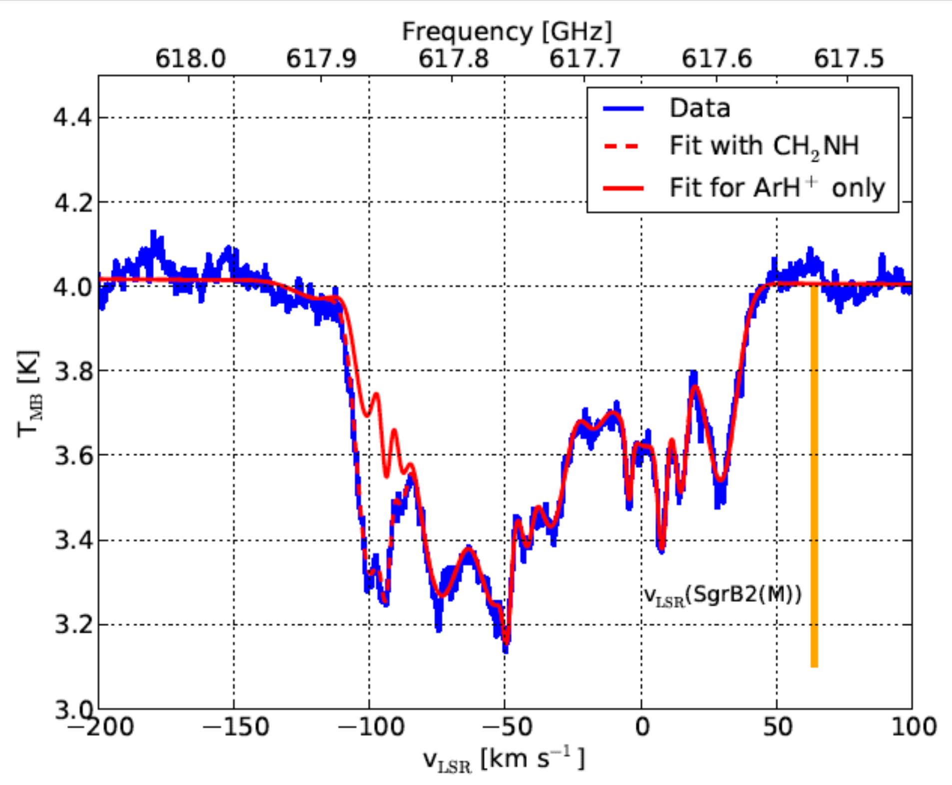


- Formation
  - $CR + Ar \rightarrow Ar^+ + e^- + CR'$
  - $Ar^+ + H_2 \rightarrow ArH^+ + H$
- Destruction
  - $ArH^+ + h\nu \rightarrow Ar^+ + H$
  - $ArH^+ + O \rightarrow OH^+ + Ar$
  - $ArH^+ + H_2 \rightarrow H_3^+ + Ar$

Argonium (ArH^+) Observations

- *J*=1-0 transition of $^{36}ArH^+$ at 617.525 GHz
- Identified in emission in Crab SNR (Barlow et al. 2013, Science, 342, 1343)
- Matched unidentified absorption line found in Galactic sight lines
- Better tracer of "pure" atomic gas than H I
- Formation relies on CR ionization of Ar

Sgr B2(M)

