Molecular Astrophysics

David Neufeld
Johns Hopkins University

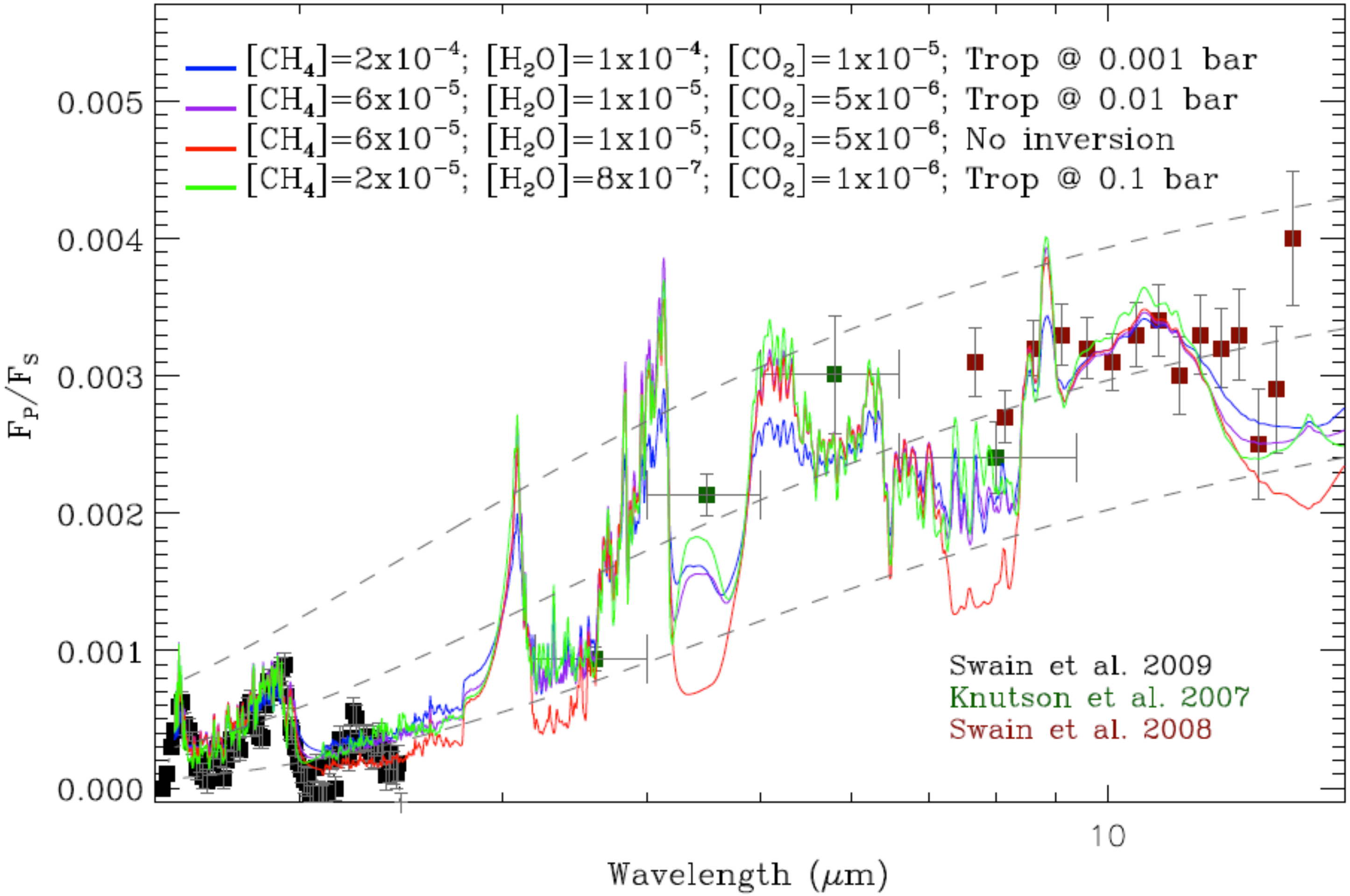
Molecular astrophysics

- Why molecular astrophysics?
- The new capabilities of *Herschel*/HIFI
- HIFI observations of interstellar hydrides
- Prospects for SOFIA

Why study molecular astrophysics?

- Molecules are ubiquitous
  - Present in interstellar, circumstellar and pregalactic gas; protostellar disks, circumnuclear gas in AGN, the atmospheres of stars and planets (including exoplanets)
  - More than 150 molecules currently known
- Molecules as diagnostic probes
  - Reveal key information by their excitation, kinematics, chemistry
- Molecules as coolants
  - Facilitate the collapse of clouds to form galaxies and stars
- The astrophysical Universe as a unique laboratory for the study of molecular physics
- Molecules as the precursors of life
  - Interstellar ices supply a rich inventory of water and organic molecules

IR spectroscopy of the exoplanet HD 209458b



Swain et al. 2009, ApJ

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2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms
H2	C3*	c-C3H	C5*	C5H	C6H	CH3C3N	CH3C4H	CH3C5N	HC9N	C6H6*(?)	HC11N
AlF	C2H	l-C3H	C4H	l-H2C4	CH2CHCN	HC(O)OCH3	CH3CH2CN	(CH3)2CO	CH3C6H	C2H5OCH3	
AlCl	C2O	C3N	C4Si	C2H4*	CH3C2H	CH3COOH	(CH3)2O	(CH2OH)2	C2H5OCHO	n-C3H7CN	
C2**	C2S	C3O	l-C3H2	CH3CN	HC5N	C7H	CH3CH2OH	CH3CH2CHO			
CH	CH2	C3S	c-C3H2	CH3NC	CH3CHO	H2C6	HC7N				
CH+	HCN	C2H2*	H2CCN	CH3OH	CH3NH2	CH2OHCHO	C8H				
CN	HCO	NH3	CH4*	CH3SH	c-C2H4O	l-HC6H*(?)	CH3C(O)NH2				
CO	HCO+	HCCN	HC3N	HC3NH+	H2CCHOH	CH2CHCHO(?)	C8H–				
CO+	HCS+	HCNH+	HC2NC	HC2CHO	C6H–	CH2CCHCN	C3H6				
CP	HOC+	HNCO	HCOOH	NH2CHO		H2NCH2CN					
SiC	H2O	HNCS	H2CNH	C5N							
HCl	H2S	HOCO+	H2C2O	l-HC4H*(?)							
KCl	HNC	H2CO	H2NCN	l-HC4N							
NH	HNO	H2CN	HNC3	c-H2C3O							
NO	MgCN	H2CS	SiH4*	H2CCNH(?)							
NS	MgNC	H3O+	H2COH+	C5N-							
NaCl	N2H+	c-SiC3	C4H								
OH	N2O	CH3*	HC(O)CN								
PN	NaCN	C3N									
SO	OCS	PH3(?)									
SO+	SO2	HCNO									
SiN	c-SiC2	HOCN									
SiO	CO2 *	HSCN									
SiS	NH2										
CS	H3+*										
HF	H2D+										
HD	HD2+										
FeO(?)	SiCN										
O2	AlNC										
CF+	SiNC										
SiH(?)	HCP										
PO	CCP										
	AlOH										

* vibrational spectra only
** electronic spectra only

150 interstellar/circumstellar molecules listed on the Cologne Database for Molecular Spectroscopy (CDMS) as of May 2010

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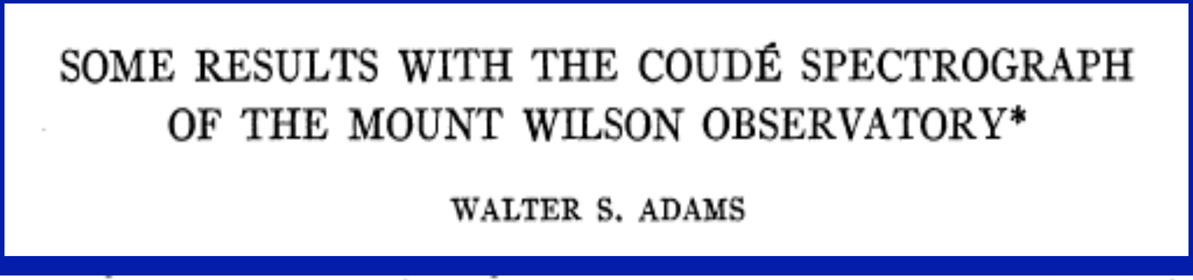
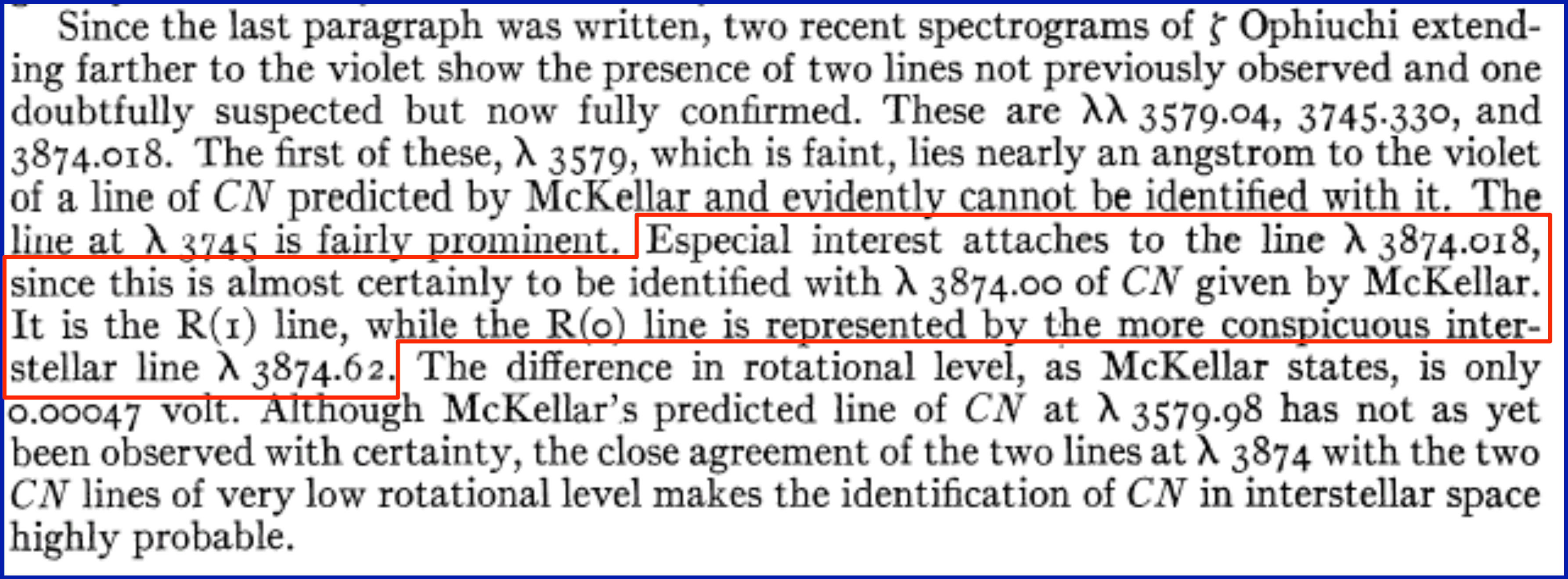
Molecular excitation as a diagnostic probe



SOME RESULTS WITH THE COUDÉ SPECTROGRAPH OF THE MOUNT WILSON OBSERVATORY*

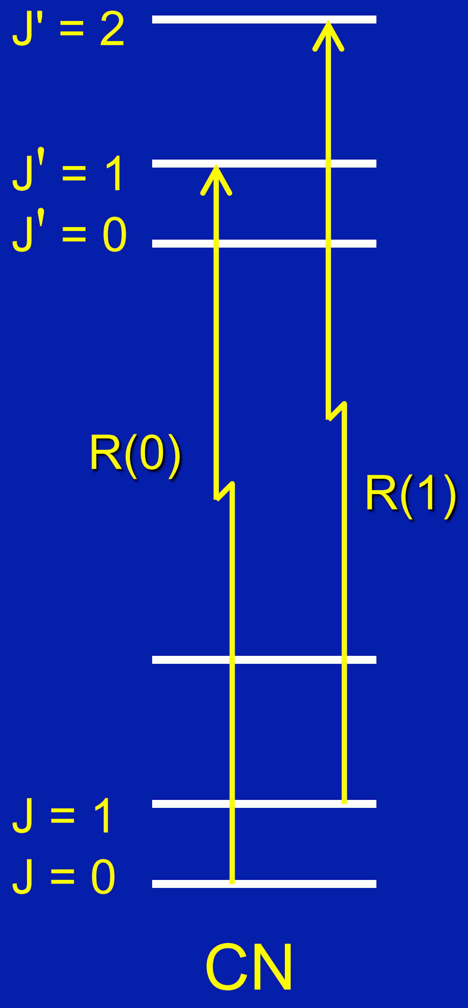
WALTER S. ADAMS



Since the last paragraph was written, two recent spectrograms of ζ Ophiuchi extending farther to the violet show the presence of two lines not previously observed and one doubtfully suspected but now fully confirmed. These are λλ 3579.04, 3745.330, and 3874.018. The first of these, λ 3579, which is faint, lies nearly an angstrom to the violet of a line of *CN* predicted by McKellar and evidently cannot be identified with it. The line at λ 3745 is fairly prominent. Especial interest attaches to the line λ 3874.018, since this is almost certainly to be identified with λ 3874.00 of *CN* given by McKellar. It is the R(1) line, while the R(0) line is represented by the more conspicuous interstellar line λ 3874.62. The difference in rotational level, as McKellar states, is only 0.00047 volt. Although McKellar's predicted line of *CN* at λ 3579.98 has not as yet been observed with certainty, the close agreement of the two lines at λ 3874 with the two *CN* lines of very low rotational level makes the identification of *CN* in interstellar space highly probable.

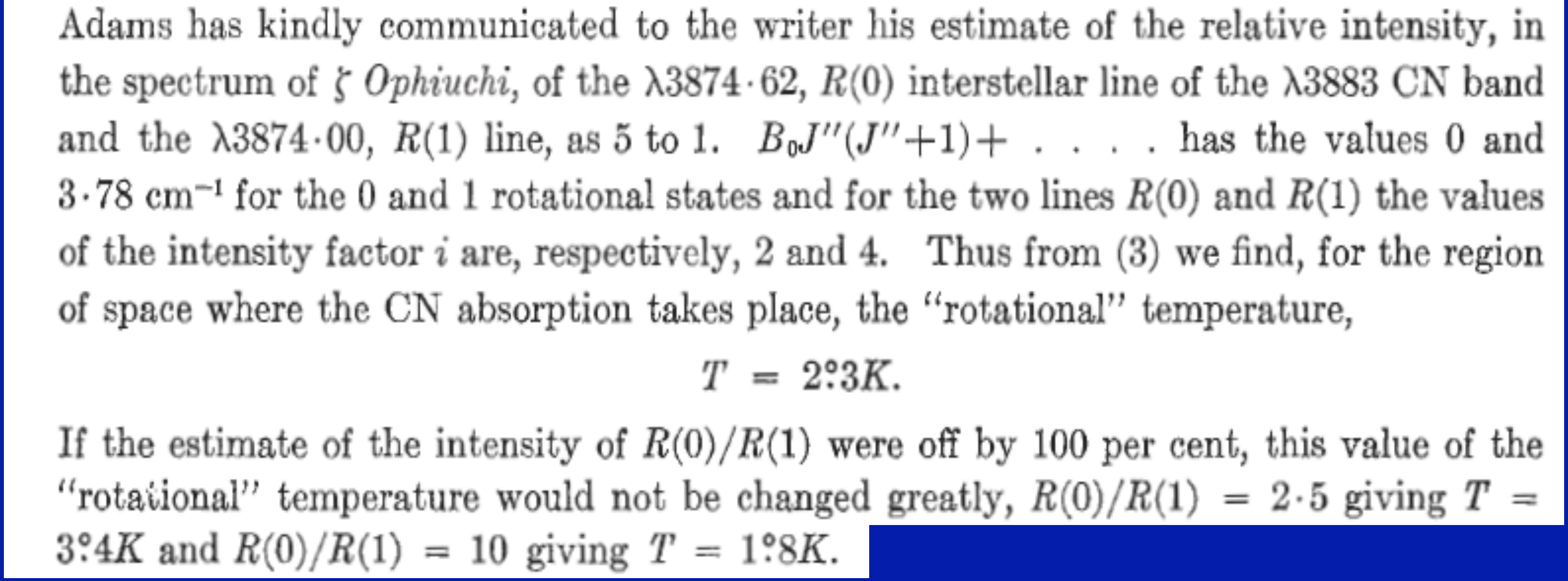
ApJ, 1941

Interstellar cyanogen absorption



Ratio of near-ultraviolet absorption line strengths, R(1)/R(0), probes the excitation of a state (J = 1) just 0.00047eV above the ground state

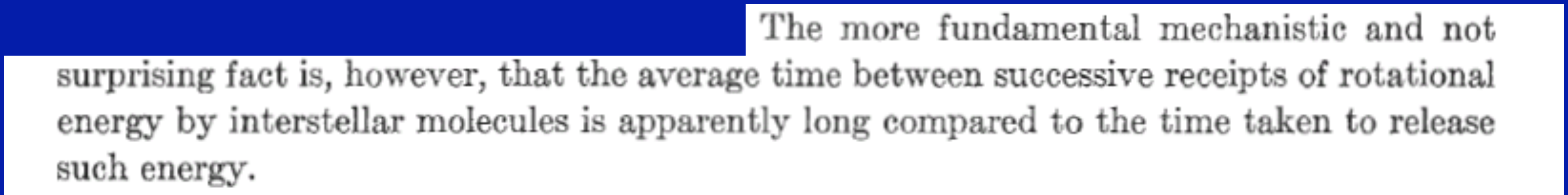
Rotational temperature of CN estimated by McKellar (1943)



Adams has kindly communicated to the writer his estimate of the relative intensity, in the spectrum of ζ *Ophiuchi*, of the $\lambda 3874 \cdot 62$, $R(0)$ interstellar line of the $\lambda 3883$ CN band and the $\lambda 3874 \cdot 00$, $R(1)$ line, as 5 to 1. $B_0 J''(J''+1)+ \ . \ . \ . \ .$ has the values 0 and $3 \cdot 78 \text{ cm}^{-1}$ for the 0 and 1 rotational states and for the two lines $R(0)$ and $R(1)$ the values of the intensity factor i are, respectively, 2 and 4. Thus from (3) we find, for the region of space where the CN absorption takes place, the "rotational" temperature,

$$T = 2\overset{\circ}{.}3K.$$

If the estimate of the intensity of $R(0)/R(1)$ were off by 100 per cent, this value of the "rotational" temperature would not be changed greatly, $R(0)/R(1) = 2 \cdot 5$ giving $T = 3\overset{\circ}{.}4K$ and $R(0)/R(1) = 10$ giving $T = 1\overset{\circ}{.}8K$.



