# Water in the diffuse interstellar medium

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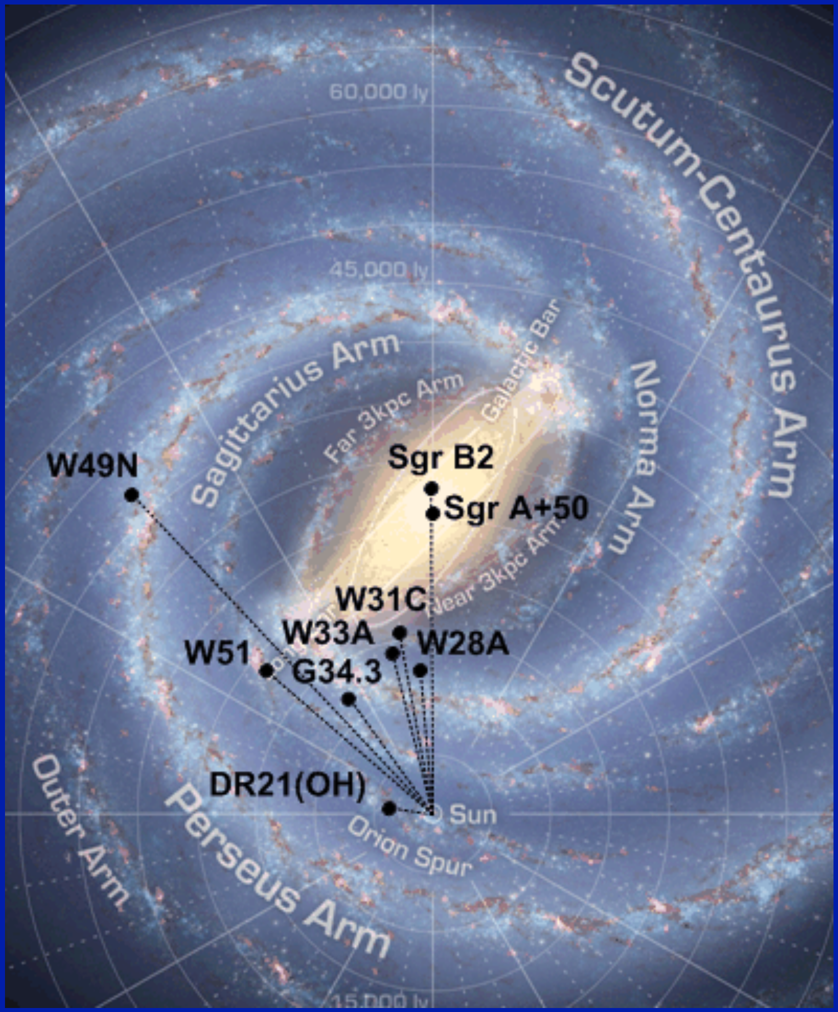
# Absorption line observations of diffuse clouds

Absorption line observations of stars – at visible wavelengths – led to the first detections of interstellar molecules in the 1940's:

$CH$, $CH^+$, and $CN$ detected in diffuse molecular clouds (with $A_V$ less than ~ 1 – 2 along the sight-line)

# Absorption line observations of diffuse clouds

- Extensive observations of molecules in diffuse clouds have now been performed at millimeter and submillimeter wavelengths
- We can use a very luminous region of massive star formation as a distant background source
- This allows us to search for absorption by gas in foreground material
- A very "clean" experiment that provides robust measurements of molecular column densities