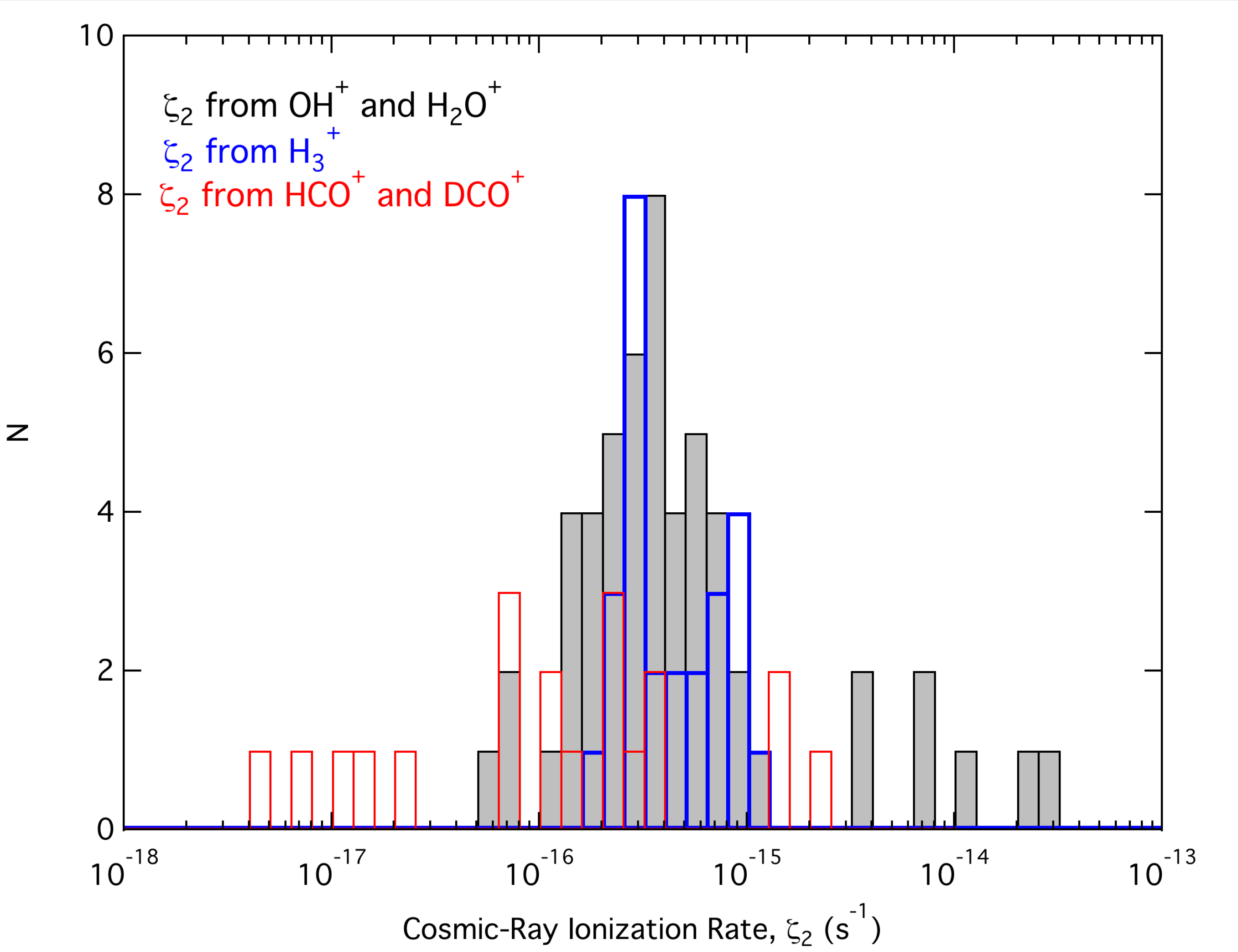


Schilke et al. 2014 A&A, 566, A29

Utility of Various Molecules

- In diffuse purely atomic ($f(H_2)<10^{-4}$) gas, ArH^+ may act as a tracer of the rate at which Ar is ionized by cosmic rays.
- In diffuse mostly atomic ($f(H_2)<0.1$) gas, OH^+ and H_2O^+ constrain the ionization rate of atomic H
- In diffuse molecular clouds, H_3^+ traces the cosmic-ray ionization rate of H_2
- In dense molecular clouds, HCO^+ and DCO^+ abundances constrain the ionization rate of H_2

