

A far-infrared study of oxygen chemistry in diffuse clouds

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The Hydride Toolbox
Paris, 2016 December 14

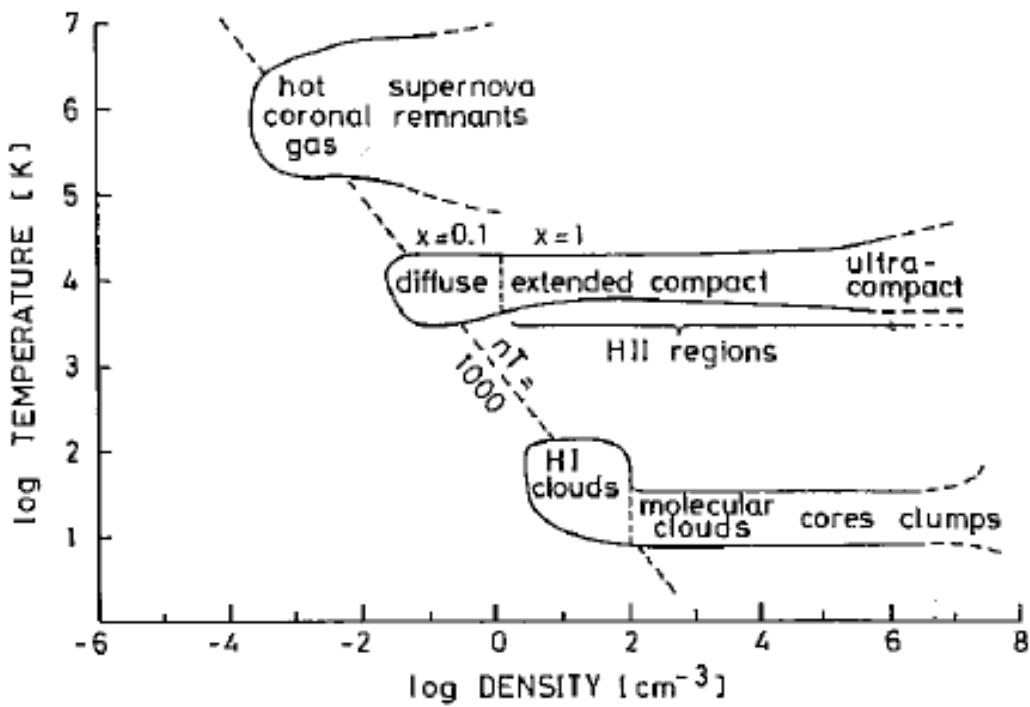
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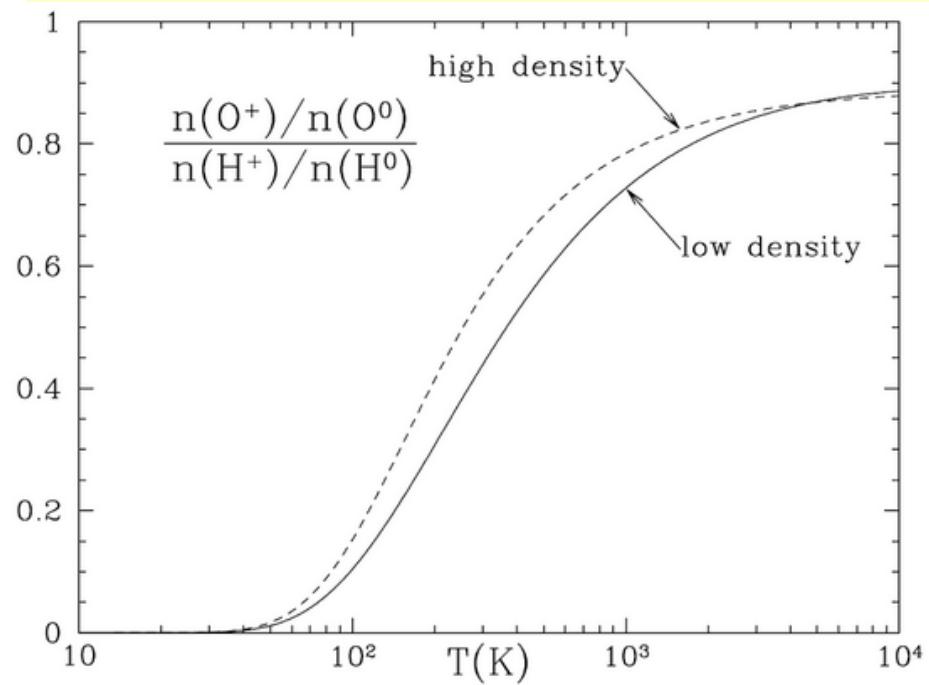
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Oxygen/Hydrogen Charge Transfer

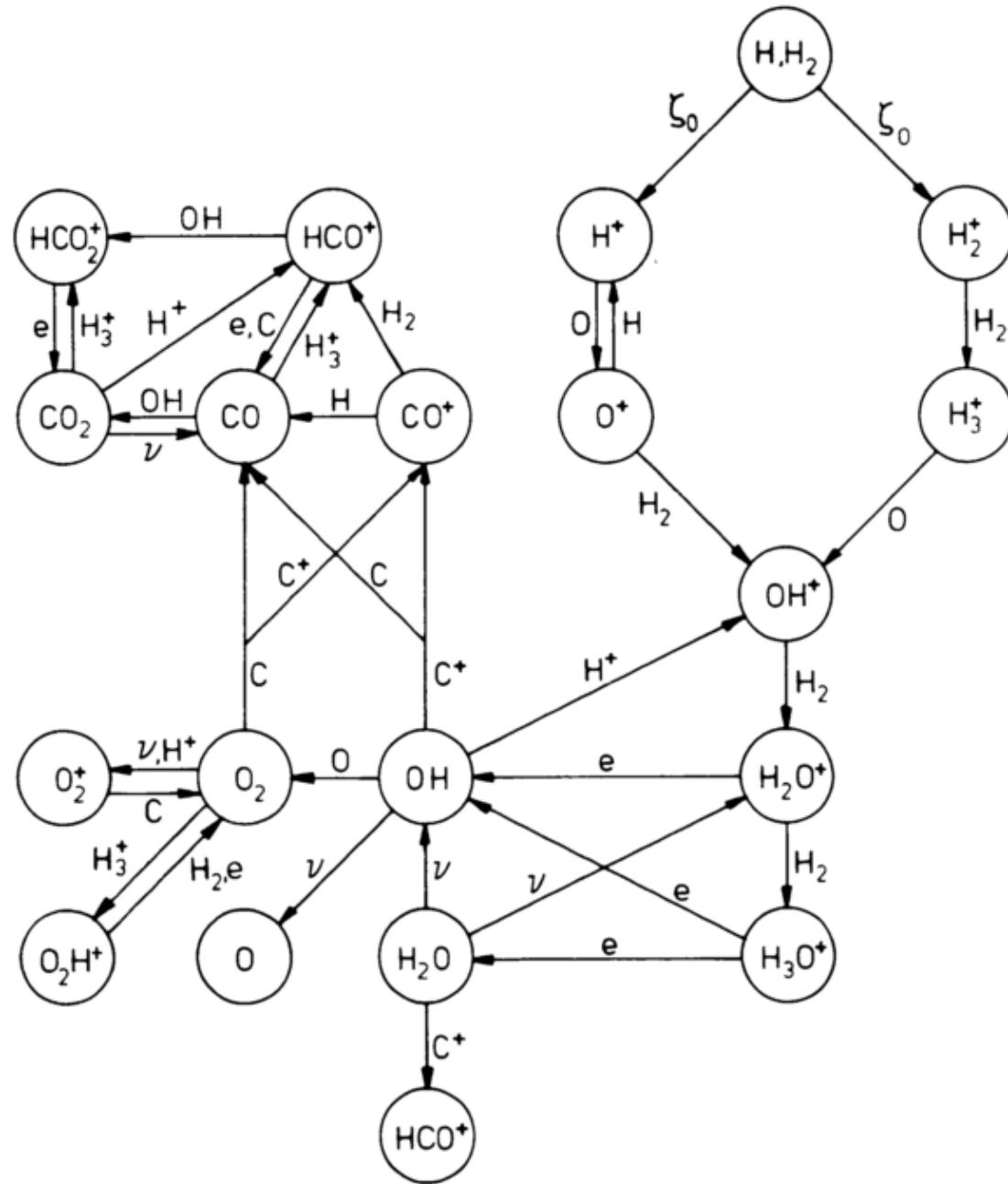


← Yorke, Saas-Fee Lecture 1988



Oxygen ionization fraction (from Draine, Physics of the ISM), →
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Reaction network of oxygen bearing molecules