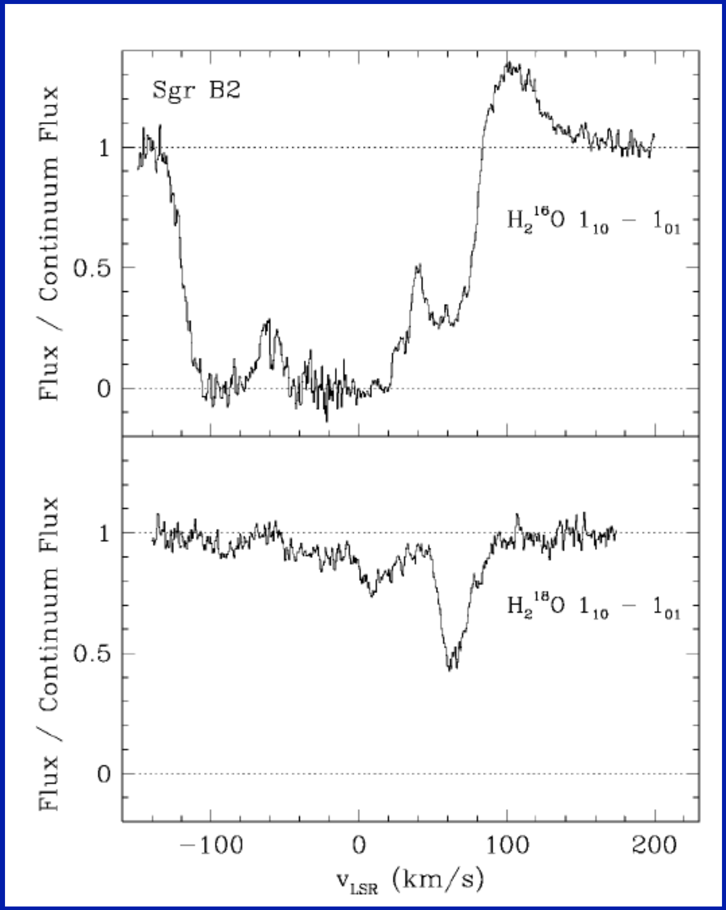


# Absorption line observations of diffuse clouds

Water detected by SWAS in foreground diffuse clouds along several sight-lines:

Sgr B2, W49, W51

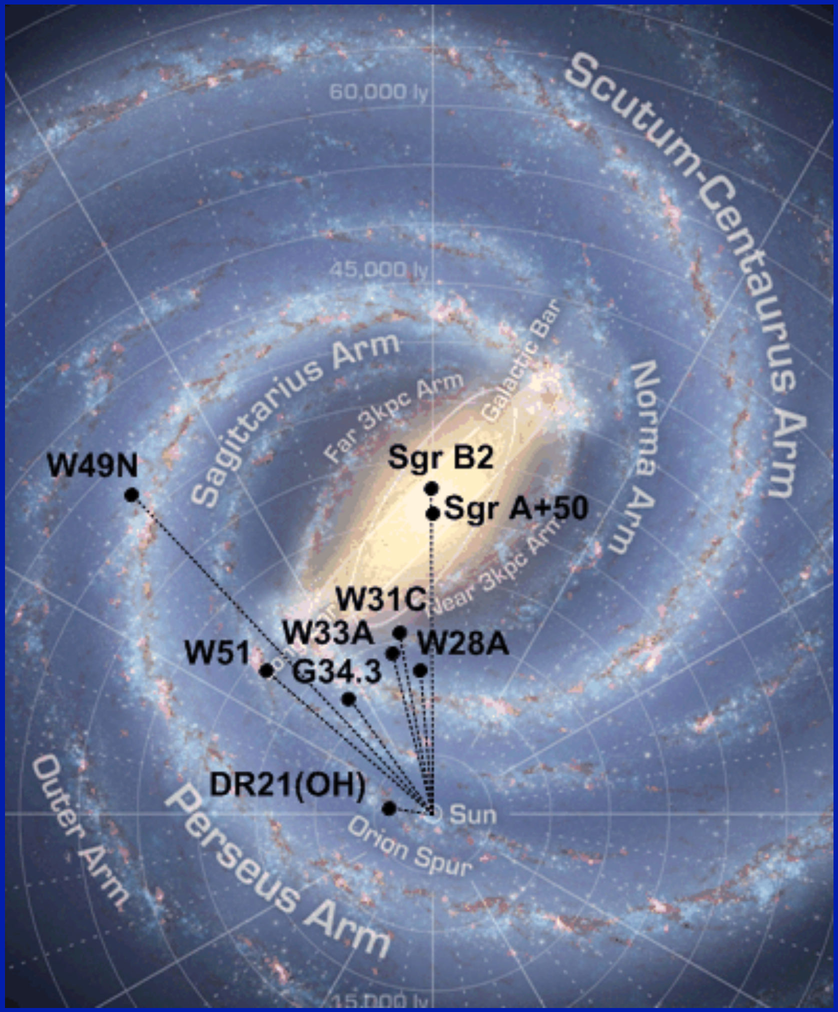
Neufeld et al. (2000, 2002); Plume et al. (2004)




Neufeld et al. 2000, ApJ

# Absorption line observations of diffuse clouds

- Past five years: diffuse cloud observations greatly expanded by Herschel/HIFI and SOFIA/GREAT
- Main focus of the PRISMAS key program (P.I. Maryvonne Gerin)
- Additional data from HEXOS and WISH programs, plus several Open Time programs
- Many small hydride molecules observed in diffuse clouds, several for the first time



# Interstellar hydrides observed in diffuse clouds at submillimeter wavelengths

| IA | IIA | IIIA | IVA | VA | VIA | VIIA | VIIIA |
|---|---|---|---|---|---|---|---|
| | | | CH<br>$CH^+$<br>$CH_2$ | NH<br>$NH_2$<br>$NH_3$ | OH<br>$H_2O$<br>$OH^+$<br>$H_2O^+$<br>$H_3O^+$ | HF | |
| | | | | | SH<br>$SH^+$<br>$H_2S$ | HCl<br>$HCl^+$<br>$H_2Cl^+$ | $ArH^+$ |