Summary of Ionization Rates



Regional Ionization Rates

- How does the cosmic-ray ionization rate change throughout the Galaxy?
- Multiple concentrated regions have been targeted in H_3^+ including
  - Sco-Oph: *d*~100 pc
  - Per OB2: *d*~250 pc
  - IC 443: *d*~1.5 kpc
  - Galactic center: *d*~8.3 kpc

Fermi-LAT Year 5 All Sky Map

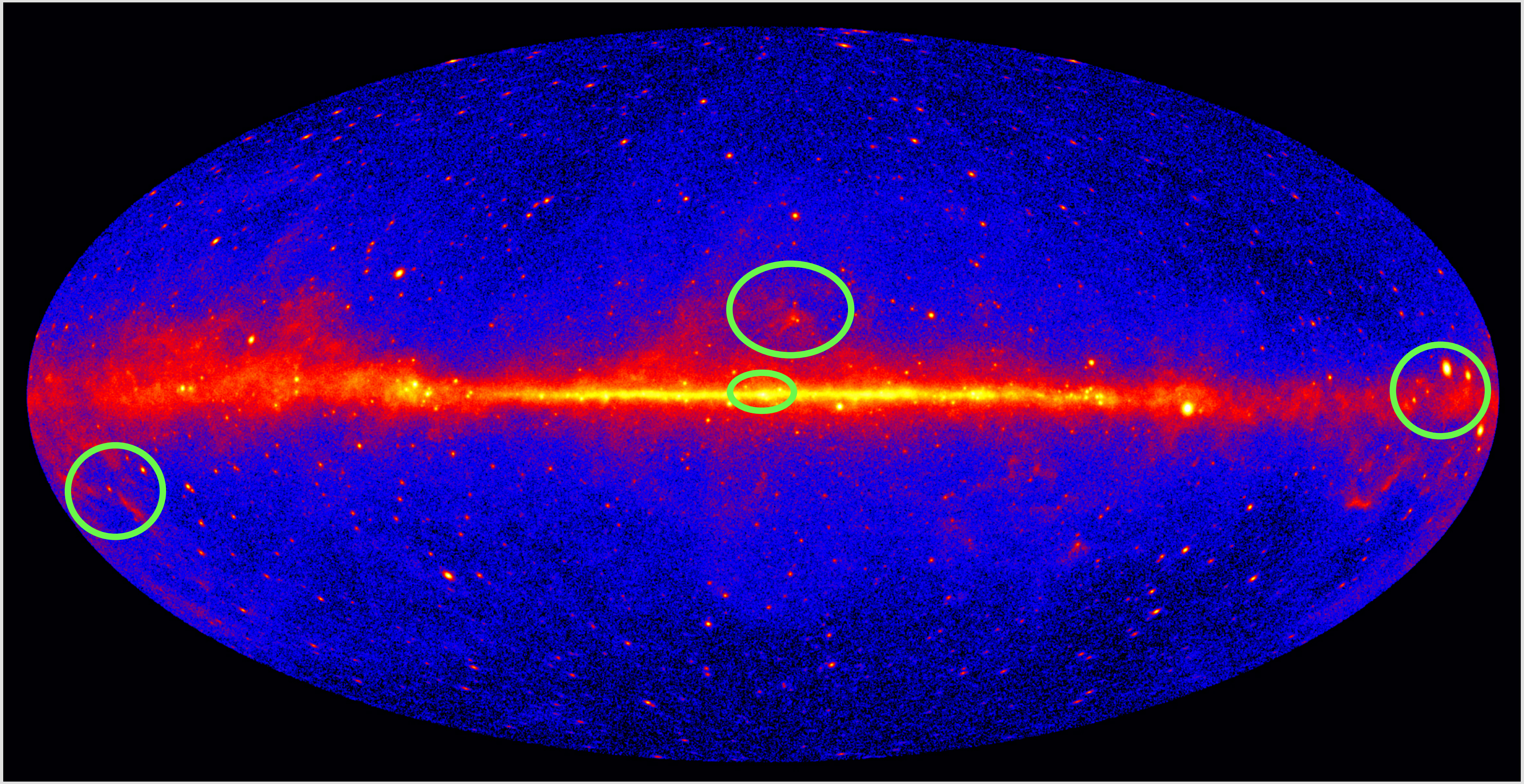
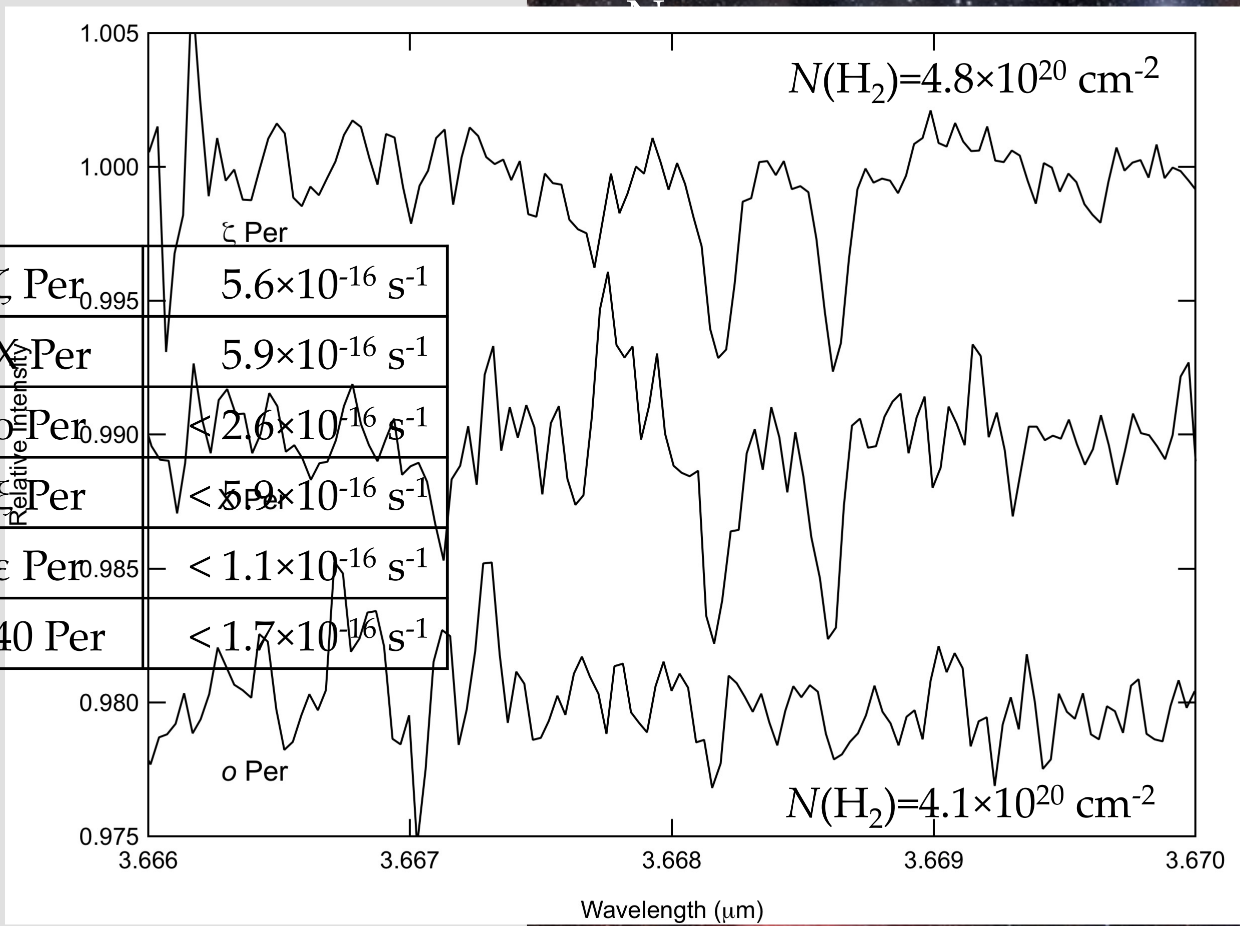