van Dishoeck
& Black 1986,
ApJ Supp. 62, 109

UV/Optical Spectroscopy

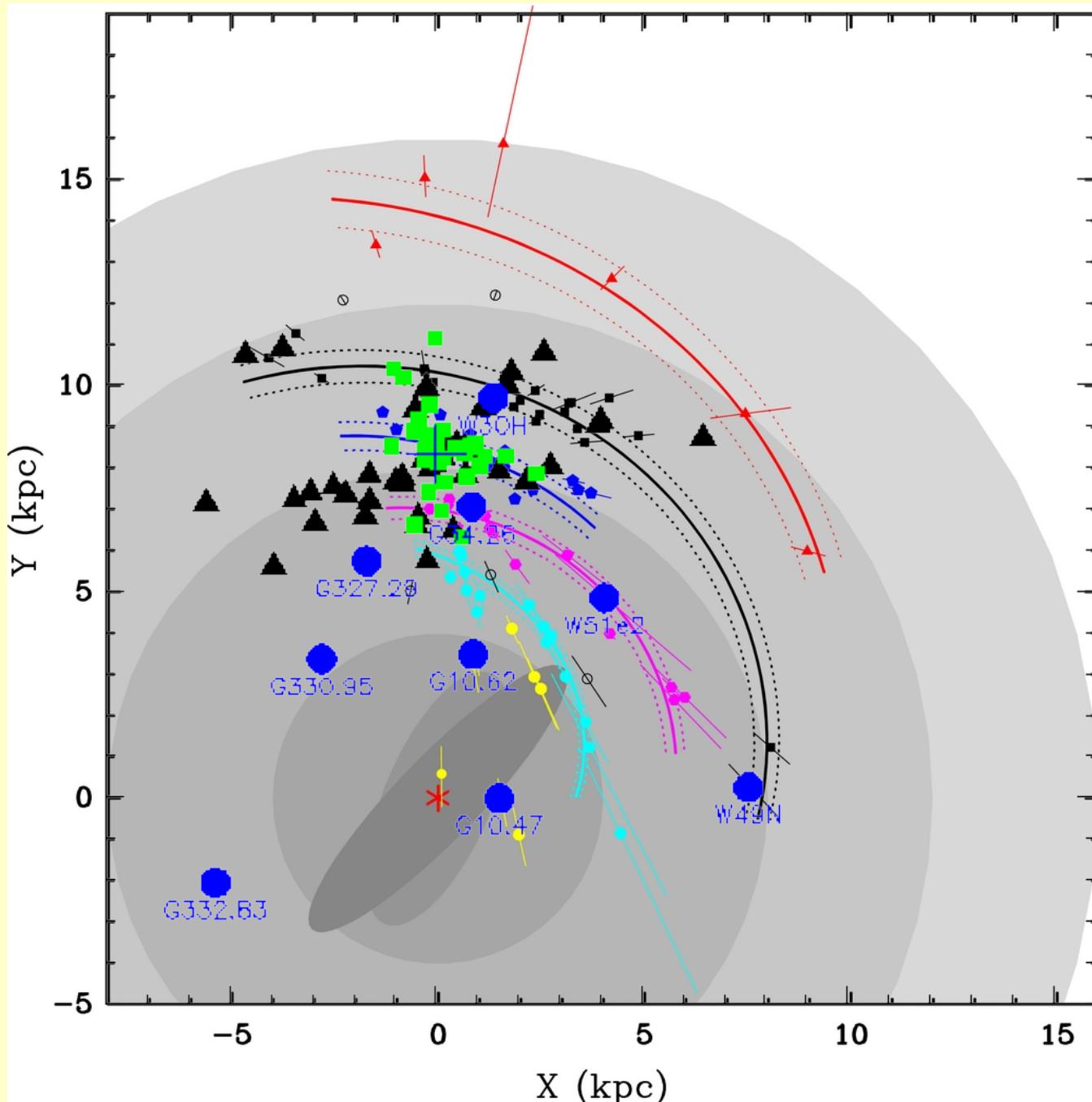
- Restricted to local arm ± a few kpc.
- Spectral resolution:
FUSE: $R \sim 10^4$
HST (STIS): $R \sim 6 \times 10^4$
Optical: $R \sim 1.7 \times 10^5$
- Needs excitation modeling and extinction corrections.

FIR Spectroscopy

- Needs FIR-bright background sources.
- Spectral resolution: $R \sim 10^7$ (upGREAT, LFA)
- Ground state transitions: Column densities from first principles:

$$\tau_{ij,v} = \sqrt{\frac{\ln 2}{\pi}} \frac{A_{E,j} c^3}{4\pi \Delta v_i v_j^3} \frac{g_{u,j}}{g_{l,j}} N w_j \exp\left(-4 \ln 2 \left(\frac{v - v_{0,ij}}{\Delta v_i}\right)^2\right),$$

Absorption spectroscopy through Galactic spiral arms



Galactic cartography:
Reid et al., 2014

- ▲ Sheffer (2008), far-UV/optical (CH)
- Jensen (2005), UV (OI)
- Wiesemeyer (2016), FIR (OI, OH, OH⁺)

outer arm
Perseus arm
local arm
Sagittarius arm
Scutum arm
inner Galaxy

OH^+ (Wyrowski et al. 2010, APEX),
 OH and OI (Wiesemeyer et al. 2016, GREAT),
PRISMAS data: H_2O (Sonnentrucker et al., 2010, 2015),
 H_2O^+ (Indriolo et al., 2015)

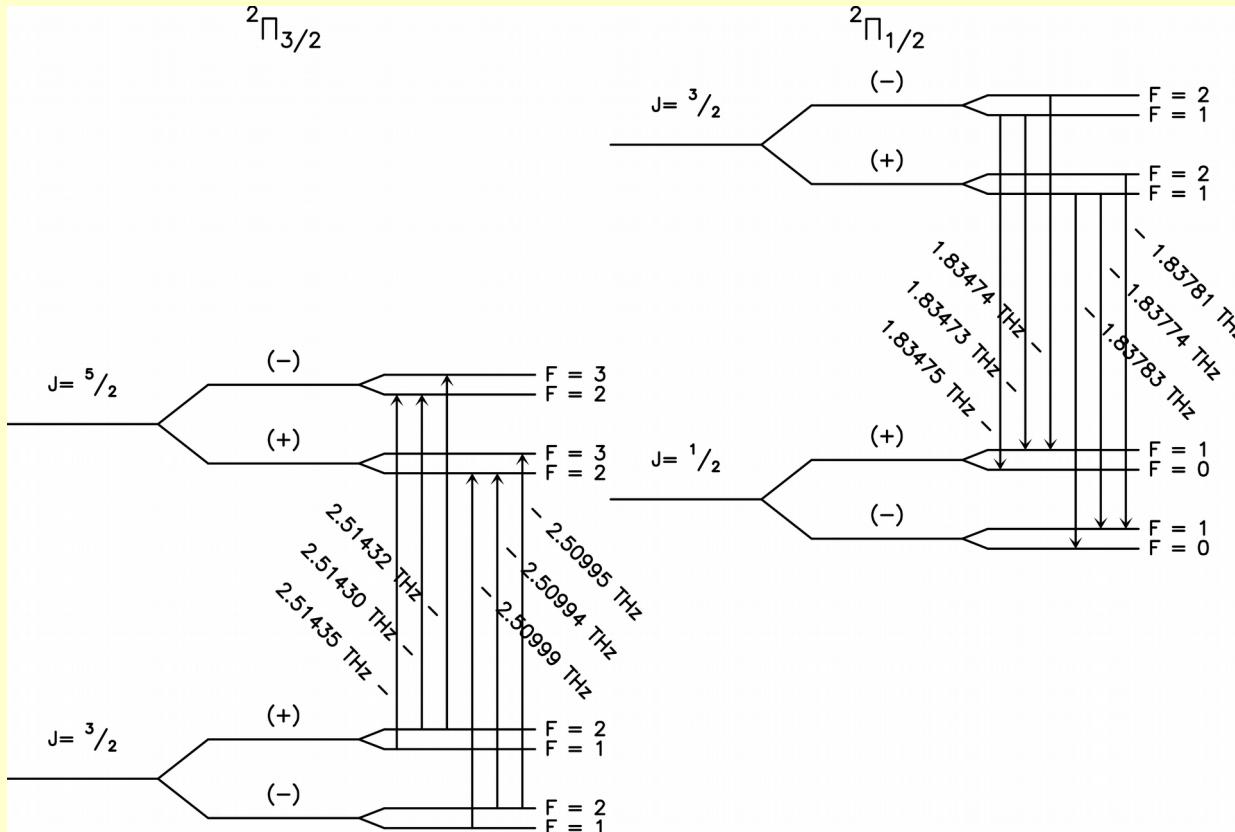


Table 3. Conditions in diffuse cloud models and coefficients for departure from LTE of the population in $\text{OH} \ ^2\Pi_{3/2}, J = 3/2$ levels. The FUV field is parametrized in units of the Habing field (Draine field = 1.7 Habing, Draine 1978).

	Model 1 diffuse molecular	Model 2 translucent
χ [Habing]	1.7	1.7
A_V	0.2	1
n_H [cm^{-3}]	100	1000
$f_{\text{H}_2}^n$	0.1	0.5
T_{gas} [K]	100	15
T_{dust} [K]	16	12
departure coefficients		
$F = 1-$	1.7580	0.9966
$F = 2-$	1.7565	0.9963
$F = 1+$	1.7398	0.9991
$F = 2+$	1.7384	0.9987

Notes. Defining quantities are from Snow & McCall (2006) and from Voshchinnikov et al. (1999) for the dust temperature. The clouds are immersed in the interstellar radiation field as given by Mathis et al. (1983) and the cosmic microwave background. Departure coefficients are defined as the fractional level population with respect to the population for thermalization at the CMB temperature, 2.73 K.