Blue entries: first detected in diffuse clouds after 2010, all with Herschel/HIFI except SH (SOFIA/GREAT) and $OH^+$ (APEX)

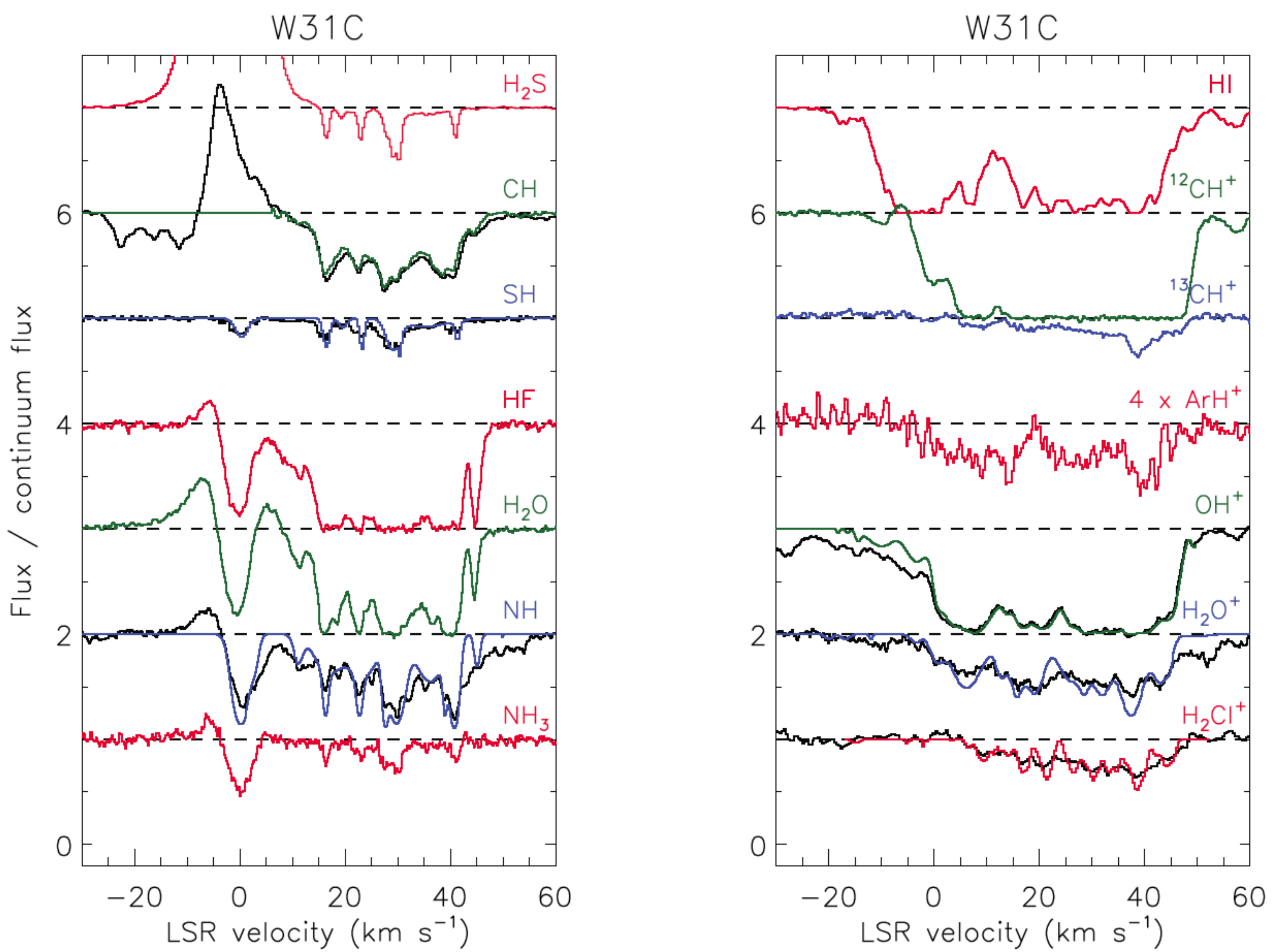
For references, see Gerin, Neufeld & Goicoechea (2016, ARAA: GNG16)

# Outline

- The distribution of water relative to other molecules found in diffuse clouds
- The abundance of water in diffuse clouds
- The abundance of other O-bearing hydrides
- The origin of water in diffuse clouds

