Chemistry of the Interstellar Medium

David Neufeld

Johns Hopkins University

Outline

- Introduction: the rich chemistry of the interstellar medium
- Probing the diffuse ISM with small hydride molecules
- Determining the “oxygen budget” in the dense ISM

Astrochemistry

A rich chemistry operates in the denser, cooler regions of the interstellar medium

More than 190 interstellar molecules have been discovered over the past 80 years

Cologne Database for Molecular Spectroscopy (CDMS)
list of interstellar and circumstellar molecules

2 atoms

- H_2
- AlF
- AlCl
- C_2**
- CH
- CH^+
- CN
- CO
- CO^+
- CP
- SiC
- HCl
- KCl
- NH
- NO
- NS
- NaCl
- OH
- PN
- SO
- SO^+
- SiN
- SiO
- SiS
- CS
- HF
- HD
- FeO ?
- O_2
- CF^+
- SiH ?
- PO
- AlO
- OH^+
- CN^-
- SH^+
- SH
- HCl^+
- TiO
- ArH^+
- NO^+ (?)

3 atoms

- C_3 *
- C_2H
- C_2O
- C_2S
- CH_2
- HCN
- HCO
- HCO^+
- HCS^+
- HOC^+
- H_2O
- H_2S
- HNC
- HNO
- MgCN
- MgNC
- N_2H^+
- N_2O
- NaCN
- OCS
- SO_2
- c-SiC_2
- CO_2 *
- NH_2
- H_3^+ (*)
- SiCN
- AlNC
- SiNC
- HCP
- CCP
- AlOH
- H_2O^+
- H_2Cl^+
- KCN
- FeCN
- HO_2
- TiO_2
- C_2N
- Si_2C

4 atoms

- c-C_3H
- l-C_3H
- C_3N
- C_3O
- C_3S
- C_2H_2 *
- NH_3
- HCCN
- $HCNH^+$
- HNCO
- HNCS
- $HOCO^+$
- H_2CO
- H_2CN
- H_2CS
- H_3O^+
- c-SiC_3
- CH_3 *
- C_3N^-
- PH_3
- HCNO
- HOCN
- HSCN
- H_2O_2
- C_3H^+
- HMgNC
- HCCO

5 atoms

- C_5 *
- C_4H
- C_4Si
- l-C_3H_2
- c-C_3H_2
- H_2CCN
- CH_4 *
- HC_3N
- HC_2NC
- HCOOH
- H_2CNH
- H_2C_2O
- H_2NCN
- HNC_3
- SiH_4 *
- H_2COH^+
- C_4H^-
- HC(O)CN
- HNCNH
- CH_3O
- NH_4^+
- H_2NCO^+ (?)
- $NCCNH^+$

6 atoms

- C_5H
- l-H_2C_4
- C_2H_4*
- CH_3CN
- CH_3NC
- CH_3OH
- CH_3SH
- HC_3NH^+
- HC_2CHO
- NH_2CHO
- C_5N
- l-HC_4H *
- l-HC_4N
- c-H_2C_3O
- H_2CCNH
- C_5N^-
- HNCHCN

7 atoms

- C_6H
- CH_2CHCN
- CH_3C_2H
- HC_5N
- CH_3CHO
- CH_3NH_2
- c-C_2H_4O
- H_2CCHOH
- C_6H^-
- CH_3NCO

8 atoms

- CH_3C_3N
- $HC(O)OCH_3$
- CH_3COOH
- C_7H
- C_6H_2
- CH_2OHCHO
- l-HC_6H *
- CH_2CHCHO (?)
- CH_2CCHCN
- H_2NCH_2CN
- CH_3CHNH

9 atoms

- CH_3C_4H
- CH_3CH_2CN
- $(CH_3)_2O$
- CH_3CH_2OH
- HC_7N
- C_8H
- $CH_3C(O)NH_2$
- C_8H^-
- C_3H_6
- CH_3CH_2SH (?)

10 atoms

- CH_3C_5N
- $(CH_3)_2CO$
- $(CH_2OH)_2$
- CH_3CH_2CHO
- CH_3CHCH_2O

11 atoms

- HC_9N
- CH_3C_6H
- C_2H_5OCHO
- $CH_3OC(O)CH_3$

12 atoms

- c-C_6H_6 *
- n-C_3H_7CN
- i-C_3H_7CN
- $C_2H_5OCH_3$ (?)

> 12 atoms

- $HC_{11}N$
- C_{60} *
- C_{70} *
- C_{60}^+ *

*vibrational spectra only **electronic spectra only (updated Aug. 2016)

Astrochemistry

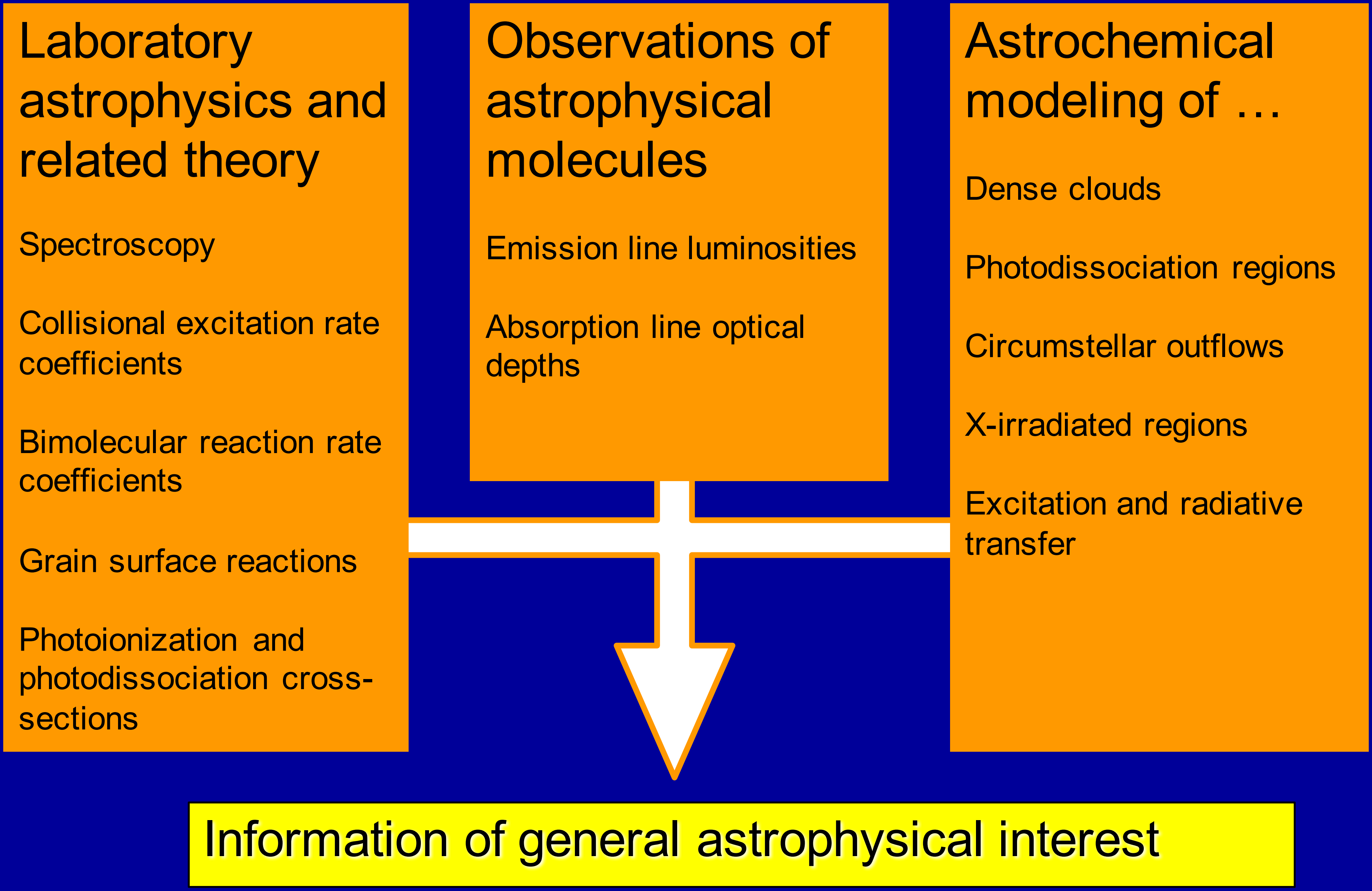
A rich chemistry operates in the denser, cooler regions of the interstellar medium

More than 190 interstellar molecules have been discovered over the past 80 years

Carefully interpreted, observations of interstellar molecules can provide unique information of general astrophysical interest

Arguably, the simplest interstellar molecules show the greatest promise for advancing our understanding

The astrochemistry game plan



Laboratory astrophysics and related theory

Spectroscopy

Collisional excitation rate coefficients

Bimolecular reaction rate coefficients

Grain surface reactions

Photoionization and photodissociation cross-sections

Observations of astrophysical molecules

Emission line luminosities

Absorption line optical depths

Astrochemical modeling of …

Dense clouds

Photodissociation regions

Circumstellar outflows

X-irradiated regions

Excitation and radiative transfer

Information of general astrophysical interest

Collaborators

- PRISMAS Key Program Team (P.I. Maryvonne Gerin)
- HEXOS Key Program Team (P.I. Ted Bergin)

- SOFIA/GREAT team (P.I. Rolf Güsten)
- SOFIA/EXES team (P.I. Matt Richter)

- Ground-based observations: Nick Indriolo (STScI)

- Theory: M. Wolfire, M. Kaufman, J. Goicoechea, E. Falgarone, D. Hollenbach, B. Godard, G. Pineau des Forêts

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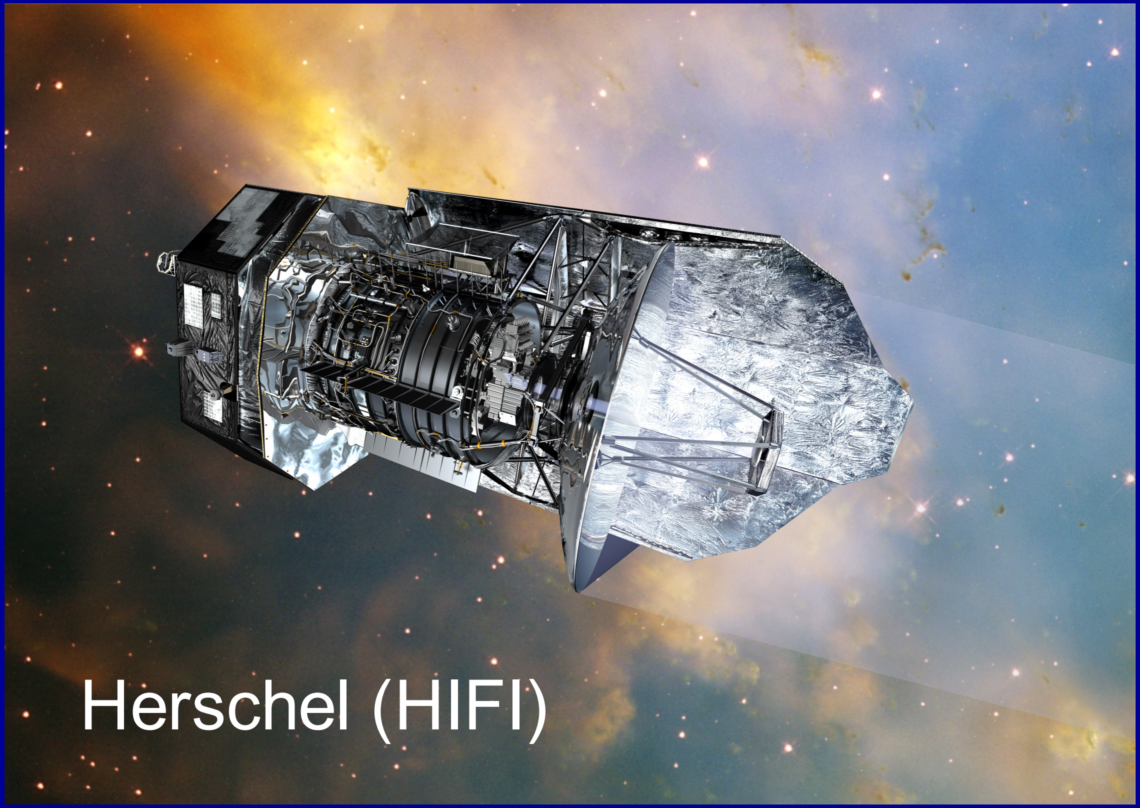
Recent discoveries of molecules in the diffuse ISM

Key facilities for submillimeter spectroscopy over the past 7 years



Herschel (HIFI)

APEX

SOFIA (GREAT)

Recent discoveries of molecules in the diffuse ISM

OH^+	Wyrowski et al. 2010	APEX
SH^+	Menten et al. 2011	APEX
H_2O^+	Gerin et al. 2010	Herschel
HF	Neufeld et al. 2010	Herschel
HCl^+	de Luca et al. 2013	Herschel
H_2Cl^+	Lis et al. 2010	Herschel
SH	Neufeld et al. 2012	SOFIA
ArH^+	Schilke et al. 2014	Herschel

All hydrides with high frequency rotational transitions that are unobservable from the ground or observable only from superb submillimeter sites

Additional discoveries of small molecules in the *dense* ISM

OD Parise et al. 2012 SOFIA

(OD/OH probes chemistry)

para-H_2D^+ Brünken et al. 2012 SOFIA

(ortho-H_2D^+ known previously, but ortho/para-H_2D^+ ratio serves as a molecular clock → cloud age ~ 1Myr)

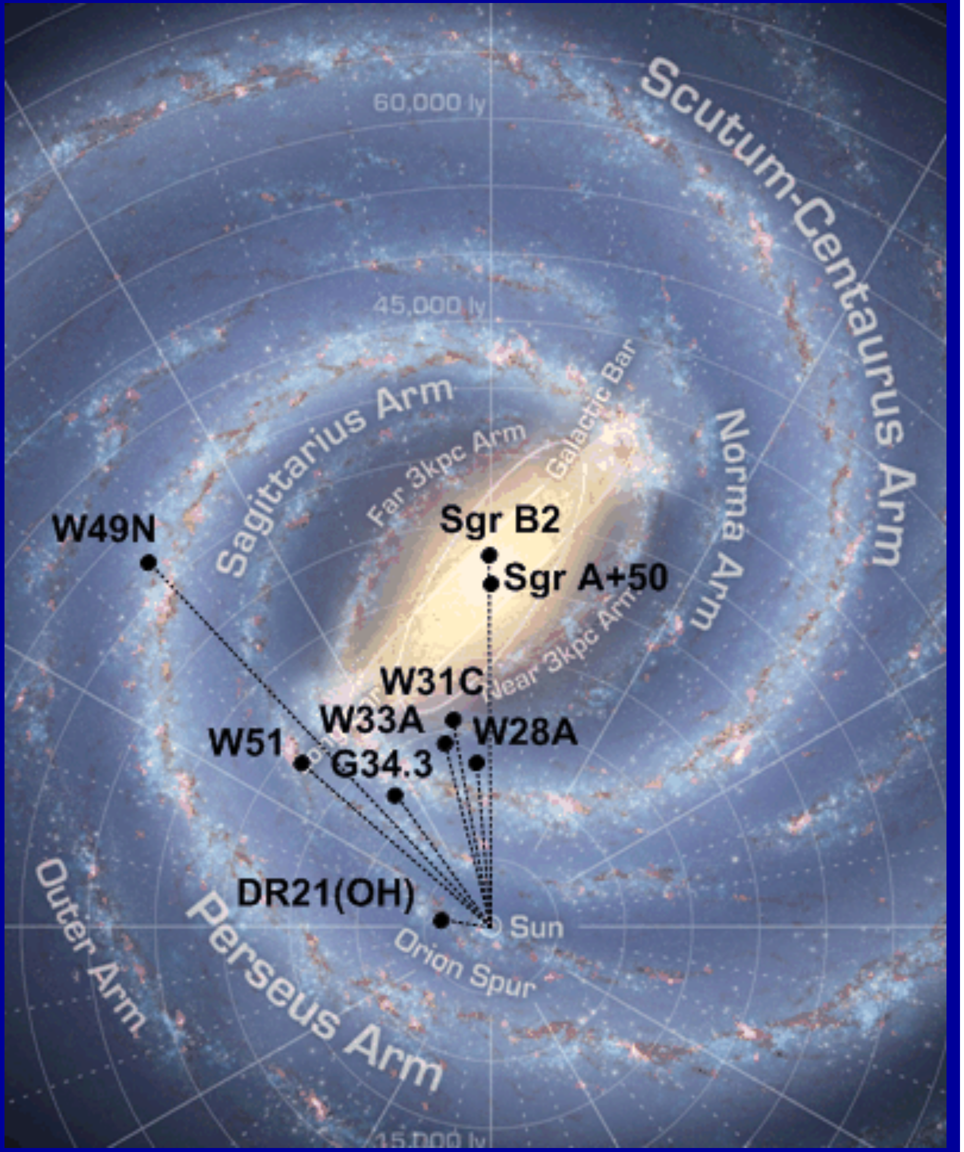
All hydrides with high frequency rotational transitions that are unobservable from the ground or observable only from superb submillimeter sites

Absorption line observations

- We can use a very luminous region of massive star formation as a background THz source

- This allows us to search for absorption by gas in foreground material

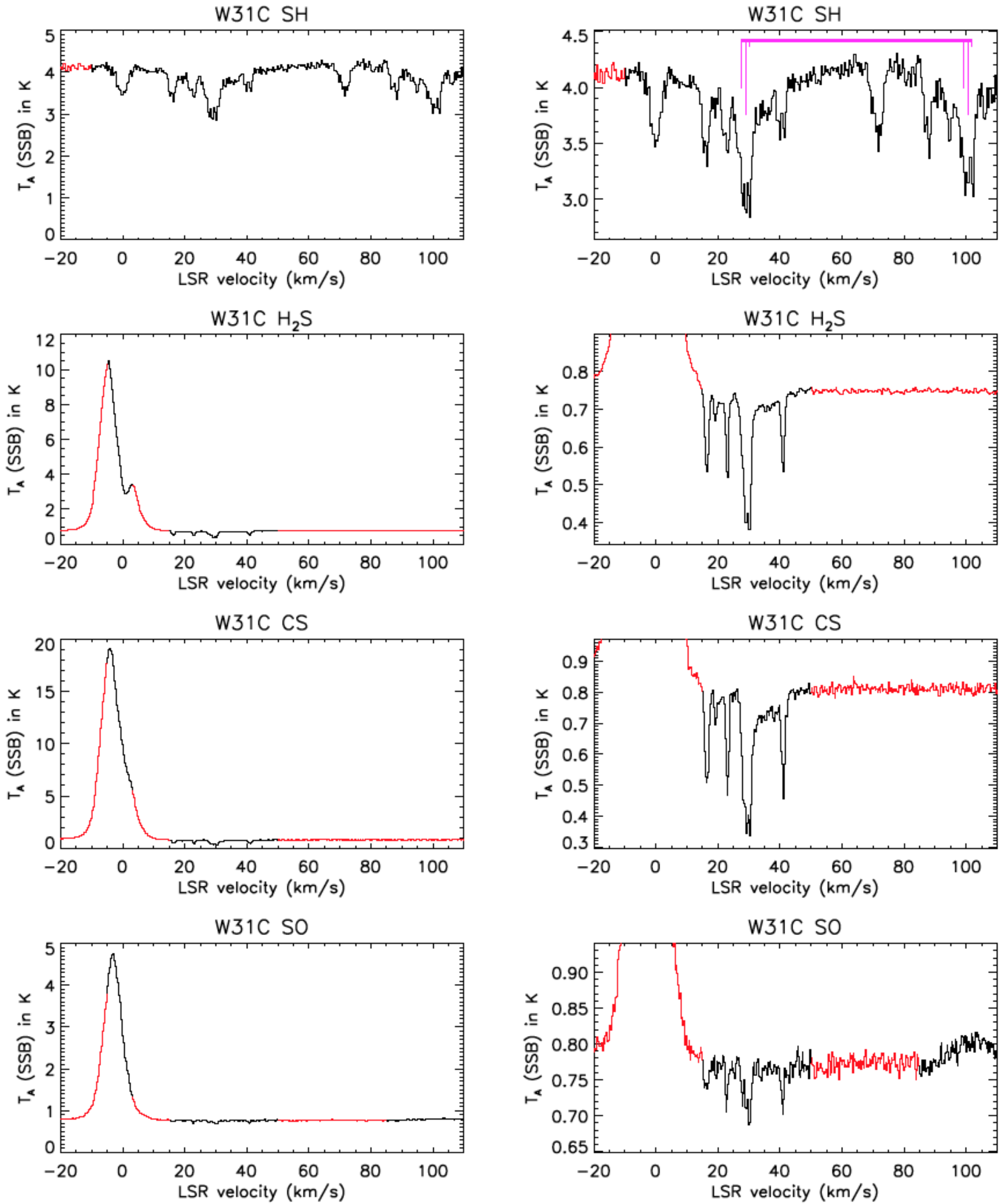
- A very “clean” experiment that provides robust measurements of molecular column densities