The more fundamental mechanistic and not surprising fact is, however, that the average time between successive receipts of rotational energy by interstellar molecules is apparently long compared to the time taken to release such energy.

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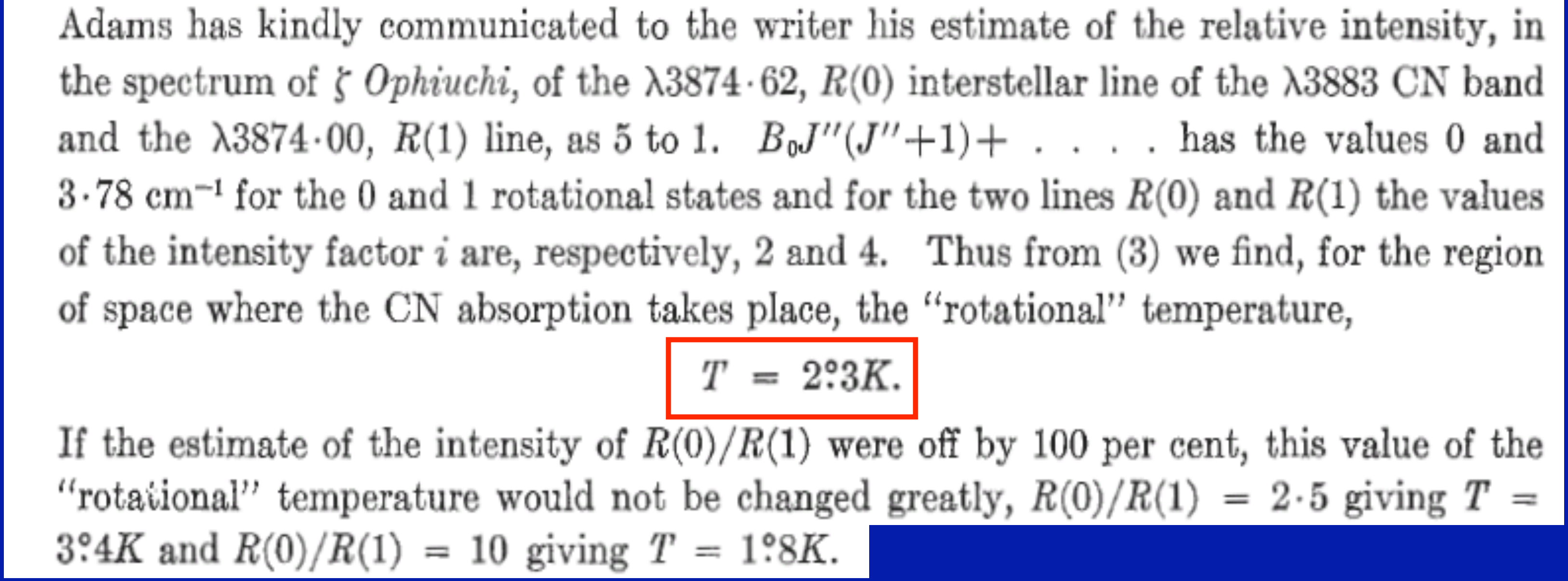

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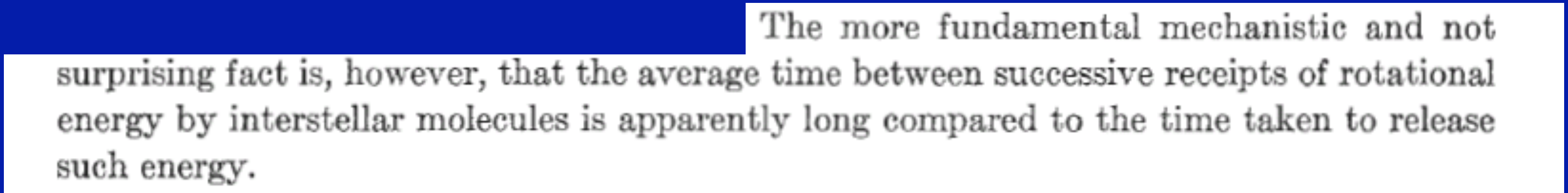

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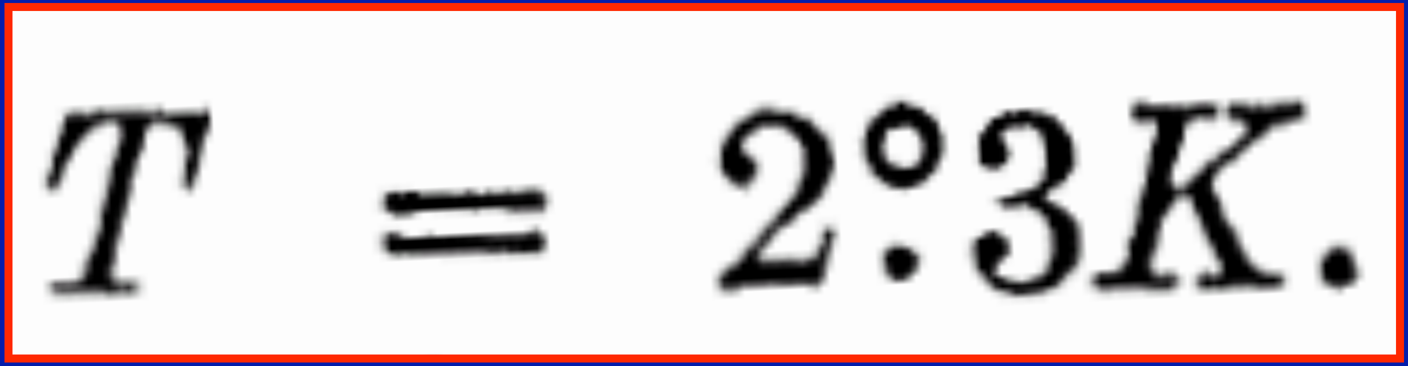

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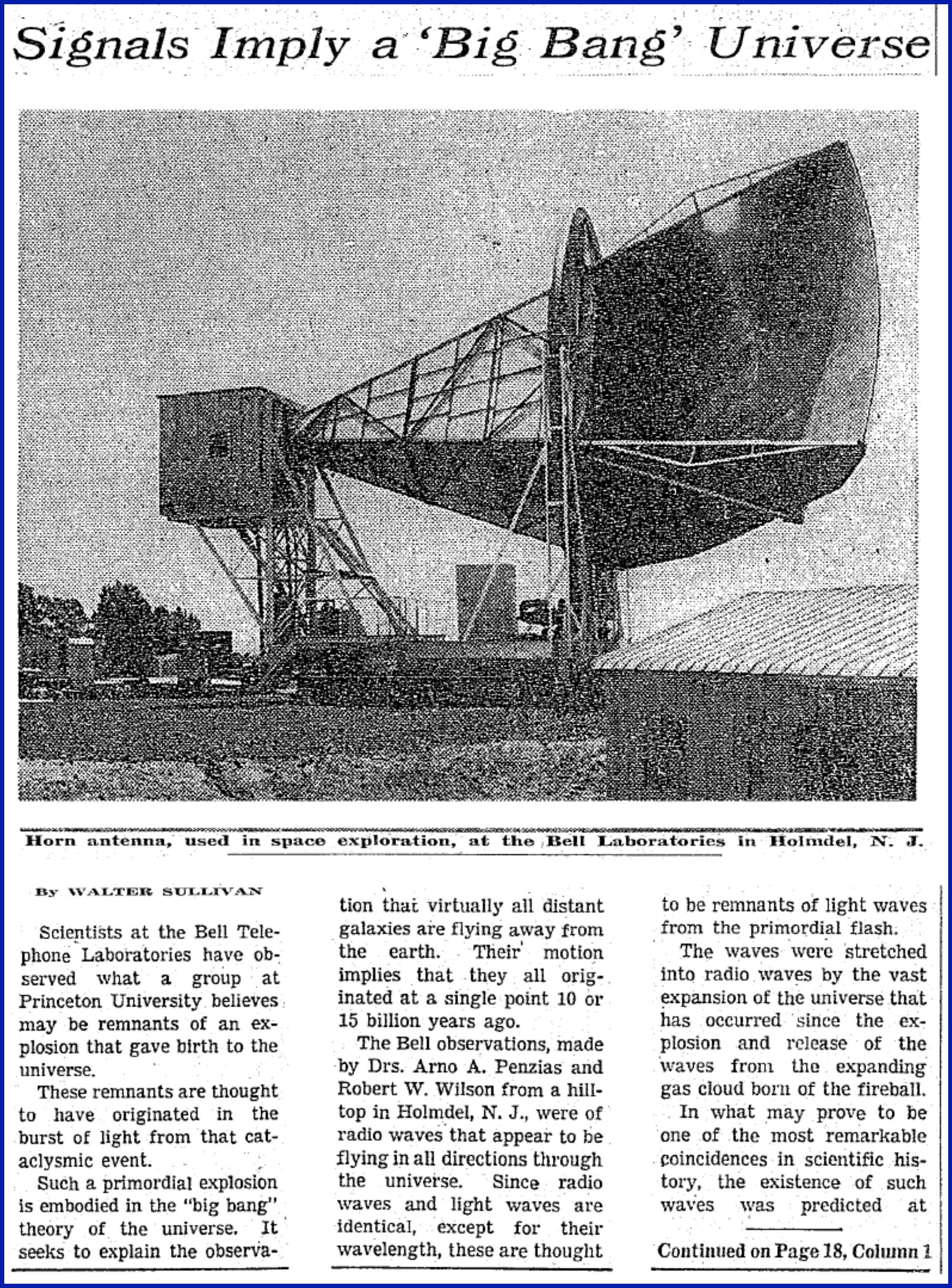


Signals Imply a 'Big Bang' Universe

Horn antenna, used in space exploration, at the Bell Laboratories in Holmdel, N. J.

By WALTER SULLIVAN

Scientists at the Bell Telephone Laboratories have observed what a group at Princeton University believes may be remnants of an explosion that gave birth to the universe.

These remnants are thought to have originated in the burst of light from that cataclysmic event.

Such a primordial explosion is embodied in the "big bang" theory of the universe. It seeks to explain the observation that virtually all distant galaxies are flying away from the earth. Their motion implies that they all originated at a single point 10 or 15 billion years ago.

The Bell observations, made by Drs. Arno A. Penzias and Robert W. Wilson from a hilltop in Holmdel, N. J., were of radio waves that appear to be flying in all directions through the universe. Since radio waves and light waves are identical, except for their wavelength, these are thought to be remnants of light waves from the primordial flash.

The waves were stretched into radio waves by the vast expansion of the universe that has occurred since the explosion and release of the waves from the expanding gas cloud born of the fireball.

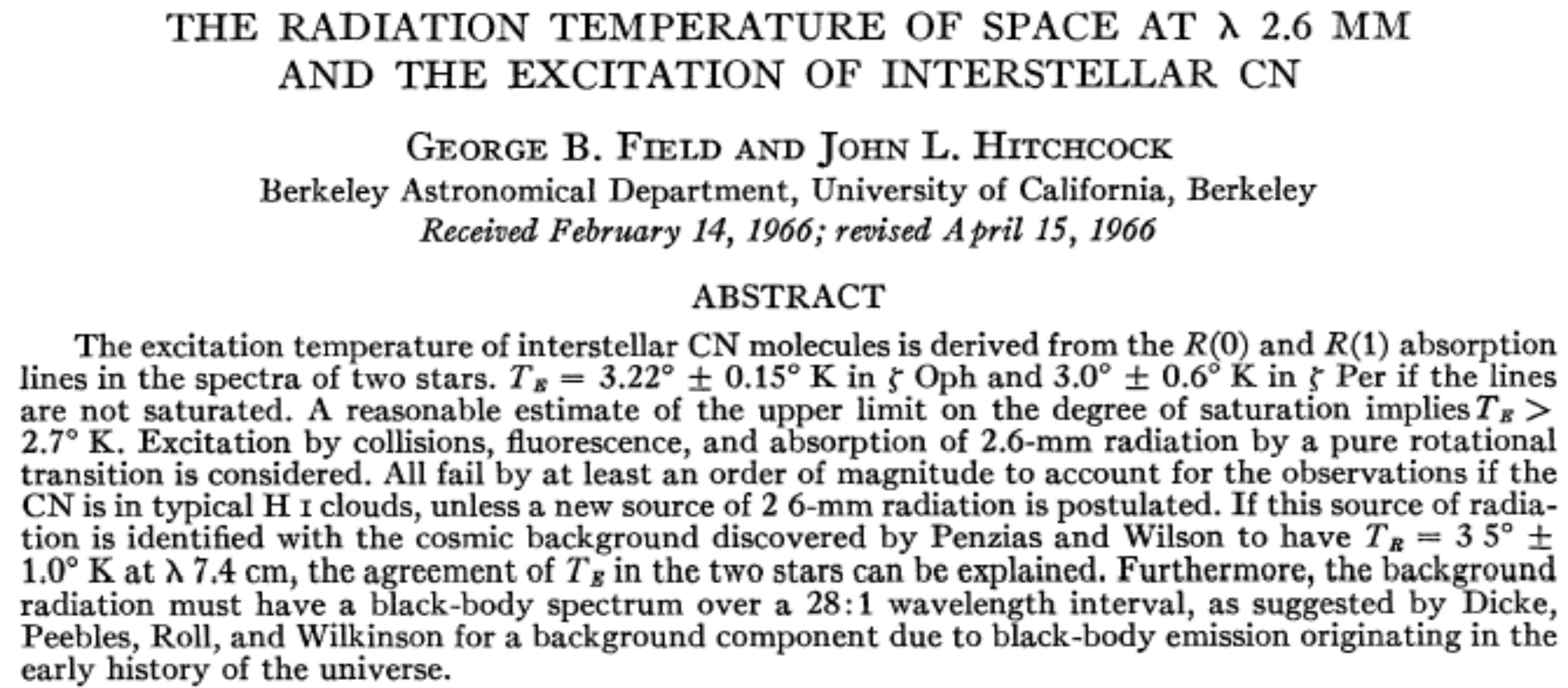
In what may prove to be one of the most remarkable coincidences in scientific history, the existence of such waves was predicted at

Continued on Page 18, Column 1

New York Times
May 21, 1965

Anomalous excitation explained

(Field & Hitchcock 1966; Thaddeus & Claussen 1966)



THE RADIATION TEMPERATURE OF SPACE AT λ 2.6 MM AND THE EXCITATION OF INTERSTELLAR CN

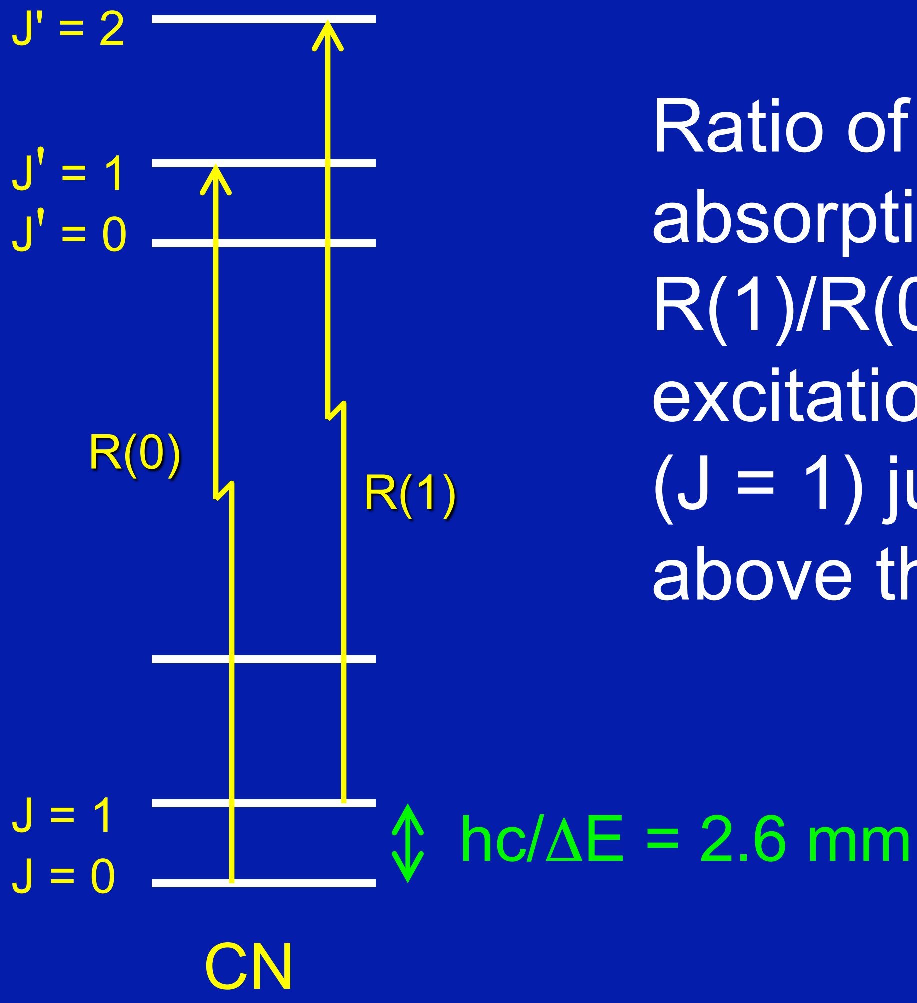
GEORGE B. FIELD AND JOHN L. HITCHCOCK
Berkeley Astronomical Department, University of California, Berkeley

Received February 14, 1966; revised April 15, 1966

ABSTRACT

The excitation temperature of interstellar CN molecules is derived from the $R(0)$ and $R(1)$ absorption lines in the spectra of two stars. $T_E = 3.22° \pm 0.15°$ K in ζ Oph and $3.0° \pm 0.6°$ K in ζ Per if the lines are not saturated. A reasonable estimate of the upper limit on the degree of saturation implies $T_E >$ 2.7° K. Excitation by collisions, fluorescence, and absorption of 2.6-mm radiation by a pure rotational transition is considered. All fail by at least an order of magnitude to account for the observations if the CN is in typical H I clouds, unless a new source of 2 6-mm radiation is postulated. If this source of radiation is identified with the cosmic background discovered by Penzias and Wilson to have $T_R = 3\ 5° \pm$ 1.0° K at λ 7.4 cm, the agreement of T_E in the two stars can be explained. Furthermore, the background radiation must have a black-body spectrum over a 28:1 wavelength interval, as suggested by Dicke, Peebles, Roll, and Wilkinson for a background component due to black-body emission originating in the early history of the universe.