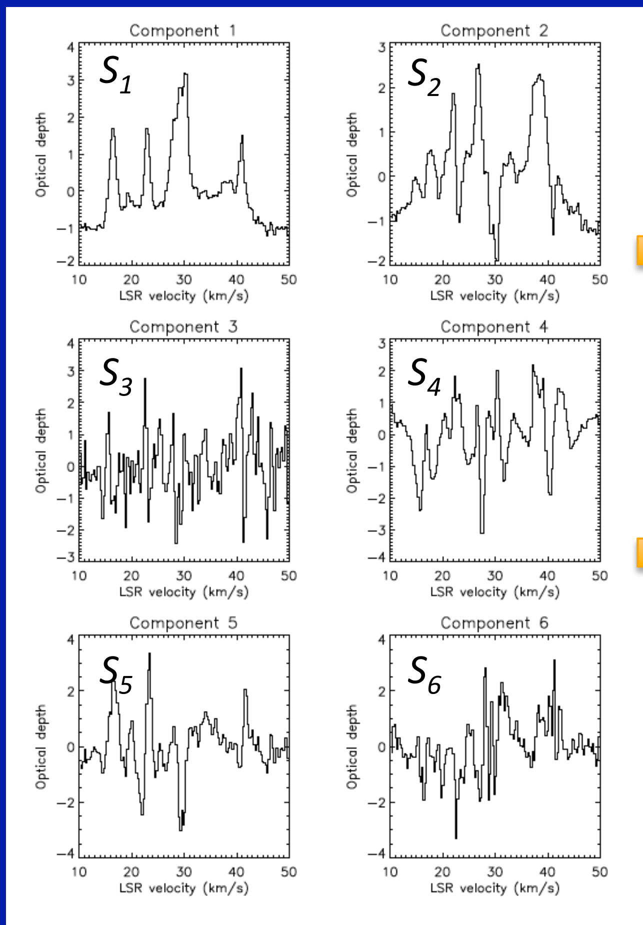
# Absorption line spectra toward W31C

Compiled by GNG16 – see references therein



# Principal component analysis

The optical depth spectra, shown by the black histograms on the right, are written as a linear combination of the six principal components shown at left. These six components are mutually orthogonal (uncorrelated) and listed in decreasing order of their contribution. The first two components are sufficient to yield a good fit to the data (red histogram on right) .




6 terms in Σ → black

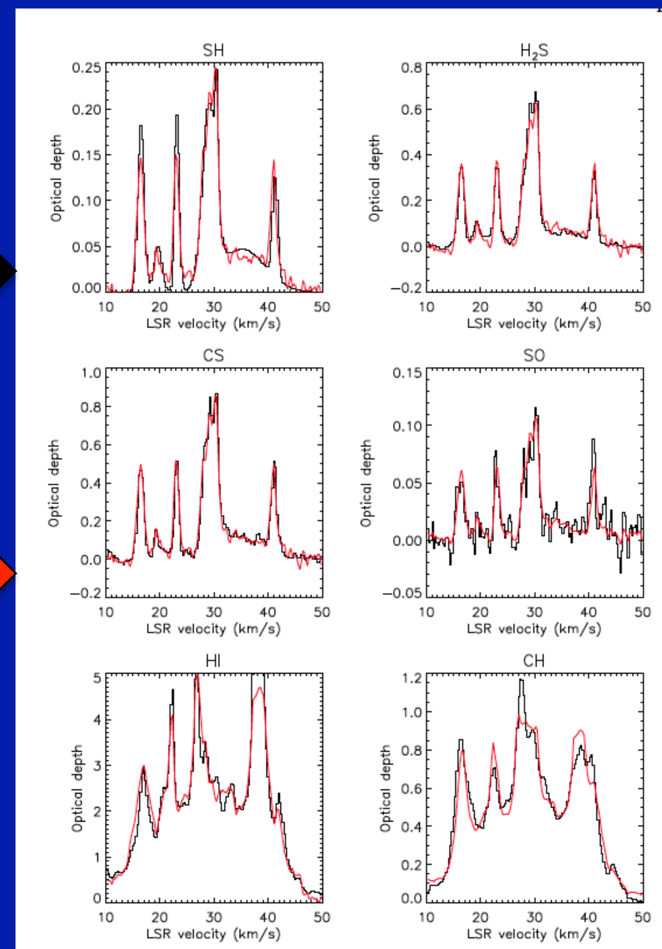
$$\tau_i(v) = a_i + b_i \sum_{j=1}^{6} C_{ij} S_j(v)$$

Gives an exact fit

2 terms in Σ → red

$$\tau_i(v) = a_i + b_i \sum_{j=1}^{2} C_{ij} S_j(v)$$

Good approximation



# Principal component analysis

A plot of the first two coefficients, $C_{i1}$ and $C_{i2}$, for each absorption line shows the similarities and differences graphically.