Absorption line observations

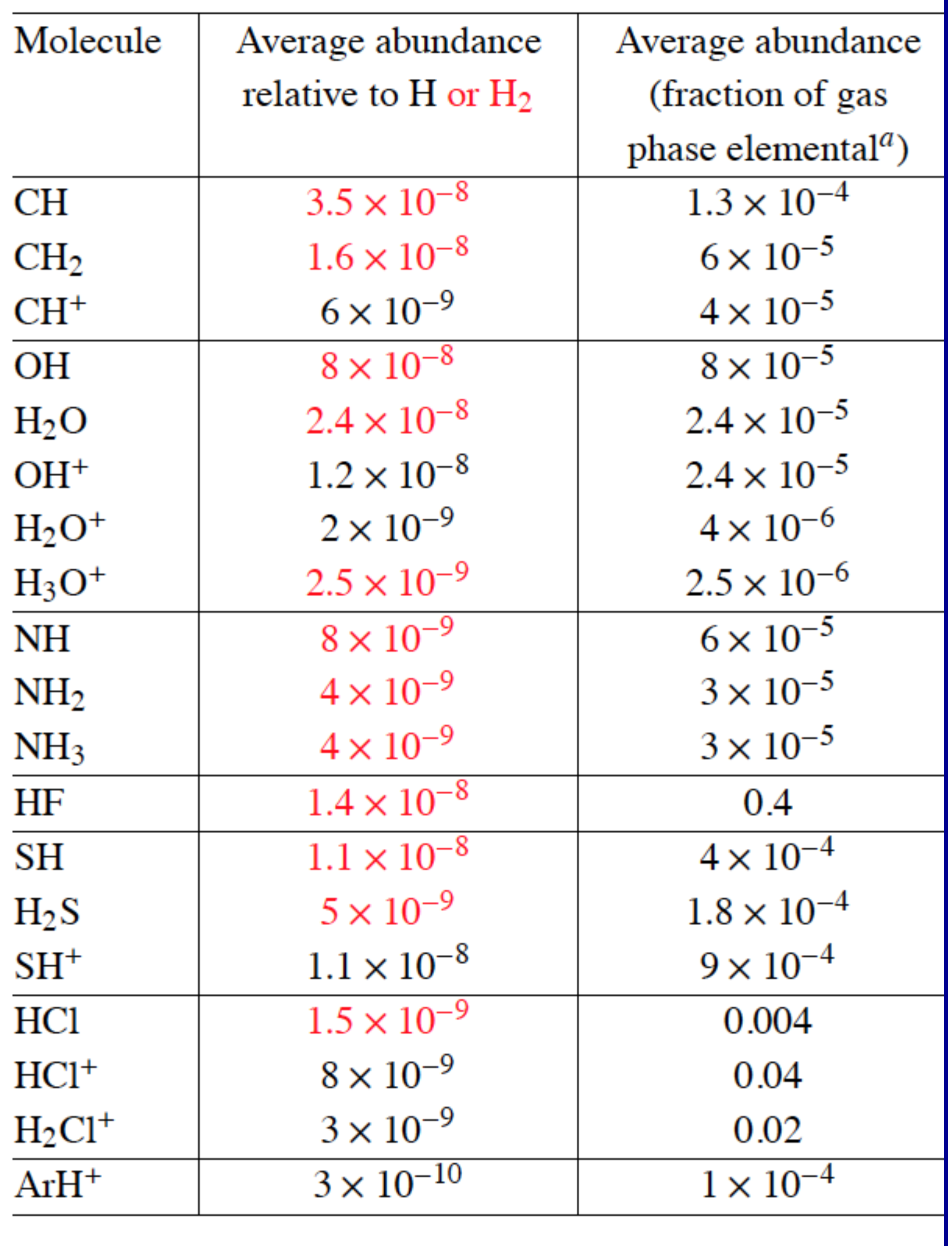
Example

SOFIA/GREAT spectrum of SH toward the W31C star-forming region, along with IRAM 30 m observations of related molecules (H_2S, CS, SO)



Hydrides in the diffuse interstellar medium

First diffuse ISM detection obtained in the past seven years



Molecule	Average abundance relative to H or H_2	Average abundance (fraction of gas phase elemental[a])
CH	3.5×10^{-8}	1.3×10^{-4}
CH_2	1.6×10^{-8}	6×10^{-5}
CH^+	6×10^{-9}	4×10^{-5}
OH	8×10^{-8}	8×10^{-5}
H_2O	2.4×10^{-8}	2.4×10^{-5}
OH^+	1.2×10^{-8}	2.4×10^{-5}
H_2O^+	2×10^{-9}	4×10^{-6}
H_3O^+	2.5×10^{-9}	2.5×10^{-6}
NH	8×10^{-9}	6×10^{-5}
NH_2	4×10^{-9}	3×10^{-5}
NH_3	4×10^{-9}	3×10^{-5}
HF	1.4×10^{-8}	0.4
SH	1.1×10^{-8}	4×10^{-4}
H_2S	5×10^{-9}	1.8×10^{-4}
SH^+	1.1×10^{-8}	9×10^{-4}
HCl	1.5×10^{-9}	0.004
HCl^+	8×10^{-9}	0.04
H_2Cl^+	3×10^{-9}	0.02
ArH^+	3×10^{-10}	1×10^{-4}

Gerin et al, ARAA 2016

Using hydride molecules as diagnostic probes

Small molecules, especially hydride molecules, have simple formation mechanisms

➔ carefully interpreted, they provide unique information of general astrophysical interest

Surrogate tracers for H_2

Tracers of gas heated by shocks and turbulence

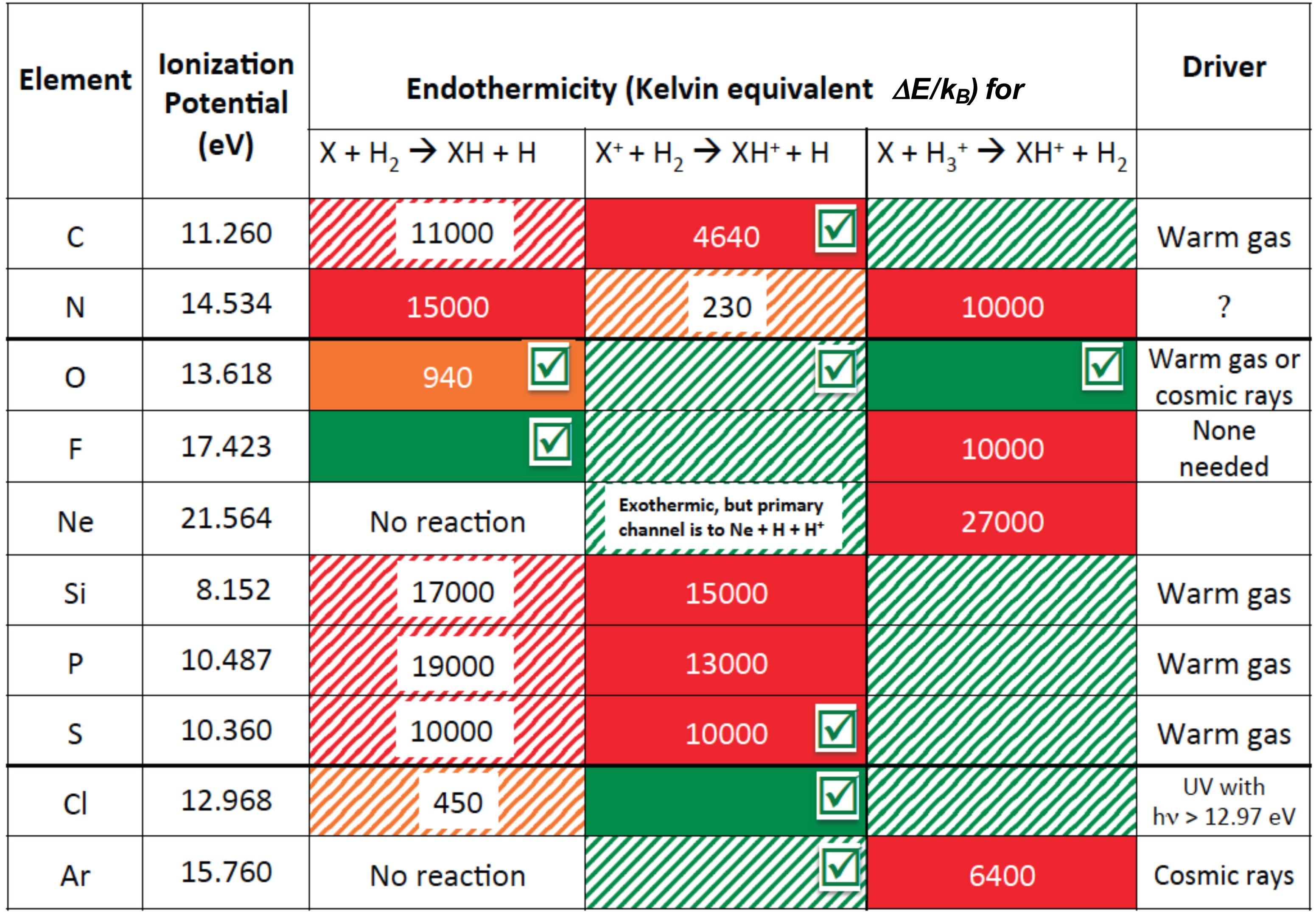
Measuring the cosmic-ray ionization rate

Measuring the H_2 fraction

Small thermochemical differences lead to large differences in chemical behavior

Thermochemistry for different elements

☑ Important formation pathway



Element	Ionization Potential (eV)	Endothermicity (Kelvin equivalent $\Delta E/k_B$) for			Driver
		$X + H_2 \rightarrow XH + H$	$X^+ + H_2 \rightarrow XH^+ + H$	$X + H_3^+ \rightarrow XH^+ + H_2$	
C	11.260	▨ 11000	🟥 4640 ☑	▨	Warm gas
N	14.534	🟥 15000	▨ 230	🟥 10000	?
O	13.618	🟧 940 ☑	▨ ☑	🟩 ☑	Warm gas or cosmic rays
F	17.423	🟩 ☑	▨	🟥 10000	None needed
Ne	21.564	No reaction	▨ Exothermic, but primary channel is to $Ne + H + H^+$	🟥 27000	
Si	8.152	▨ 17000	🟥 15000	▨	Warm gas
P	10.487	▨ 19000	🟥 13000	▨	Warm gas
S	10.360	▨ 10000	🟥 10000 ☑	▨	Warm gas
Cl	12.968	▨ 450	🟩 ☑	▨	UV with hν > 12.97 eV
Ar	15.760	No reaction	▨ ☑	🟥 6400	Cosmic rays

🟩 Exothermic reaction of element in its main ionization state

🟧🟥 Endothermic reaction of element in its main ionization state

▨ Exothermic reaction of element **not** in main ionization state

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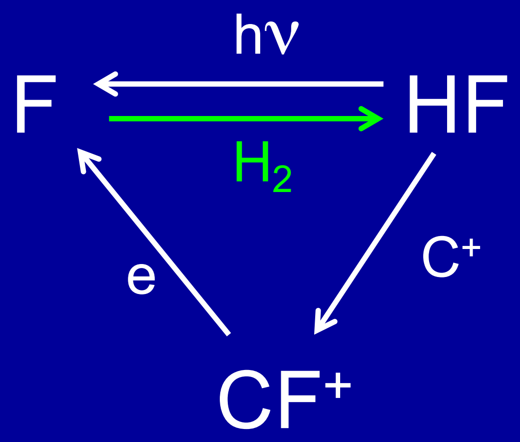
Interstellar hydrogen fluoride:

a surrogate for molecular hydrogen

Fluorine chemistry is very simple



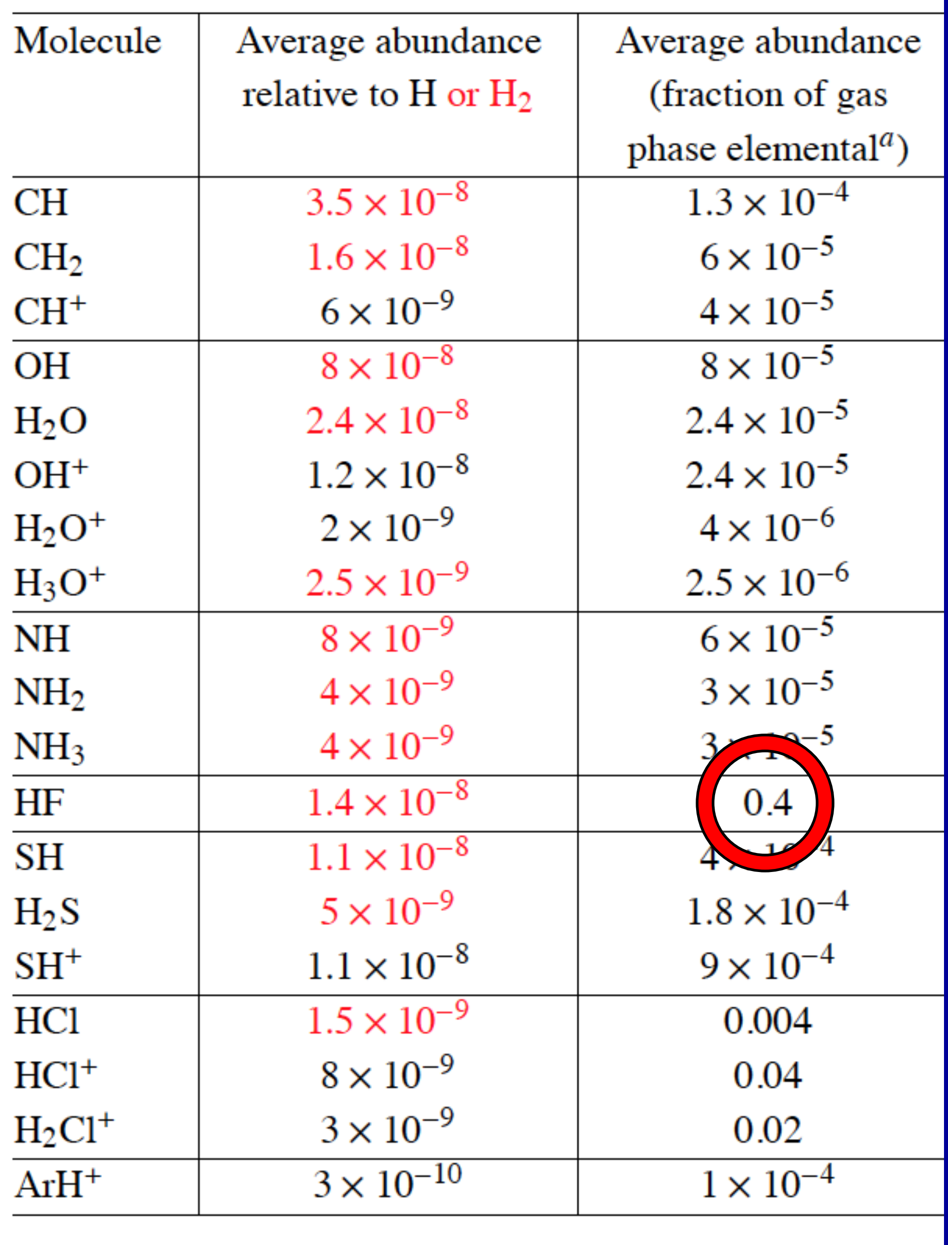
HF is rapidly produced by the exothermic reaction

$HF + H_2 \rightarrow HF + H$ and only slowly destroyed

It is a major reservoir of F wherever H_2 is abundant

Hydrides in the diffuse interstellar medium

First diffuse ISM detection obtained in the past five years



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H_3O^+	2.5×10^{-9}	2.5×10^{-6}
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SH^+	1.1×10^{-8}	9×10^{-4}
HCl	1.5×10^{-9}	0.004
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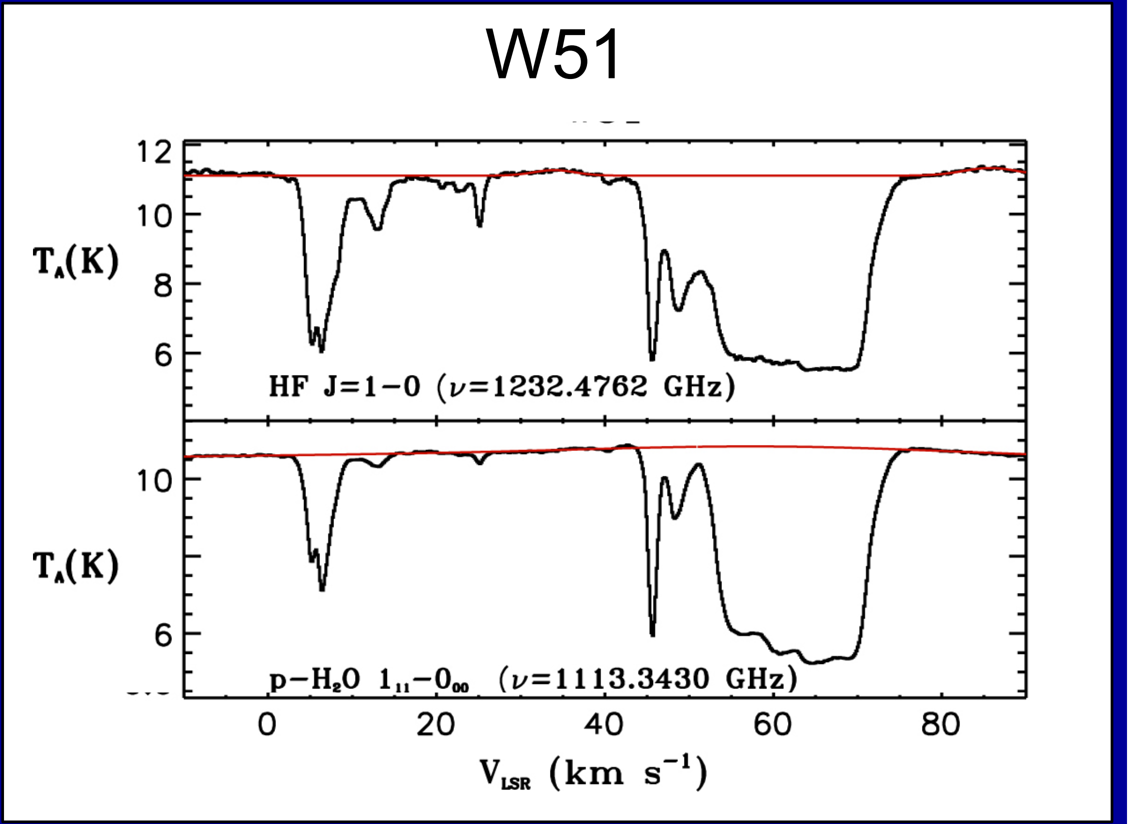
Gerin et al, ARAA 2016