Interstellar cyanogen absorption



Ratio of near-ultraviolet absorption line strengths, R(1)/R(0), probes the excitation of a state (J = 1) just 0.00047eV above the ground state

Observations of astrophysical molecules, carefully interpreted, provide unique information of general astrophysical interest.

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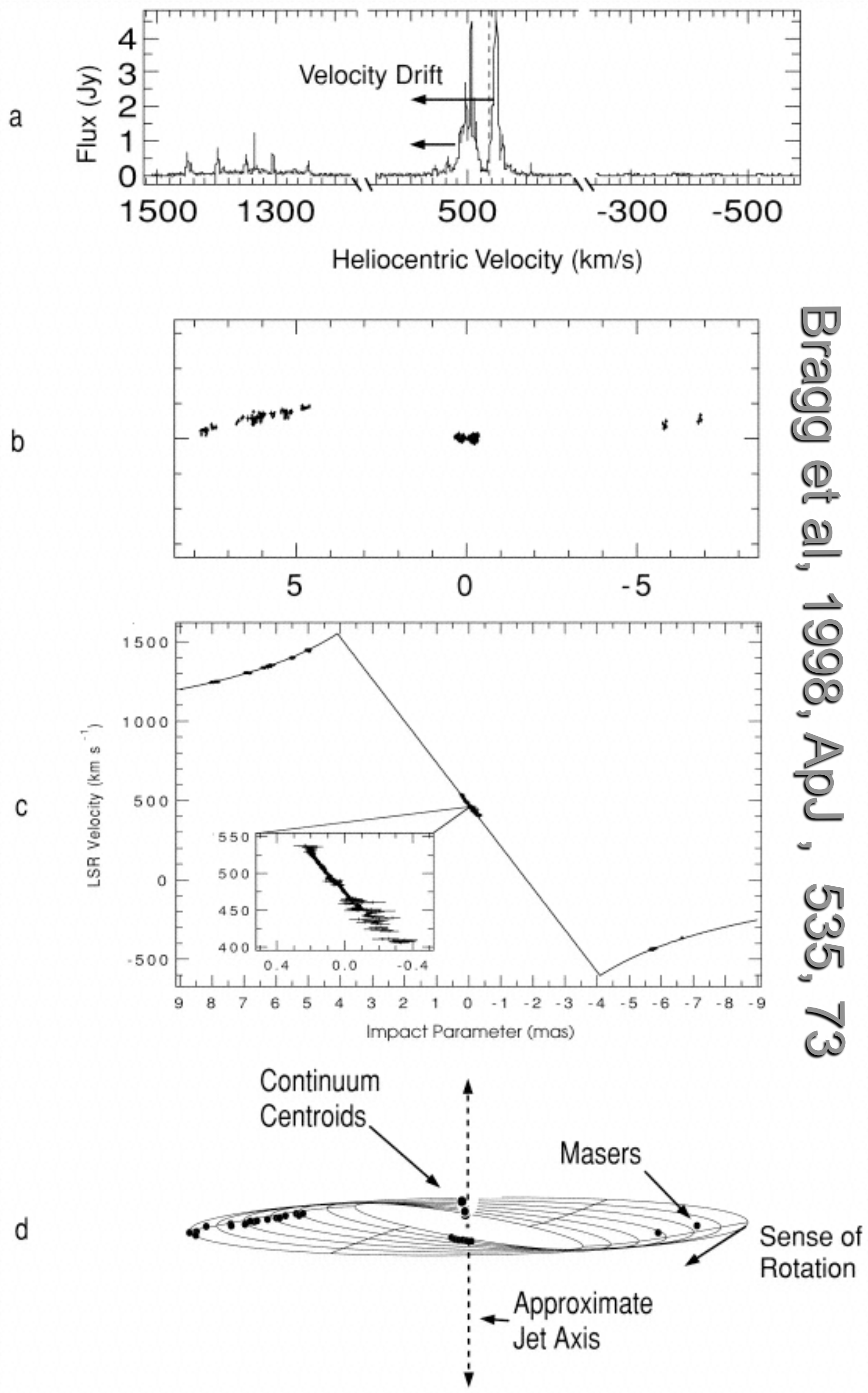
Water masers as kinematic probes: AGN accretion disks



Bragg et al, 1998, ApJ , 535, 73

Water maser observations provide the best evidence we currently have for the existence of supermassive black holes

Derived dynamical mass in NGC 4258 is 4 x 10^7 $M_\odot$ within a region of radius 0.13 pc.

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Observing astrophysical molecules

- Electronic transitions:

  $E \sim 1$ Rydberg = $m_e e^4/\hbar^2 = 13.6$ eV

  $\lambda \sim 0.1$ μm (ultraviolet)
- Vibrational transitions:

  $E \sim (m_e/m_N)^{1/2}$ Rydberg

  $\lambda \sim 4$ μm (near- to mid-IR)
- Rotational transitions:

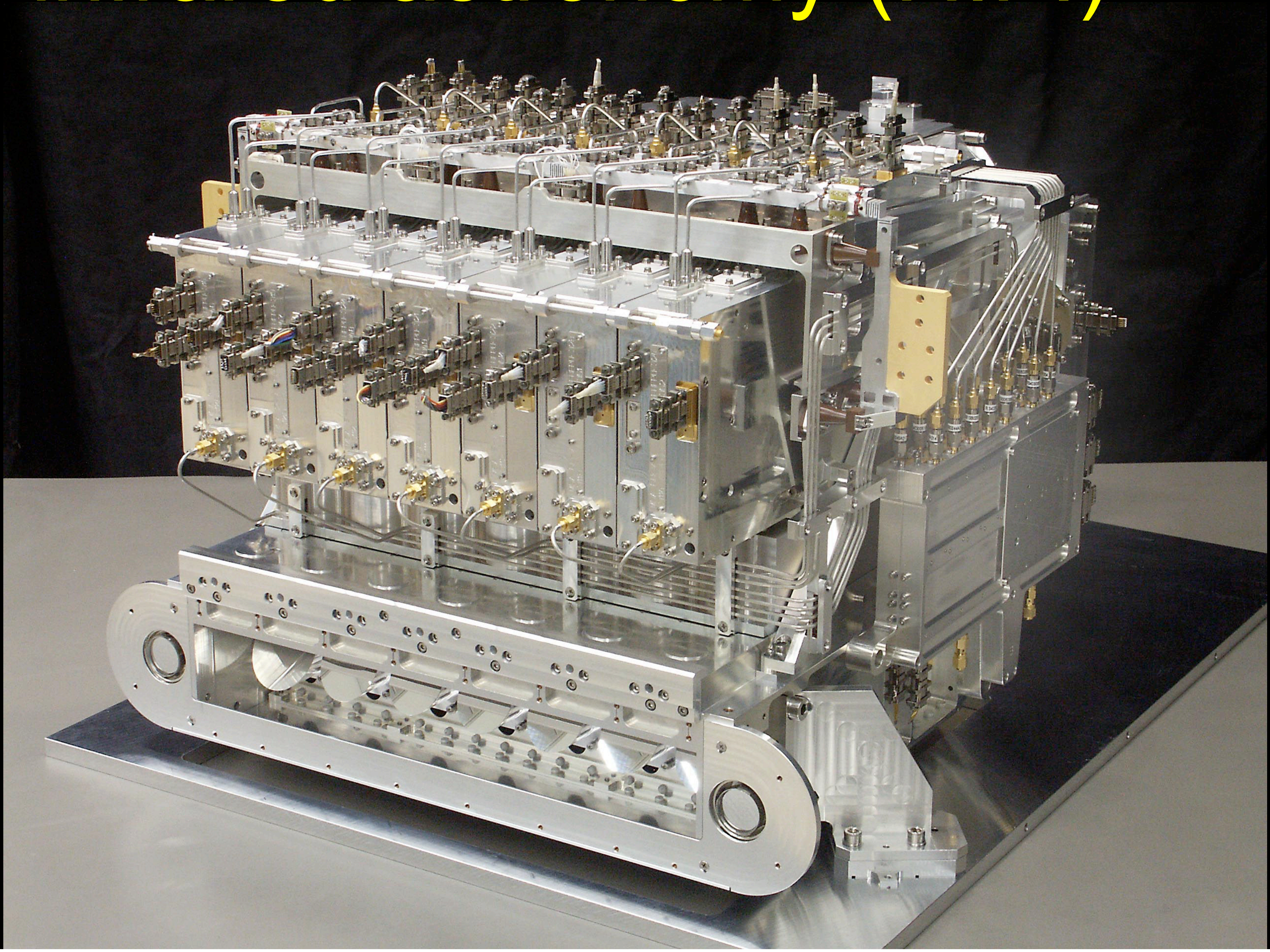
  $E \sim (m_e/m_N)$ Rydberg

  $\lambda \sim$ 200 μm for hydrides (far-IR/submillimeter)

  $\sim$ 2000 μm for non-hydrides (millimeter/centimeter)

Herschel Space Observatory

Heterodyne instrument for infrared astronomy (HIFI)



Heterodyne instrument for infrared astronomy (HIFI)

PI: Frank Helmich (SRON)

Co-PIs: Thijs de Graauw (ALMA), Tom Phillips (Caltech), Emmanual Caux (CESR), Jürgen Stutzki, (Köln)

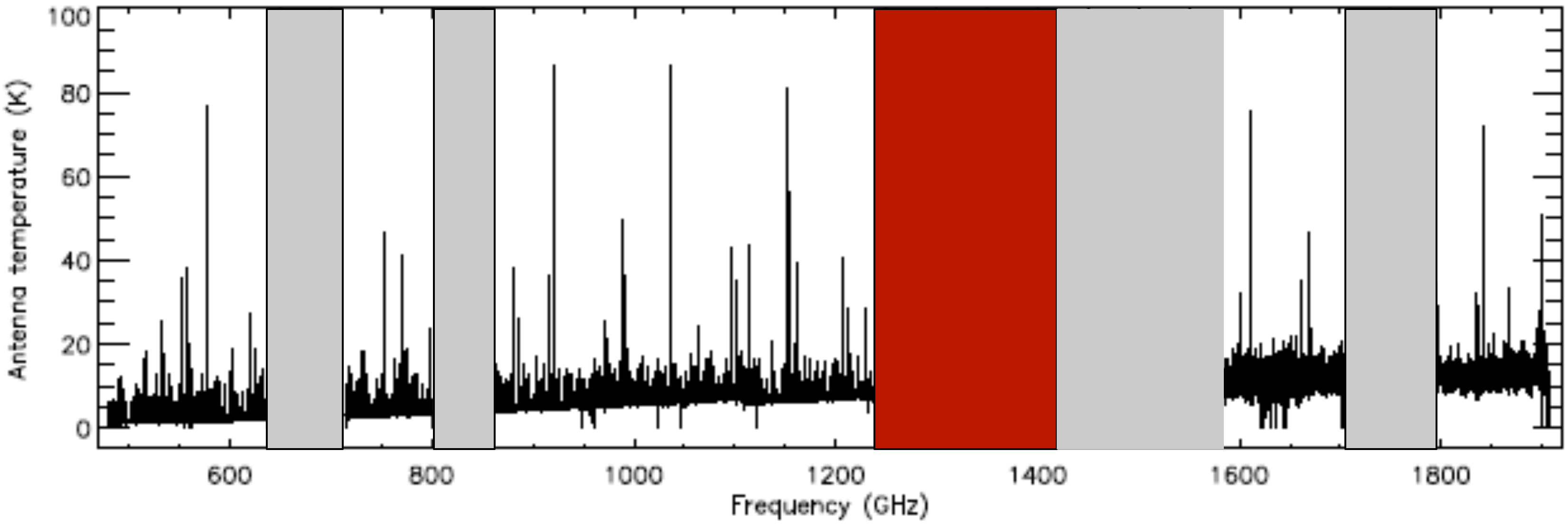
Spectral coverage: 480 – 1250 and 1410 – 1910 GHz
(157 – 212 and 240 – 625 micron)

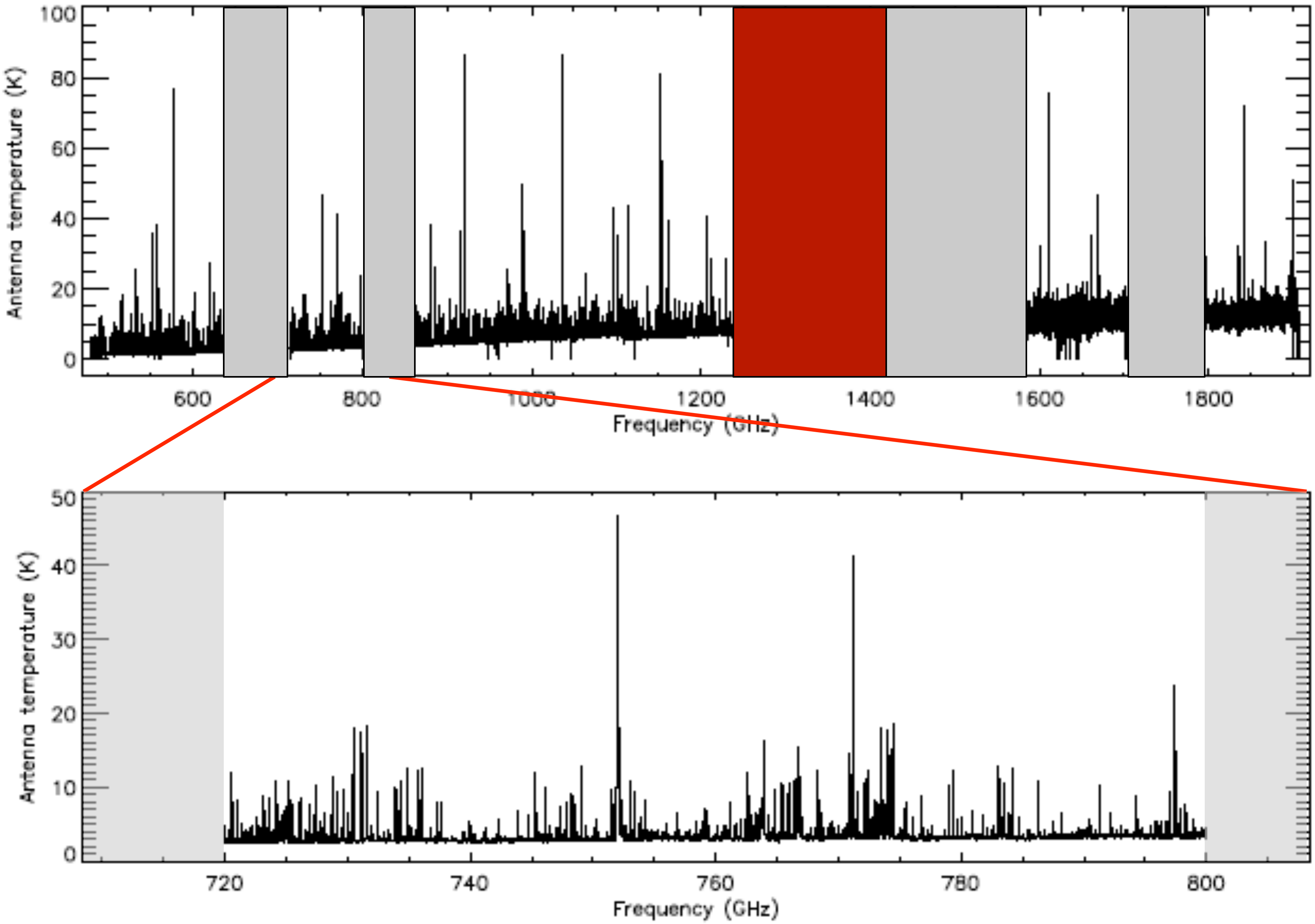
Spectral resolution: 1.1 MHz (wide band spectrometer)

Simultaneous bandwidth: 4 GHz

Heterodyne instrument for infrared astronomy (HIFI)

- A complete spectral scan produces ~ 1 million spectral samples
- In the HEXOS Key Program (PI Ted Bergin) such a scan is underway towards a massive protostellar core in the Orion Molecular Cloud


Antenna temperature (K)
0
20
40
60
80
100
600
800
1000
1200
1400
1600
1800
Frequency (GHz)