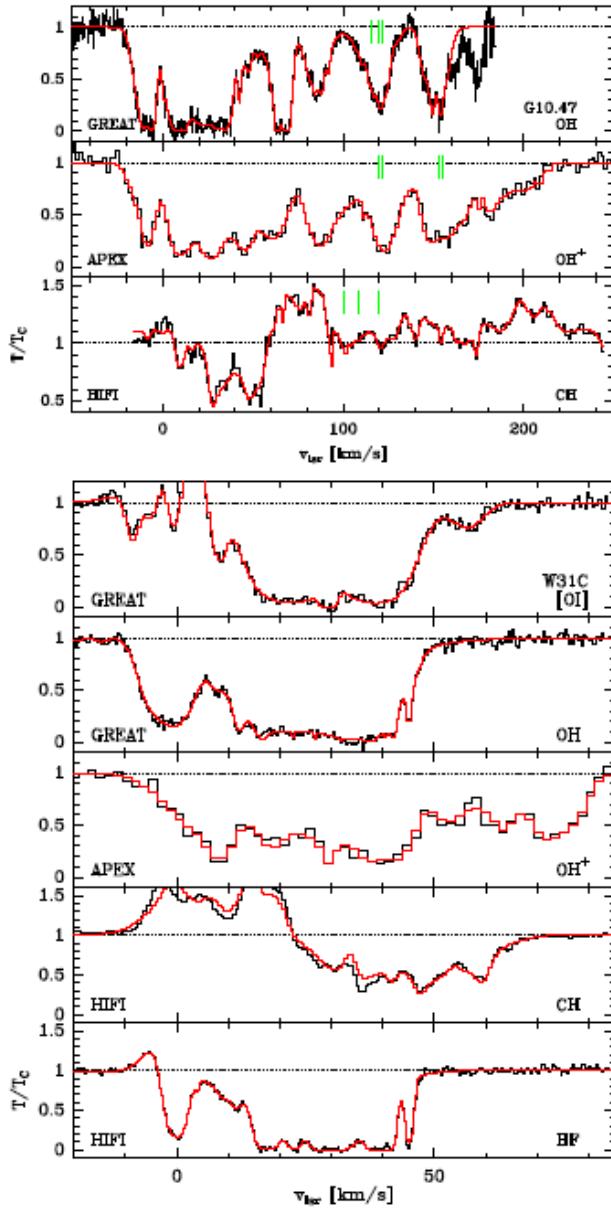


Fig. 1. $\text{O}_1^3P_1 \leftarrow {}^3P_2$, $\text{OH}^2\Pi_{3/2} J = 5/2 \leftarrow 3/2$ and $\text{OH}^+ N = 1 \leftarrow 0$ spectra of sightlines in the first quadrant, along with $\text{CH}^2\Pi_{3/2} J = 3/2 \leftarrow 1/2$ and $\text{HF} J = 1 \leftarrow 0$ spectra. All five transitions are only available for W31C and W49N. Model fits are overlaid in red. For O_1 , CH and HF one emission line component was added where needed. For

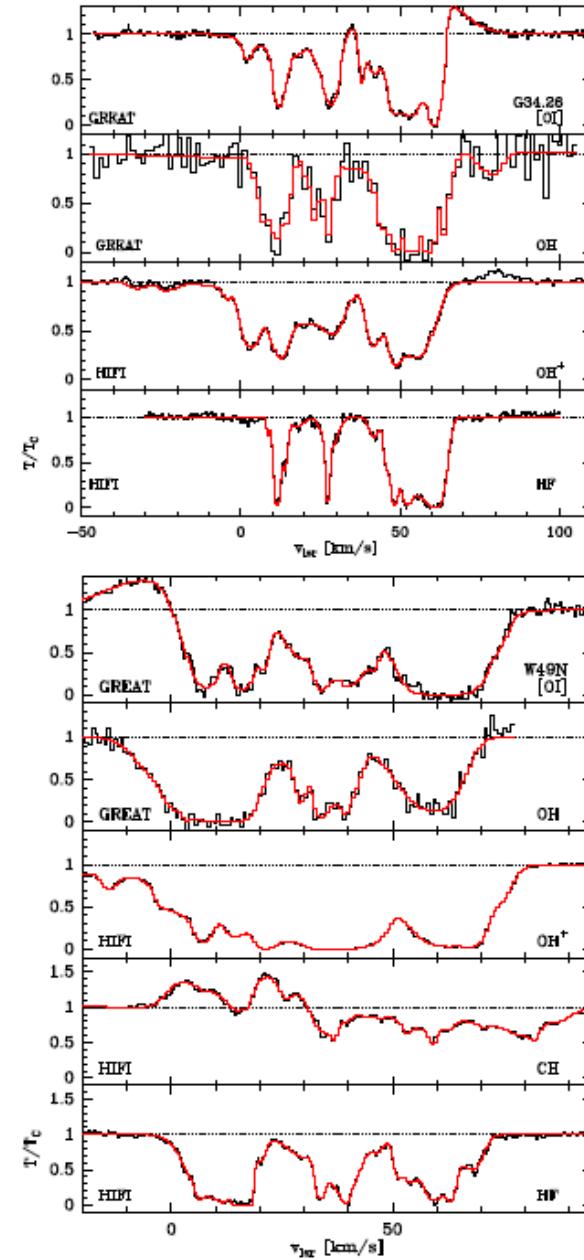


Fig. 1. continued.

OI, OH, OH^+ spectra and H_2 proxies in the 1st quadrant

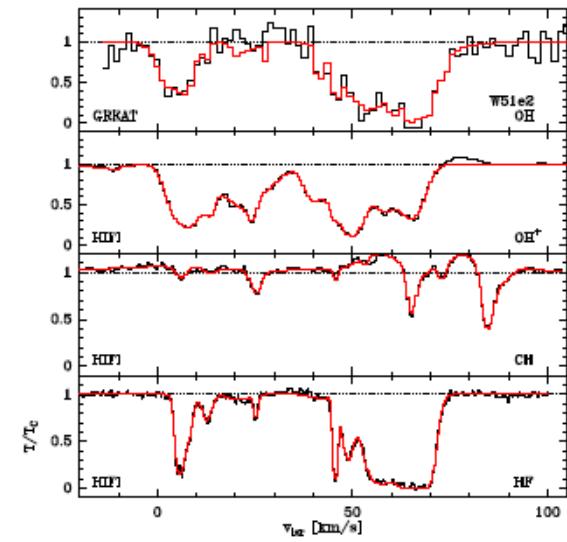


Fig. 1. continued.

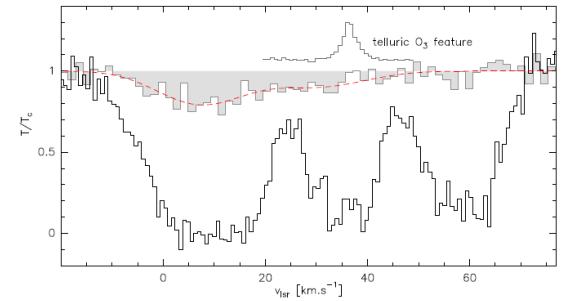
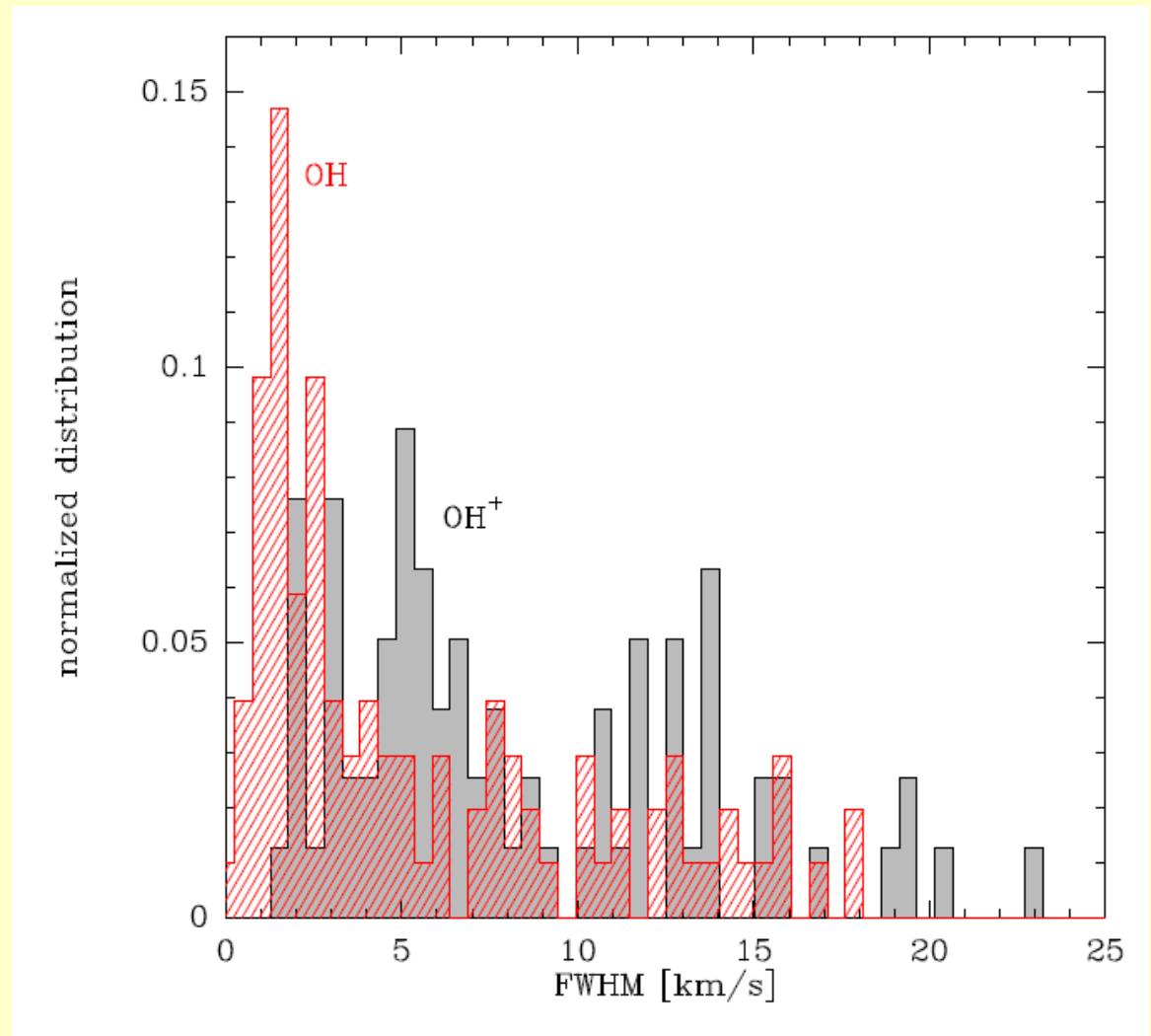
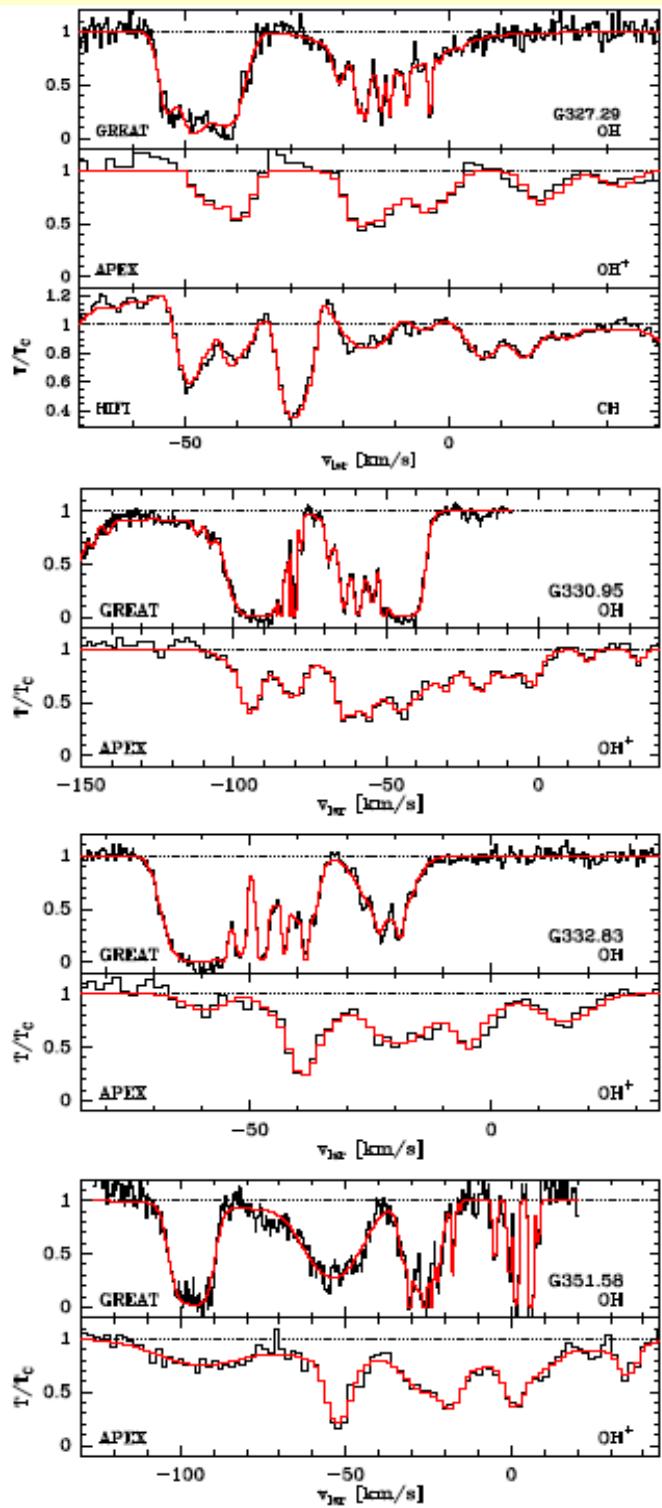