Herschel has provided an extensive database of HF $J = 1 – 0$ spectra

Recent study by Sonnentrucker et al. 2015, ApJ

→HF observed in 47 diffuse clouds in the disk

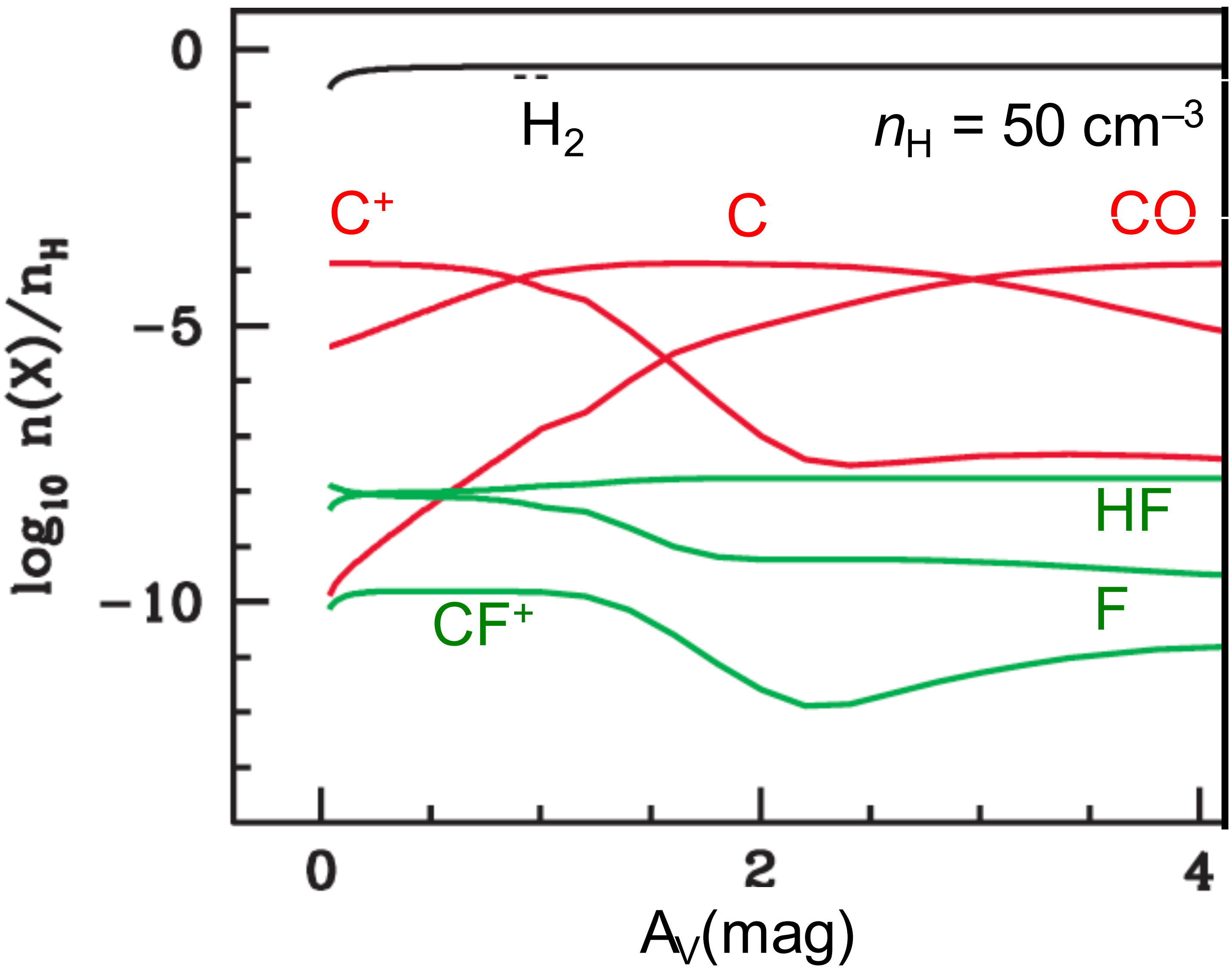
Remarkably, the optical depth for HF is typically larger than that for H_2O, even though the elemental abundance of fluorine is 10^4 times smaller than that of oxygen



$\tau(HF) / \tau(p–H_2O) \sim 2$

➔ $N(HF) / N(H_2O) \sim 0.7$

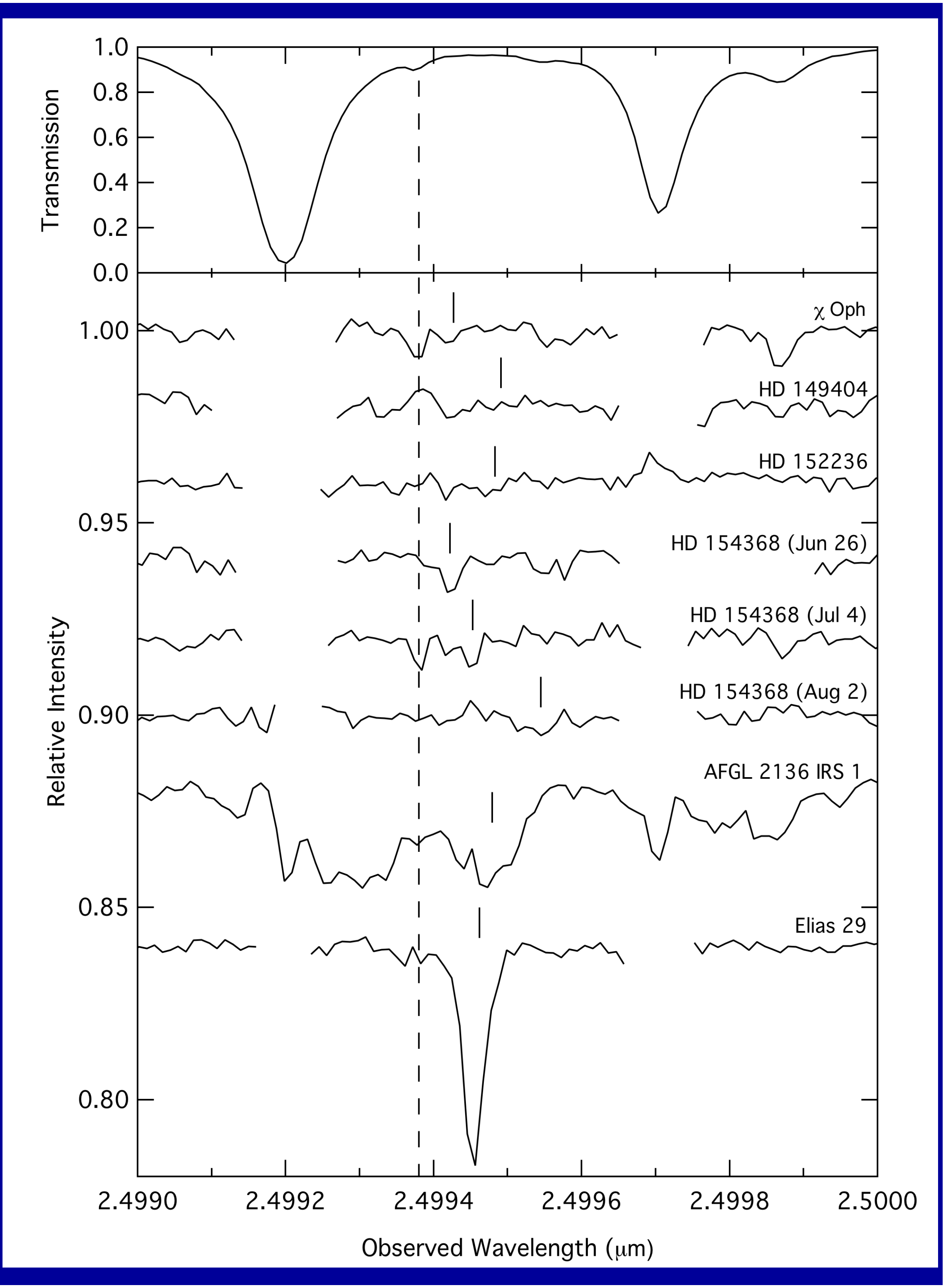
HF is present in CO-dark molecular gas



Neufeld and Wolfire (2009)

Calibrating HF using ground-based near-IR observations from VLT

- Indriolo et al. (2012) observed the v = 1 – 0 vibrational band of HF at 2.5 μm
- Detected in 3 sources where we have direct measurements of H_2 (in UV or near-IR): Elias 29, AFGL 2136, **HD 154368**
- Diffuse ISM abundance **~ 1.2 x 10^{-8} ~ 40% of fluorine** in excellent agreement with astrochemical models



CH^+, SH^+ and SH as probes of "warm chemistry"

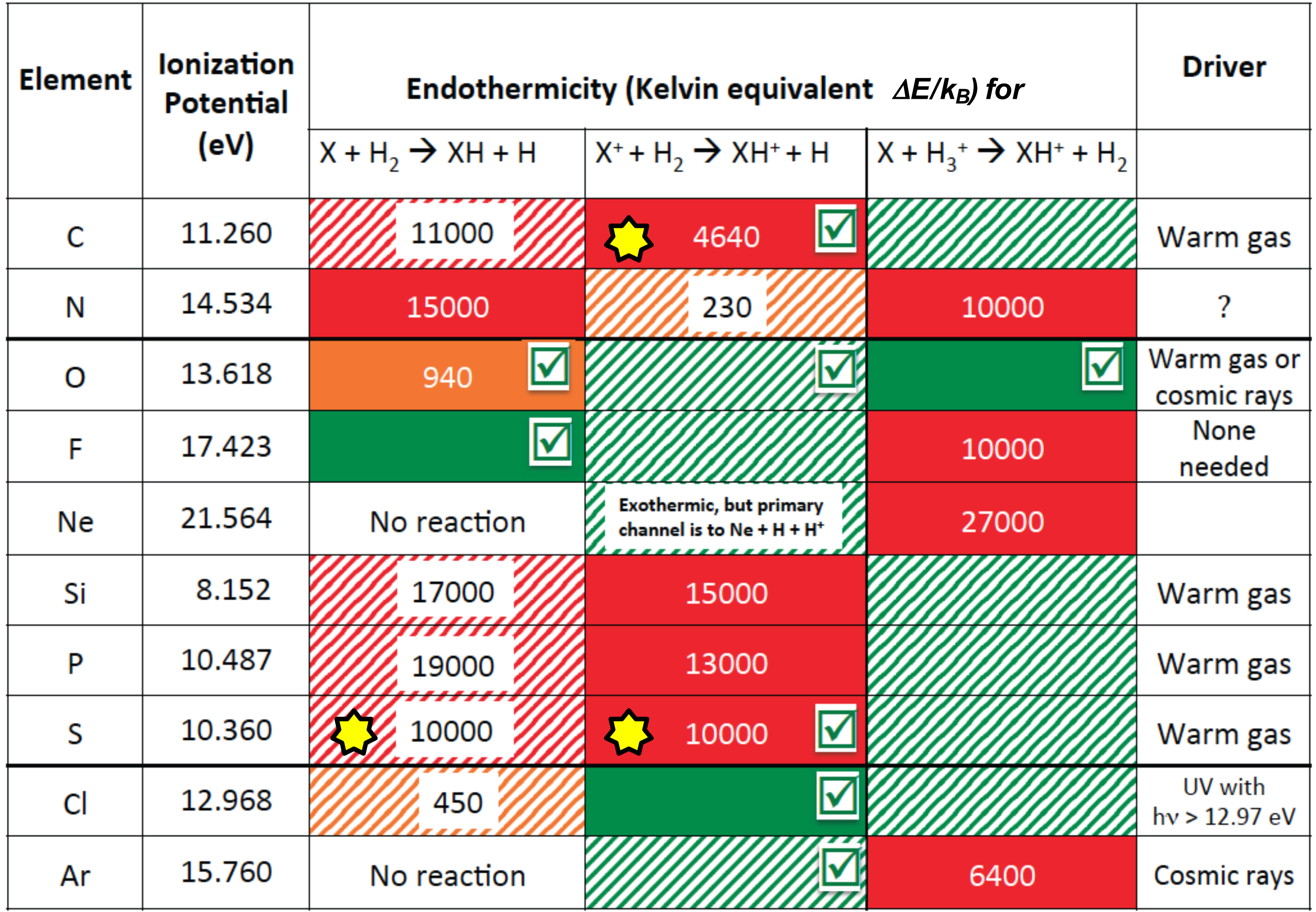
- Neither of C^+, S^+ nor S can react exothermically with $H_{2,}$ but have reaction endothermicities of 4640K, 10^4 K and 10^4K respectively

- Observed CH^+, SH^+ and SH abundances are much greater than what would be expected at the average temperature of the diffuse ISM (Godard et al. 2012; Neufeld et al. 2015)

→ Evidence for ion-neutral drift or elevated temperatures in material affected by shocks or the dissipation of turbulence.

Thermochemistry for different elements

☑ Important formation pathway



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C	11.260	11000	★ 4640 ☑	▨	Warm gas
N	14.534	15000	230	10000	?
O	13.618	940 ☑	▨ ☑	🟩 ☑	Warm gas or cosmic rays
F	17.423	🟩 ☑	▨	10000	None needed
Ne	21.564	No reaction	**Exothermic, but primary channel is to $Ne + H + H^+$**	27000	
Si	8.152	17000	15000	▨	Warm gas
P	10.487	19000	13000	▨	Warm gas
S	10.360	★ 10000	★ 10000 ☑	▨	Warm gas
Cl	12.968	450	🟩 ☑	▨	UV with hν > 12.97 eV
Ar	15.760	No reaction	▨ ☑	6400	Cosmic rays

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- Neither of C^+, S^+ nor S can react exothermically with H_2, but have reaction endothermicities of 4640, 10^4 and 10^4K respectively

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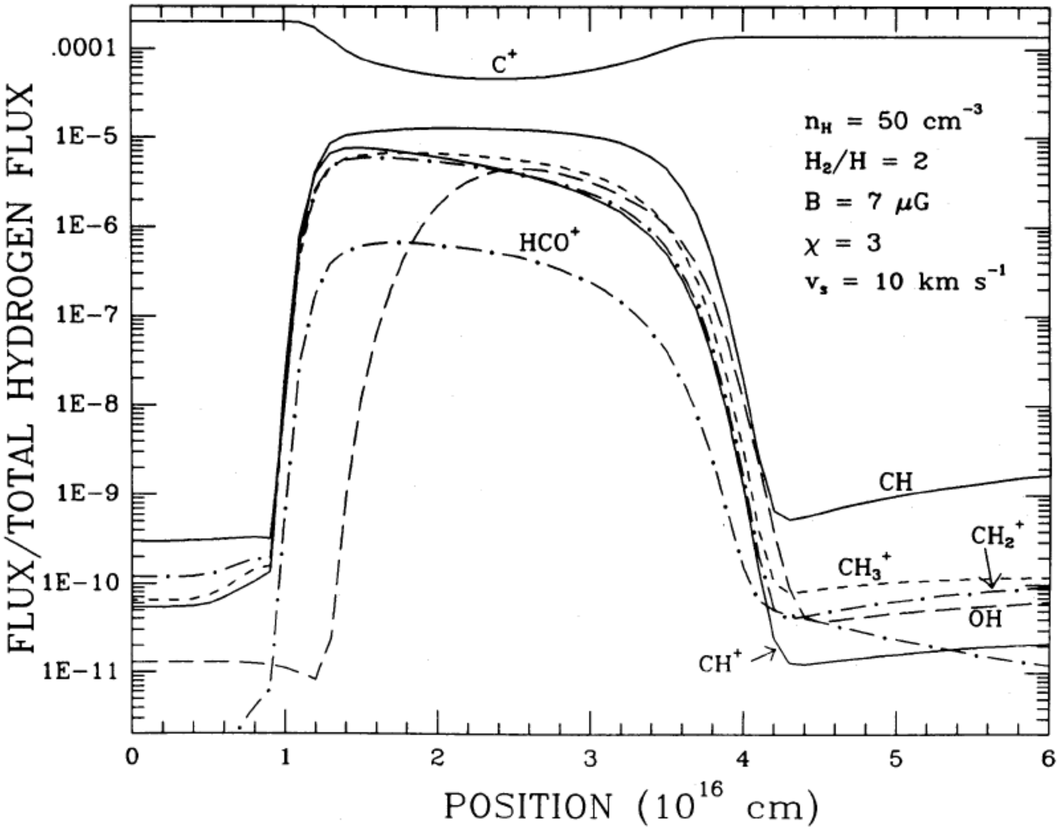
→ Evidence for ion-neutral drift or elevated temperatures in material affected by shocks or the dissipation of turbulence.

CH^+, SH^+ and SH as probes of “warm chemistry”

The abundance of CH^+ has long been recognized as anomalous, but recent observations of SH^+ and SH corroborate the presence of a ubiquitous “warm chemistry.”



