EVOLVED STARS (II)
LINE SURVEYS IN THE ALMA ERA

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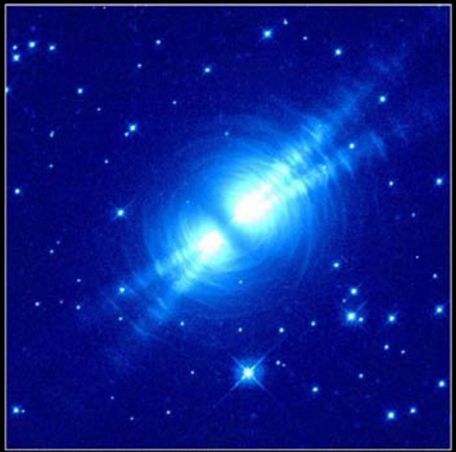
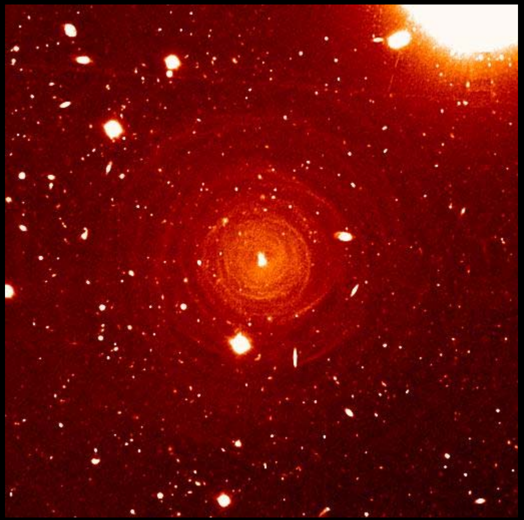
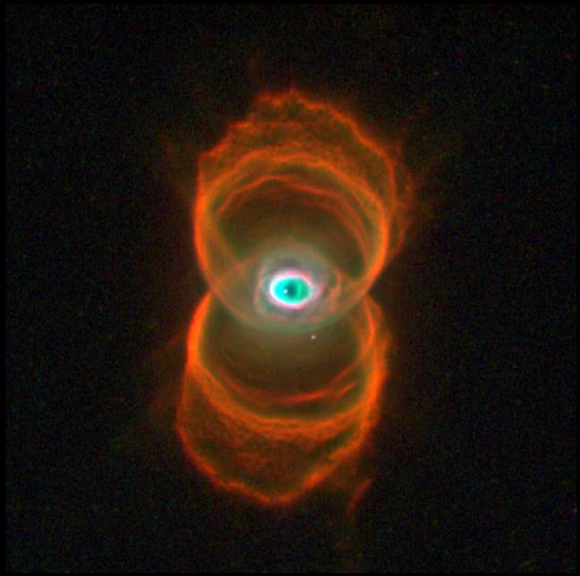
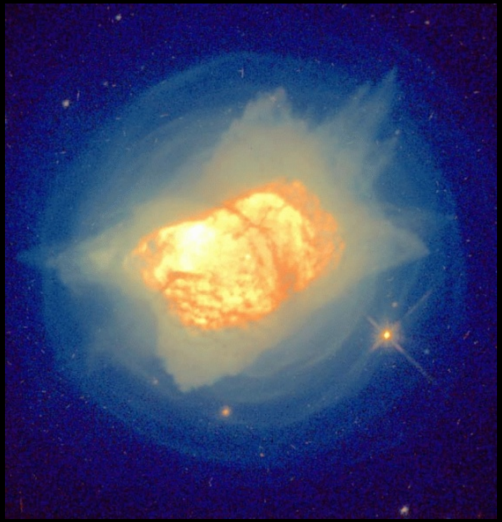


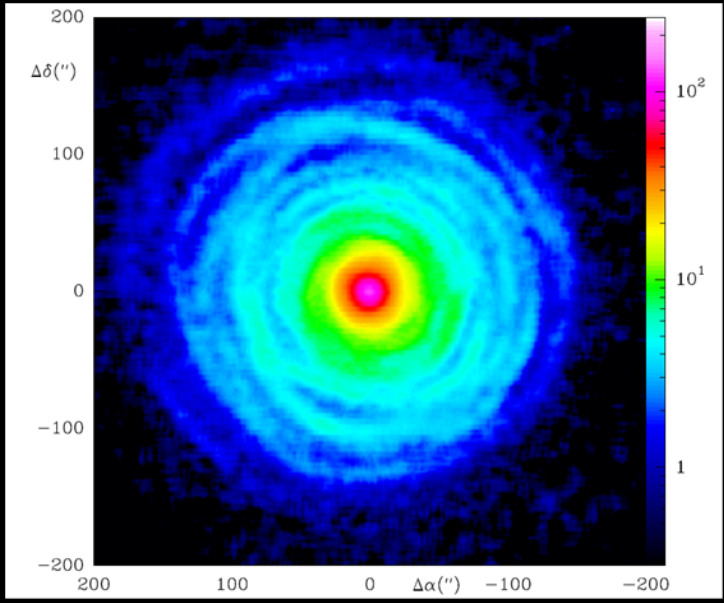
Egg Nebula · CRL 2688 HST · WFPC2
PRC96-03 · ST ScI OPO · January 16, 1996
R. Sahai and J. Trauger (JPL), the WFPC2 Science Team and NASA