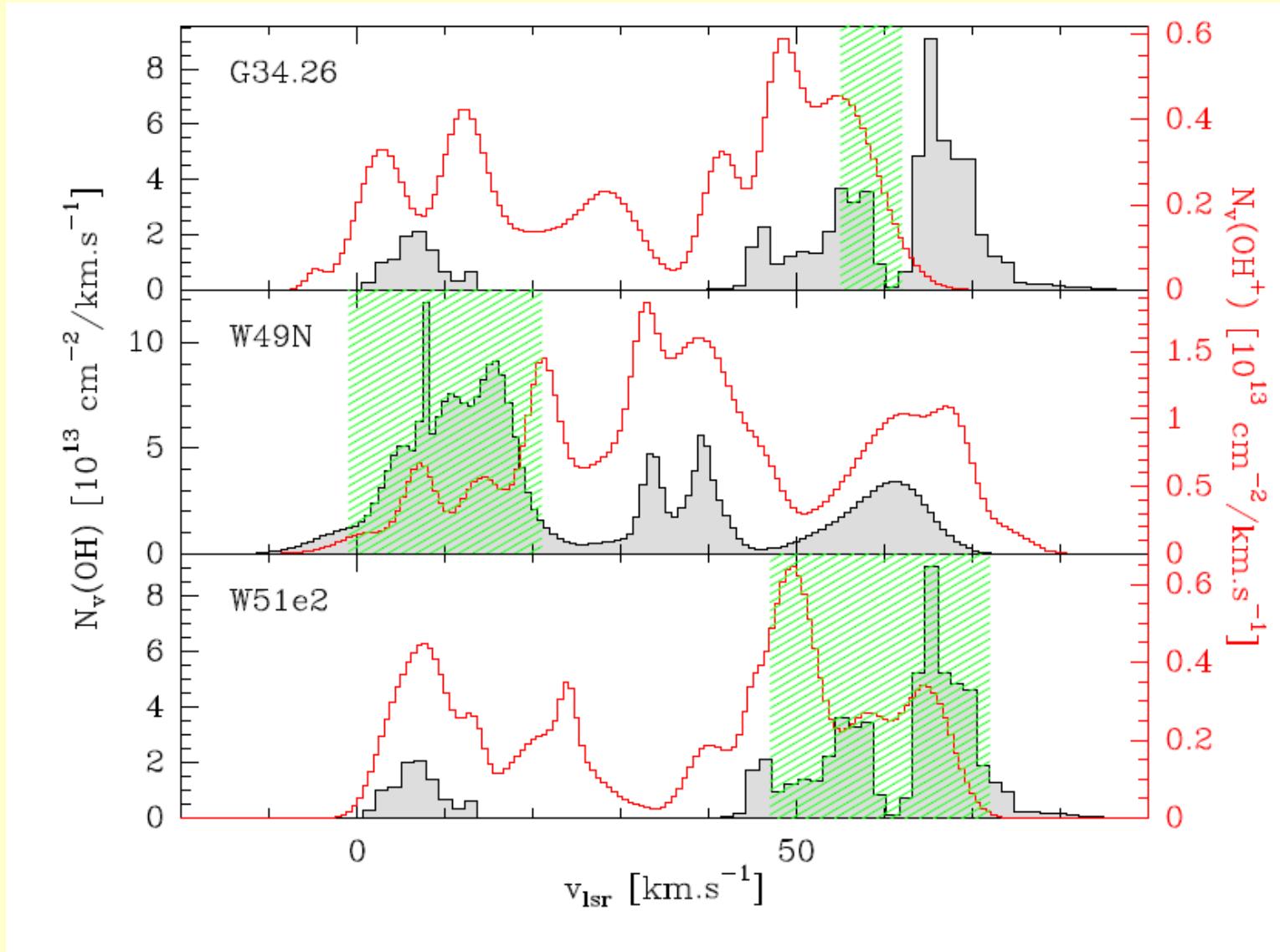
Fig. 3. ^{18}OH absorption (top, grey-shaded), a least-squares, two-component fit to it (dashed line) and OH absorption towards W49N. The spectra are scaled by the corresponding continuum level, to facilitate a comparison. The insert at the top shows a telluric ozone feature (as observed in total power), where the calibration is more uncertain.