100
80
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Antenna temperature (K)
600
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1200
1400
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Frequency (GHz)
50
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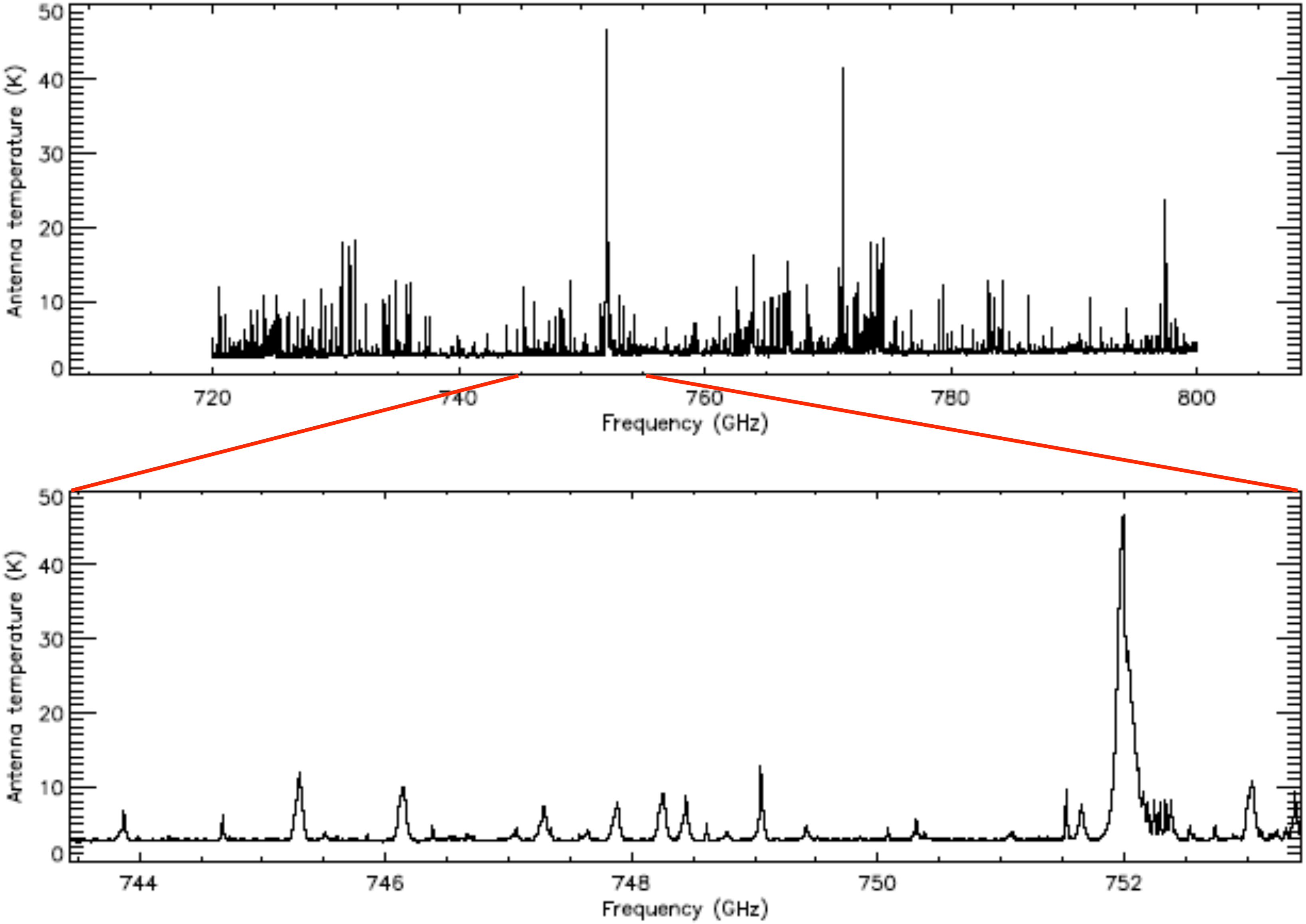
Antenna temperature (K)
720
740
760
780
800
Frequency (GHz)


Antenna temperature (K)
0
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50
720
740
760
780
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Frequency (GHz)
Antenna temperature (K)
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10
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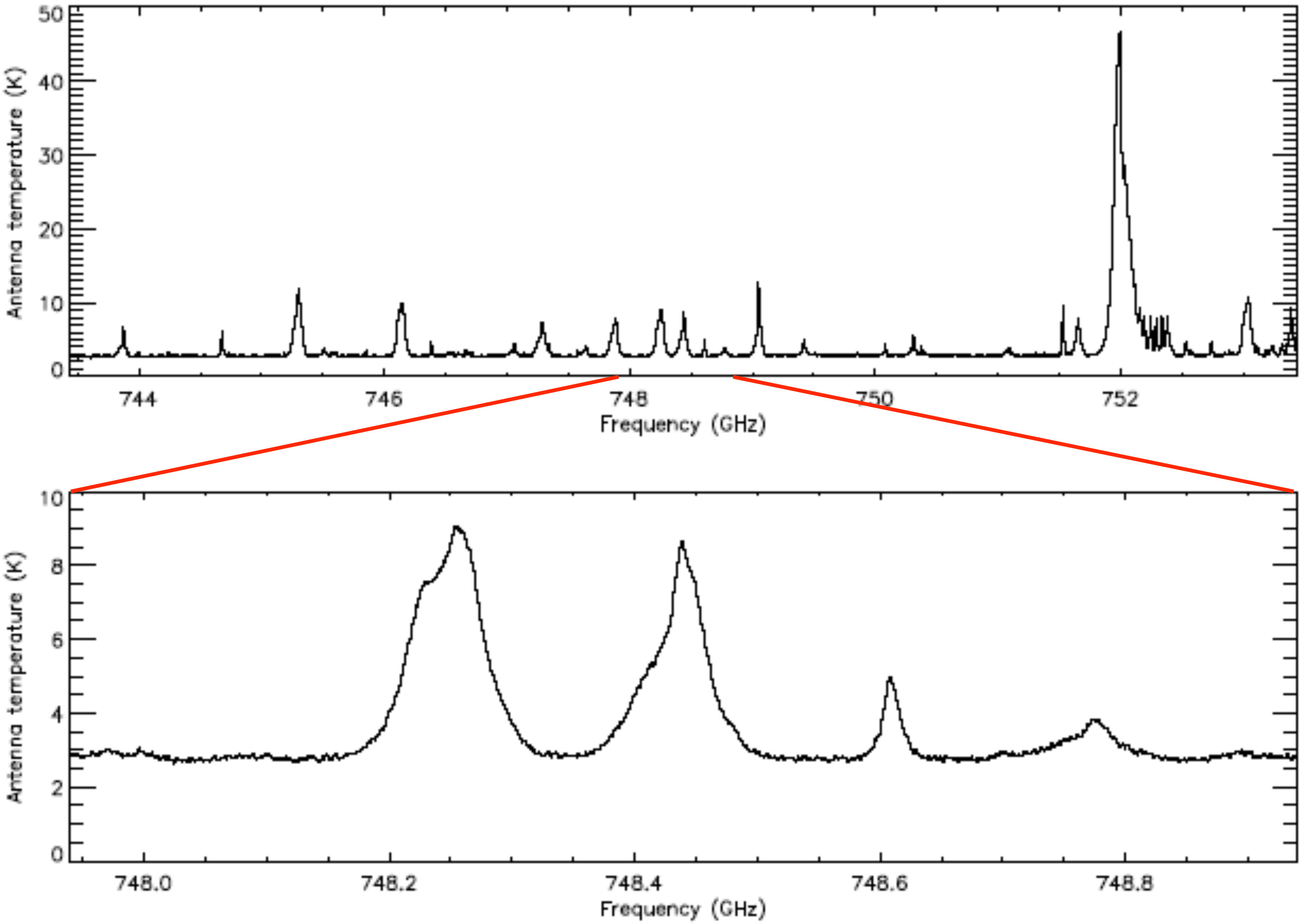
30
40
50
744
746
748
750
752
Frequency (GHz)



50
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Antenna temperature (K)
744
746
748
750
752
Frequency (GHz)
10
8
6
4
2
0
Antenna temperature (K)
748.0
748.2
748.4
748.6
748.8
Frequency (GHz)

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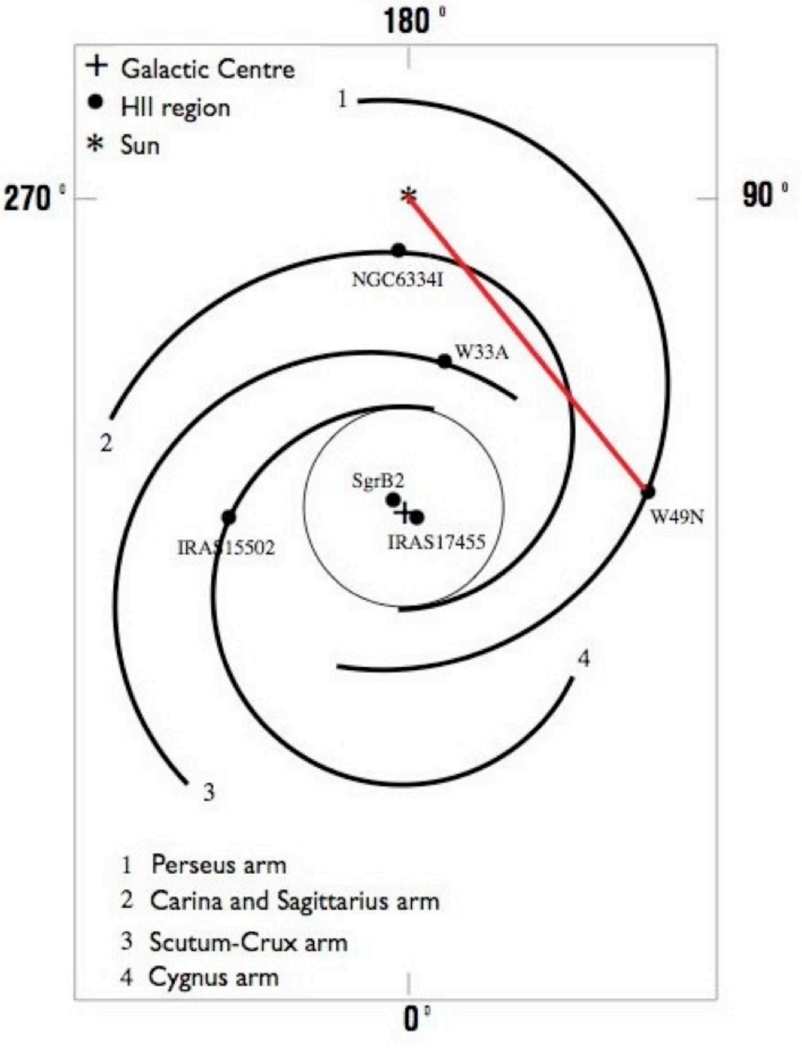
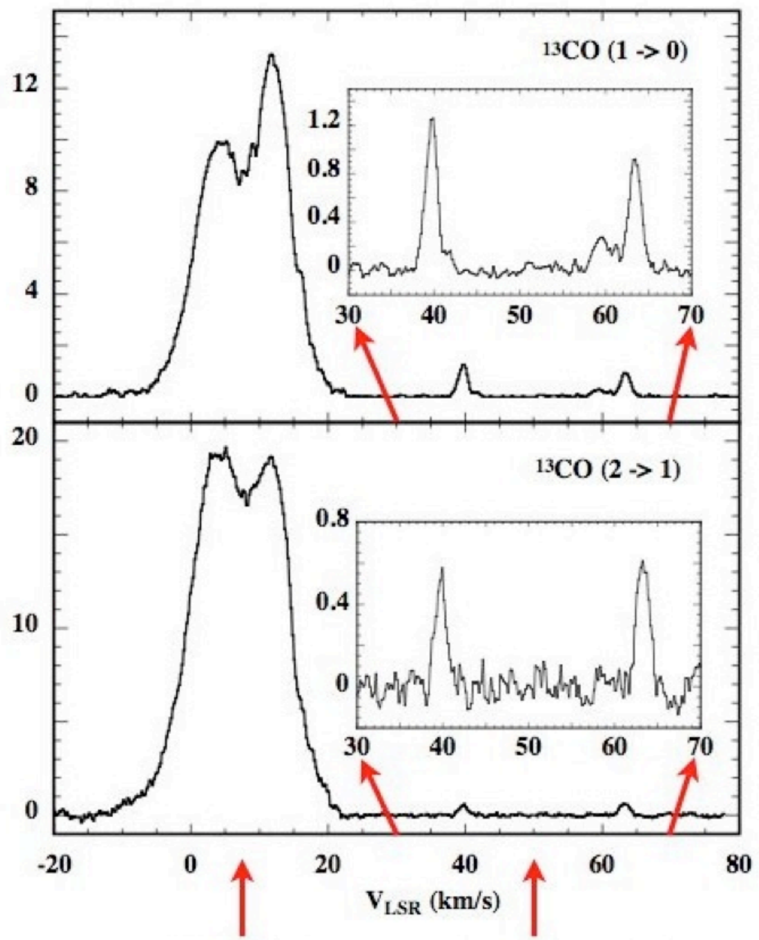
Interstellar hydrides

- It is natural to expect that hydrides will be major constituents of the ISM
- HIFI provides a unique opportunity to study interstellar hydrides
- The PRISMAS key program has carried out absorption line studies of foreground clouds along the sight-lines to bright Galactic continuum sources

Observing geometry





W49N

clouds in the line of sight

http://astro.ens.fr/index.cgi?exe=217263

Interstellar hydrides

- The first observations, of very short duration, have provided spectacular spectra that reveal the presence of:

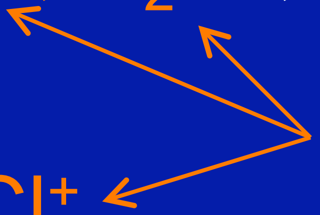
CH, CH^+

NH, NH_2, NH_3

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

HF

H_2Cl^+



“new” interstellar molecules

Interstellar hydrogen fluoride:

a surrogate for molecular hydrogen

Dissociation energy of the diatomic hydrides (eV)

H_2 4.48							
LiH 2.41	BeH 2.24	BH 3.44	CH 3.49	NH 3.22	OH 4.39	HF 5.87	
NaH 2.04	MgH 1.99	AlH 2.95	SiH 2.98	PH 2.87	SH 3.65	HCl 4.43	
KH 1.87	CaH 1.77	GaH 2.78	GeH 2.73	AsH 2.66	SeH 3.11	HBr 3.76	

ScH 2.09	TiH 2.08	VH 1.67	CrH 2.27	MnH 1.27	FeH 1.59	CoH 1.97	NiH 2.57	CuH 2.64	ZnH 0.83

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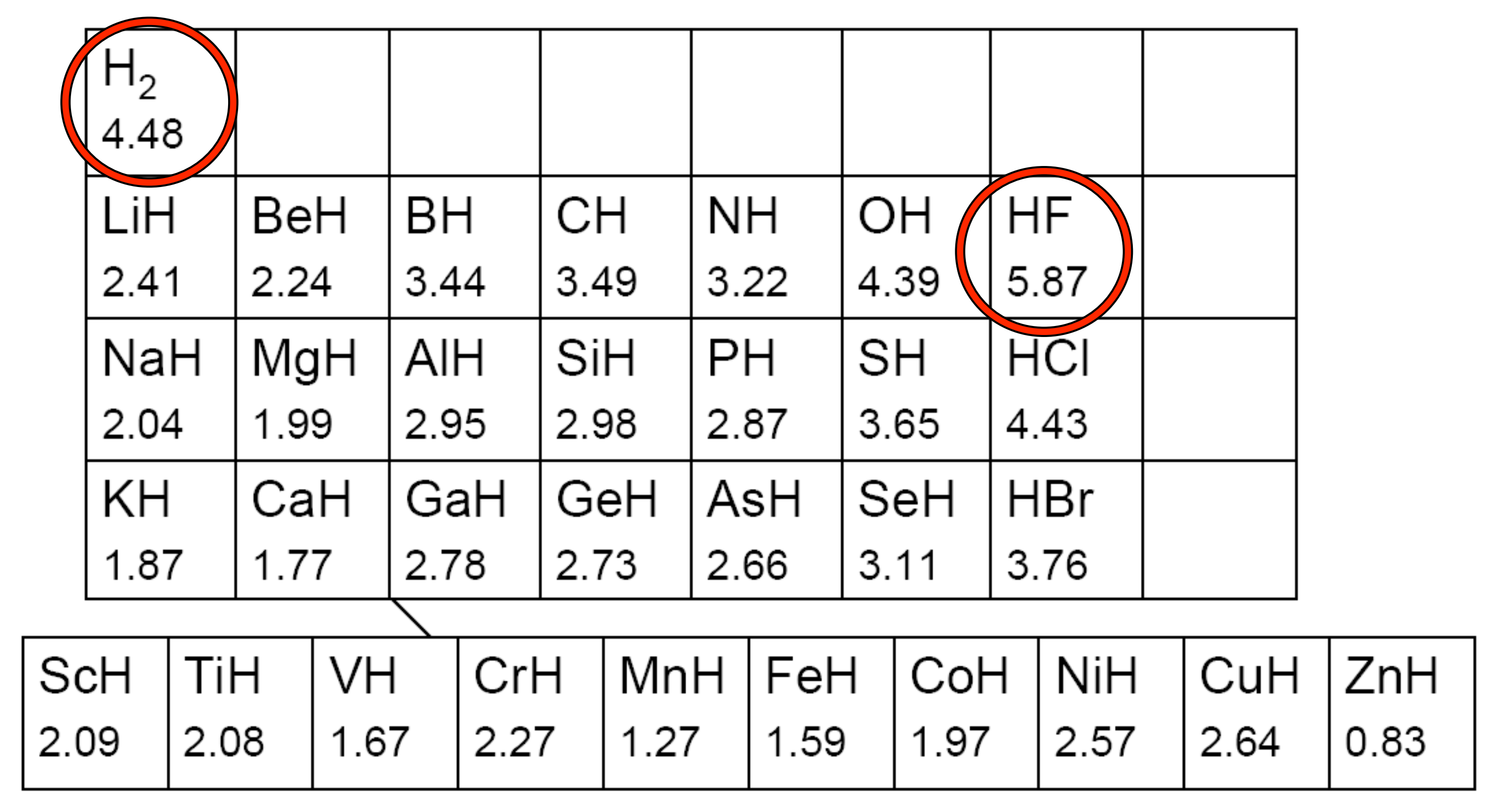