CH^+ prediction

Draine and Katz1986, ApJ

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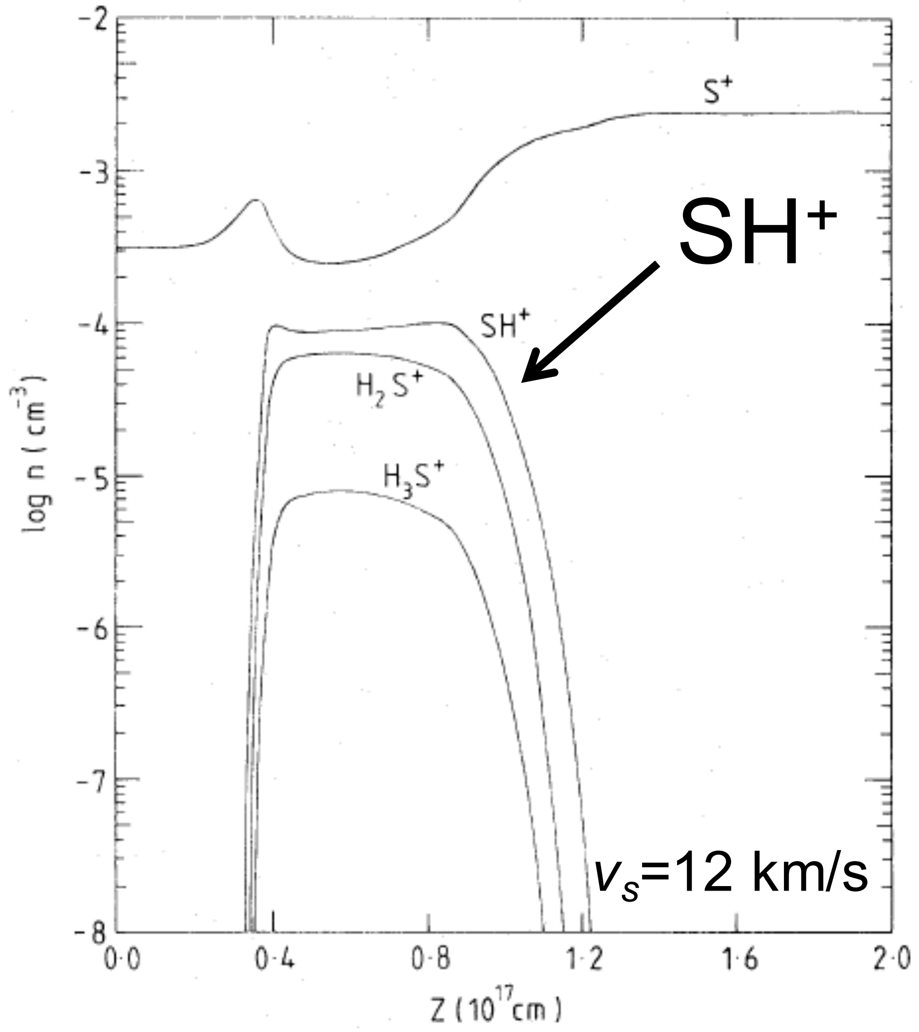

Pineau des Forets et al. 1986, MNRAS

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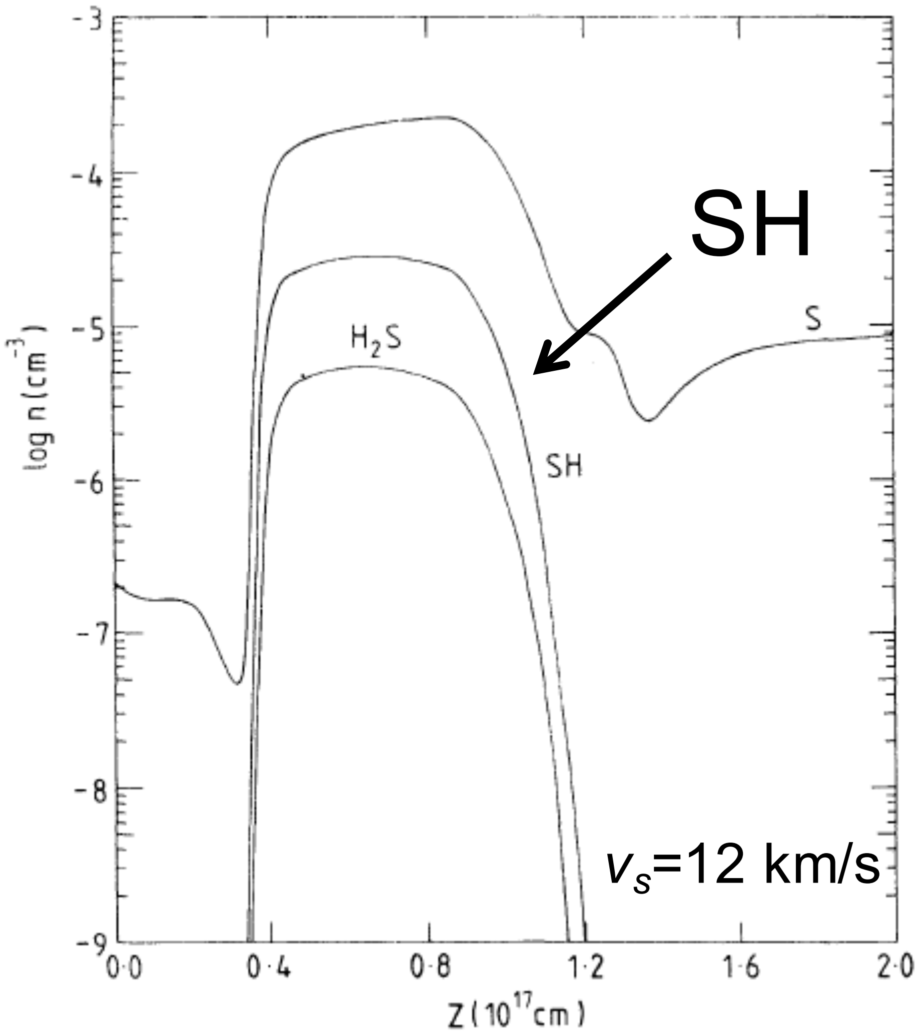


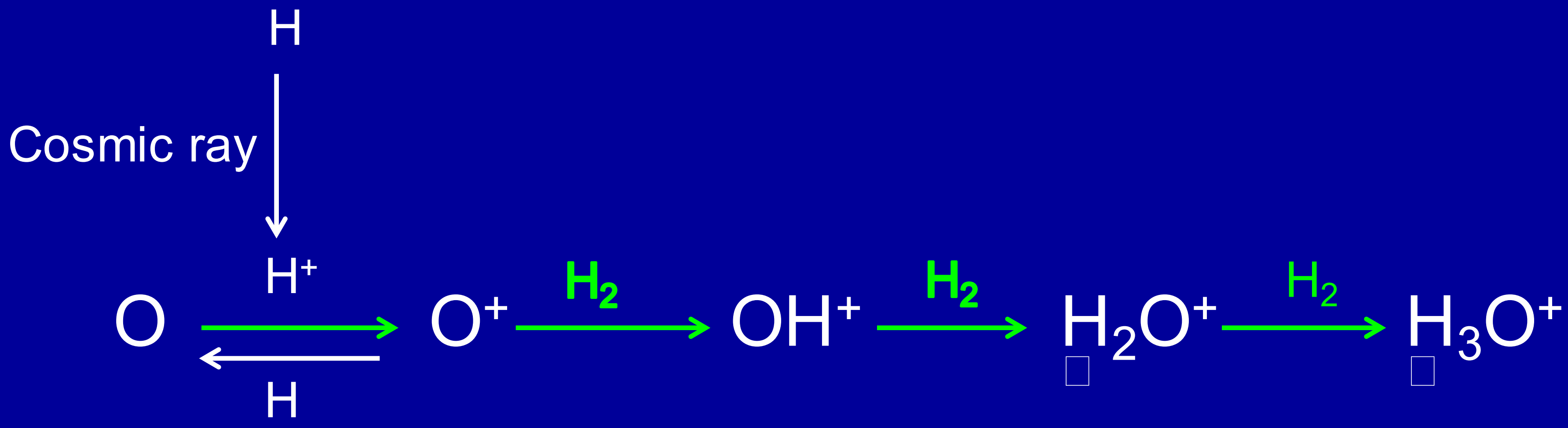
SH

v_s=12 km/s

Pineau des Forets et al. 1986, MNRAS

Measuring the cosmic-ray ionization rate with OH^+ and H_2O^+

Unlike C^+ and S^+, O^+ does react with H_2 at low temperature. But O is not ionized by UV radiation longward of the Lyman limit, so OH^+ and H_2O^+ formation must be initiated by cosmic ray ionization



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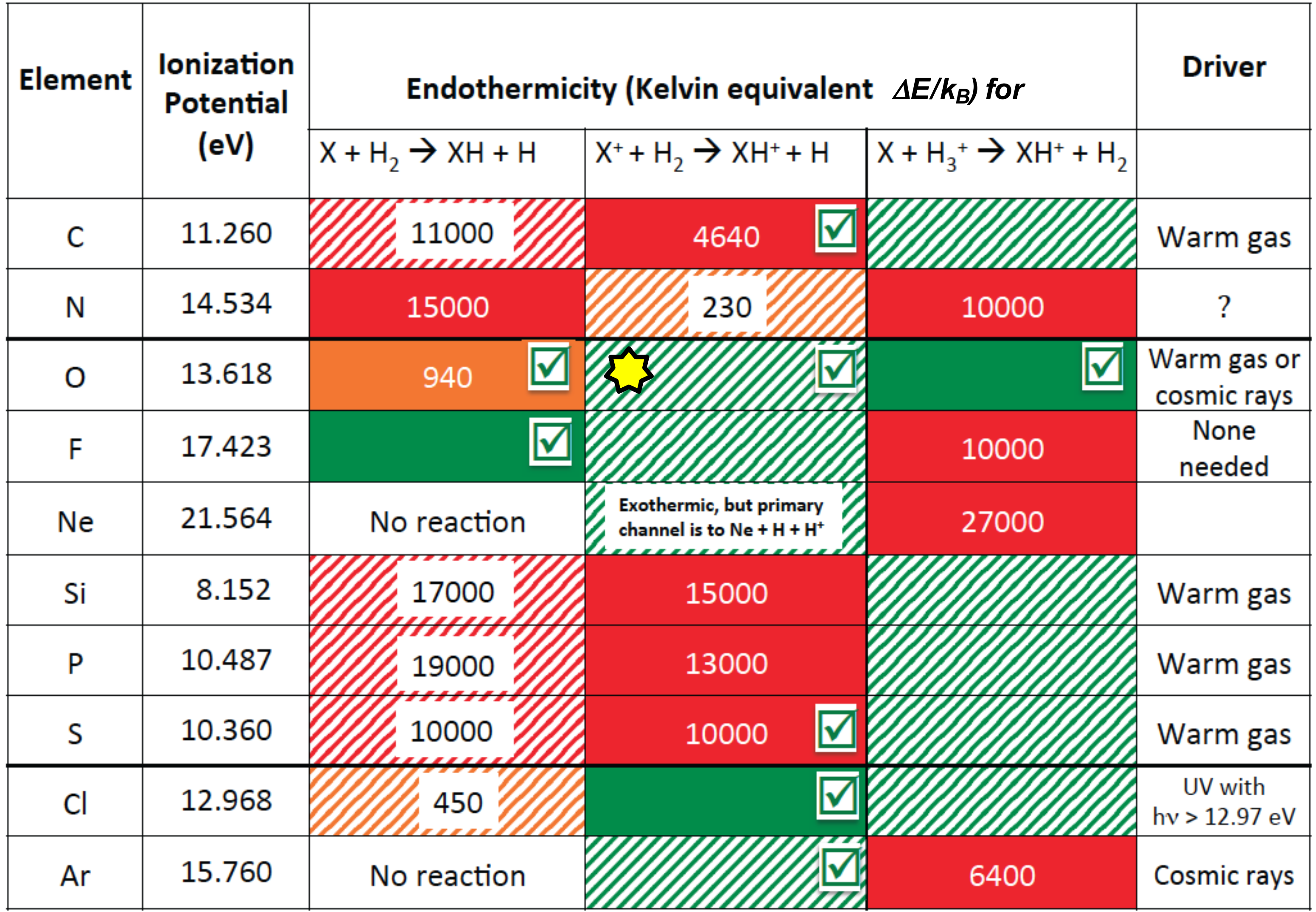

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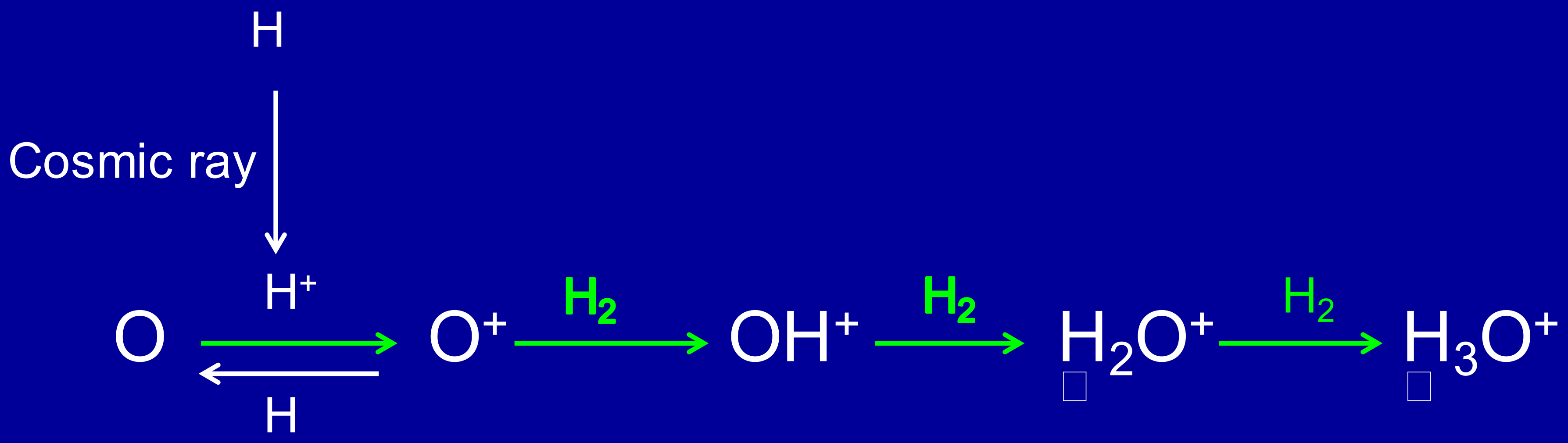


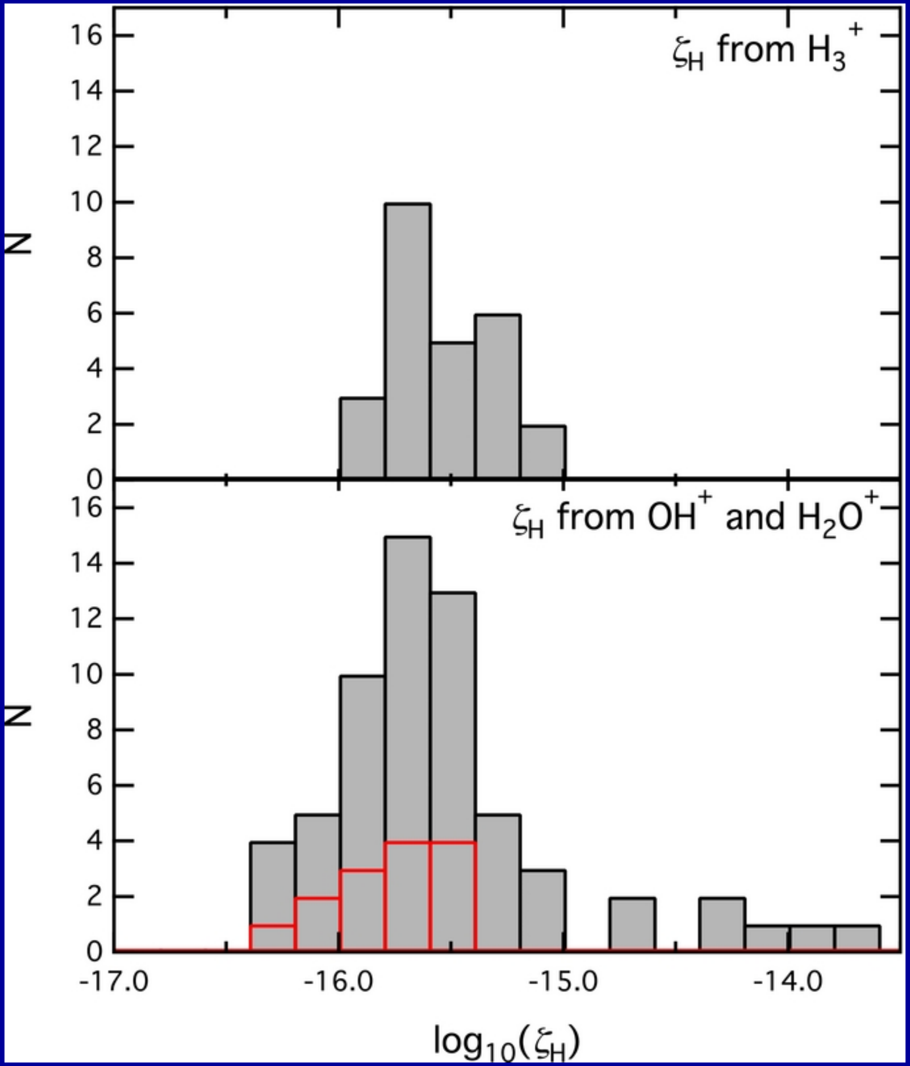
$$\mathrm{H} \xrightarrow{\text{Cosmic ray}} \mathrm{H}^+$$

$$\mathrm{O} \underset{\mathrm{H}}{\overset{\mathrm{H}^+}{\rightleftarrows}} \mathrm{O}^+ \xrightarrow{\mathrm{H}_2} \mathrm{OH}^+ \xrightarrow{\mathrm{H}_2} \mathrm{H}_2\mathrm{O}^+ \xrightarrow{\mathrm{H}_2} \mathrm{H}_3\mathrm{O}^+$$

Measuring the cosmic-ray ionization rate with OH^+ and H_2O^+

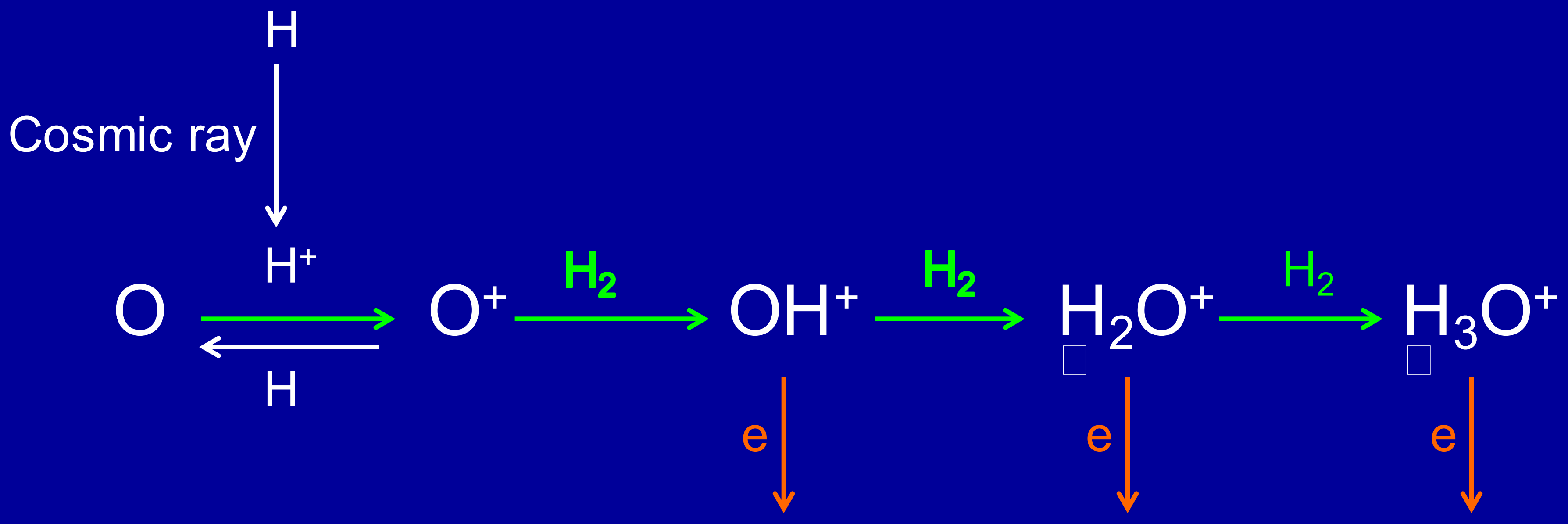
OH^+ and H_2O^+ abundances measured by Herschel/HIFI allow the CR ionization rate to be measured. Indriolo et al. (2015) surveyed OH^+ and H_2O^+ in ~ 100 diffuse clouds

Confirm typical ionization rates ~ 2 x 10^{-16} s^{-1} inferred from recent H_3^+ observations (which are ~ 10 times the "canonical value" assumed previously)