← OI, OH, OH⁺ spectra and H₂ proxies in quadrant IV



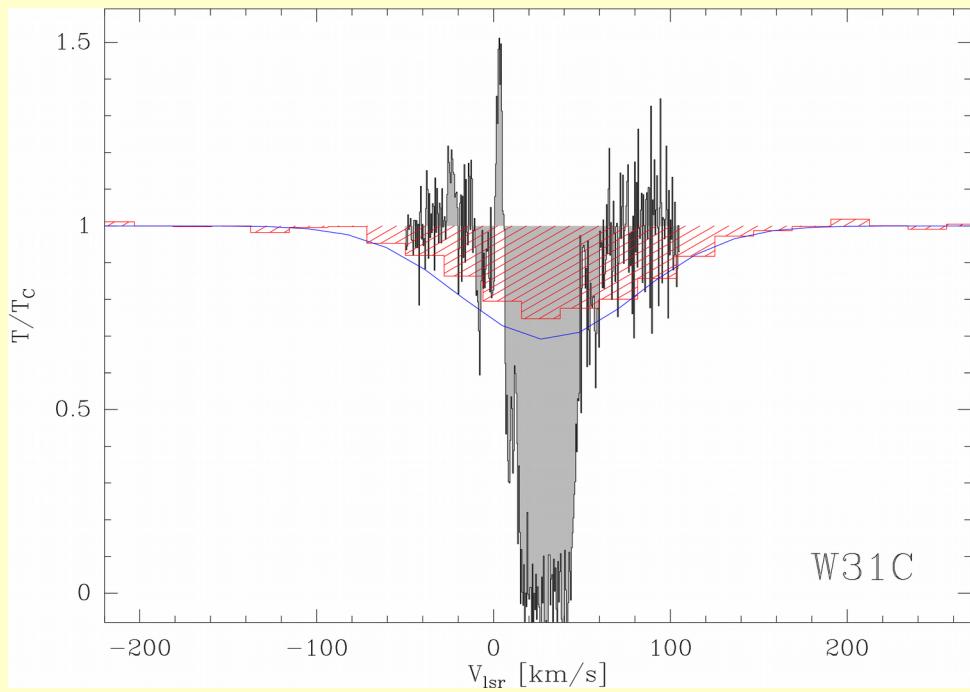
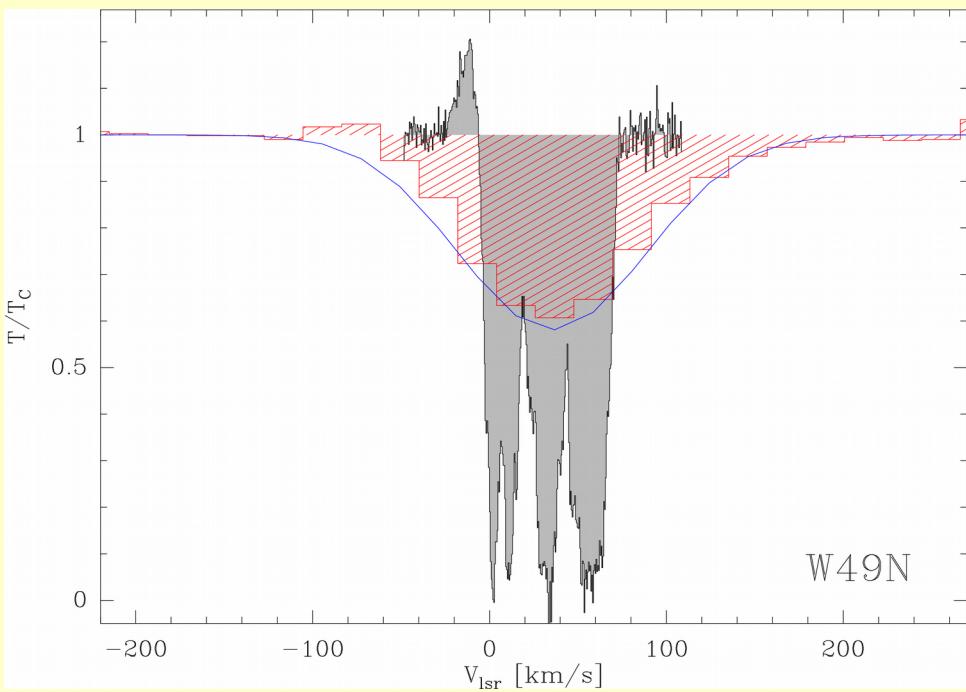
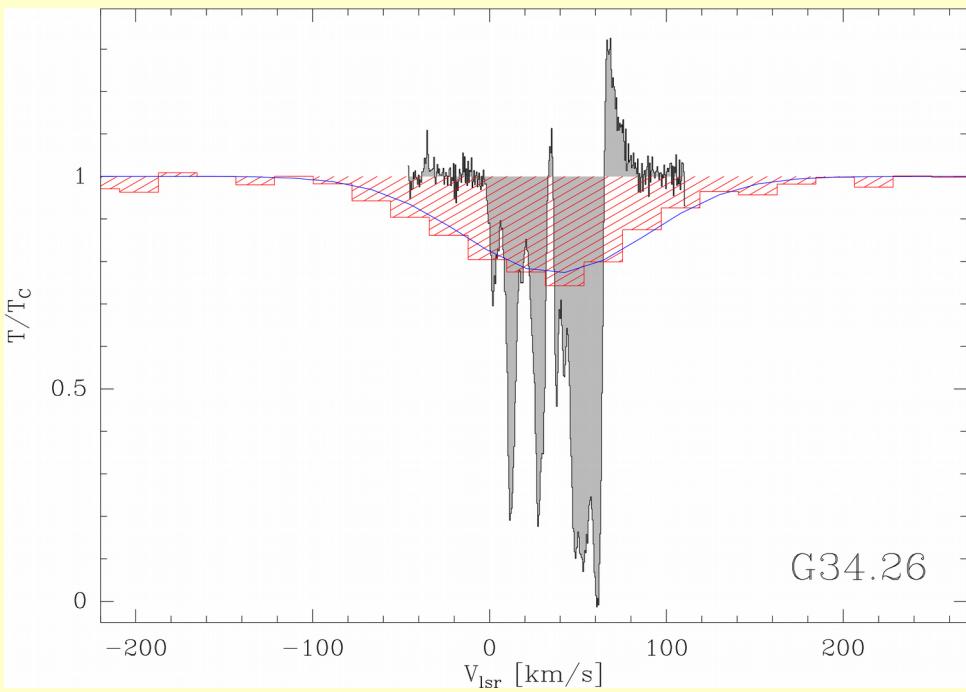
Distribution of fitted linewidths ↑

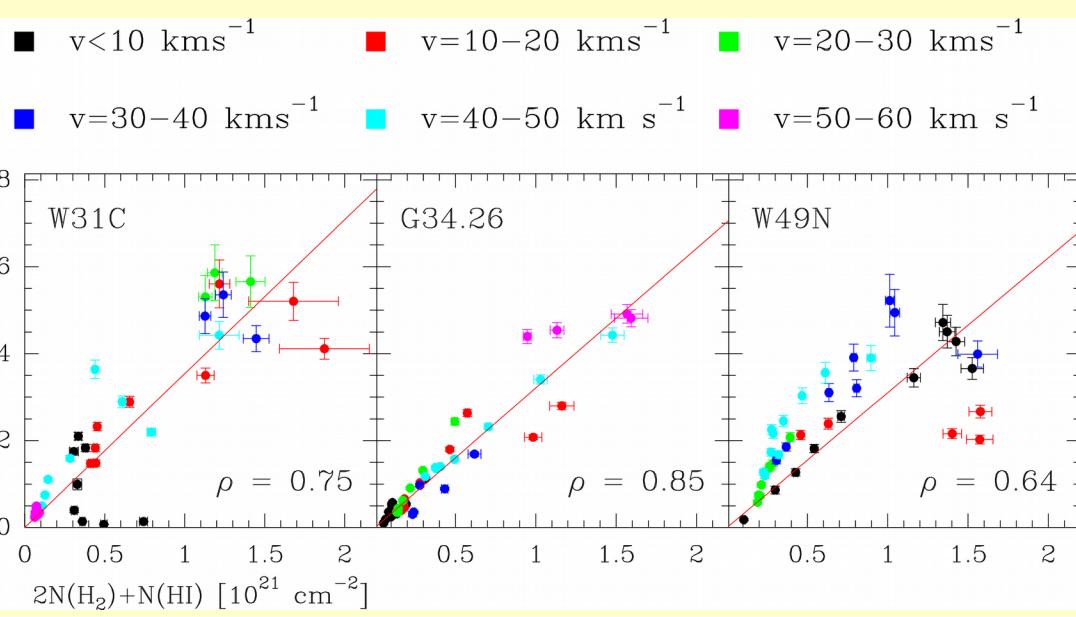
Arm-to-interarm contrast



Sagittarius arm/interarm ratio: 5 (OH), 2 (OH⁺)
Cf. Terebey & Heyer (1998): 28 (CO), 2.5 (HI)

[OI] spectroscopy: GREAT vs. PACS





[OI] traces atomic & molecular hydrogen reservoir (HF spectra from PRISMAS, HI from Winkel et al., 2016):

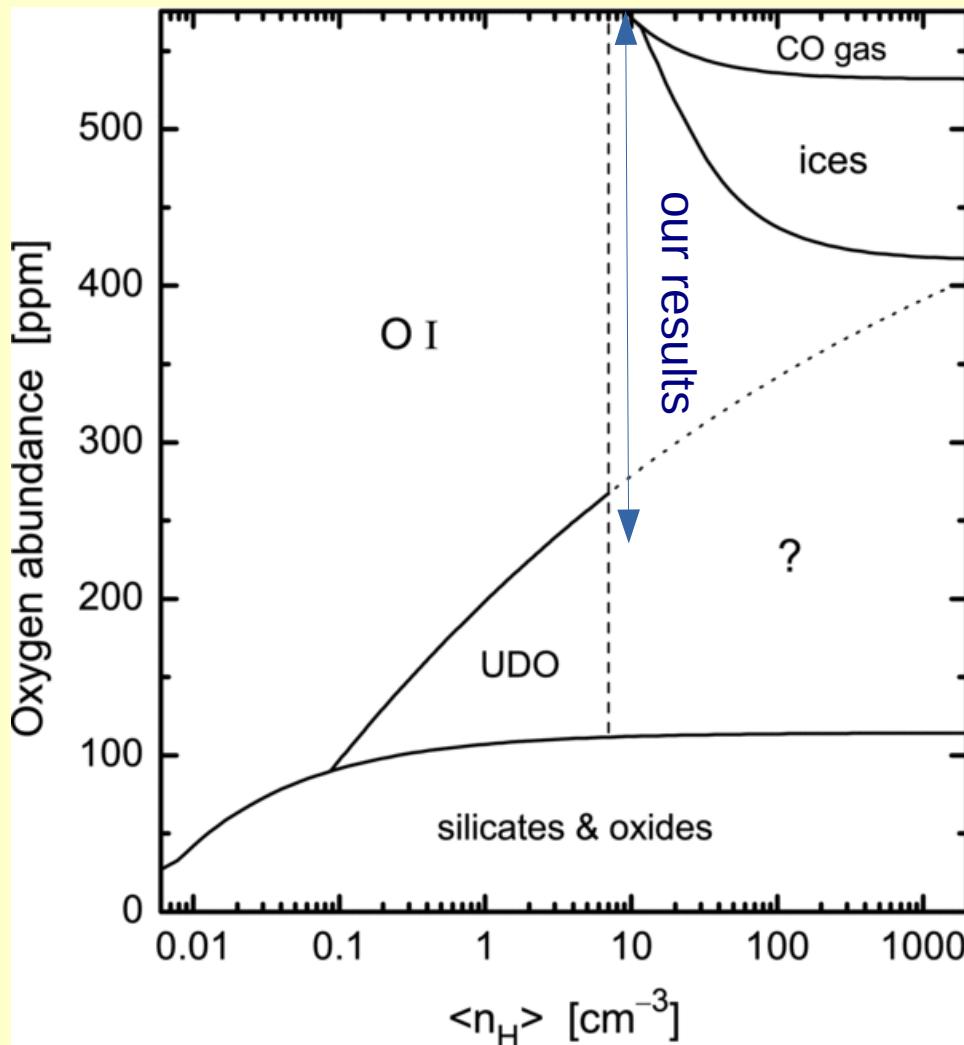
$X(\text{OI}) = 350, 320, 310 \text{ ppm}$ towards W31C, G35.26, W49N