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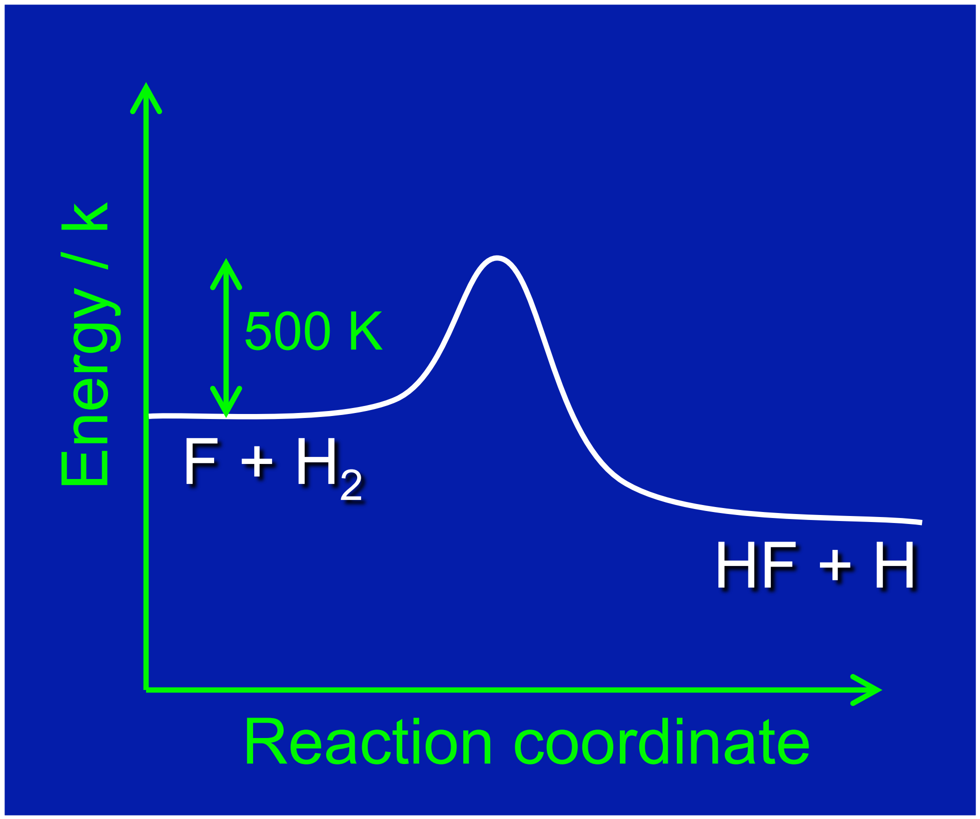
Neufeld and Wolfire 2009, ApJ

Reaction of H_2 with F

One of the most extensively studied bimolecular chemical reactions

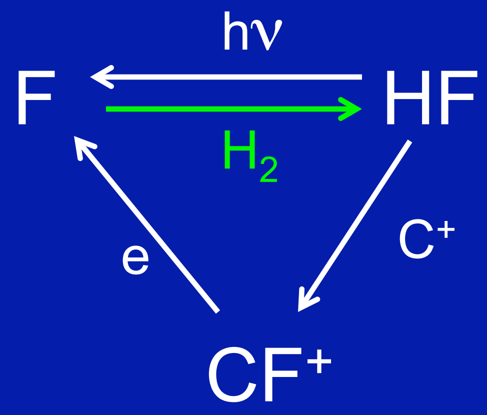
Room temperature experiments suggest a barrier, $E_A/k \sim 500$ K

Theory suggests a substantial tunneling probability at low T



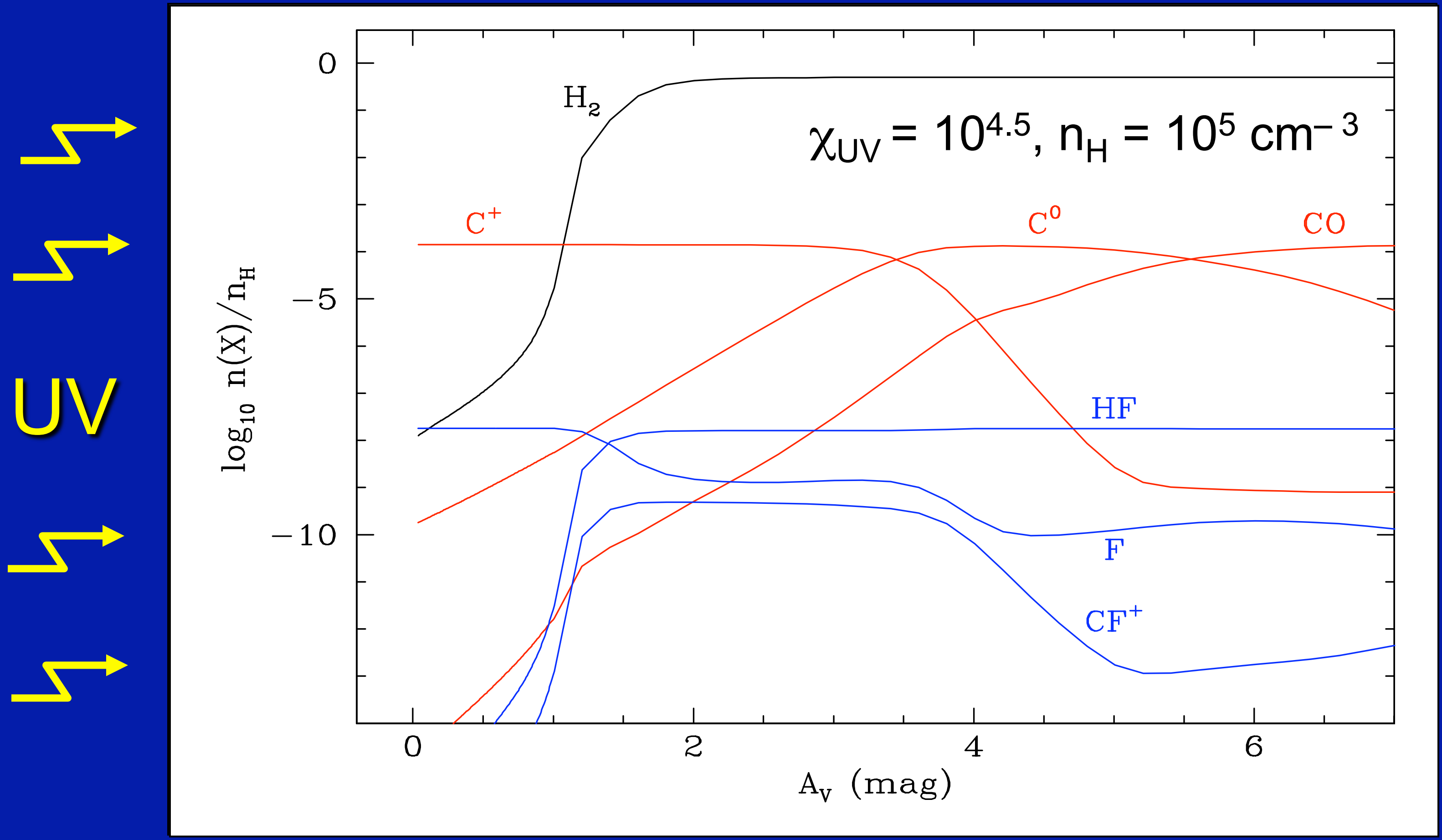
Chemistry of interstellar fluorine

- Fluorine chemistry is very simple



Predicted abundance profiles

(Neufeld, Wolfire & Schilke 1995)



UV

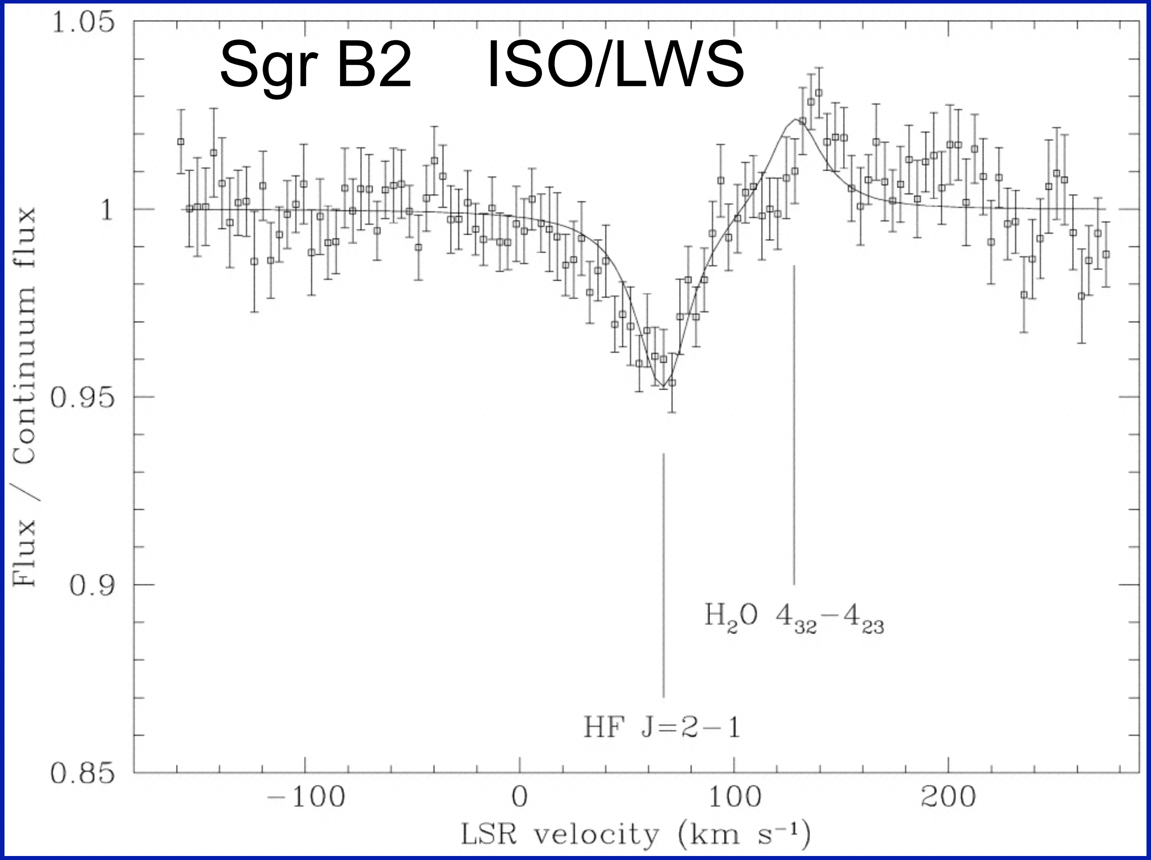
Chemistry of interstellar fluorine

- Once H_2 becomes abundant, HF is produced rapidly
- HF is destroyed slowly by photodissociation and reaction with C^+
- HF becomes the dominant reservoir of fluorine:
  - Unobservable from the ground, however: the J = 1– 0 transition is at 1.232 THz

Discovery of interstellar HF

J = 2 – 1 transition discovered by ISO

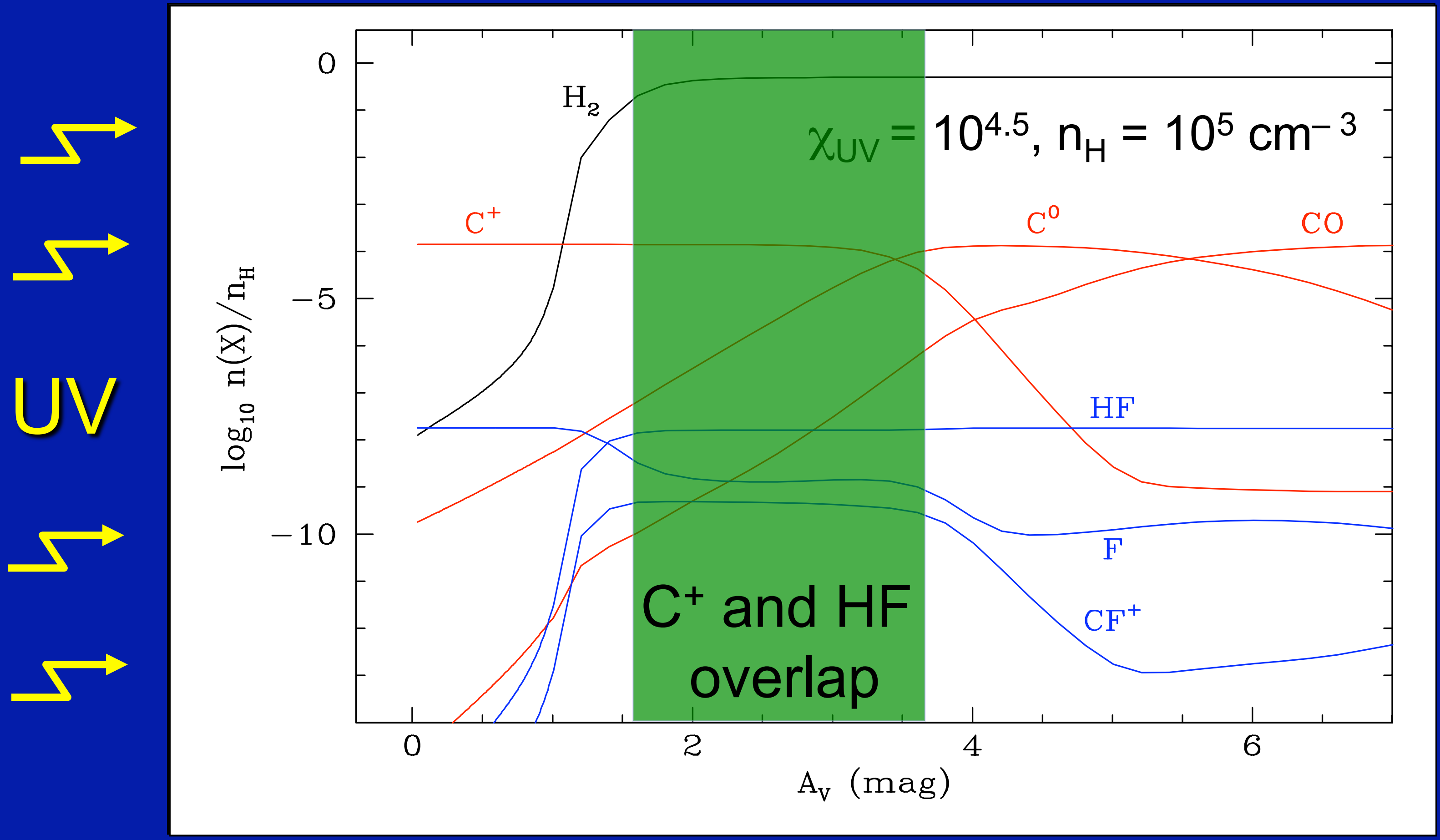
(Neufeld, Zmuidzinas, Schilke and Phillips 1997)



Lacking access to the J = 1 – 0 transition, ISO was unable to probe HF in any source other than Sgr B2

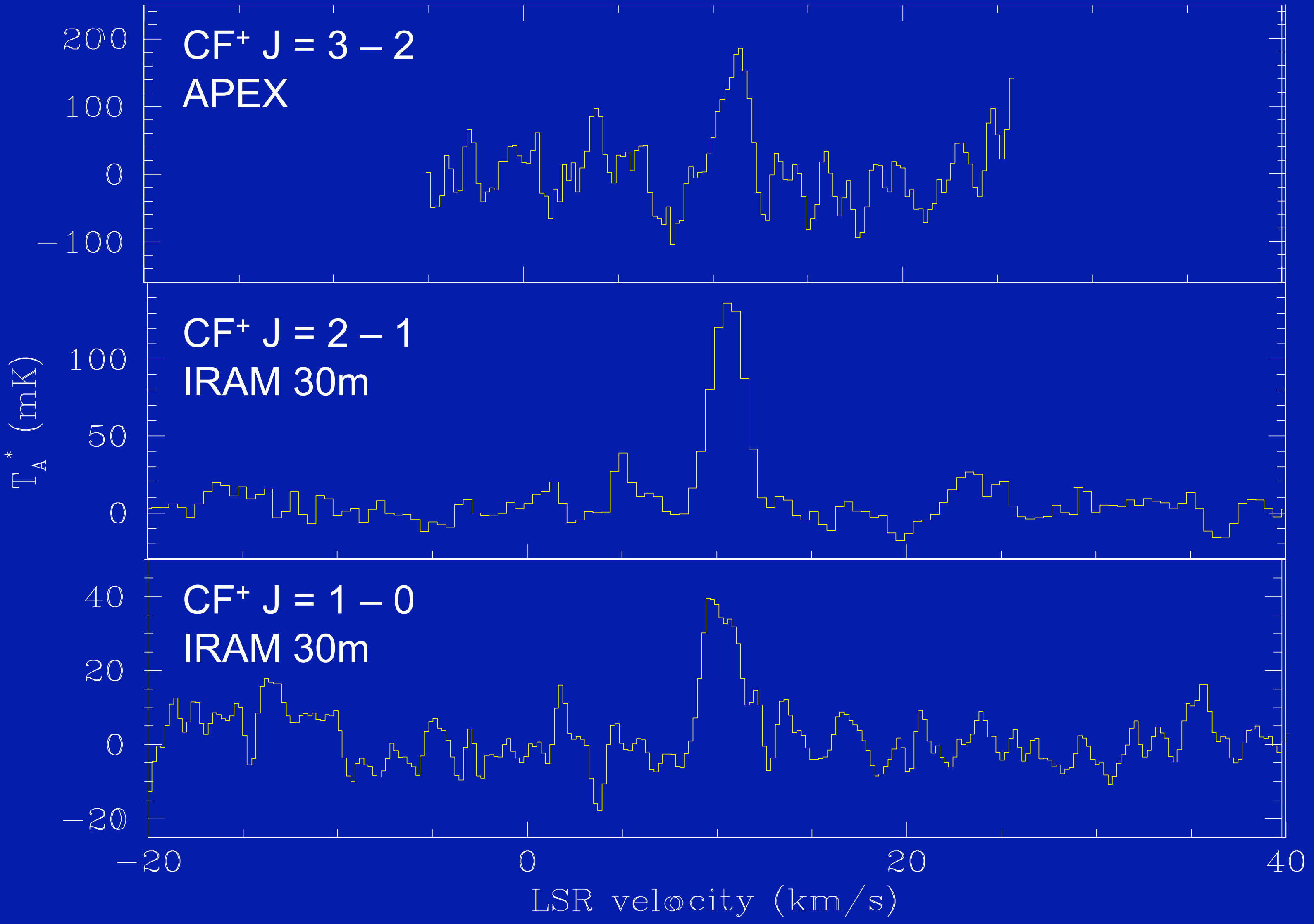
Predicted abundance profiles

(Neufeld, Wolfire & Schilke 1995)