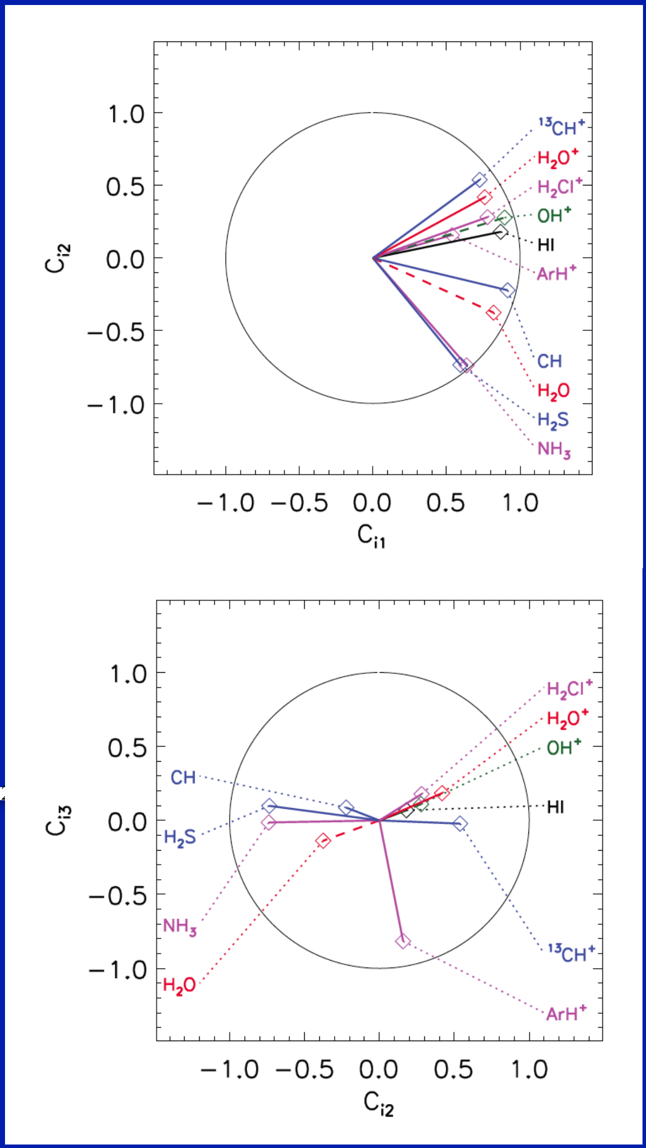
NOTES

(1) Except for $ArH^+$, all points lie close to unit circle in the upper panel , indicating that the first two components account for most of what is observed

➔ the correlation coefficient is roughly the cosine of the angle between any two vectors

(2) Except for $ArH^+$, the hydride molecular ions are very well-correlated with atomic H, but the neutral hydrides are not