cf. UV spectroscopy: $\sim 300 \text{ ppm}$ (Meyer et al. 1998, Cartledge et al. 2004, Jensen et al. 2005)

Possible indication of [OI] depletion towards W31C

Formation rate for OH vs. molecular hydrogen fraction

The “interstellar oxygen crisis” (Whittet, 2010, Jenkins 2009)

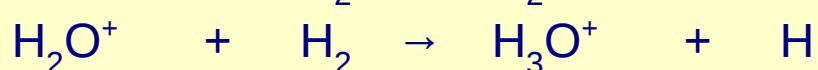
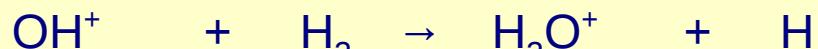


For diffuse molecular/ translucent clouds no indication of Oxygen uptake into unidentified carriers.

Cf. Meyer et al. (1998), Cartledge et al. (2004), Jensen et al. (2005): UV spectroscopy ($A_V < 1$):
Oxygen abundance ~ 300 ppm,
cf. solar value:
490 ppm (Asplund et al. 2009)

Synergies with laboratory work: Branching ratio for water formation.

Hydrogen abstraction reactions:

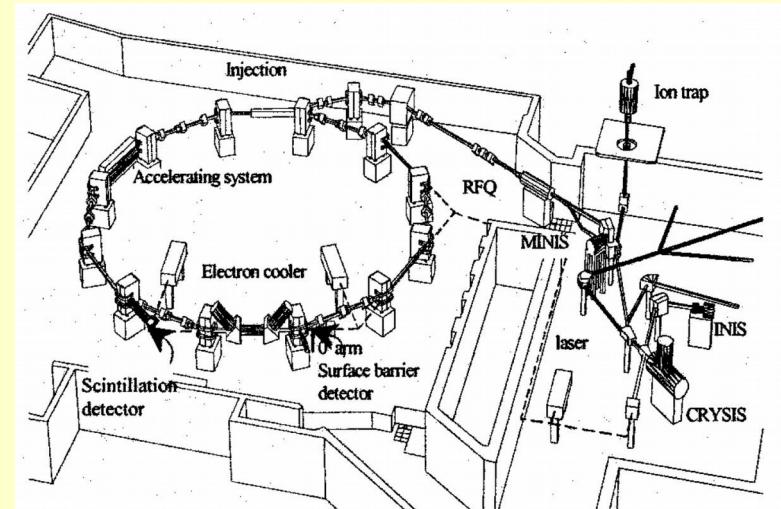
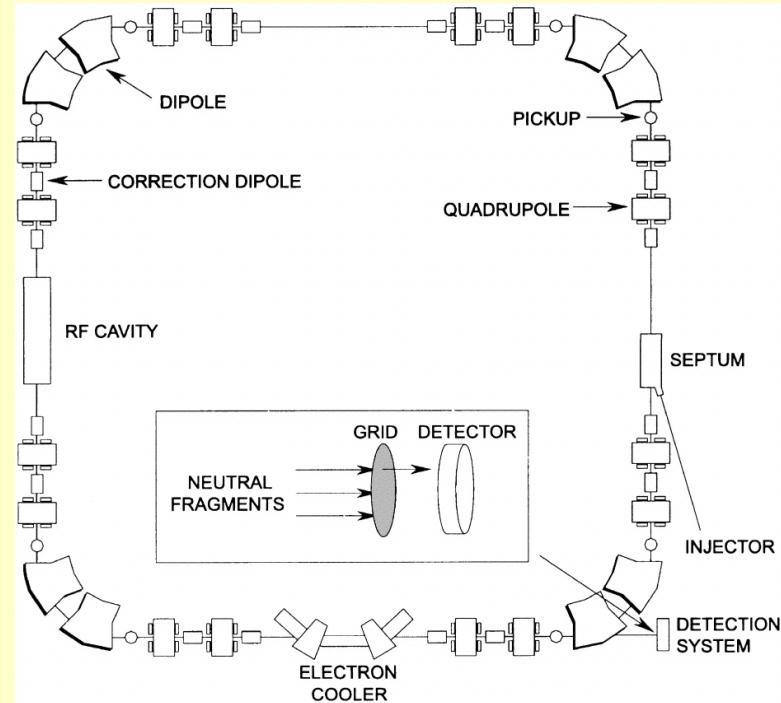


Dissociative recombination:



Reactions (2)+(3):

$\beta_{\text{OH}} = 83\%$ (Neau et al. 2000, Aarhus ion storage ring),
 $= 74\%$ (Jensen et al. 2000, Stockholm)



Determination of β_{OH} with GREAT

Gain due to dissociative recombination of H_3O^+ : γ_{DR}

Gain of OH from photodissociation of H_2O : γ_{PD}

Other processes:

Gain rates for OH and H_2O : $\Gamma_{\text{OH}}(A_V), \Gamma_{\text{H}_2\text{O}}(A_V)$

Loss rates for OH and H_2O : $\Lambda(A_V, T)_{\text{OH}}, \Lambda_{\text{H}_2\text{O}}(A_V)$

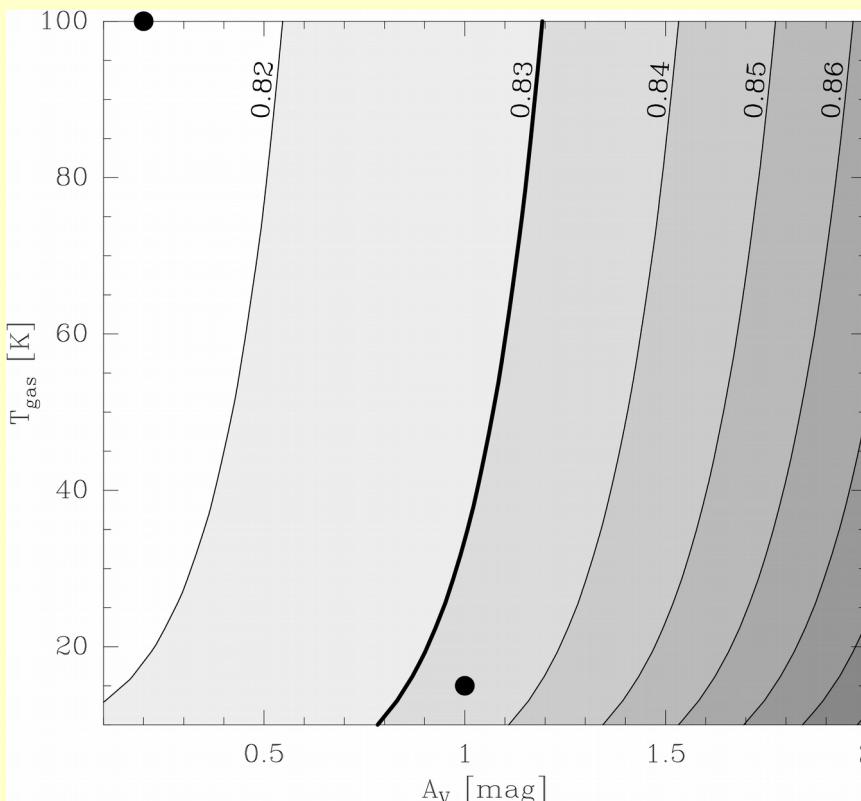
$$\begin{aligned}\frac{dn_{\text{OH}}}{dt} &= \Gamma_{\text{OH}} + \beta\gamma_{\text{DR}}n_{\text{H}_3\text{O}^+} + \gamma_{\text{PD}}n_{\text{H}_2\text{O}} - \Lambda_{\text{OH}}n_{\text{OH}}, \\ \frac{dn_{\text{H}_2\text{O}}}{dt} &= \Gamma_{\text{H}_2\text{O}} + (1 - \beta)\gamma_{\text{DR}}n_{\text{H}_3\text{O}^+} - (\Lambda_{\text{H}_2\text{O}} + \gamma_{\text{PD}})n_{\text{H}_2\text{O}},\end{aligned}$$

H_3O^+ data from Indriolo et al. (2015).