CF^+ spectra toward the Orion Bar

(Neufeld et al. 2006, A&A)



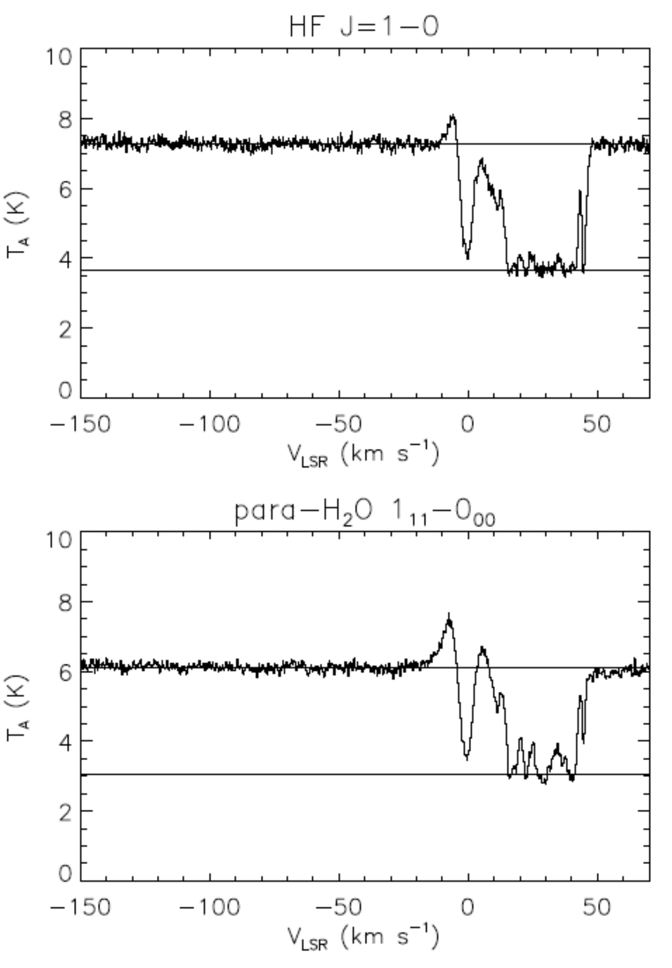
Herschel/HIFI observations of HF J = 1 – 0

- As part of the "PRobing InterStellar Molecules with Absorption line Studies (PRISMAS)" Key Program, we have observed the HF J = 1 – 0 transition toward three strong continuum sources with sight-lines that are intersected by foreground clouds:

G10.6 – 0.4 (W31C), W49, W51

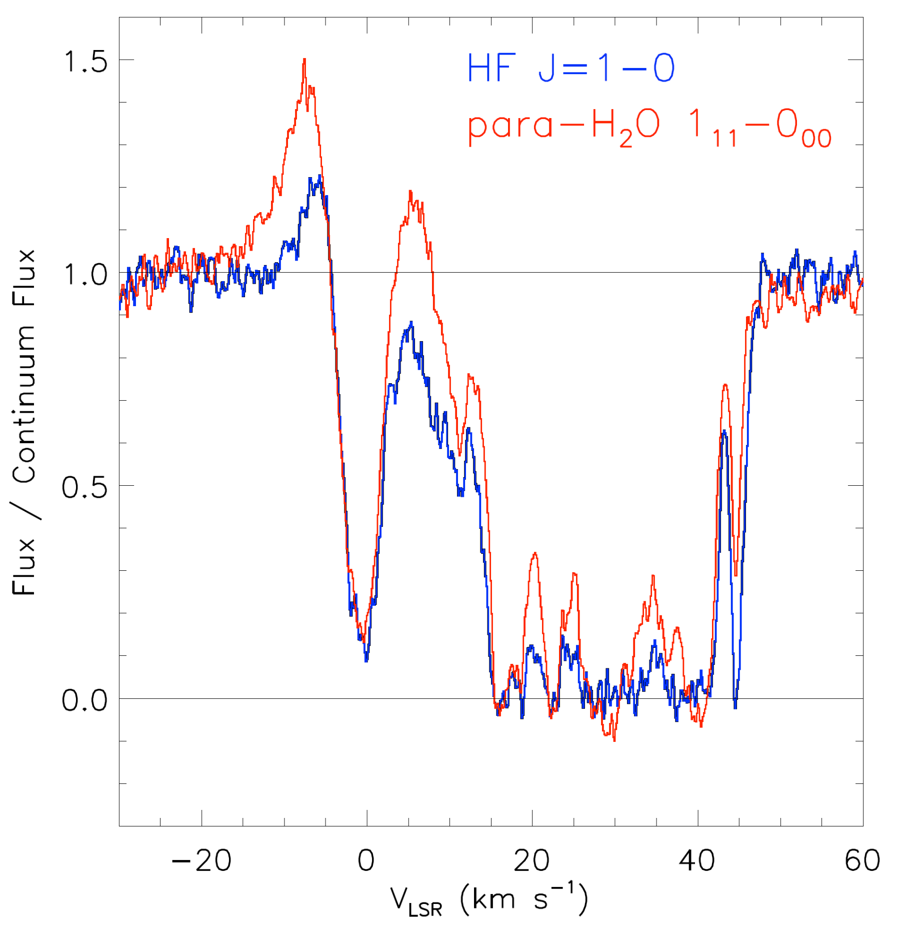
Strong HF absorption observed toward G10.6 – 0.4 (W31C)

- We observed the HF J = 1 – 0 and para-H_2O $1_{11} – 0_{00}$ transitions in mixer band 5a
- The on-source integration times were 225 s and 117 s, respectively
- The spectra are double-sideband spectra ➔ the complete absorption of radiation reduces the apparent antenna temperature by one-half (for a sideband gain ratio of unity)



Neufeld et al. 2010, A&A, accepted

Strong HF absorption observed toward G10.6 – 0.4 (W31C)



Neufeld et al. 2010, A&A, accepted

Strong HF absorption observed toward G10.6 – 0.4 (W31C)

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

$\tau(HF) / \tau(p\text{–}H_2O) \sim 2 – 3$

➔ $N(HF) / N(H_2O) \sim 1$

for an assumed H_2O ortho-to-para ratio of 3

Strong HF absorption observed toward G10.6 – 0.4 (W31C)

- Inferred column density and abundance

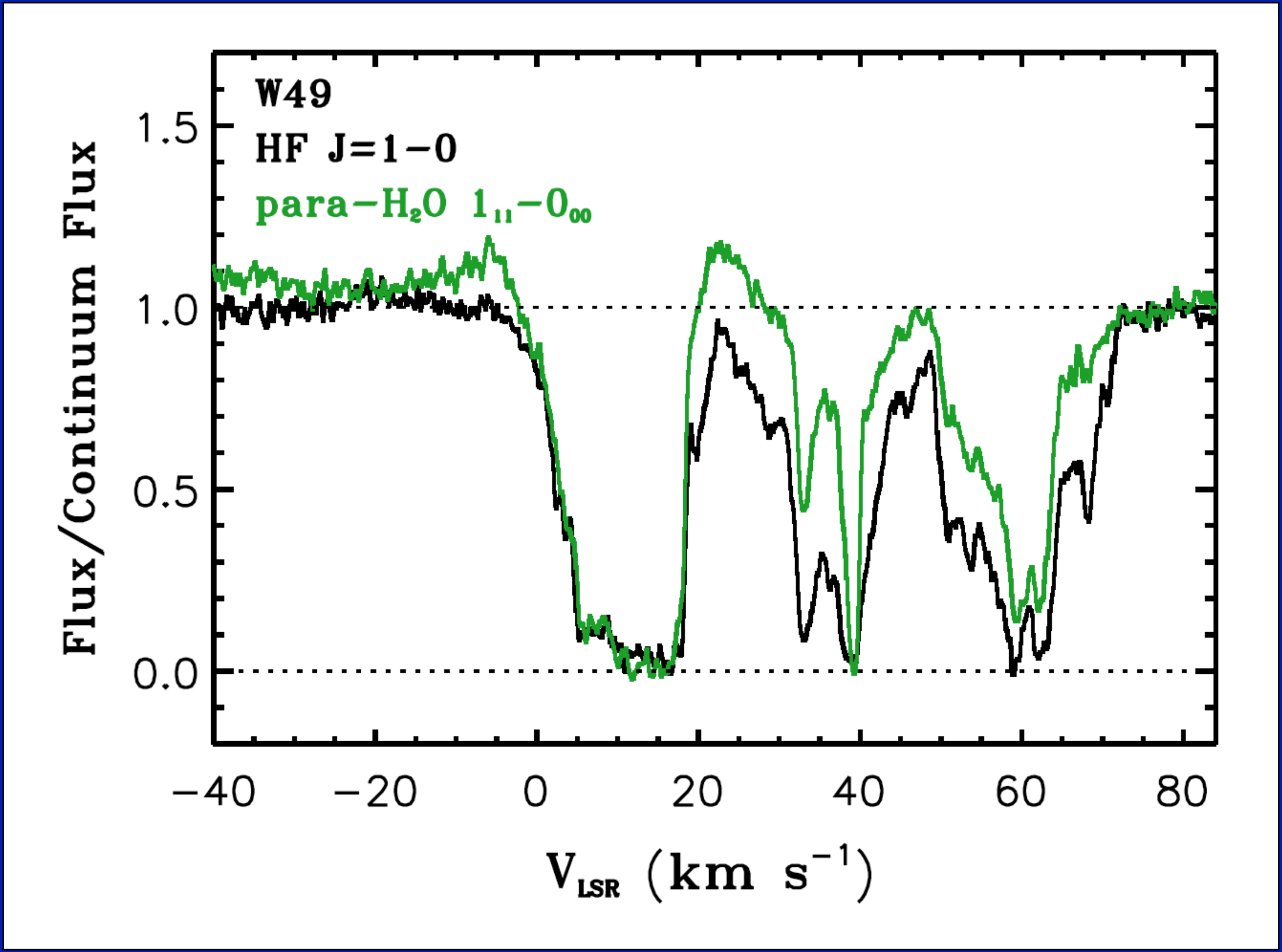
$N(HF) > 1.6 \times 10^{14}$ cm^{-2} (lower limit, because the optical depth is large)

Along this sight-line, $N_H = N(H) + 2\,N(H_2) \sim 2.7 \times 10^{22}$ cm^{-2} (based on extinction estimates)

$N(HF)/N_H > 6 \times 10^{-9}$

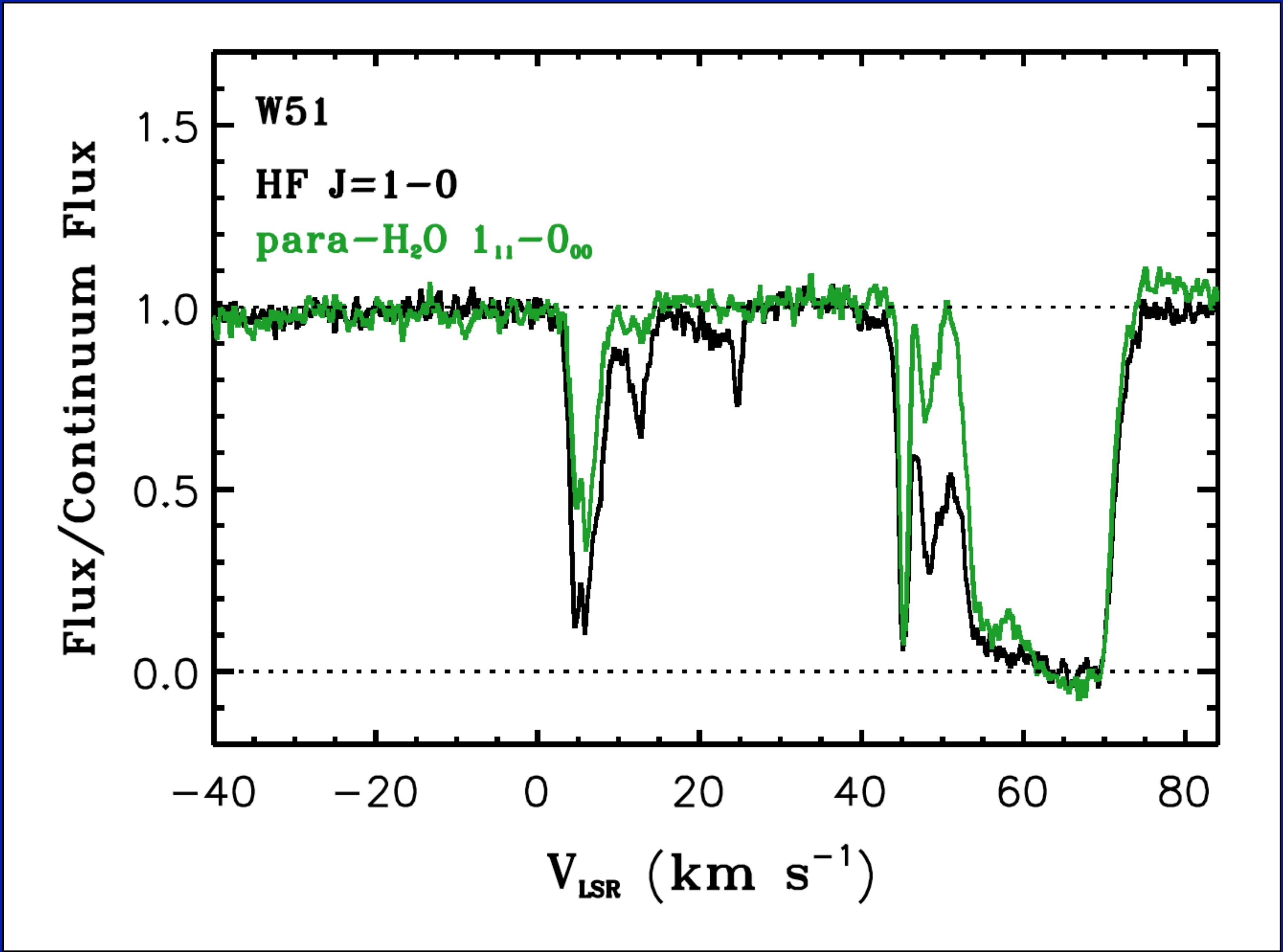
➔ HF accounts for 30 – 100% of fluorine in the gas phase

HF absorption also detected toward W49



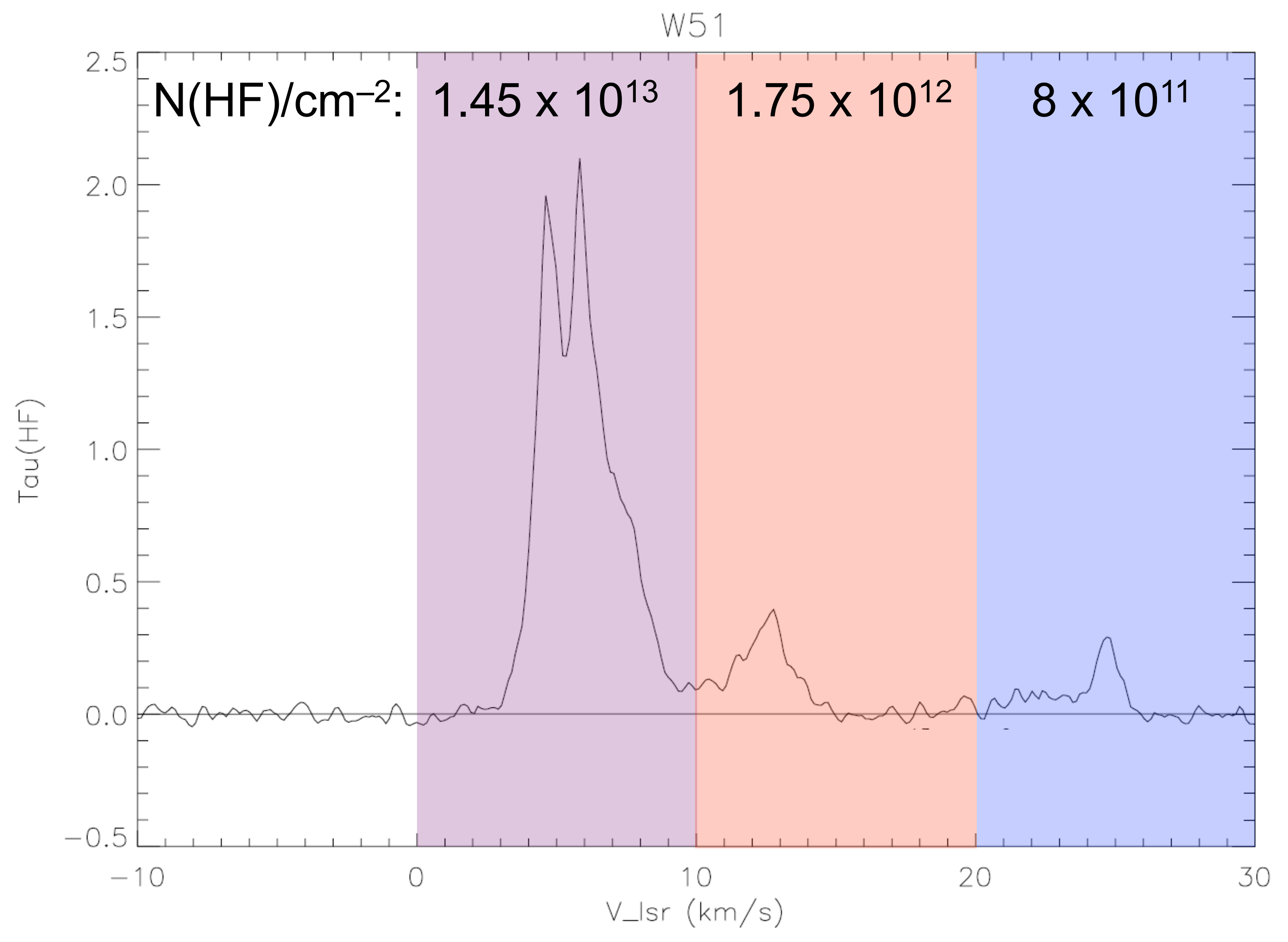
Sonnentrucker et al. 2010, A&A, submitted