GNG16, adapted from Neufeld et al. 2015, A&A

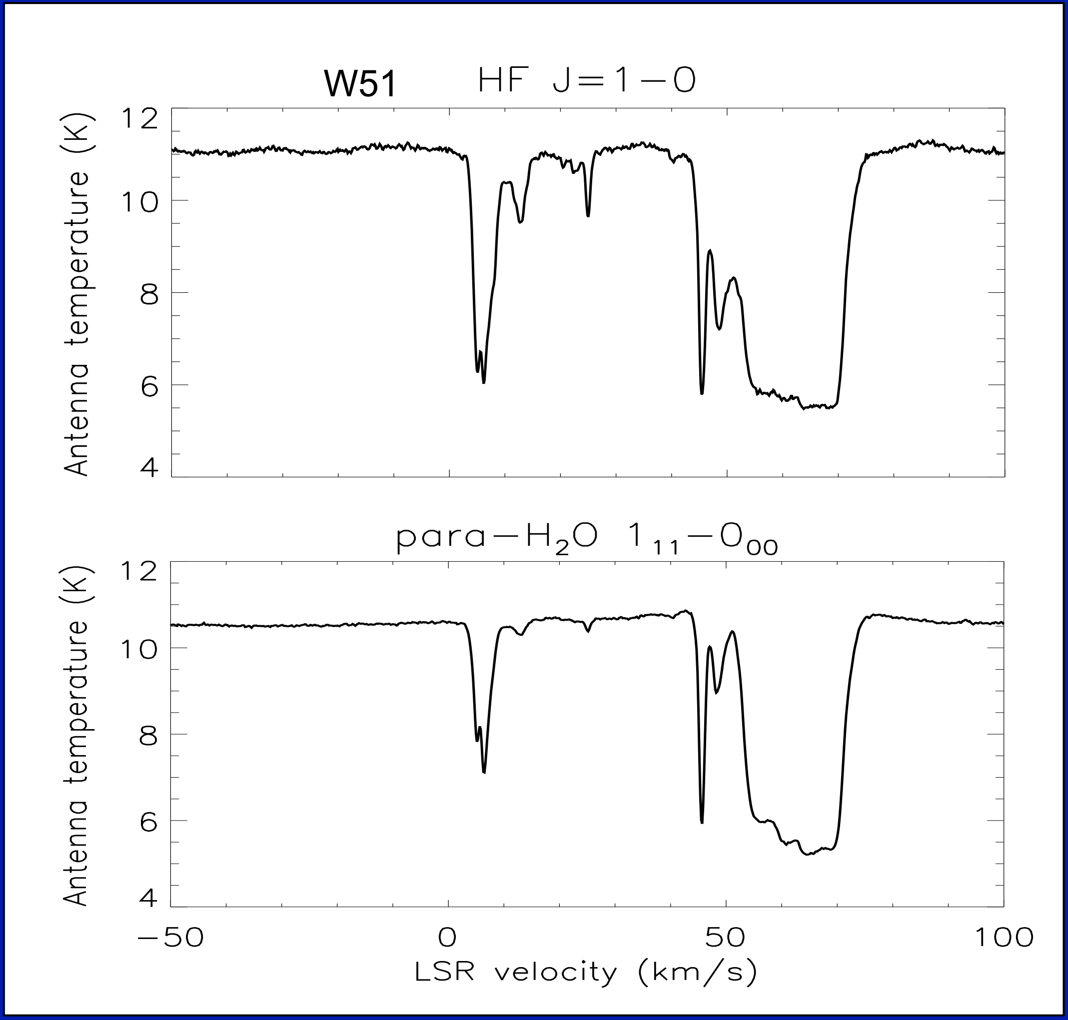


# $H_2O$ and HF are extremely well-correlated

HF is expected to have a very constant abundance relative to $H_2$, because HF can be formed directly by the exothermic reaction

$F + H_2 \rightarrow HF + H$

Suggests that the $H_2O/H_2$ ratio is also fairly constant




Adapted from Sonnentrucker et al. 2015

# The $H_2O$ abundance in diffuse clouds

Two careful analyses of the PRISMAS data on HF and $H_2O$ by Flagey et al. (2013) and Sonnentrucker et al. (2015)

These data provide measurements in ~ 50 diffuse clouds on 12 sight-lines

In determining $N(H_2O)/N(H_2)$, the greatest problem is measuring the *denominator*, because $H_2$ is not directly observable along the same sight-lines as $H_2O$ ➔ Use CH or HF as a surrogate

(1) Optical/UV observations ➔ Typical $CH/H_2 = 3.5 \times 10^{-8}$

(2) Submillimeter observations with *Herschel* ➔ HF/CH = 0.4

(3) Early theoretical expectation ➔ $HF/H_2 = 3.6 \times 10^{-8}$

(accounting for almost all gas-phase F in regions of large $H_2$ fraction)

NB: (3) is inconsistent with (1) and (2) by a factor 2.5

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Flagey et al. (2013) found

(1) Typical $N(H_2O) / N(H_2) = 5 \times 10^{-8}$ , based on measurements of $N(H_2O) / N(CH)$ and the assumptions that $N(HF) / N(CH) = 0.4$ and $N(HF) / N(H_2) = 3.6 \times 10^{-8}$

(2) $H_2O$ ortho-to-para ratios are almost always consistent with 3, the value expected in LTE in the high temperature limit

# The $H_2O$ abundance in diffuse clouds

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Sonnentrucker et al. (2015) found

(1) Direct submillimeter measurements of para-$H_2O$ and HF imply a median $N(H_2O)/N(HF)$ ratio of 1.5, for an assumed OPR of 3. Given the $N(HF)/N(H_2)$ ratio of $3.6 \times 10^{-8}$ adopted by Flagey et al., this would yield the same $N(H_2O) / N(H_2)$ ratio of $5 \times 10^{-8}$

(2) A reanalysis of F chemistry, which takes account of recent laboratory measurements of the reaction rate for HF formation, reduces the predicted $N(HF) / N(H_2)$ ratio by a factor ~ 2