Determining the molecular fraction in the diffuse ISM

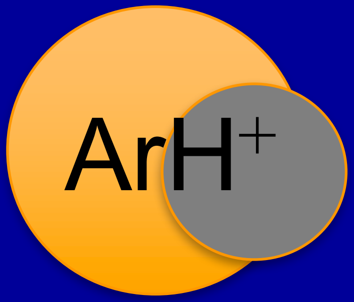
The OH^+/H_2O^+ ratio reflects a competition between reaction of OH^+ with H_2 and reaction with electrons



$$\begin{tikzcd}
H \arrow[d, "\text{Cosmic ray}"'] & & & & \\
H^+ & & & & \\
O \arrow[r, shift left, "H^+"] & O^+ \arrow[l, shift left, "H"] \arrow[r, "H_2"] & OH^+ \arrow[r, "H_2"] \arrow[d, "e"'] & H_2O^+ \arrow[r, "H_2"] \arrow[d, "e"'] & H_3O^+ \arrow[d, "e"'] \\
 & & {} & {} & {}
\end{tikzcd}$$

Observed OH^+/H_2O^+ ratios ~ 3 to 15 imply that only 2 – 10 % of the H is typically in H_2

Other molecules provide additional probes of the H_2 fraction



Argonium: the first known interstellar molecule containing a noble gas atom

Other molecules provide additional probes of the H_2 fraction

Argonium (ArH^+) has been widely observed in the diffuse ISM through its 617 GHz $J = 1 – 0$ absorption line (identified by Barlow et al. 2013 only several years after it was first detected)

It is rapidly destroyed by H_2 in the reaction

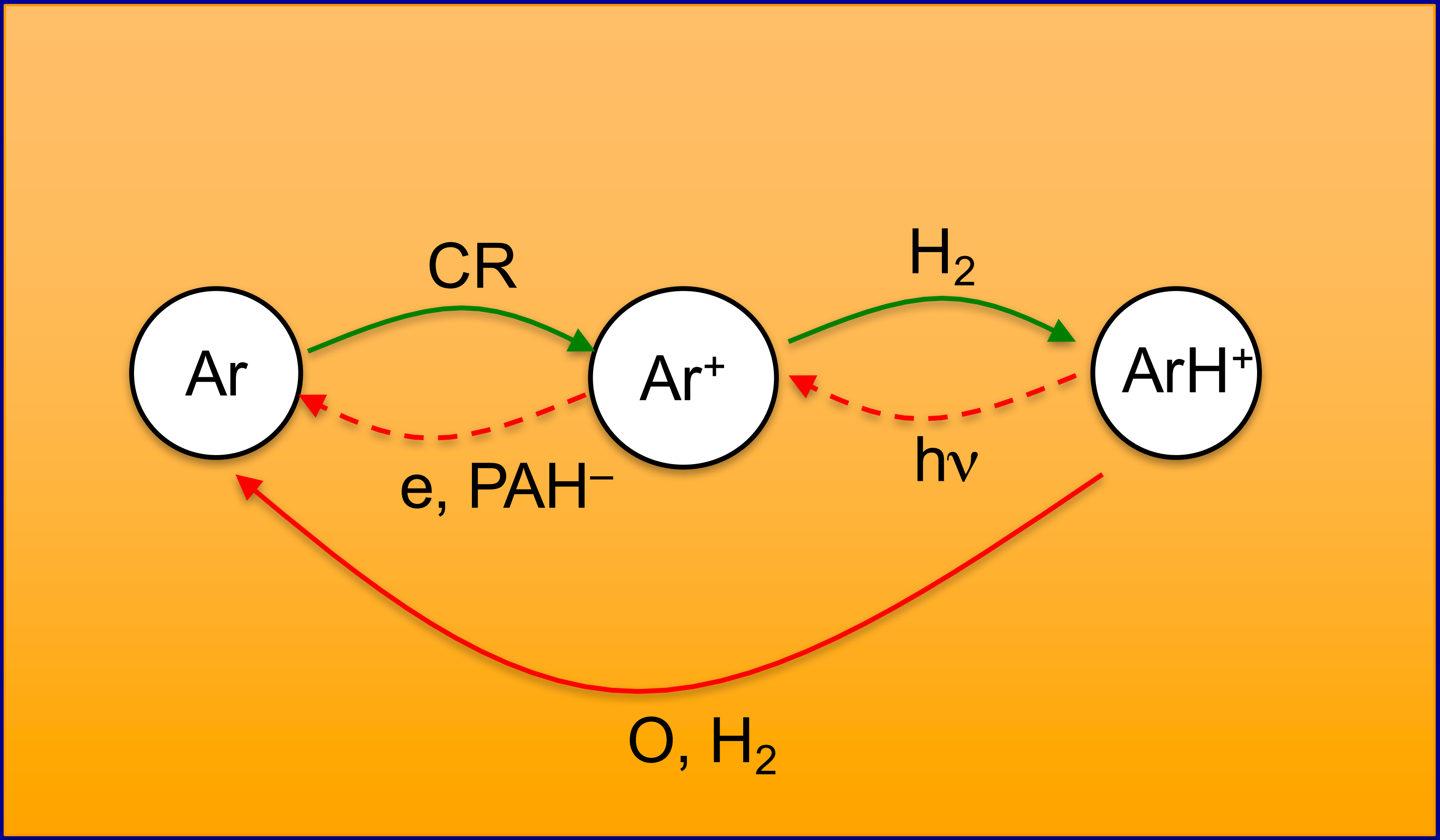
$$ArH^+ + H_2 \rightarrow Ar + H_3^+$$

and attains its maximum abundance when

$f_{H2} = 2n(H_2) / [2n(H_2) + n(H)] \sim 10^{-4}$

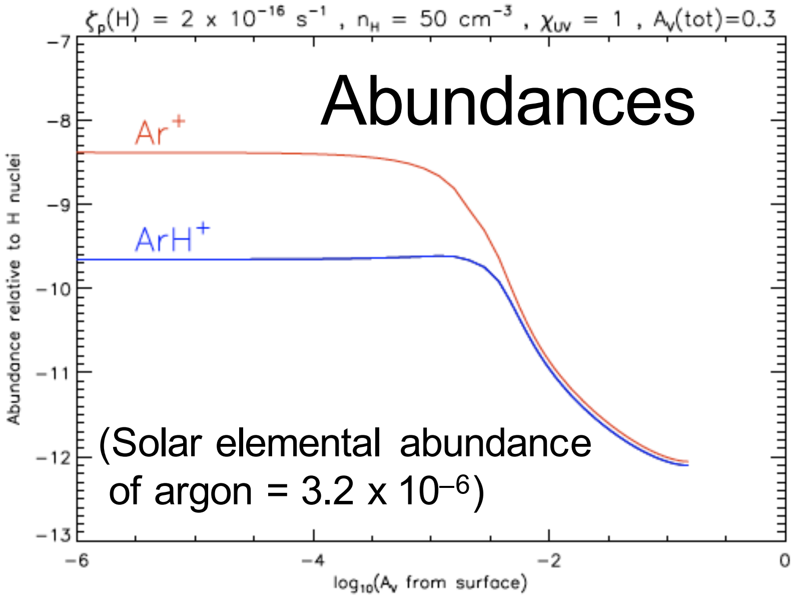
A molecular tracer of *almost purely atomic* gas

Argon chemistry



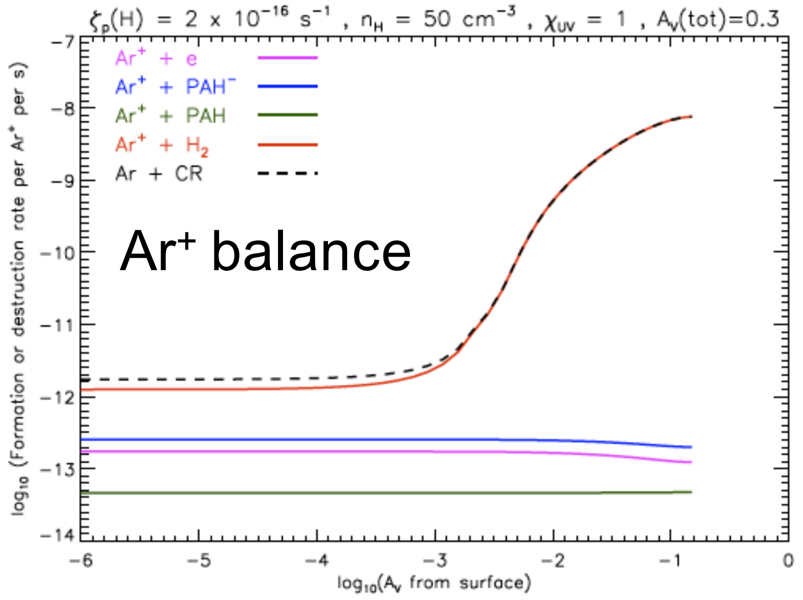
- If $n(H_2)/n_H > 10^{-5}$, almost every ionization of Ar leads to ArH^+
- Destruction of ArH^+ is usually dominated by reaction with O or H_2

Diffuse cloud model results (with Mark Wolfire)

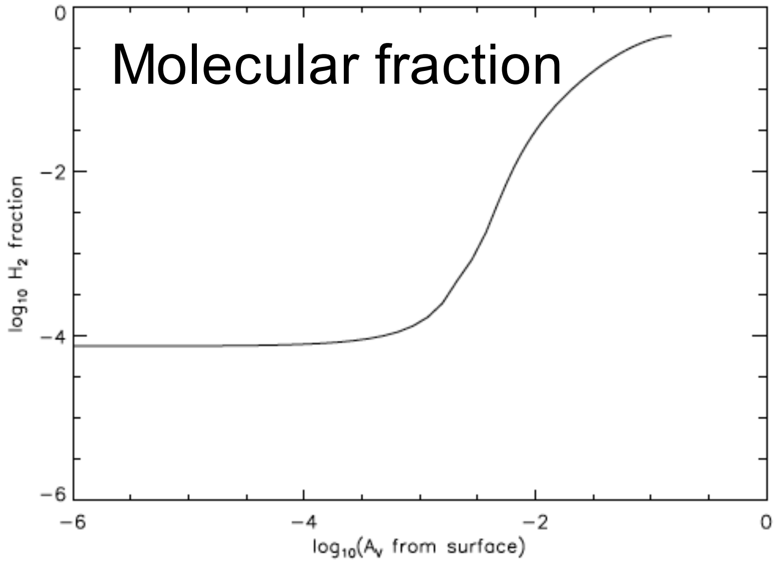


Abundances

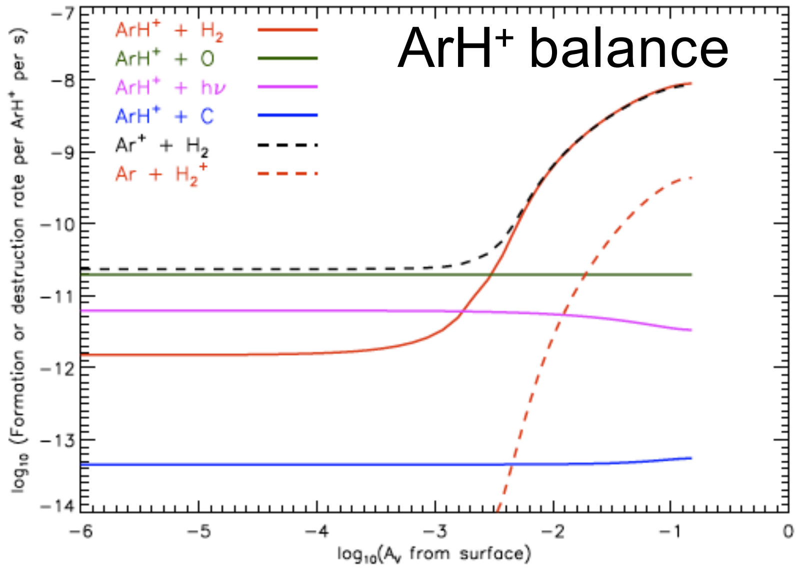
(Solar elemental abundance of argon = 3.2×10^{-6})



Ar^+ balance

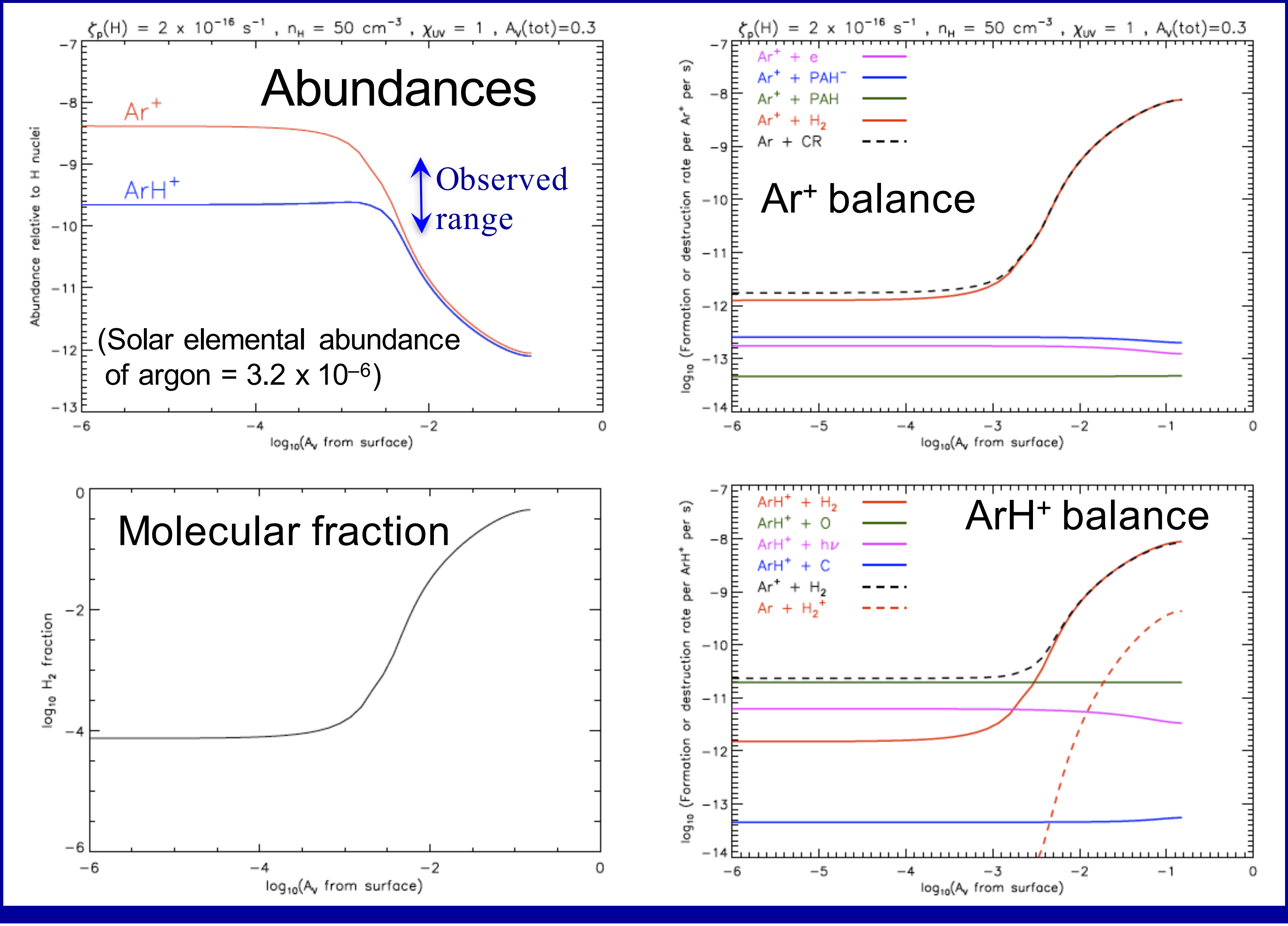


Molecular fraction



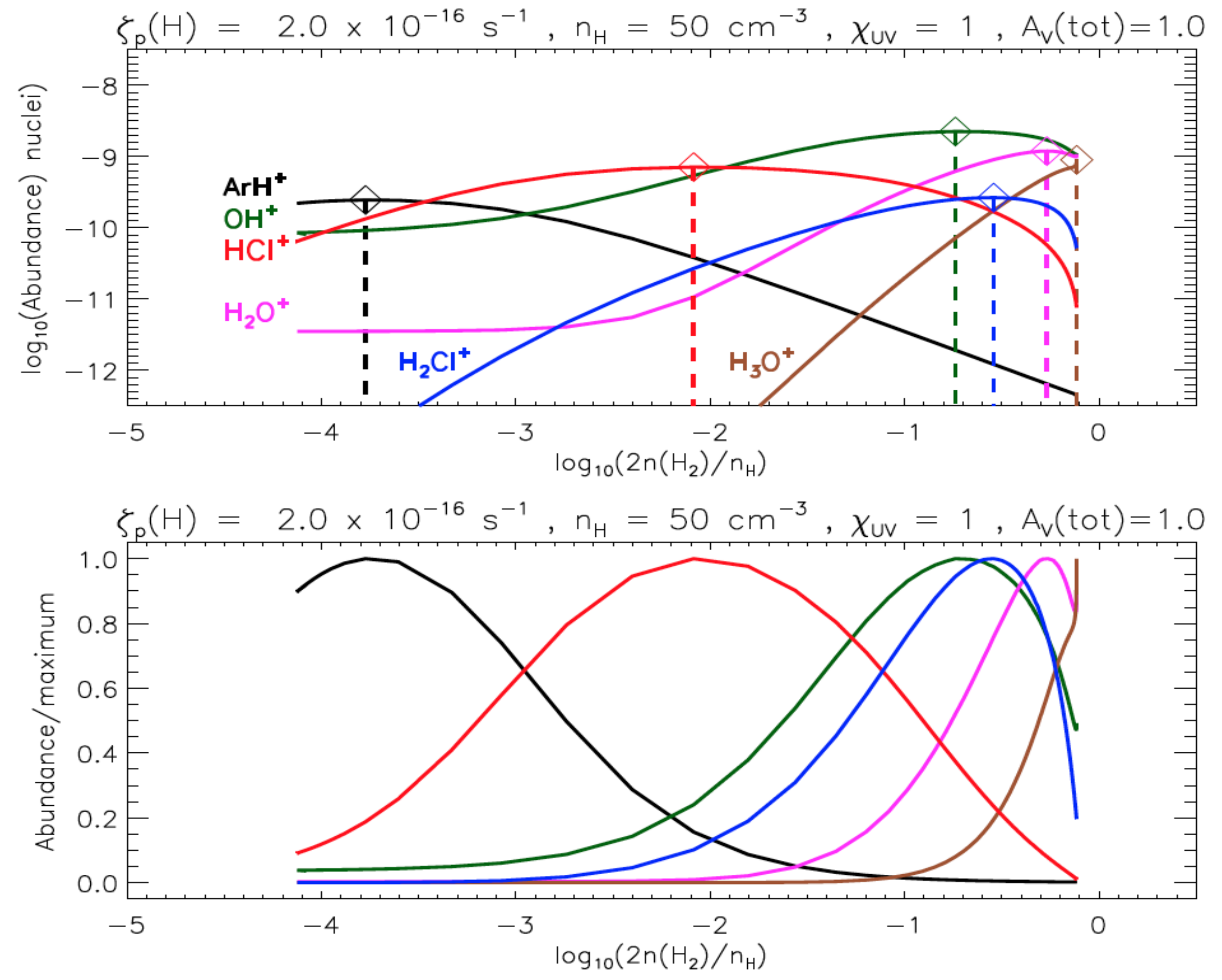
ArH^+ balance

Diffuse cloud model results (with Mark Wolfire)