…….and toward W51



Sonnentrucker et al. 2010, A&A, submitted

W51 exhibits some *optically-thin* absorption clouds



W51 absorption

Total HF column density at LSR velocities between 3 and 27 km s^{-1}: 1.7×10^{13} cm^{-2}

(a *measurement*, not a lower limit)

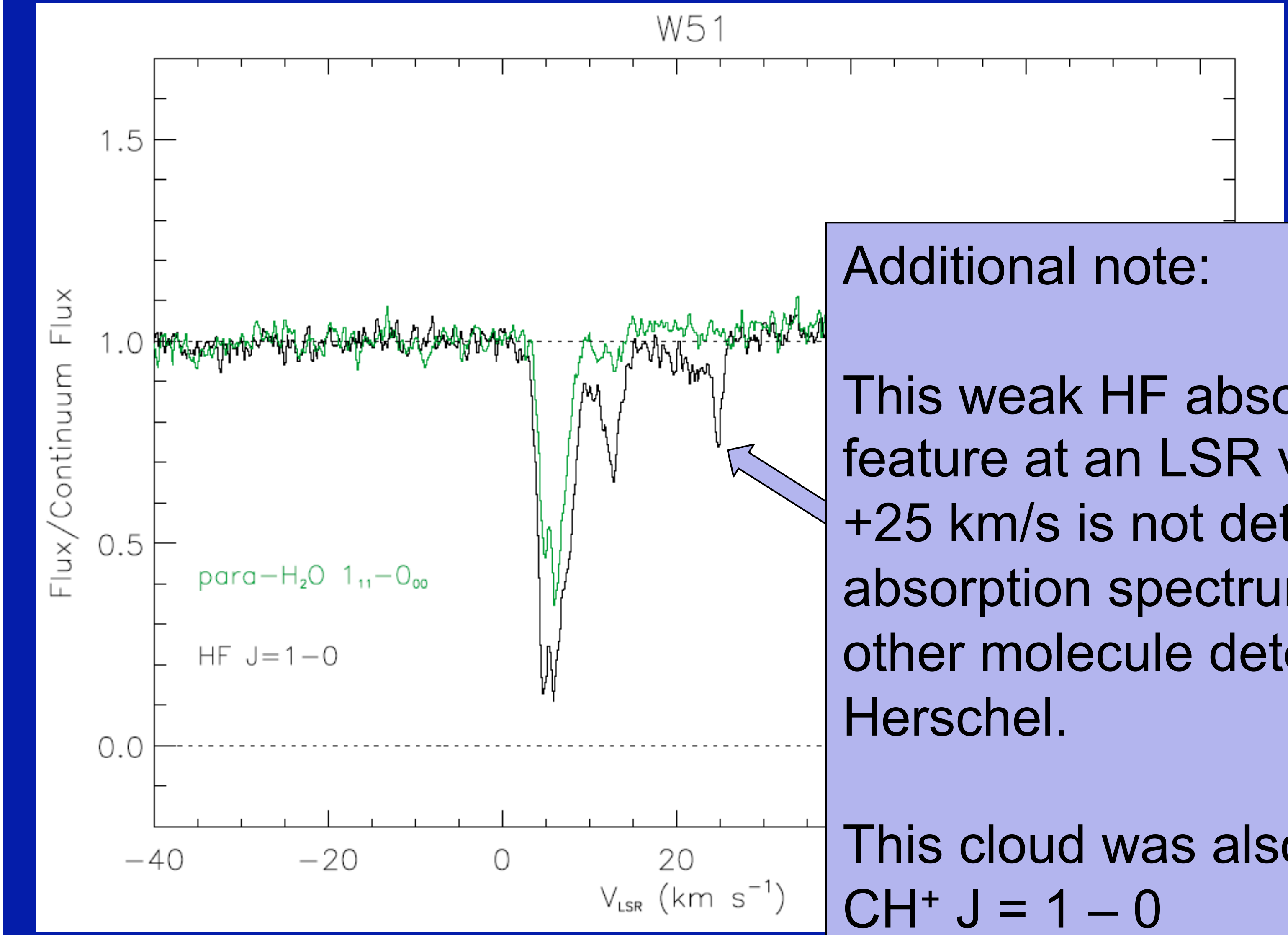
Corresponding H_2 column density ~ 6×10^{20} cm^{-2}

(based upon observations of CH by Gerin et al. 2010, and assuming $CH/H_2 = 3.5 \times 10^{-8}$)

$N(HF)/N(H_2) \sim 3 \times 10^{-8}$

By comparison: average $N_F/N_H = 1.8 \times 10^{-8}$ in diffuse atomic clouds (Snow et al. 2007)

W51 absorption



Additional note:

This weak HF absorption feature at an LSR velocity of +25 km/s is not detected in the absorption spectrum of any other molecule detected before Herschel.

This cloud was also detected in CH^+ J = 1 – 0 (Falgarone et al. 2010)

Future prospects

Hydrogen fluoride could prove to be a valuable surrogate for H_2

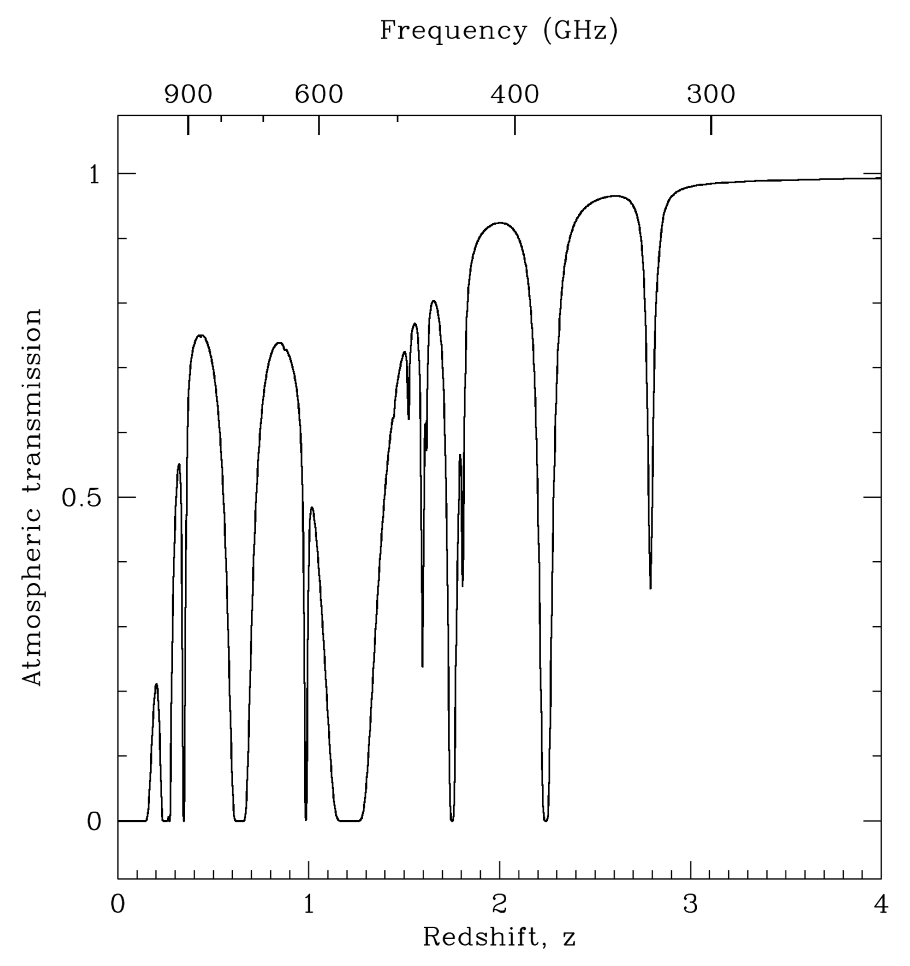
- Initial observations of diffuse clouds confirm the theoretical prediction that $N(HF)/2N(H_2)$ = gas phase elemental F/H ratio
- HF J = 1 – 0 can trace clouds of very small H_2 column density ($< 10^{20}$ cm $^{-2}$) that are difficult to detect by other means
- In the observations presented here, the on-source integration time was only 4 minutes

→ substantial sensitivity improvement will be achievable in longer integrations

Future prospects

Observations of HF J = 1 – 0 absorption might prove valuable in probing molecular hydrogen at high redshifts (e.g. in absorption toward a quasar)

Atmospheric windows appear at redshifts > 0.2

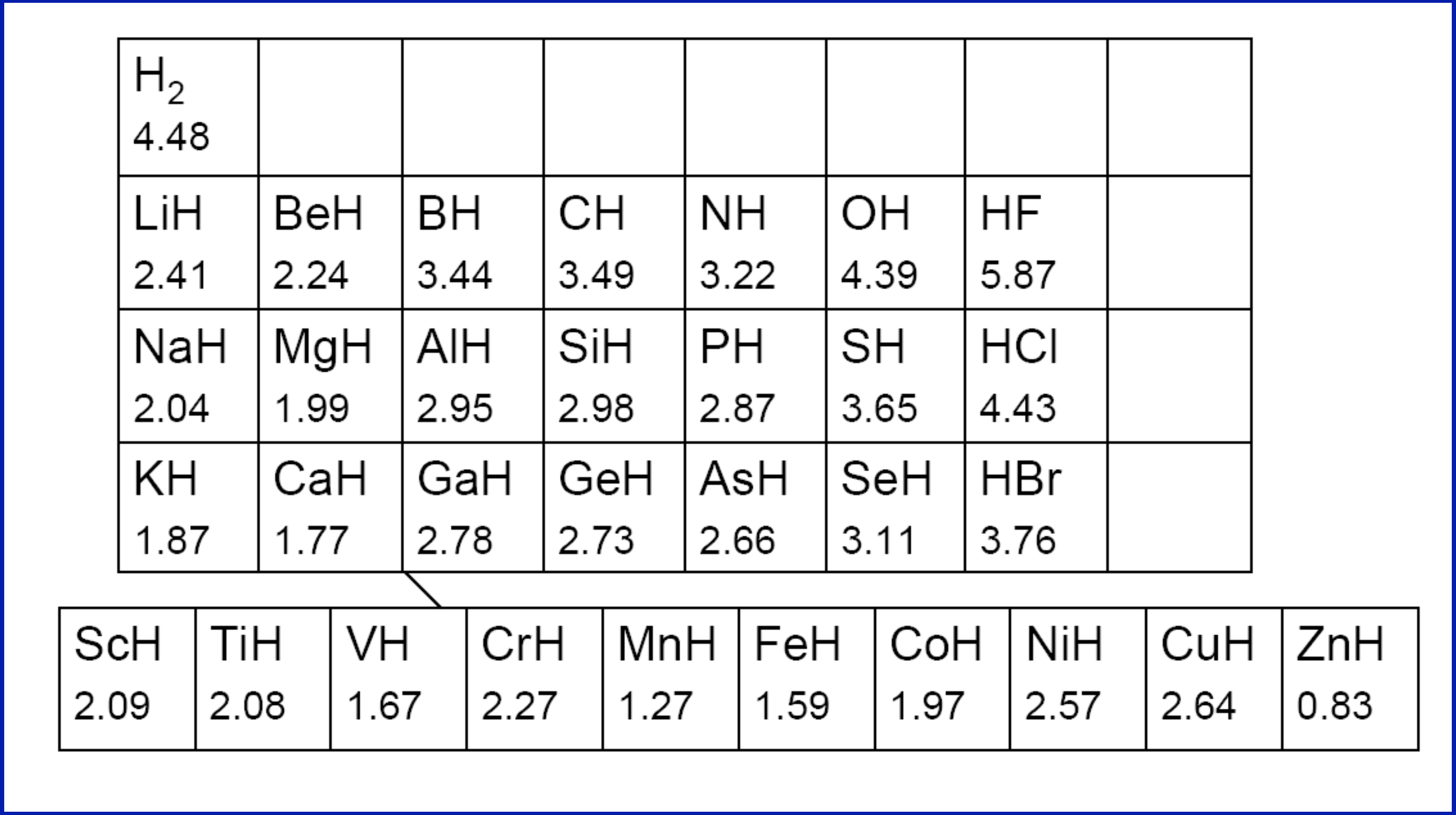


Neufeld, Wolfire & Schilke 2005

Interstellar OH^+ and H_2O^+:

probing clouds of low molecular fraction

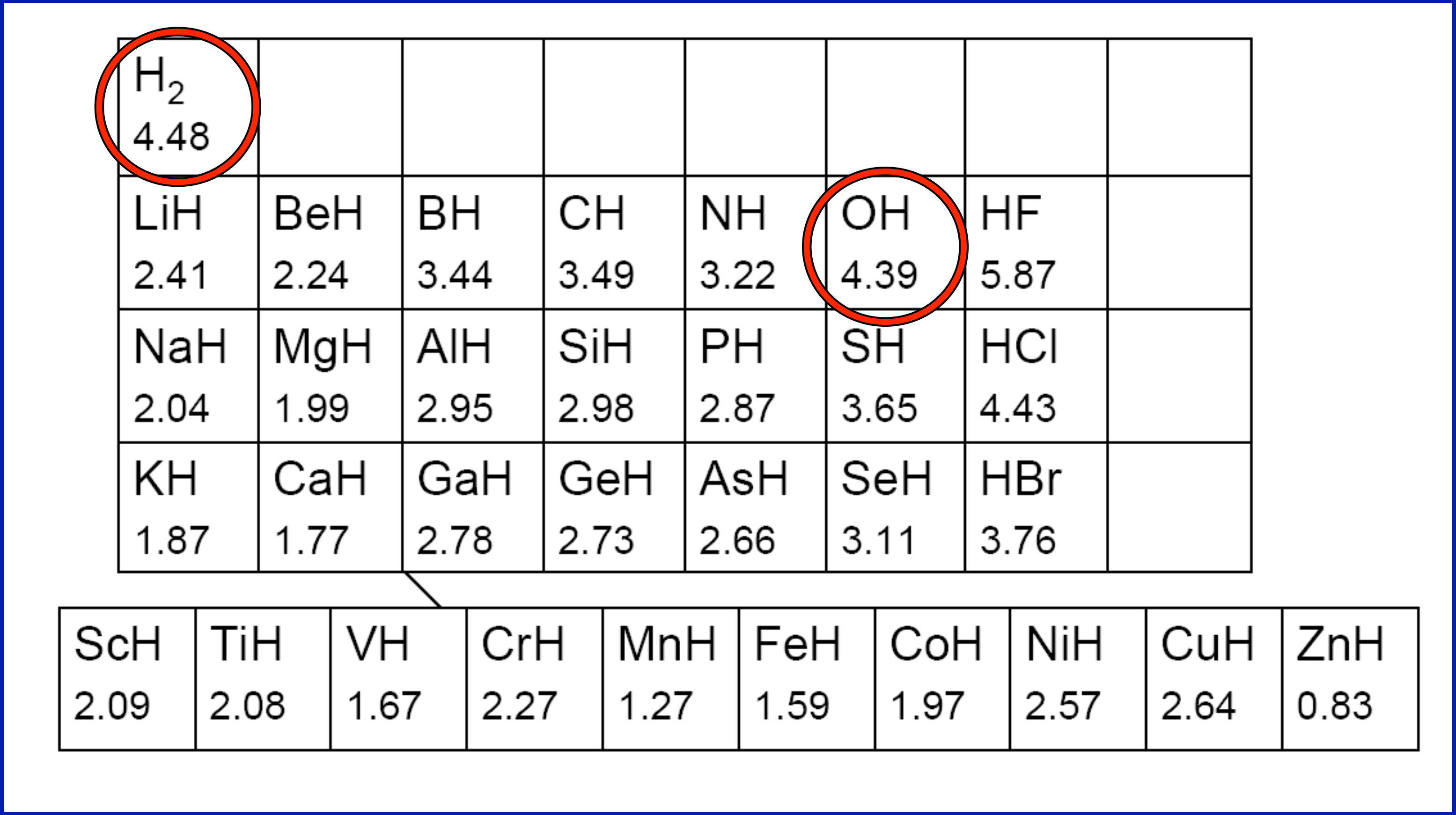
Dissociation energy of the diatomic hydrides (eV)



H_2 4.48							
LiH 2.41	BeH 2.24	BH 3.44	CH 3.49	NH 3.22	OH 4.39	HF 5.87	
NaH 2.04	MgH 1.99	AlH 2.95	SiH 2.98	PH 2.87	SH 3.65	HCl 4.43	
KH 1.87	CaH 1.77	GaH 2.78	GeH 2.73	AsH 2.66	SeH 3.11	HBr 3.76	

ScH 2.09	TiH 2.08	VH 1.67	CrH 2.27	MnH 1.27	FeH 1.59	CoH 1.97	NiH 2.57	CuH 2.64	ZnH 0.83

Dissociation energy of the diatomic hydrides (eV)



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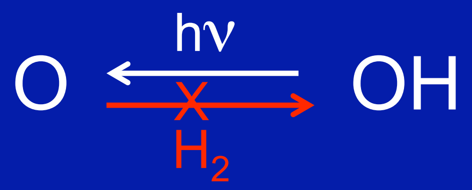
Neufeld and Wolfire 2009, ApJ