Image Credit: NASA, DOE, Fermi-LAT Collaboration

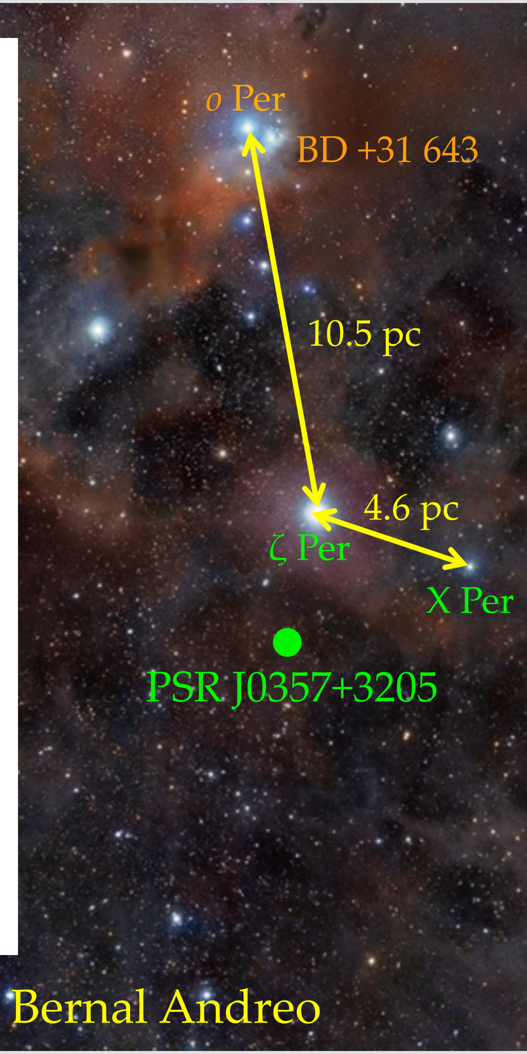
Sco-Oph Region

- No detection of H_3^+ in currently observed sight lines
- Continuum level S/N approaching 1000 in multiple spectra
- 3σ upper limits: 0.3×10^{-16} $s^{-1} < \zeta_2 < 2\times10^{-16}$ s^{-1}
- Consistent with ionization rates inferred from local interstellar proton spectrum

Per OB2 Region



ζ Per	5.6×10^{-16} s^{-1}
X Per	5.9×10^{-16} s^{-1}
o Per	$< 2.6\times10^{-16}$ s^{-1}
ξ Per	$< 5.9\times10^{-16}$ s^{-1}
ε Per	$< 1.1\times10^{-16}$ s^{-1}
40 Per	$< 1.7\times10^{-16}$ s^{-1}