A combination of molecular ions could constrain the distribution function for f_{H2}

Model predictions
(Neufeld & Wolfire, 2016, ApJ)



Summary: what we've learned from recent molecular observations of the diffuse ISM

- A substantial component of the diffuse ISM has a small H_2 fraction (few % or less)
- "Warm chemistry" (e.g. due to turbulent dissipation in shocks) is ubiquitous (and must be warm enough to produce SH and SH^+)
- The cosmic-ray ionization rate is confirmed to have a typical value of 2×10^{-16} s^{-1} in the diffuse ISM, an order of magnitude larger than was believed a decade ago

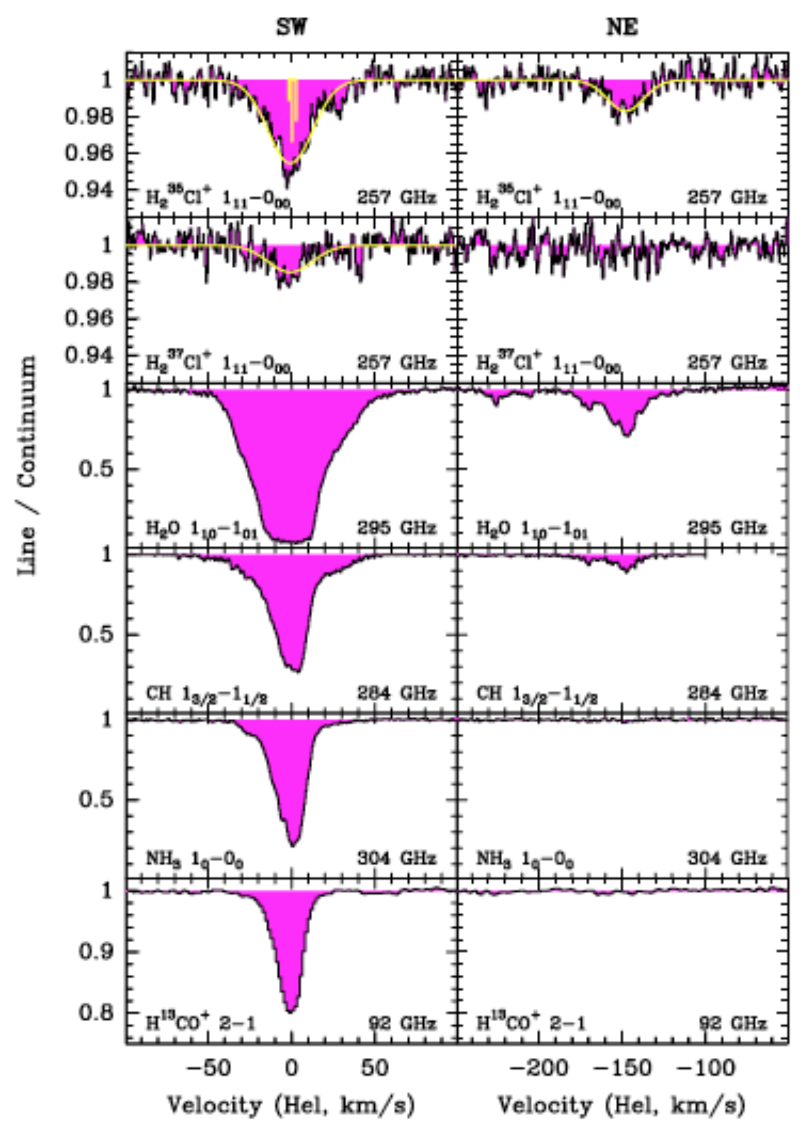
The diffuse ISM: future directions

Herschel’s helium ran out in April 2013. What’s next for spectroscopic studies of the neutral diffuse ISM?

APEX → ALMA: vastly improved sensitivity, that will facilitate observations of hydrides at high-z (including those that cannot be observed from the ground at z = 0)

Example (right): H_2Cl^+ at $z = 0.89$ with ALMA (Muller et al. 2014, A&A)

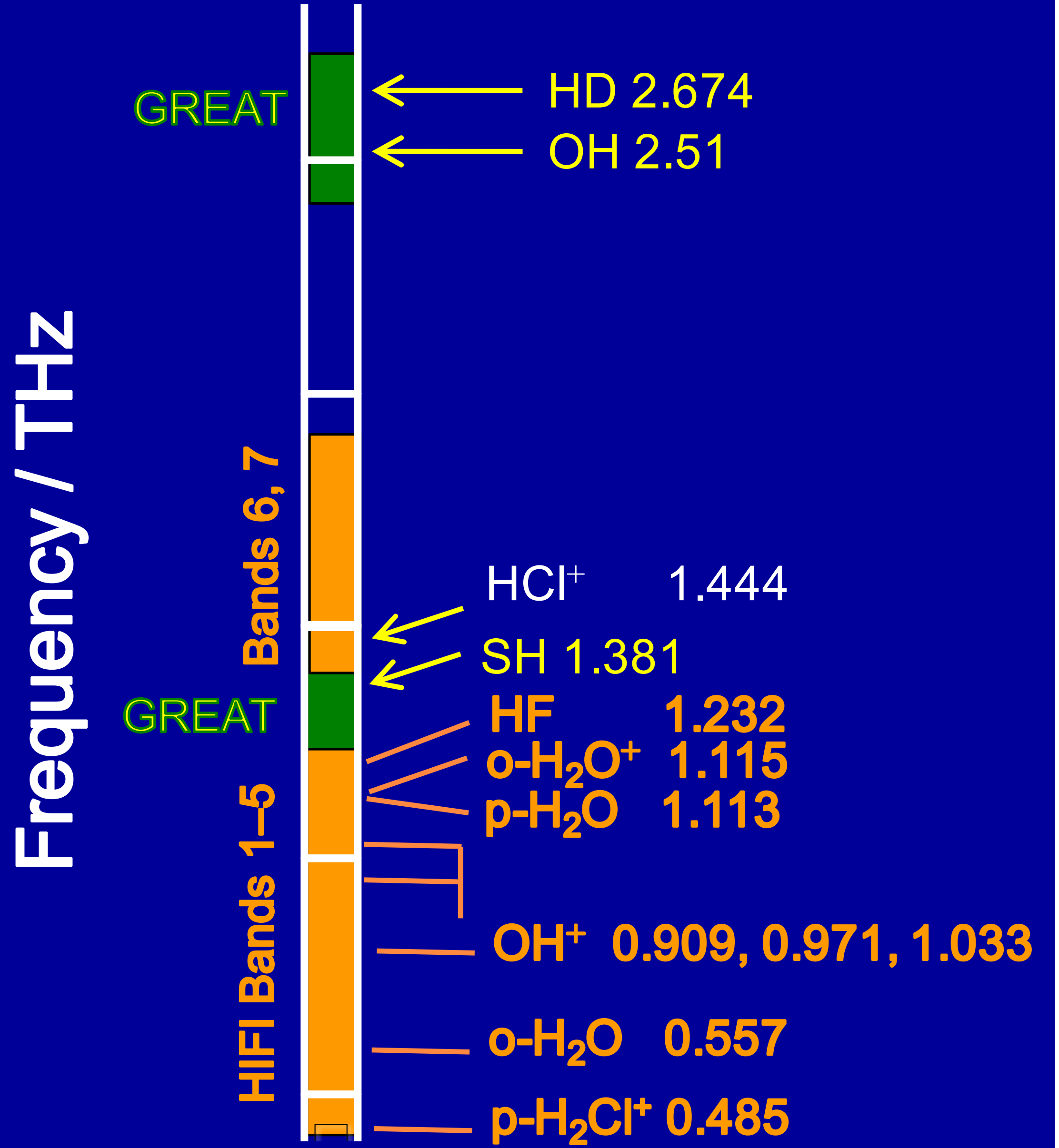
Measured ^{35}Cl/^{37}Cl (found to be the same as in the solar system), a probe of stellar nucleosynthesis



The diffuse ISM: future directions

SOFIA: heterodyne spectroscopy at frequencies inaccessible with Herschel

Future instrumentation may allow access to frequencies below 1.25 THz that were previously covered by HIFI but are unobservable from the ground



HD 2.674

OH 2.51

HCl^+ 1.444

SH 1.381

HF 1.232

o-H_2O^+ 1.115

p-H_2O 1.113

OH^+ 0.909, 0.971, 1.033

o-H_2O 0.557

p-H_2Cl^+ 0.485

Outline

- Introduction: the rich chemistry of the interstellar medium
- Probing the diffuse ISM with small hydride molecules
- Determining the “oxygen budget” in the dense ISM

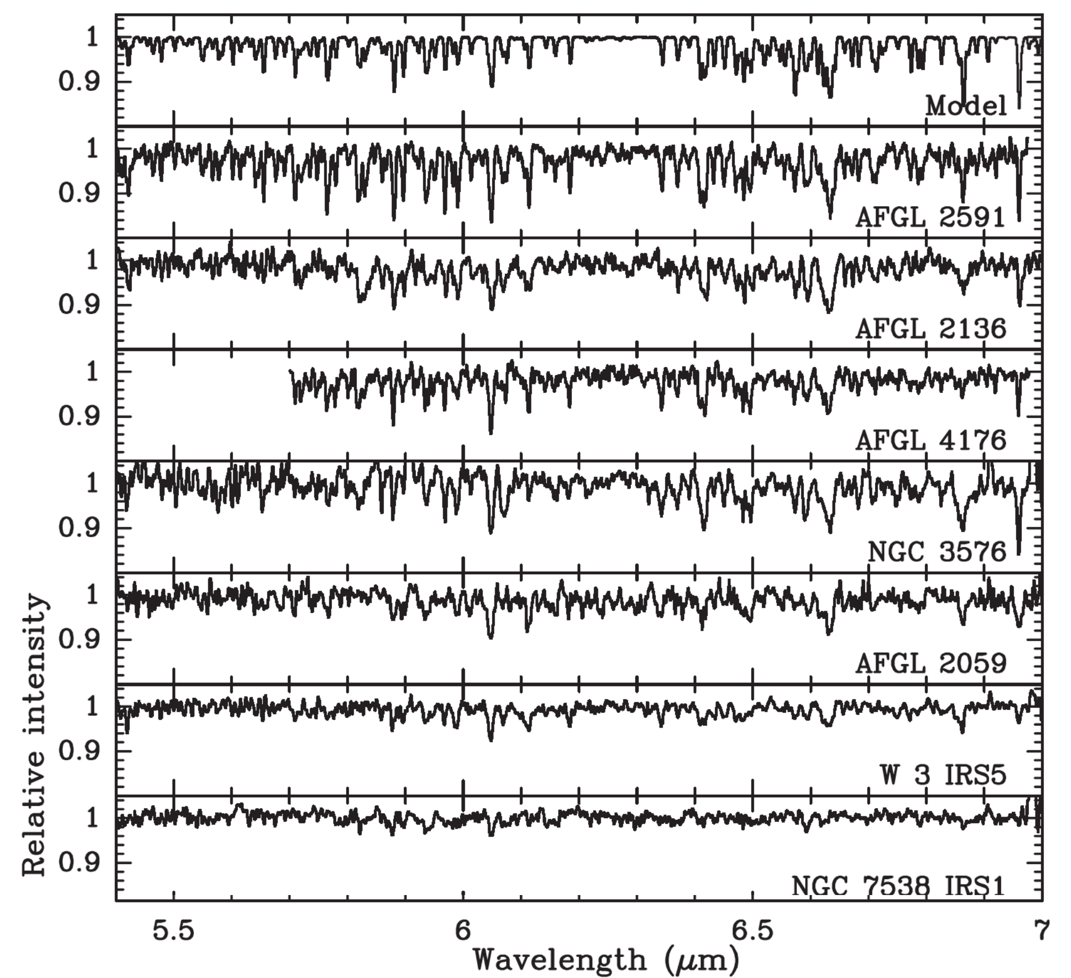
Water around deeply-embedded massive protostars

- Water ice is the major constituent of icy grain mantles, accounting for almost 10% of interstellar oxygen nuclei in cold dense clouds

- Close enough to massive protostars, the dust temperature exceeds ~ 100 K, and water ice is vaporized

Water vapor was detected by ISO in absorption toward many massive protostars

- Observations of the 6 μm ν_2 bending mode yielded clear detections of water vapor in 7 of 11 sources observed
- Inferred gas temperatures were 250 – 500 K
- Significant limitation of these observations: spectral resolving power $\lambda/\Delta\lambda \sim 1500$ was insufficient to fully resolve rotational structure

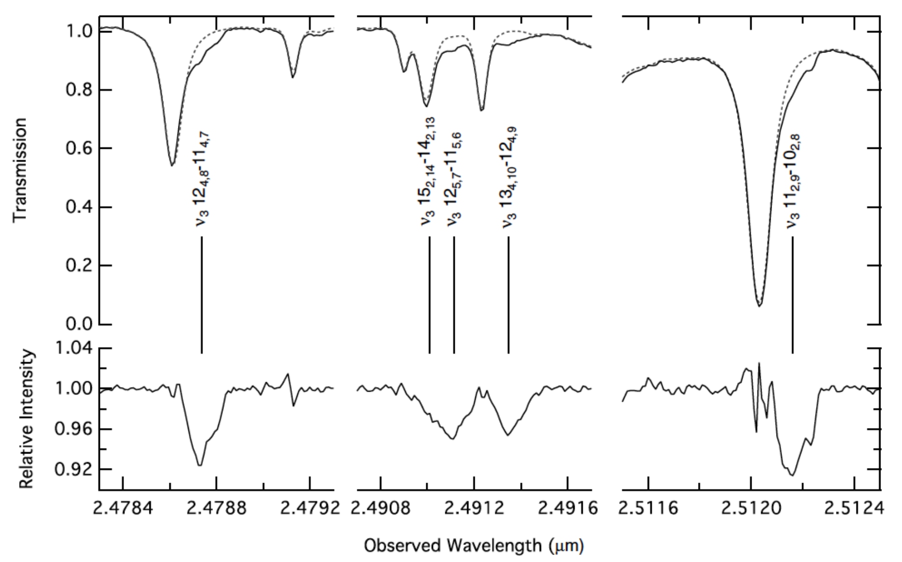


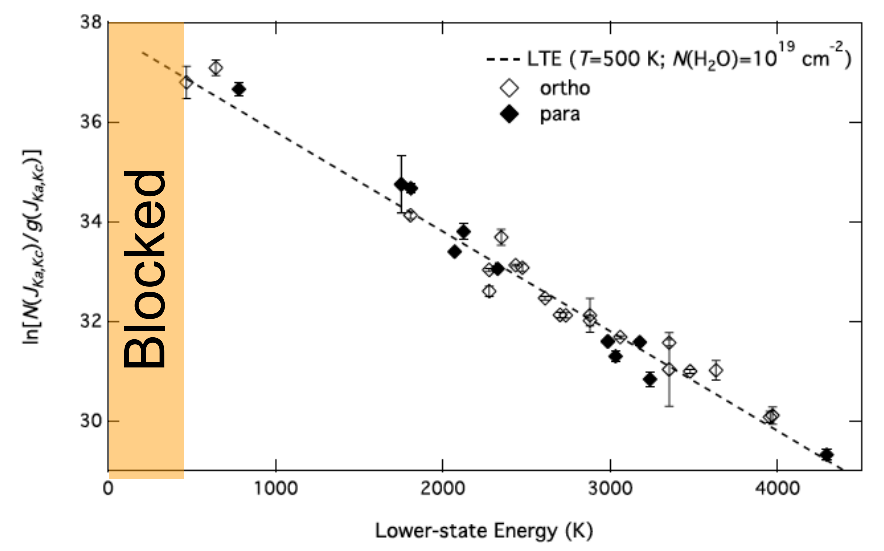
Boonman and van Dishoeck 2003, ApJ

Water vapor was detected at higher spectral resolution from the ground toward AFGL 2136

- Observations near 2.5 μm (in a search for HF) led to the fortuitous detection of 47 rovibrational lines in the ν_1 and ν_3 bands
- Resolving power $\lambda/\Delta\lambda \sim 10^5$

  ➔ rotational structure fully resolved
- Rotational diagram implies
  T = 506 ± 25 K and
  $N(H_2O) = (1.02 \pm 0.02) \times 10^{19}$ cm^{-2}
  (7 times the value inferred from the low resolution ISO spectrum)
- Significant limitation of these observations: atmosphere blocks access to states with $E_L/k < 470$ K





Indriolo et al. 2013, ApJ

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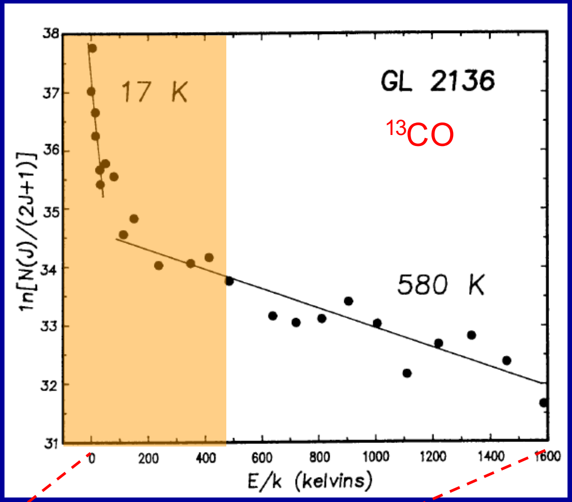
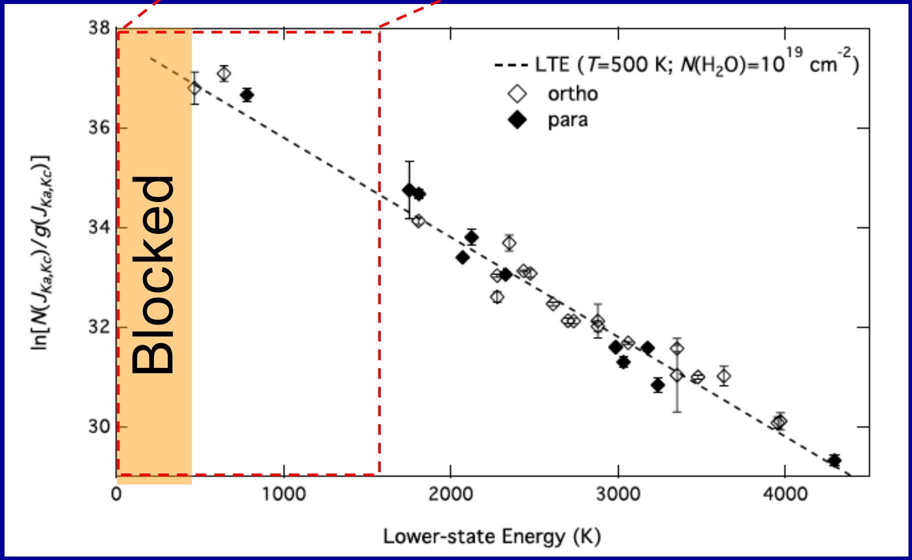
  ➔ no information about water in cold component seen in CO