Ratio $b_X = X/\text{H}_3\text{O}^+$ for $X=\text{OH}$ and H_2O yields β_{OH} :

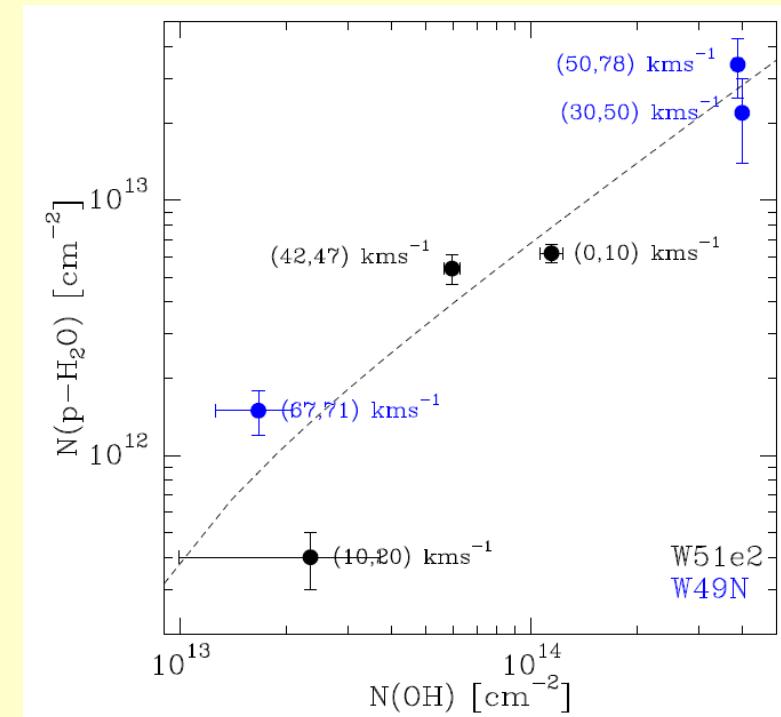
$$\frac{b_{\text{OH}}}{b_{\text{H}_2\text{O}}} = \frac{\gamma_{\text{PD}} + \beta\Lambda_{\text{H}_2\text{O}}}{(1 - \beta)\Lambda_{\text{OH}}}$$

$\rightarrow \beta_{\text{OH}} = 0.82 \text{ to } 0.88$ (Wiesemeyer et al., 2016)

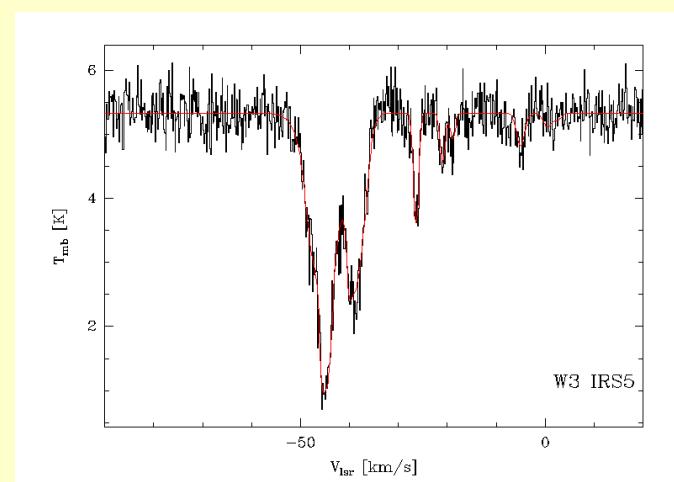
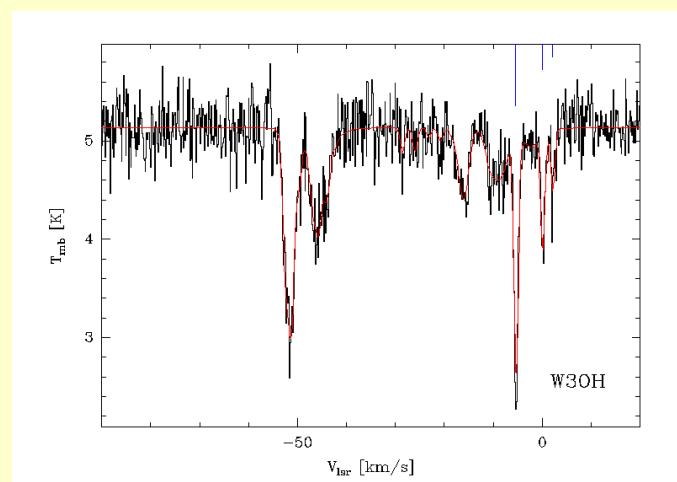
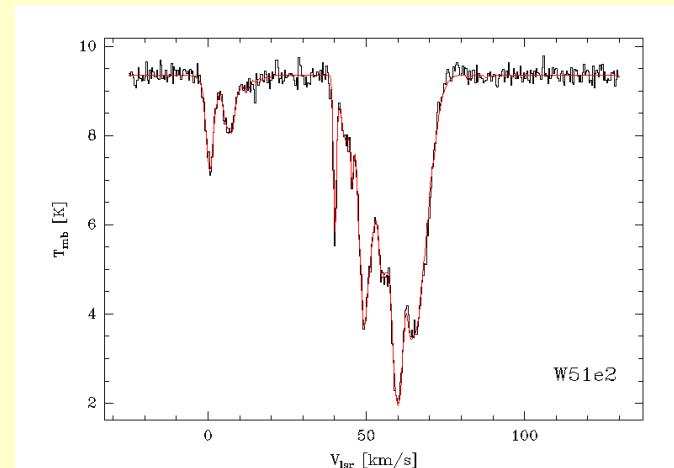
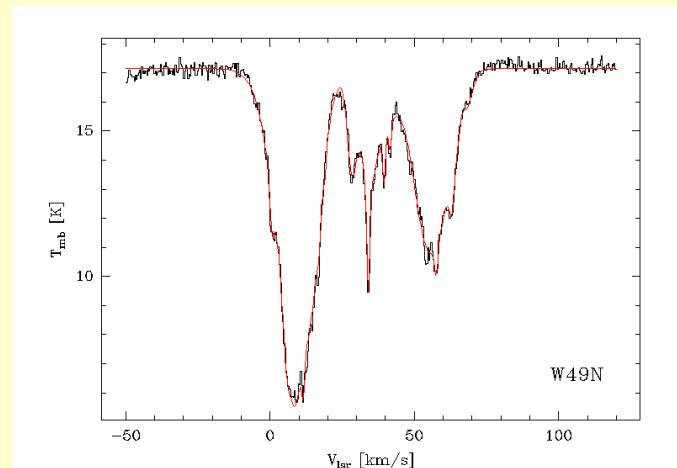
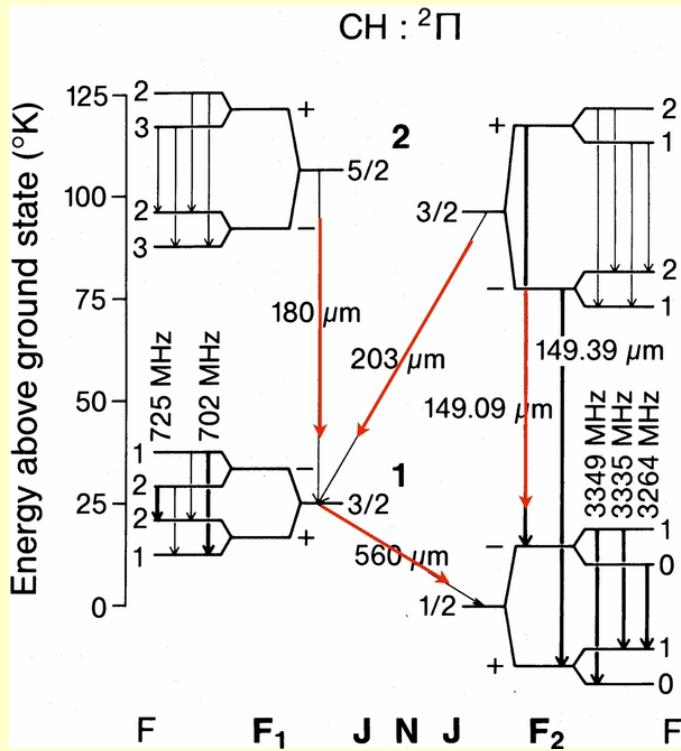


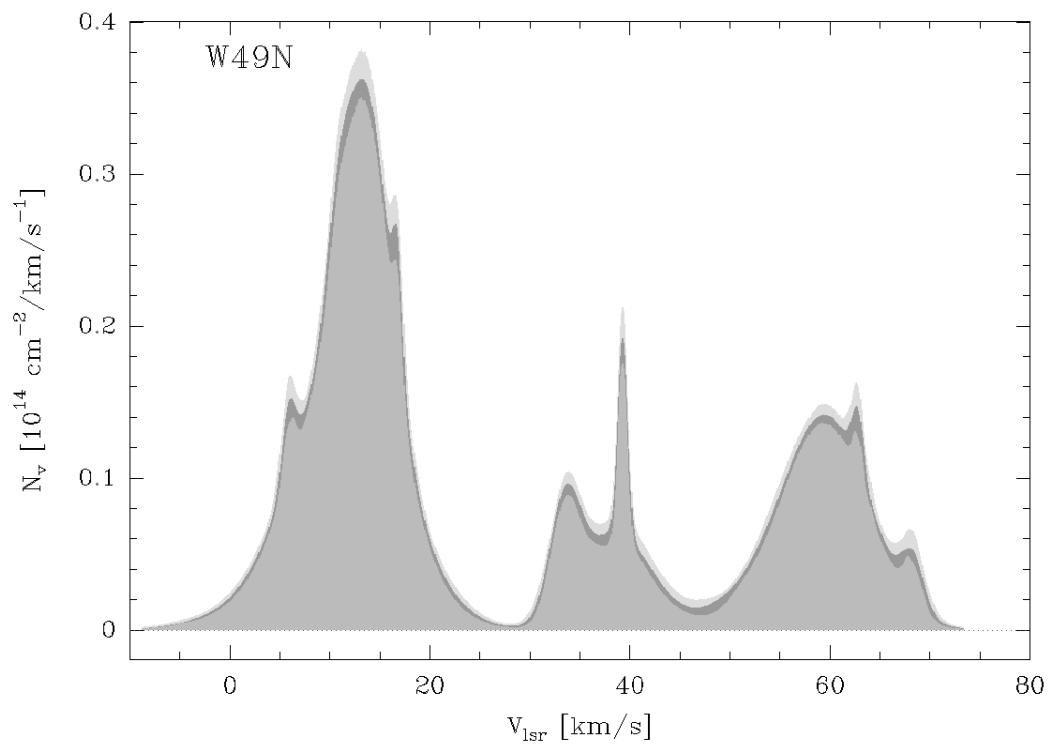
Signposts for “warm” chemistry ?