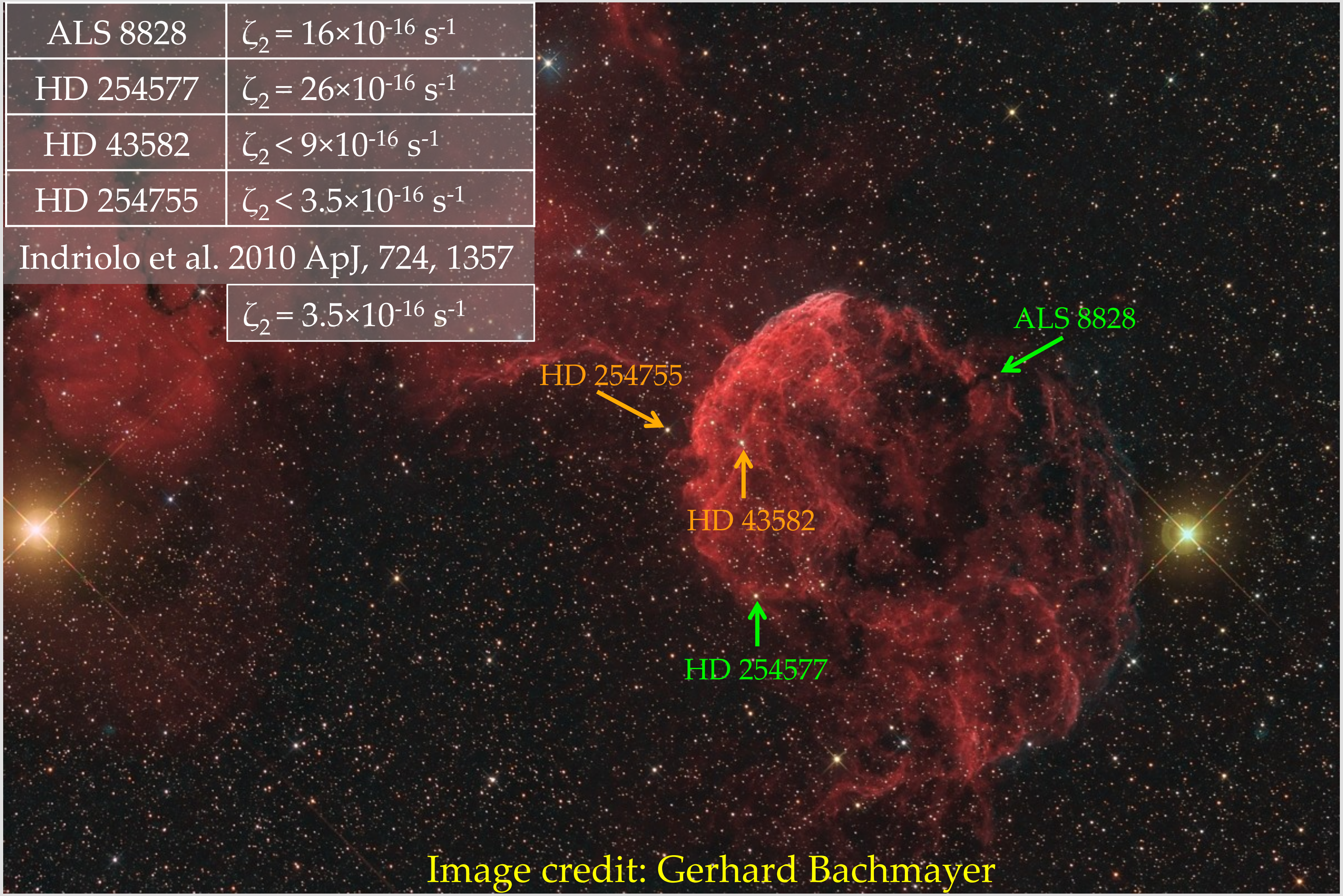


IC 443 Survey

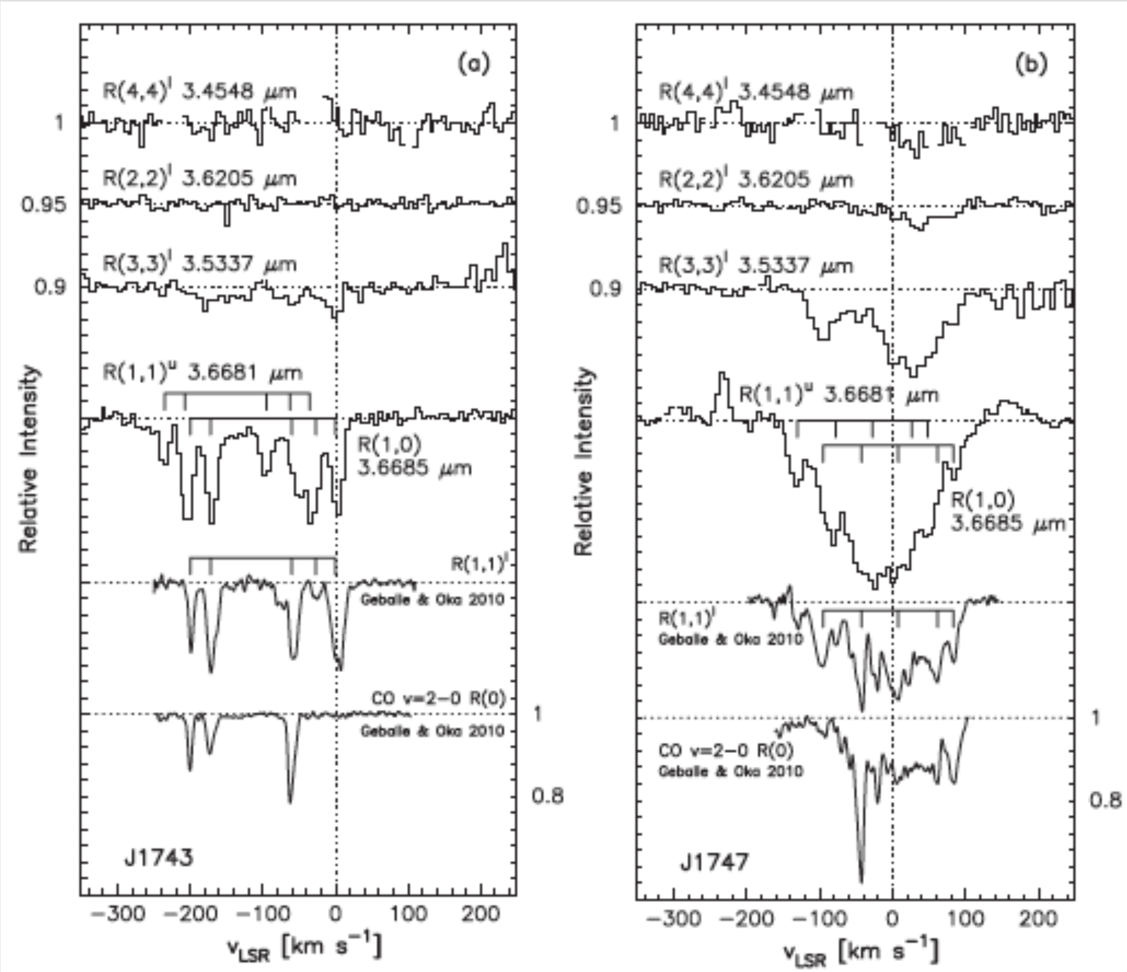
ALS 8828	$\zeta_2 = 16\times10^{-16}\ s^{-1}$
HD 254577	$\zeta_2 = 26\times10^{-16}\ s^{-1}$
HD 43582	$\zeta_2 < 9\times10^{-16}\ s^{-1}$
HD 254755	$\zeta_2 < 3.5\times10^{-16}\ s^{-1}$