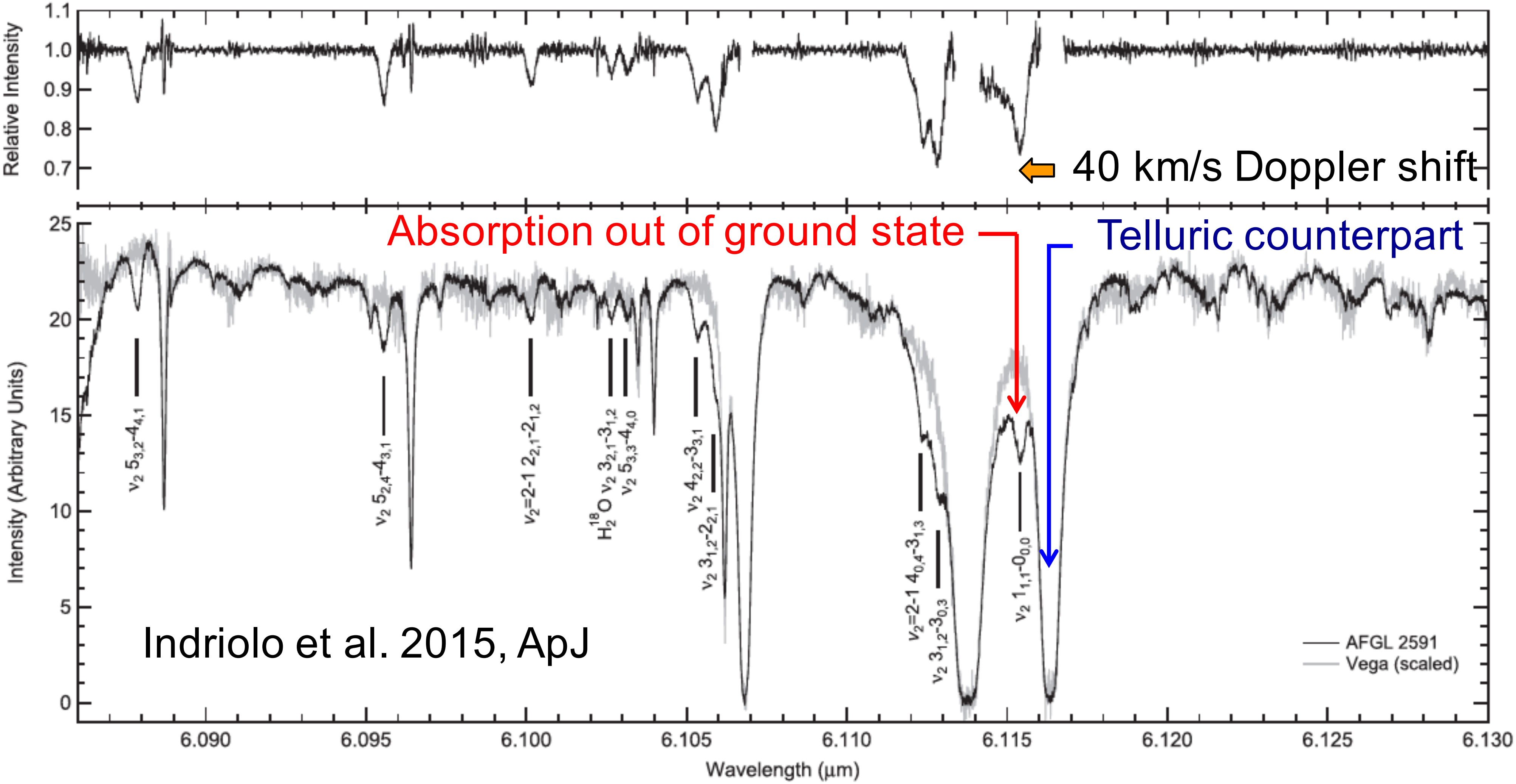
Mitchell et al. 1990, ApJ



Indriolo et al. 2013, ApJ

SOFIA/EXES observations of AFGL 2591

- Observations of the 6.3 μm band are possible from 43,000 ft, and allow even the *ground rotational state* to be observed
- This capability was demonstrated in commissioning phase observations



40 km/s Doppler shift

Absorption out of ground state

Telluric counterpart

Indriolo et al. 2015, ApJ

SOFIA/EXES observations of AFGL 2591

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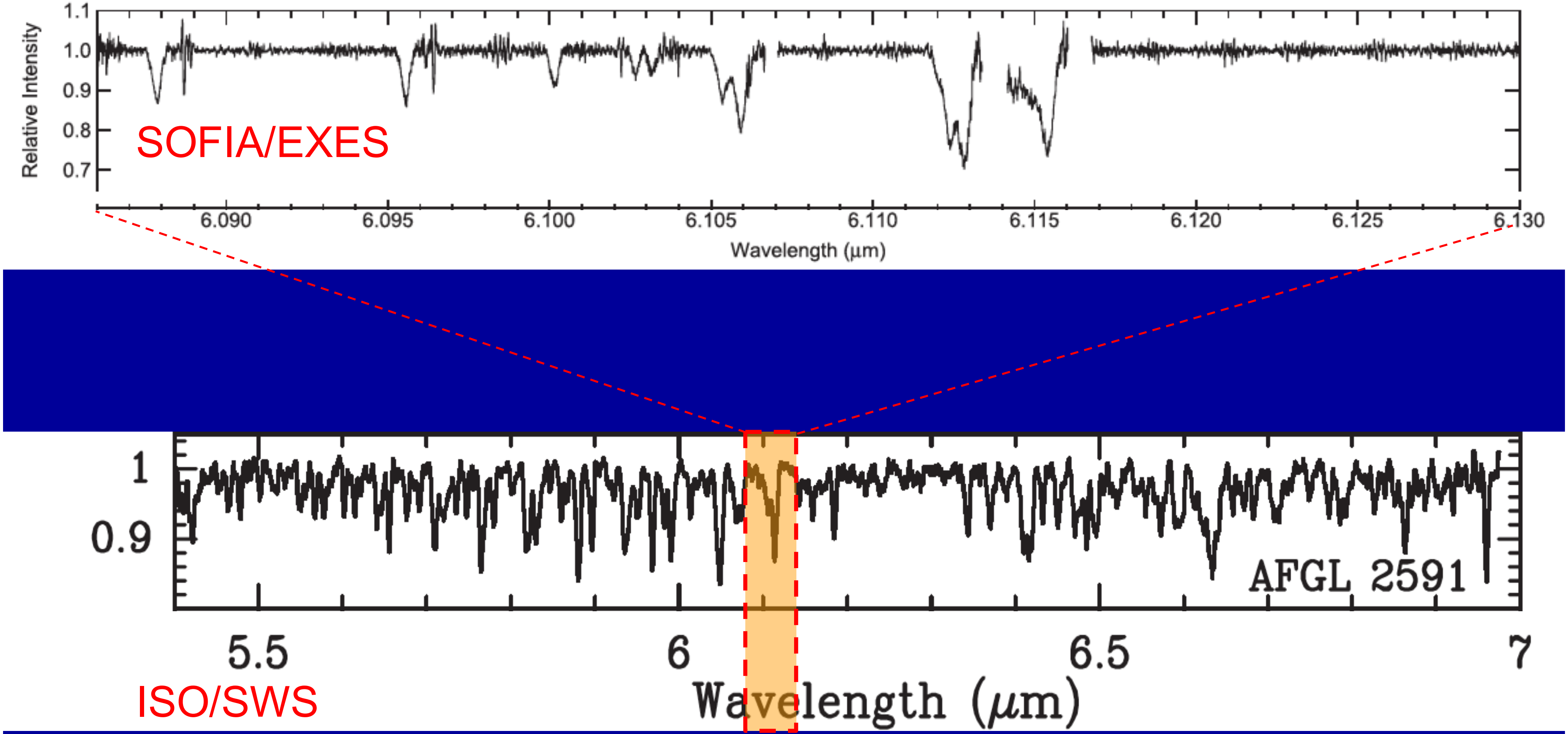


SOFIA/EXES observations of AFGL 2591

- No evidence for cold water component

- In hot component,

  $N(H_2O)/N(^{13}CO) = 35$

  ➔ $N(H_2O)/N(^{12}CO) = 0.58$

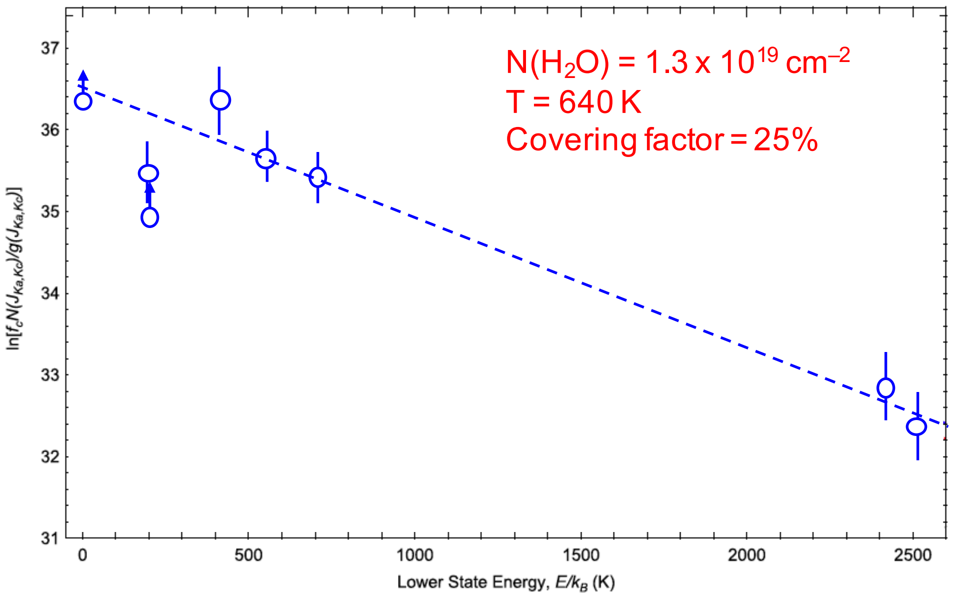
- Similar to result obtained for AFGL 2136

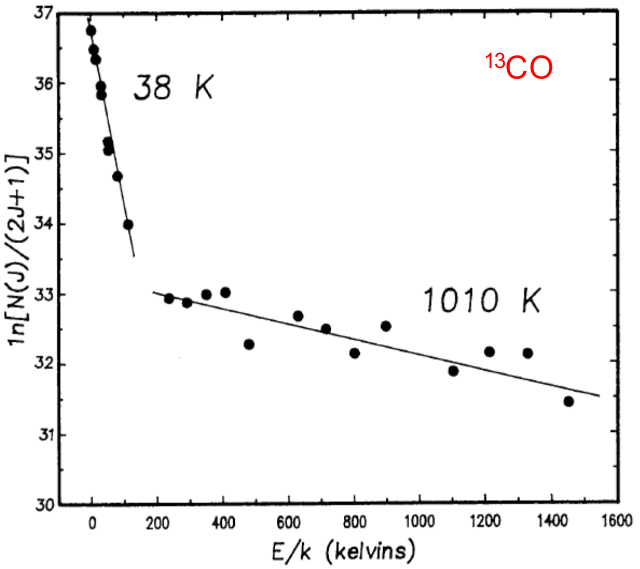
  $N(H_2O)/N(^{13}CO) = 40$

  ➔ $N(H_2O)/N(^{12}CO) = 0.67$

- $N(H_2O)$ is 3 – 4 orders of magnitude larger than that inferred from submm/far-IR Herschel observations

  ➔ probing gas much closer to the protostar

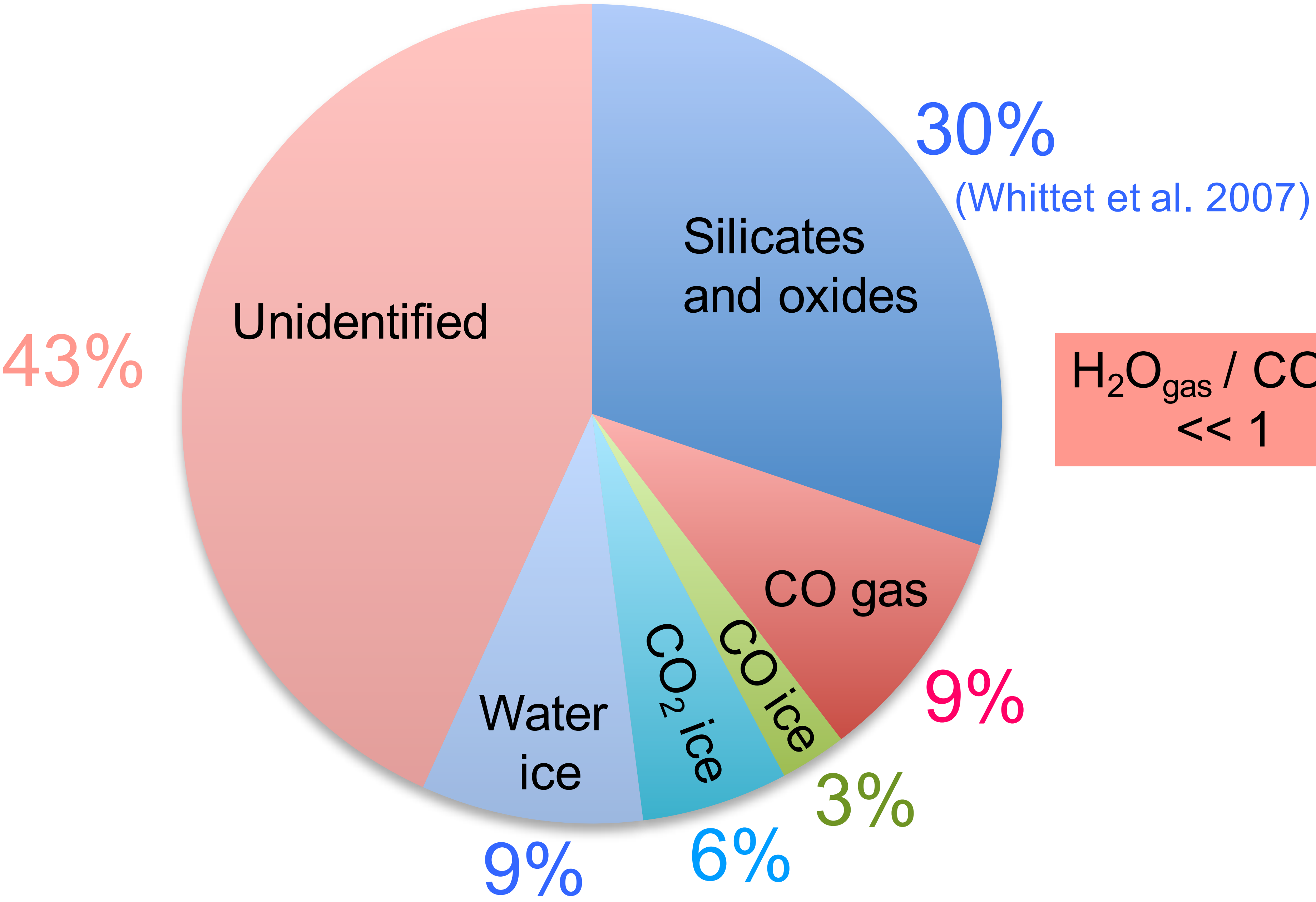




Mitchell et al. 1990, ApJ

Oxygen budget for cold dense ISM

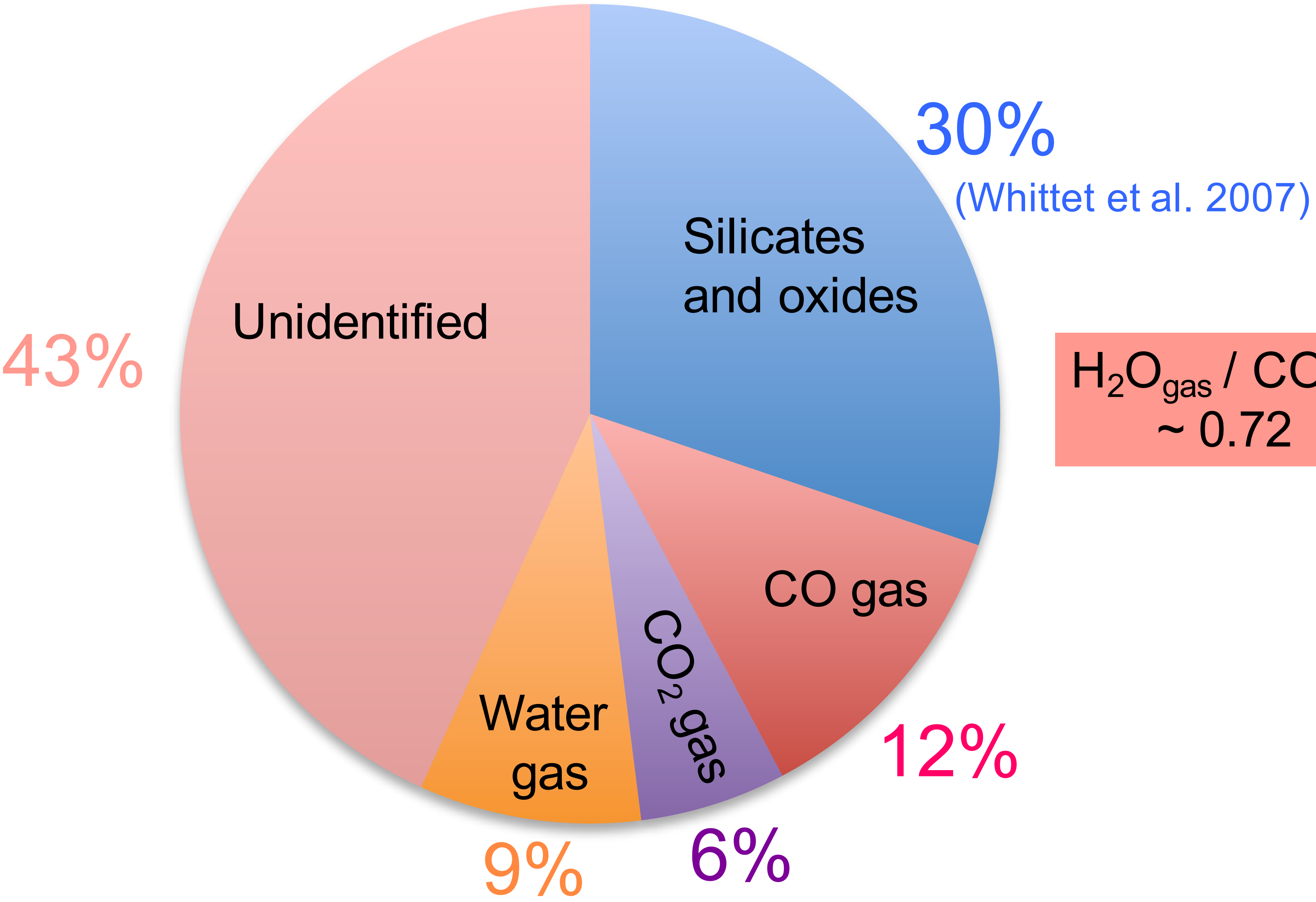
(ices from Boogert et al. 2015 ARAA)