➔ Average $N(H_2O) / N(H_2) = 2.4 \times 10^{-8}$

➔ $N(H_2O)$ / N (gas-phase O nuclei) = $4 \times 10^{-5}$

# The $H_2O$ abundance in diffuse clouds

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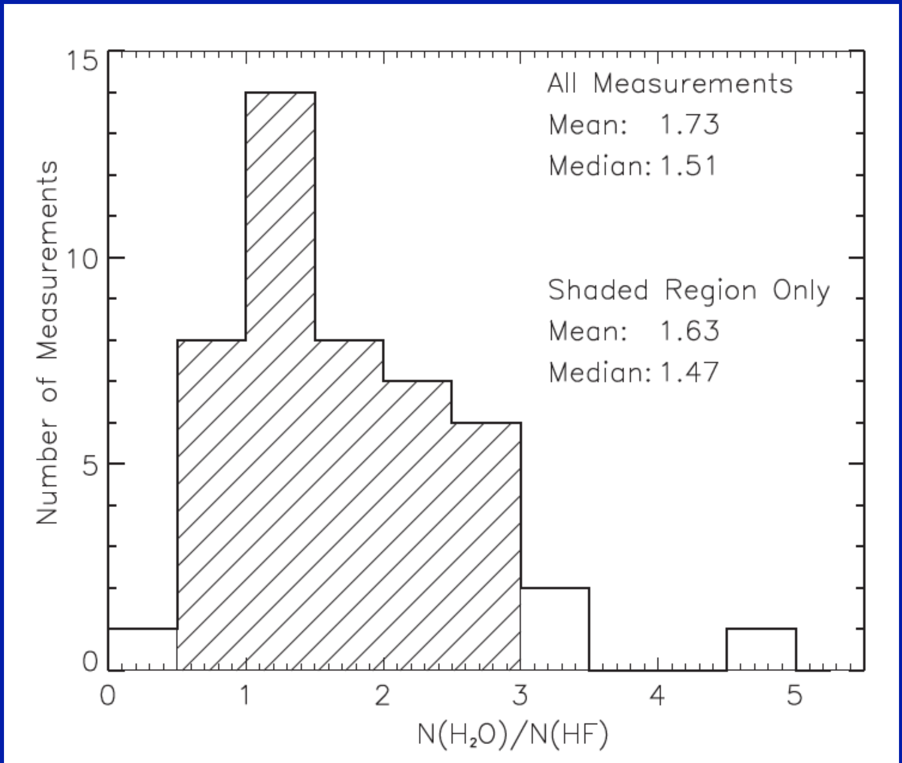
Sonnentrucker et al. (2015) found

(3) The $H_2O$/HF ratio shows real variations: may reflect variations in the CR ionization rate




Sonnentrucker et al. 2015, ApJ

# Five other O-bearing hydrides have been detected in diffuse clouds

| Molecule | Average abundance relative to H or $H_2$ | Average abundance (fraction of gas phase elemental[a]) | Method | Reference for hydride column densities |
|---|---|---|---|---|
| OH | $1 \times 10^{-7}$ | $1.6 \times 10^{-4}$ | UV, submm, cm | Wiesemeyer et al. (2015); Lucas & Liszt (1996) |
| $H_2O$ | $2.4 \times 10^{-8}$ | $4 \times 10^{-5}$ | submm | Flagey et al. (2013) |
| $OH^+$ | $1.2 \times 10^{-8}$ | $4 \times 10^{-5}$ | UV, submm | Indriolo et al. (2015) |
| $H_2O^+$ | $2 \times 10^{-9}$ | $6.5 \times 10^{-6}$ | submm | Indriolo et al. (2015) |
| $H_3O^+$ | $2.5 \times 10^{-9}$ | $4 \times 10^{-6}$ | submm | Lis et al. (2014) |

All are trace constituents, accounting together for ~ 0.025% of gas-phase oxygen nuclei. Most of the oxygen is in OI and CO.

$OH^+$ and $H_2O^+$ have a distribution similar to that of atomic hydrogen
$H_3O^+$, OH and $H_2O$ have a distribution similar to that of $H_2$

# The origin of water vapor in diffuse clouds

Three formation mechanisms have been considered in the literature

(1) Cosmic-ray driven chemistry

$H$ (cr,e) $H^+$ (O,H) $O^+$ ($H_2$,H) $OH^+$ ($H_2$,H) $H_2O^+$ ($H_2$,H) $H_3O^+$ (e,H) $H_2O$

(2) Grain surface catalysis

H and O atoms adsorbed and react on grain surface to make $H_2O$, which is subsequently desorbed

(3) Warm chemistry (in some fraction of the gas at $T > 400$ K)