Indriolo et al. 2010 ApJ, 724, 1357

	$\zeta_2 = 3.5\times10^{-16}\ s^{-1}$



Galactic Center

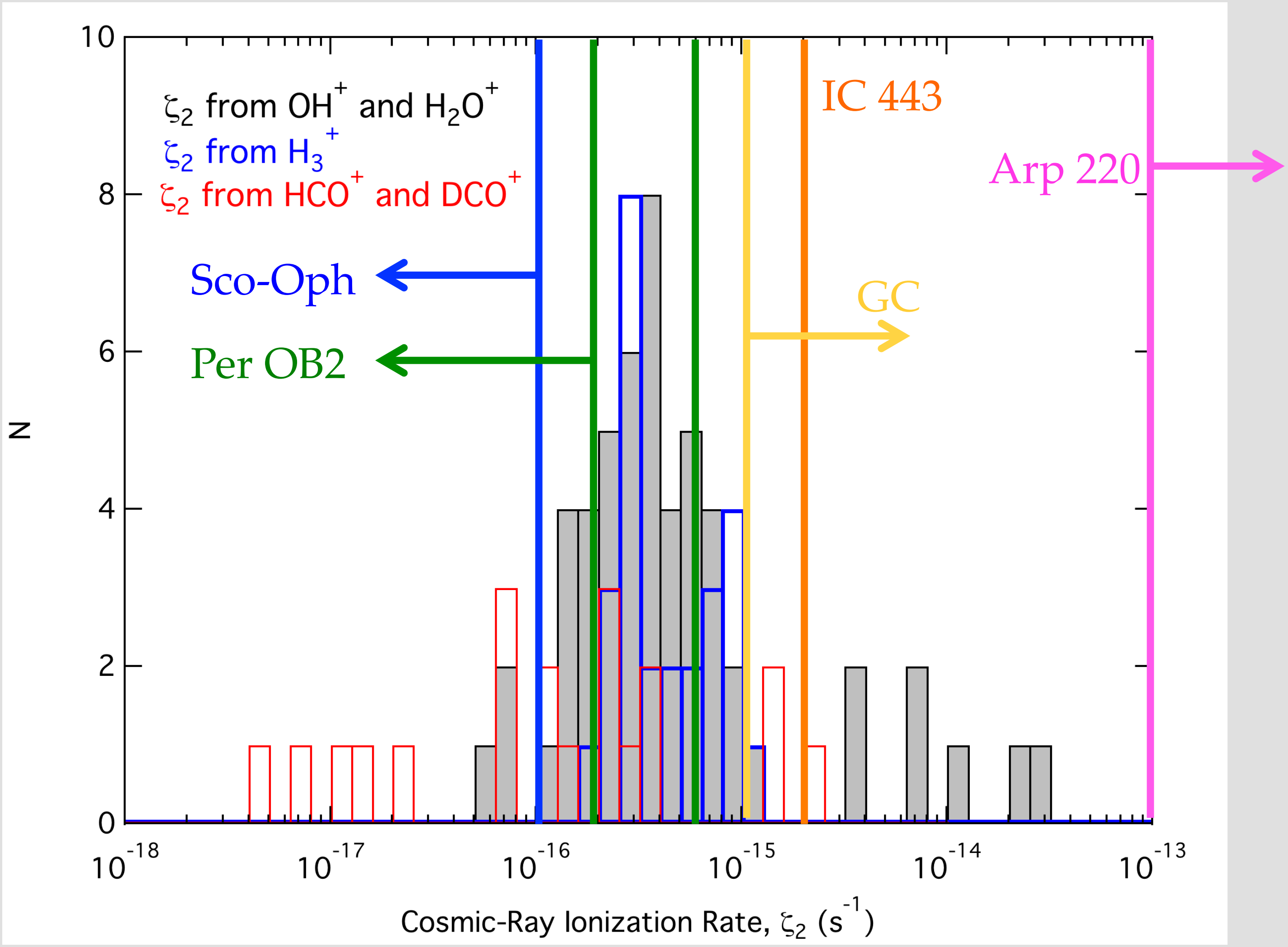


Goto et al. 2011 PASJ, 63, 13

$\zeta_2 > 10^{-15}$ s^{-1}

Consistent with high ionization rates inferred from OH^+ and H_2O^+ abundances

Summary of Ionization Rates



Key Points

- Observations of molecular ions yield a mean cosmic-ray ionization rate of a few times 10^{-16} s^{-1} in diffuse clouds
- The distribution of ionization rates ranges from about 10^{-17} s^{-1} to 10^{-15} s^{-1}
- Cosmic-ray flux appears to vary on length scales of about 10 pc
- SNRs show enhanced ionization rates
- Different molecules will allow us to track the cosmic-ray flux across many environments

Future Prospects

- Expand survey of HCO^+ and DCO^+ in dense cores to improve sample
- Mine *Herschel* archive for ArH^+ coverage to study diffuse, neutral, atomic gas
- Target molecular ions in more supernova remnants (e.g., RX J1713.7)
- Combine with gamma-ray analysis to constrain particle spectrum