H_2O_{gas} / CO_{gas} << 1

Expected budget near protostar

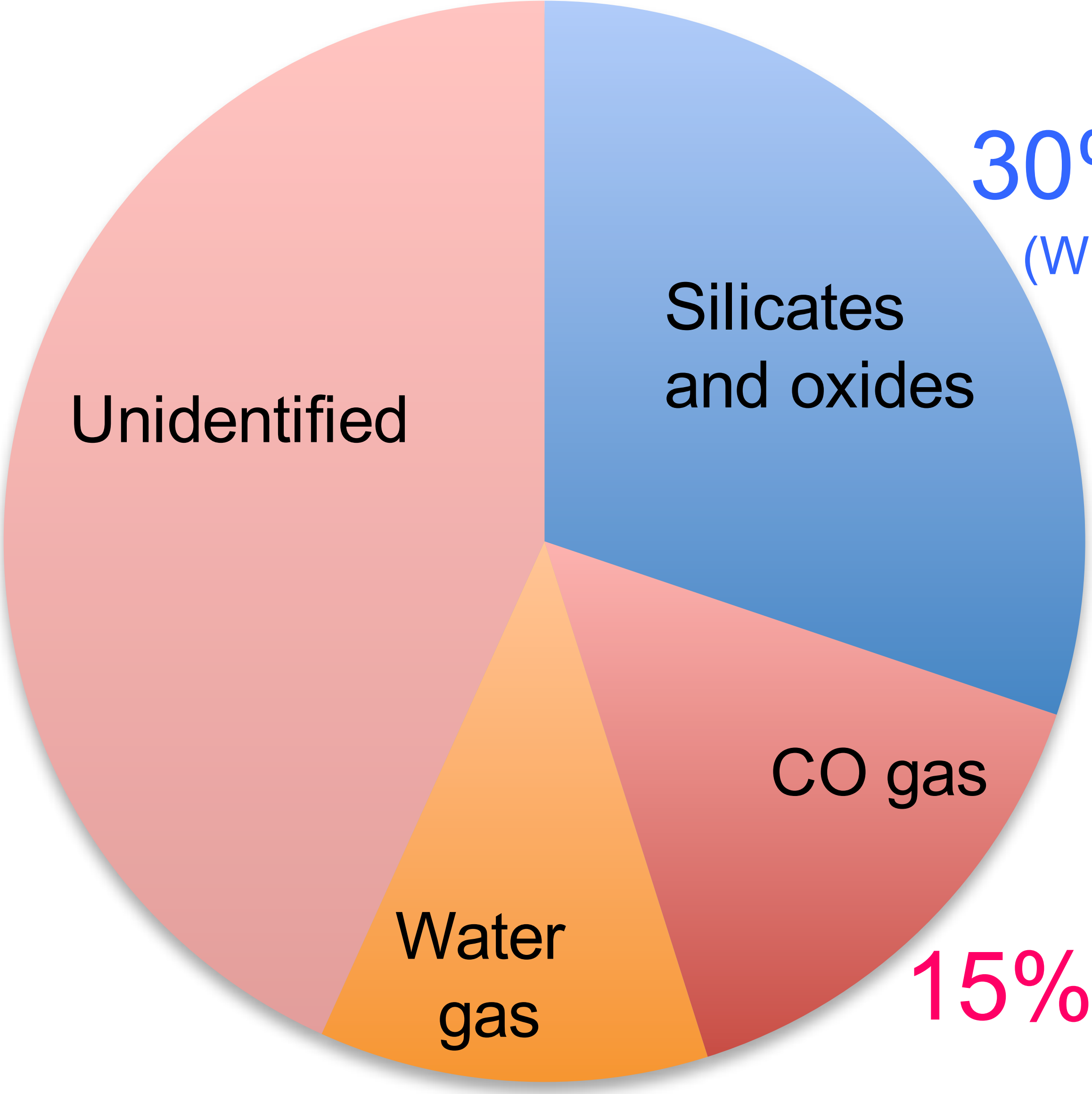
(after vaporization of ices)



H_2O_{gas} / CO_{gas} ~ 0.72

Expected budget near protostar

(after vaporization of ices and CO_2 destruction)



(Whittet et al. 2007)

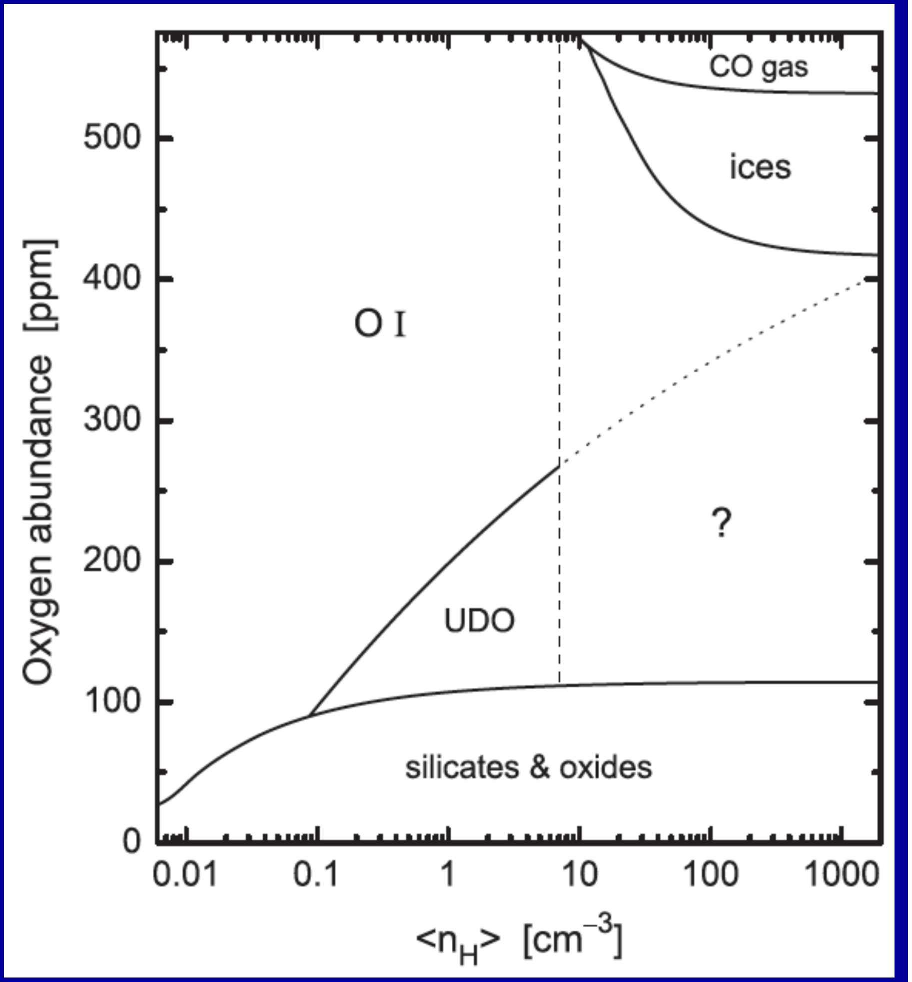
H_2O_{gas} / CO_{gas} ~ 0.78

Result of $CO_2 + H_2 \rightarrow CO + H_2O$

Key conclusions

- The observed column densities of warm water (with $N(H_2O)/N(^{12}CO) = 0.6 – 0.7$) are consistent with the hypothesis that the water vapor originates from the vaporization of H_2O ice

- Because atomic oxygen reacts rapidly with H_2 to form water, the observed column densities of warm water argue against a significant fraction of the "missing oxygen" in dense gas being atomic oxygen or any other material (e.g. O_2 ice) that could be processed rapidly at high temperature to form water vapor



Whittet 2010, ApJ

*UDO = unidentified depleted oxygen

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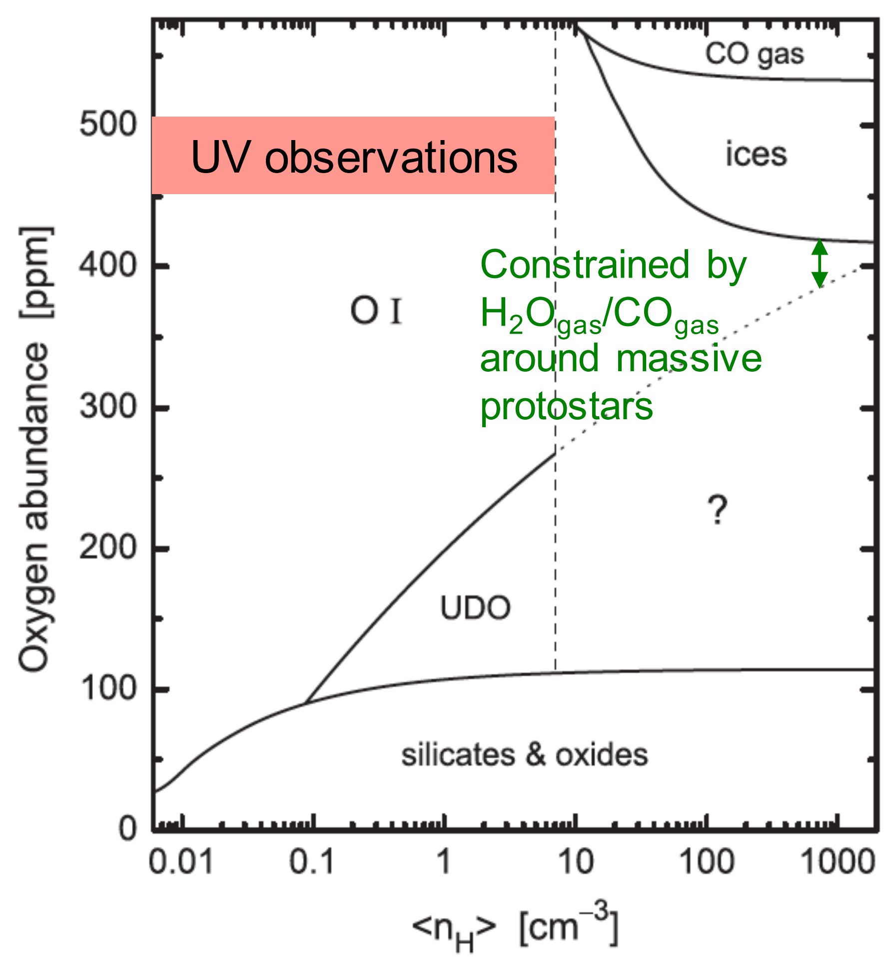


Whittet 2010, ApJ

*UDO = unidentified depleted oxygen

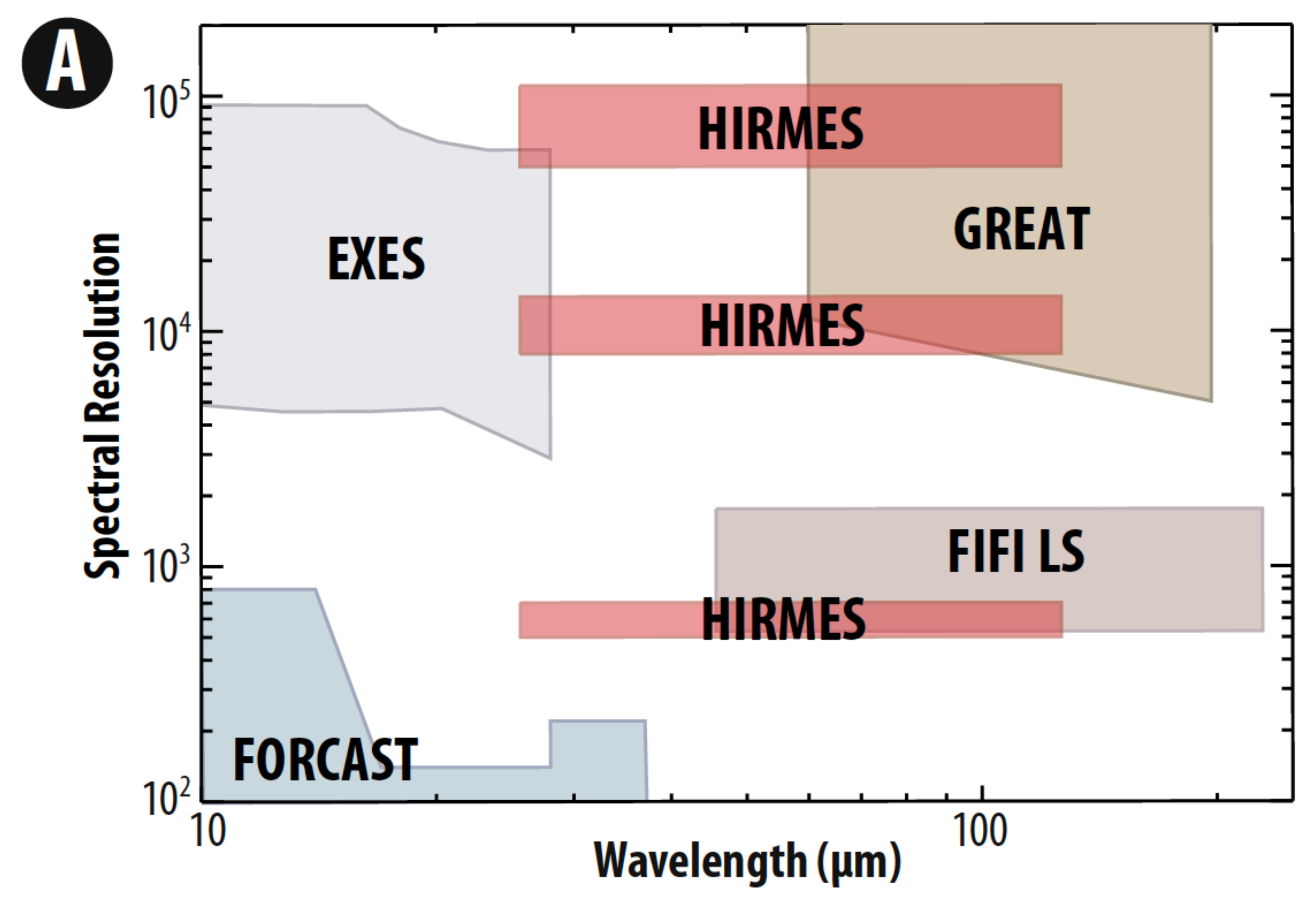
The dense ISM: future directions

- SOFIA/EXES provides a unique probe of water vapor

  Advantages:
  - can probe water in rotational states all the way down to the ground state
  - spectral resolution allows the rotational structure to be resolved
  - levels of widely varying excitation observed at nearly the same wavelength
  - Individual absorption lines resolved → kinematic information
- Ice abundances are variable ➔ need water vapor observations toward a larger sample of protostars to draw stronger conclusions about the oxygen budget
- Many other molecules have vibrational modes in the range accessible to EXES: Adwin Boogert will discuss CH_4 and SO_2

The dense ISM: future directions

- SOFIA/HIRMES will bridge the gap between the two current high-resolution SOFIA instruments



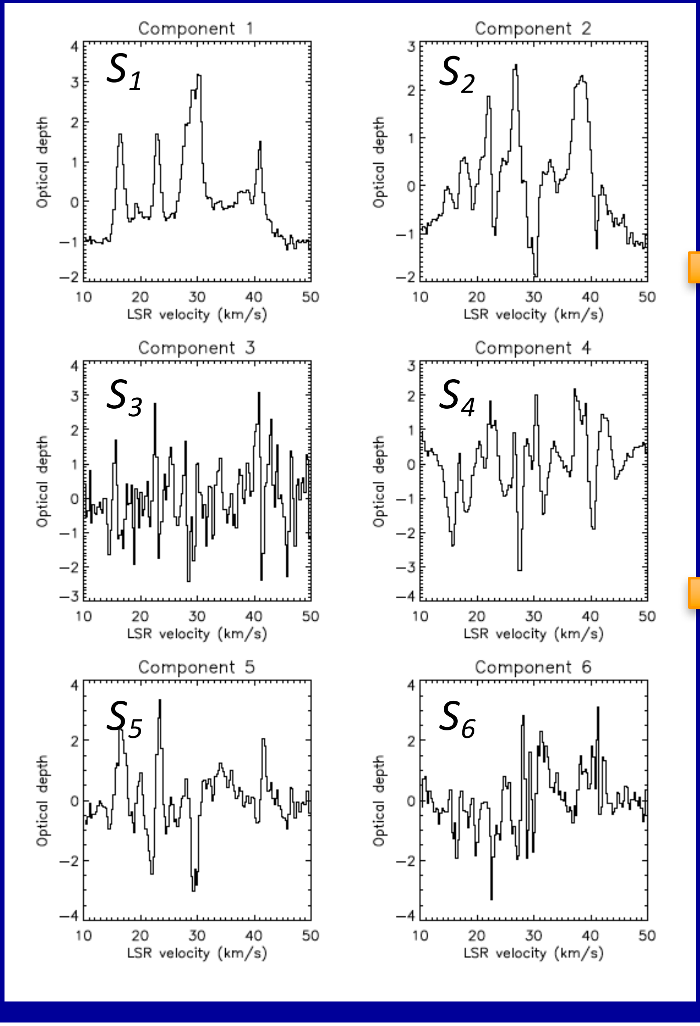
The dense ISM: future directions

- SOFIA/HIRMES will bridge the gap between the two current high-resolution SOFIA instruments
- Access to many rotational emission lines of water, CO, H_2O , OH, and HD that are excited in warm dense gas.
- Primary science driver is the chemistry of protostellar disks, but will provide valuable constraints on interstellar chemistry as well.
- Gordon Stacey will talk about this on Thursday

Extra slides

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

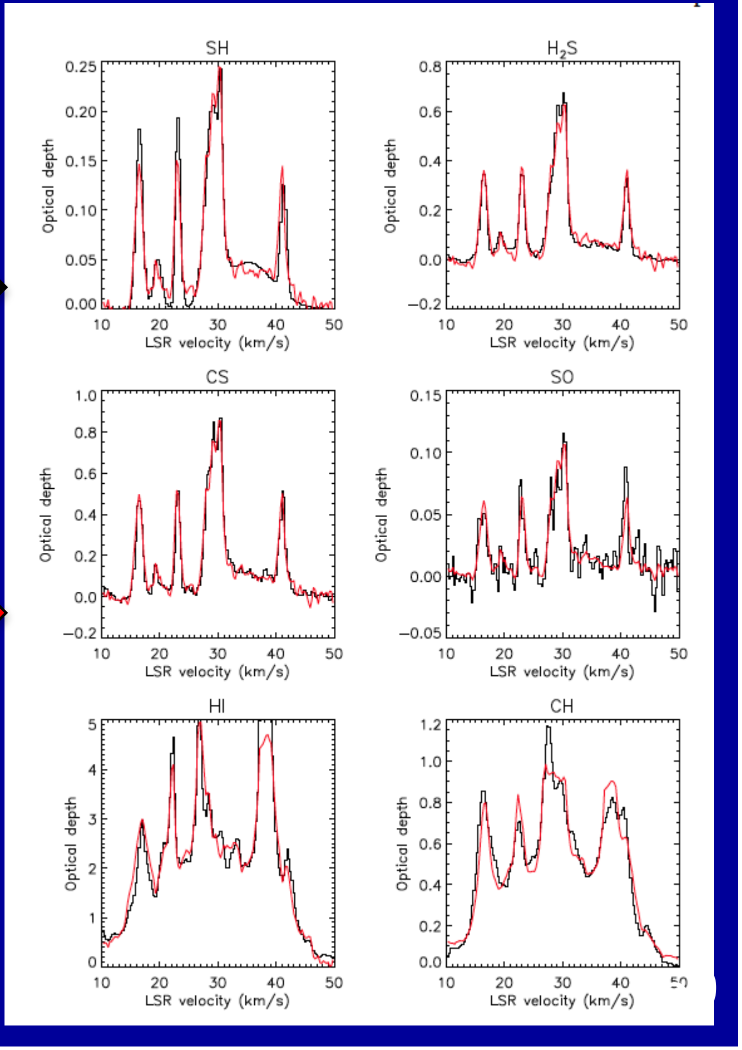
$$\tau_i(v) = a_i + b_i \sum_{j=1}^{6} C_{ij} S_j(v)$$

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, 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) The position of the neutral sulphur-bearing molecules relative to H, CH and the other species may suggest that they are present mainly in material with a large molecular fraction (since HI traces atomic gas and CH traces H_2 in partially- or fully-molecular gas)