- Derived OH abundance $N(OH)/N(H_2) \sim (0.3 - 2.2) \times 10^{-7}$
- Model predictions (Albertsson et al. 2014): $X(OH) = (0.3 - 1.6) \times 10^{-7}$
Ion-neutral & gas-grain chemistry, varying ortho/para ratio, Meudon PDR code.
- Comparison of $X(OH)$ and $X(H_2O)$: Signpost of “warm” chemistry ?
Endothermic reaction chain: $O(H_2,H)OH(H_2,H)H_2O$
Model yields: $X(H_2O)/X(OH) \sim 0.16$
(Godard et al. 2012)
- Observationally: $X(H_2O)/X(OH) \sim 0.3$
(p- H_2O from Sonnentrucker et al. 2010)
- Timescale to reach chemical equilibrium:
 ~ 10 Myr (Heck, 1992)
Timescale for density wave crossing:
 $\sim 15, 68$ and 80 Myr
 $@ R_G = 4.5, 7.2$ and 8.3 kpc, respectively.

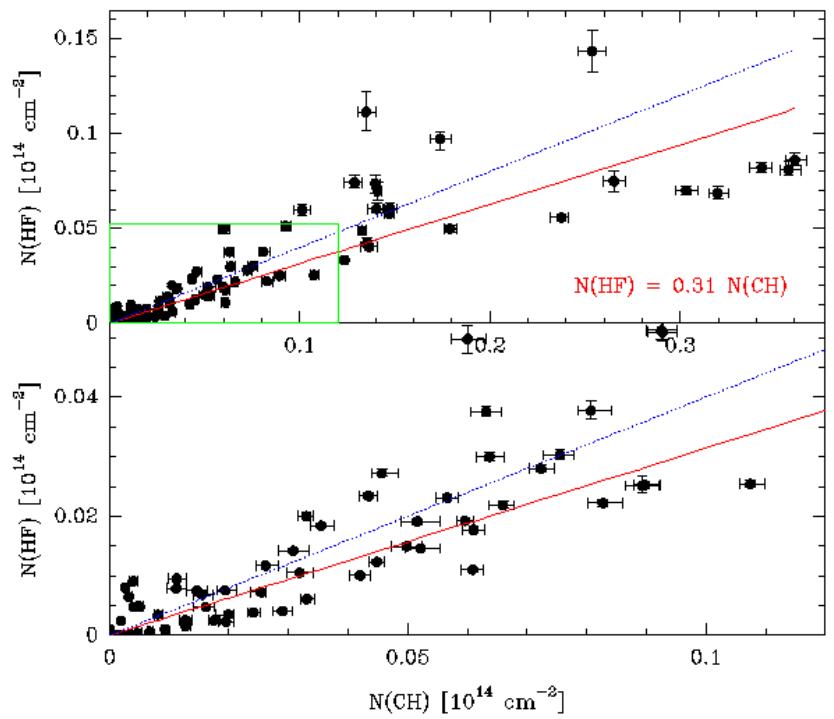


$\text{CH } ^2\Pi \text{ J} = 3/2 \rightarrow 1/2$, an H_2 proxy for SOFIA



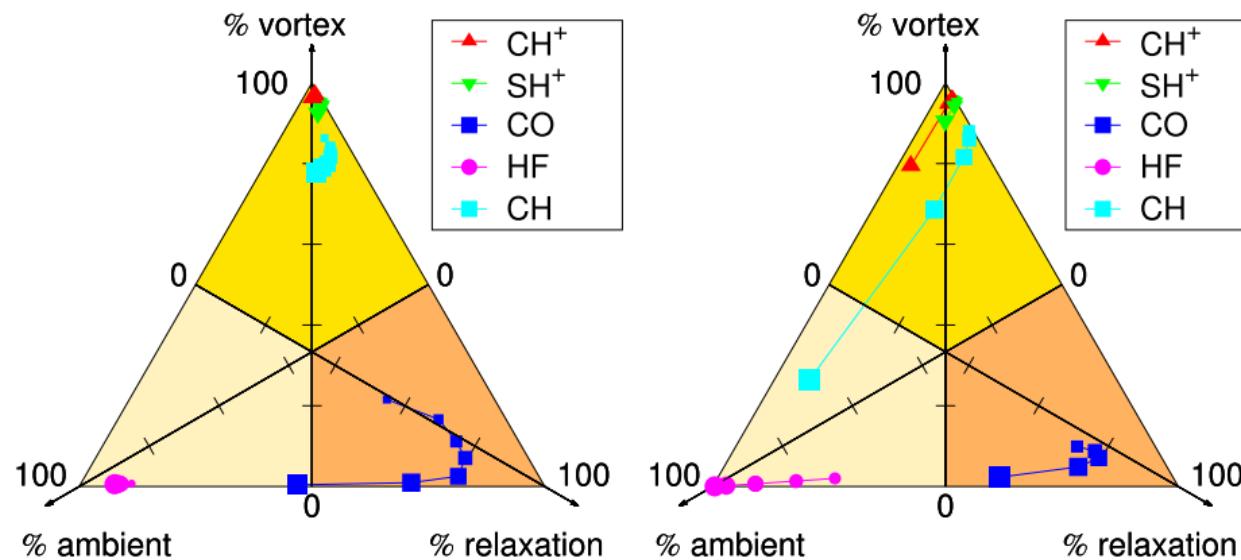


CH column density towards W49N



$N(\text{HF})/N(\text{CH})$ in 1 km/s intervals

CH vs. HF: A signpost for warm chemistry ?



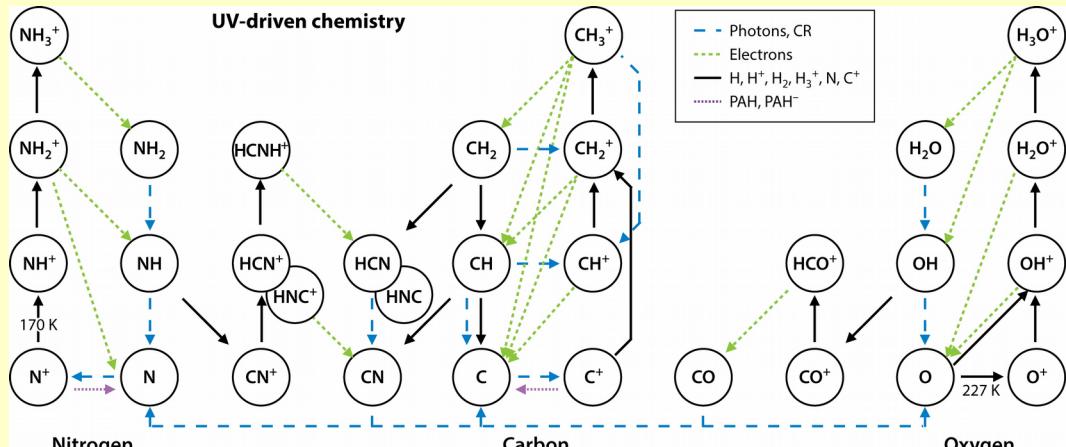
Ternary diagrams for cold, warm and relaxation chemistry.

Godard, Falgarone, Pineau des Forêts, 2014, A&A 570, A27

Cf. “canonical” values:

$$\begin{aligned} X(\text{HF}) / X(\text{CH}) &= 0.4 \\ \text{with } X(\text{CH}) &= 3.5 \times 10^{-8} \end{aligned}$$

New reaction rates from Tizniti et al. (2014).
 HF abundance modeled by Sonnentrucker et al. (2015) and measured by Indriolo et al. (2013).
 CH abundance from Sheffer et al. 2008).



Gerin M, et al. 2016.
 Annu. Rev. Astron. Astrophys. 54:181–225

SUMMARY

- Several signposts for attribution of OH⁺ and OH to lower and higher end of molecular H₂ fraction in diffuse gas.
- OI ${}^3P_1 \leftarrow {}^3P_2$ a proxy for hydrogen reservoir in diffuse clouds.
- Oxygen abundance in diffuse gas ~300 to 350 ppm, close to values from UV spectroscopy ($A_V \sim 1$). Is there an “oxygen crisis” (Jenkins 2009, Whittet 2010) ? Improved Galactic cartography may allow for determination of abundance gradients.
- OH/H₂O ratios do not rule out endothermic contributions to observed abundance patterns, but confirmation is needed.
- Scatter in OH/H₂O ratios moderate → OH a secondary H₂ proxy.
- For Sofia, CH ${}^2\Pi$ J= 3/2 → 1/2 a possible proxy for H₂ (caveat: endothermic abundance enhancement).