O ($H_2$,H) OH ($H_2$,H) $H_2O$

# The origin of water vapor in diffuse clouds

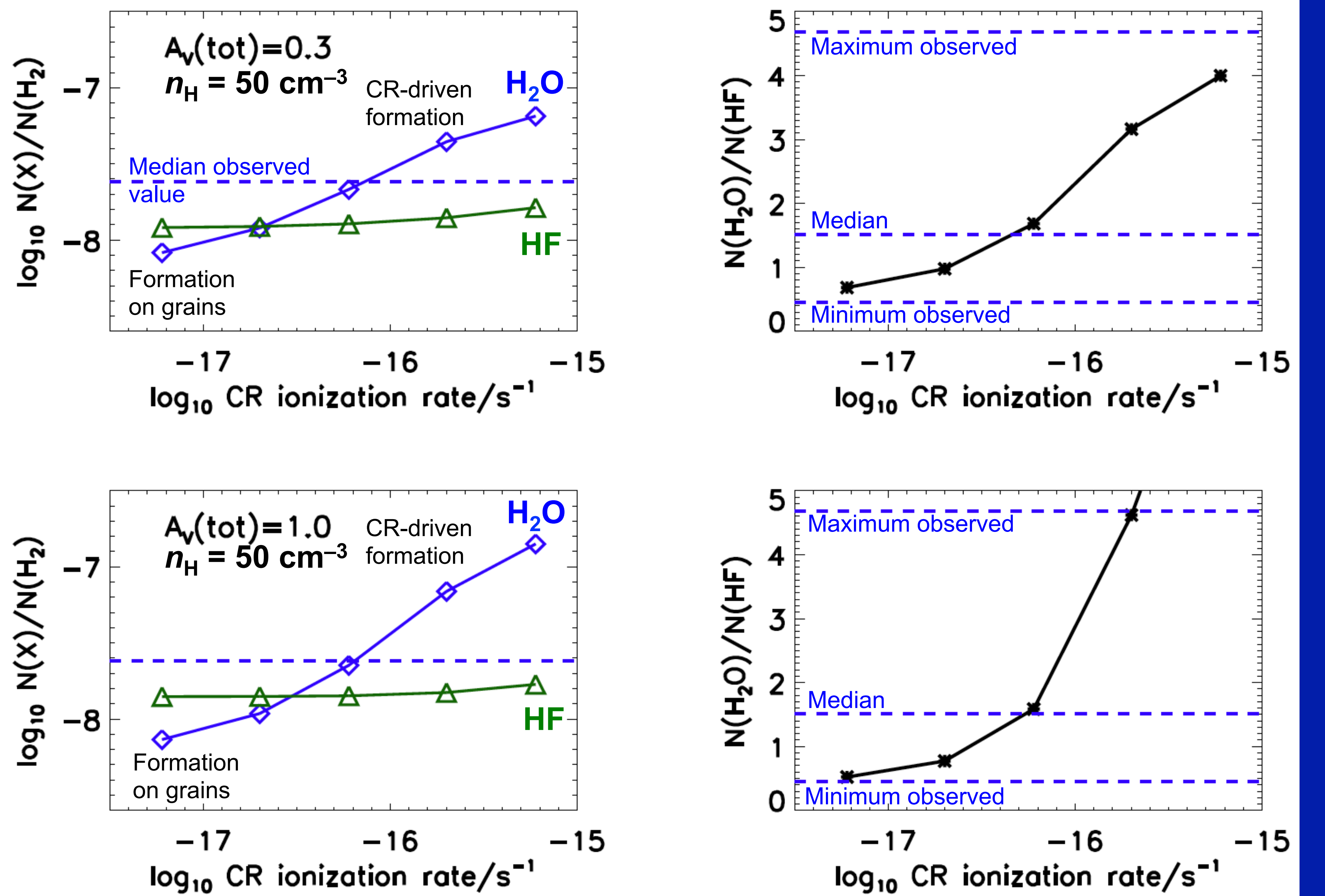
Sonnentrucker et al. (2015, ApJ, and poster P13)

Observed $H_2O$/HF ratios can be explained in models that invoke grain surface and cold gas-phase chemistry alone

In clouds with larger $H_2O$/HF ratios, the CR ionization rate is larger and gas-phase reactions dominate

In clouds with smaller $H_2O$/HF ratios, the CR ionization rate is smaller and grain surface reactions dominate

# Recent calculations with Mark Wolfire



# $H_2O$ as diagnostic probe

- $H_2O$ abundance relative to $H_2$ is only weakly dependent on the physical parameters → a useful "secondary" surrogate for $H_2$ (see Sonnentrucker et al. poster P13)

- $H_2O$ originates primarily in material of large $H_2$ fraction. By contrast, $OH^+$ and $H_2O^+$ (which are destroyed by $H_2$) originate mainly in material of small $H_2$ fraction: consistent with observed correlations revealed by PCA

- High precision measurements of $H_2O$/HF may provide useful information about the cosmic-ray ionization rate

  → values of (CR ionization rate / density) are a factor of several smaller than those inferred from $OH^+$ and $H_2O^+$ (Densities may be higher and/or CR ionization rates lower in material with a larger molecular fraction)

# Summary

- Water vapor is strongly correlated with other hydrides (CH and HF) that trace material of high molecular fraction

- Water vapor is ubiquitous in the diffuse ISM, but is a trace constituent. The median abundance ratio, $N(H_2O)/N(H_2)$, is $2.4 \times 10^{-8}$, corresponding to < 0.003% of gas-phase oxygen

- The observed distribution and abundance of water vapor in the diffuse ISM can be accounted for by models that invoke $H_2O$ production via (1) grain surface chemistry and (2) gas-phase reactions initiated by cosmic-rays