Chemistry of interstellar oxygen

- Oxygen differs from fluorine

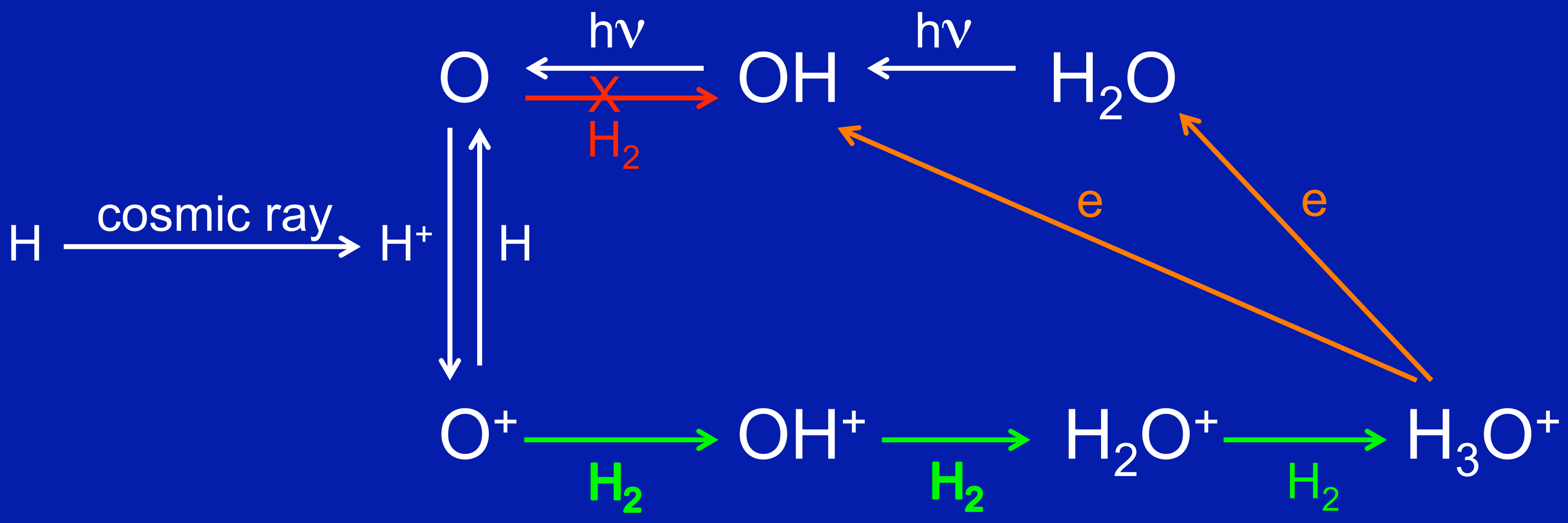


$$\mathrm{O}\ \underset{\cancel{\xrightarrow[H_2]{}}}{\xleftarrow{h\nu}}\ \mathrm{OH}$$

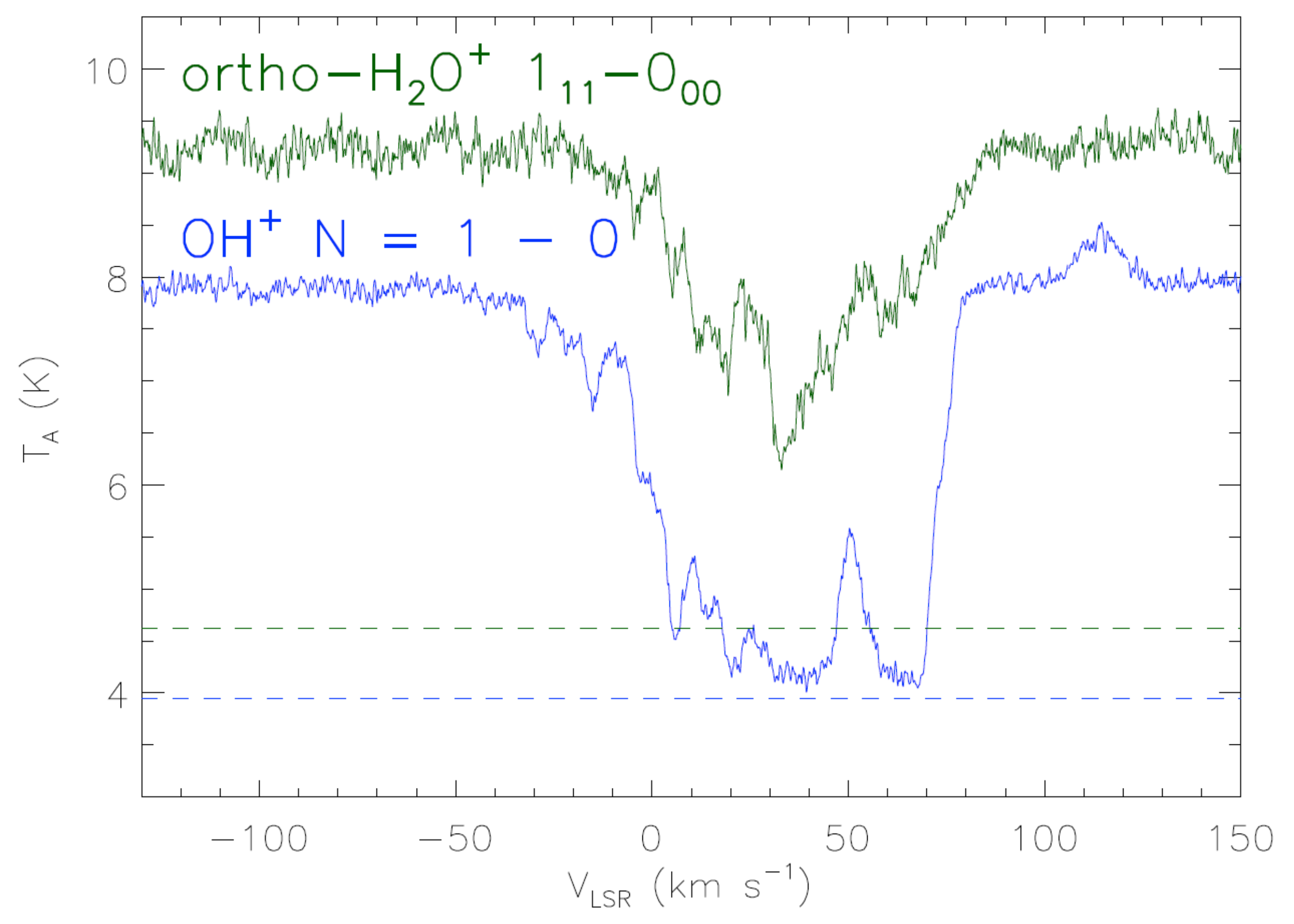
O cannot react with H_2 except at high temperature (> 300 K)

Chemistry of interstellar oxygen

- Chemistry is initiated by cosmic rays



OH^+ and H_2O^+ along the sight-line to W49N



Neufeld, Goicoechea, Sonnentrucker et al. 2010

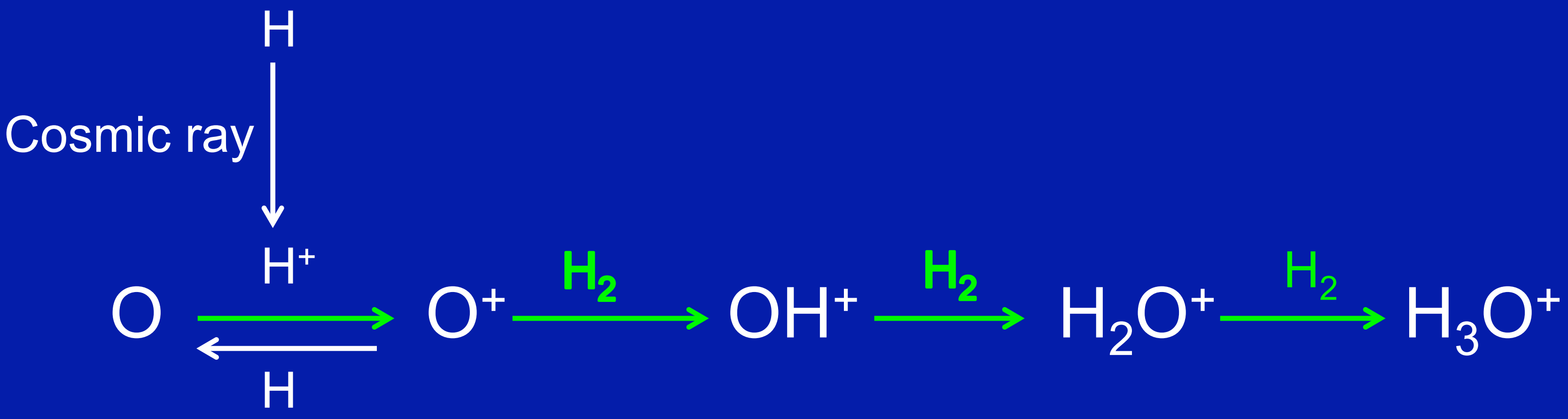
OH^+ and H_2O^+ along the sight-line to W49N

Rather surprising result:

$OH^+/H_2O^+ = 3 – 15$

We would have expected a ratio ~ 1 if reaction with H_2 dominated the destruction of H_2O^+

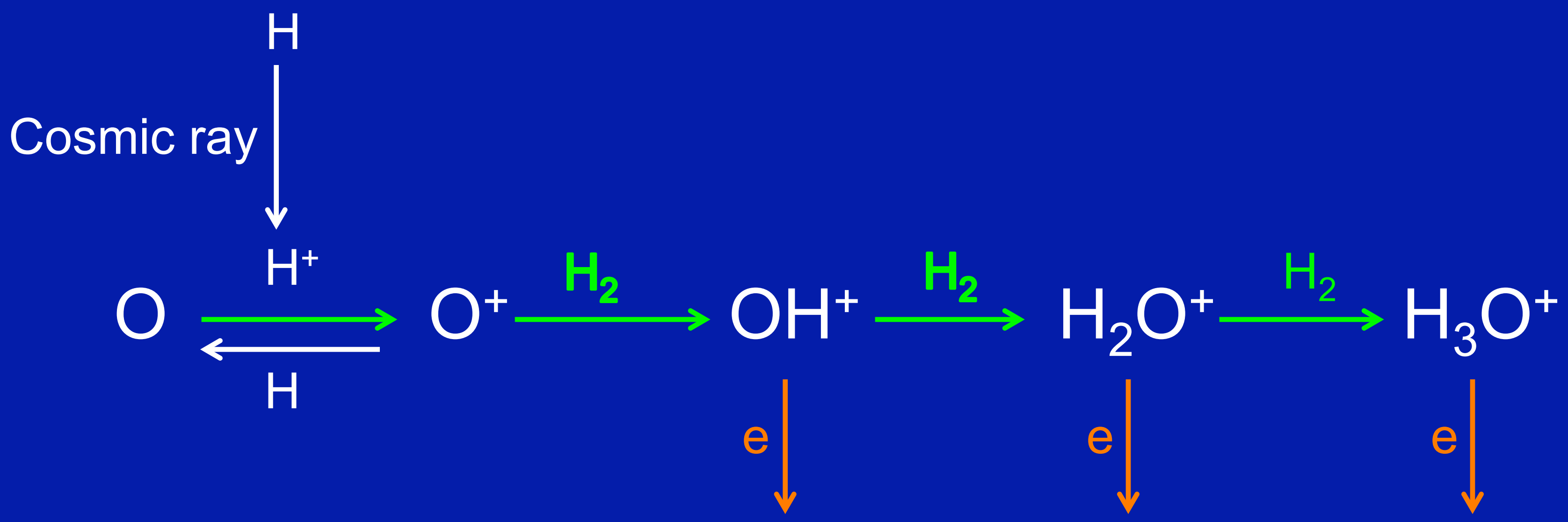
The oxygen pipeline



$$\mathrm{O} \underset{\mathrm{H}}{\overset{\mathrm{H^+}}{\rightleftharpoons}} \mathrm{O^+} \xrightarrow{\mathrm{H_2}} \mathrm{OH^+} \xrightarrow{\mathrm{H_2}} \mathrm{H_2O^+} \xrightarrow{\mathrm{H_2}} \mathrm{H_3O^+}$$

The large OH^+/H_2O^+ ratio implies that the pipeline is leaky

The oxygen pipeline



The large OH^+/H_2O^+ ratio implies that the pipeline is leaky – electrons are competing with H_2 in destroying molecular ions

Implication: the molecular fraction is only 2 – 8 %

OH^+ and H_2O^+ along the sight-line to W49N

Implications

OH^+/H_2O^+ ratio → low molecular fraction

Many small clouds along the sight-line (weakly shielded), or could represent departure from steady state

We may be witnessing the transition from atomic to molecular clouds

OH^+ and H_2O^+ along the sight-line to W49N

Implications

OH^+ column density → cosmic ray ionization rate

$\zeta_H = 0.5 - 3 \times 10^{-16}\ s^{-1}$

Confirmation of new larger values inferred by Indriolo, Geballe, Oka, & McCall from observations of H_3^+

Molecular astrophysics

- Why molecular astrophysics?
- The new capabilities of *Herschel/*HIFI
- HIFI observations of interstellar hydrides
- Prospects for SOFIA

Prospects for SOFIA

- Key capability required in many studies of astrophysical molecules:

High Spectral Resolution

Prospects for SOFIA

SOFIA can push high resolution spectroscopy forward in at least three areas

I. Heterodyne spectroscopy at frequencies above 2 THz (GREAT):

access to HD, OH, [OI] etc…

Prospects for SOFIA

SOFIA can push high resolution spectroscopy forward in at least three areas

II. Very high resolution mid-IR spectroscopy (EXES):

access to vibrational bands

Prospects for SOFIA

SOFIA can push high resolution spectroscopy forward in at least three areas

III. Spatial multiplex advantage:

Heterodyne arrays for mapping

Summary

- Observations of astrophysical molecules provide a wealth of information of broad astrophysical interest
- Infrared observations from airborne, balloon or satellite observatories are needed to study many important species
- High spectral resolution is crucial for many applications

Bonus slides

Thermochemistry in the interstellar medium

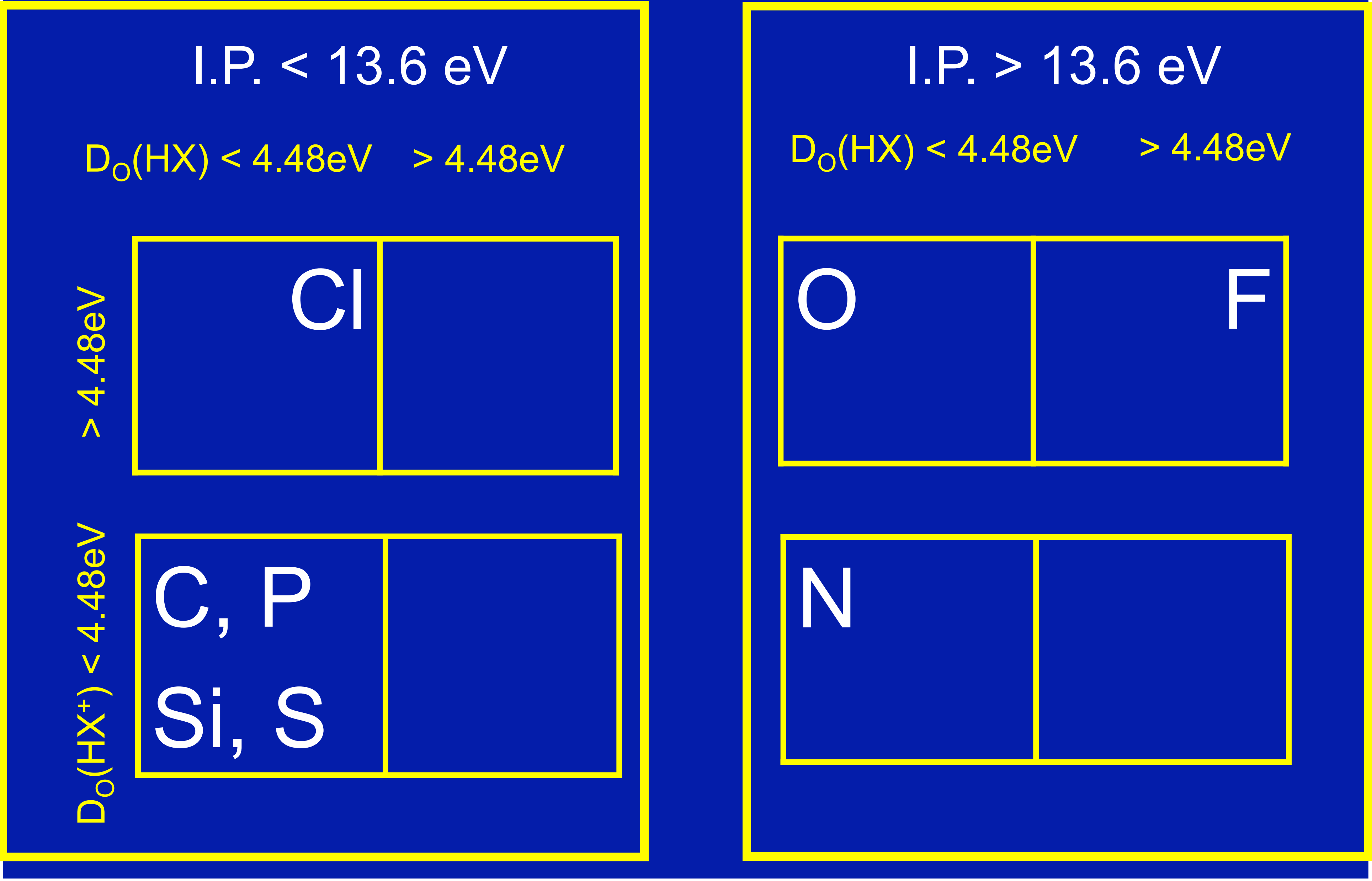
- Two or three key thermochemical parameters largely determine the chemistry of any element X

  1) The ionization potential of X
  2) The dissociation energy of XH
  3) The dissociation energy of XH^+

Thermochemical data (eV)

Element	I.P	D_0 (XH^+)	D_0 (XH)
F	17.42		5.87
N	14.53		3.22
O	13.62		4.39
H	13.598		4.48
Cl	12.97	4.65	4.43
C	11.26	4.11	3.49
S	10.36	3.49	3.65
Si	8.15	3.23	2.98

Five families of elements



I.P. < 13.6 eV

	$D_O(HX)$ < 4.48eV	> 4.48eV
> 4.48eV	Cl	
$D_O(HX^+)$ < 4.48eV	C, P Si, S	

I.P. > 13.6 eV

$D_O(HX)$ < 4.48eV	> 4.48eV
O	F
N	