Hourglass Nebula · MyCn18 HST · WFPC2
PRC96-07 · ST ScI OPO · January 16, 1996
R. Sahai and J. Trauger (JPL), the WFPC2 Science Team and NASA





The case of IRC+10216

ANATOMY OF AN AGB STAR

- THE DUST FORMATION ZONE
- THE INTERMEDIATE ENVELOPE
- THE EXTERNAL LAYERS
- PHOTOCHEMISTY, SHOCKS AND

THE ROLE OF BINARITY IN SHAPING

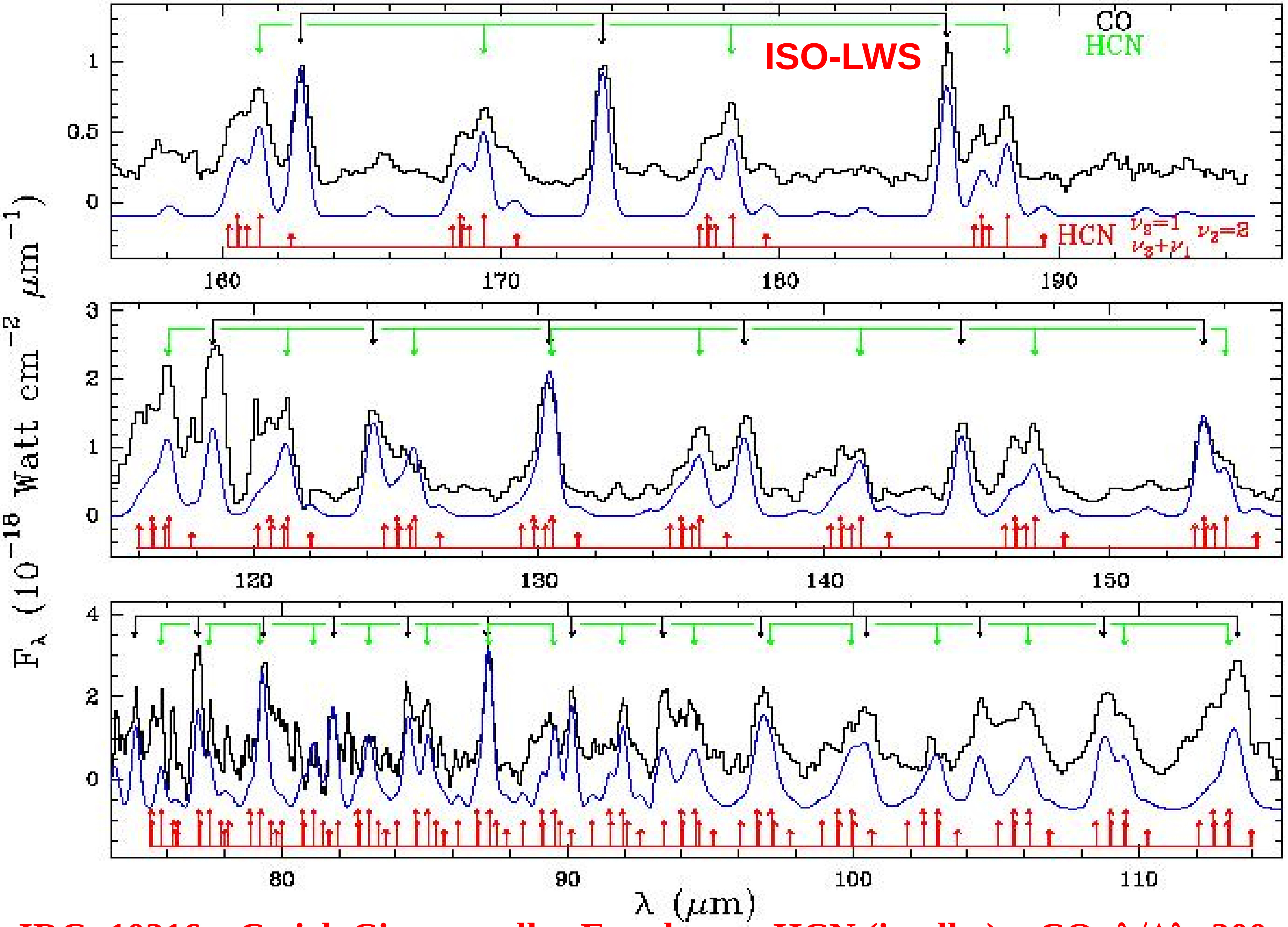
THE CIRCUMSTELLAR ENVOLOPE

The Physical and Chemical Conditions in the dust formation zone in IRC+10216

The first step to understand the chemistry of the whole envelope

Tools: Line Surveys in the Mid and Near Infrared with ISO & Ground Based Telescopes

Cernicharo et al., 1996, A.&A., 315, 201



IRC+10216 a C-rich Circumstellar Envelope :: HCN (in all ν) + CO; λ/Δλ~300

A&A 529, L3 (2011)
DOI: 10.1051/0004-6361/201116717

Astronomy & Astrophysics

Letter to the Editor

Probing the dust formation region in IRC +10216 with the high vibrational states of hydrogen cyanide⋆,⋆⋆

J. Cernicharo[1], M. Agúndez[2], C. Kahane[3], M. Guélin[4], J. R. Goicoechea[1], N. Marcelino[1], E. De Beck[5], and L. Decin[5]

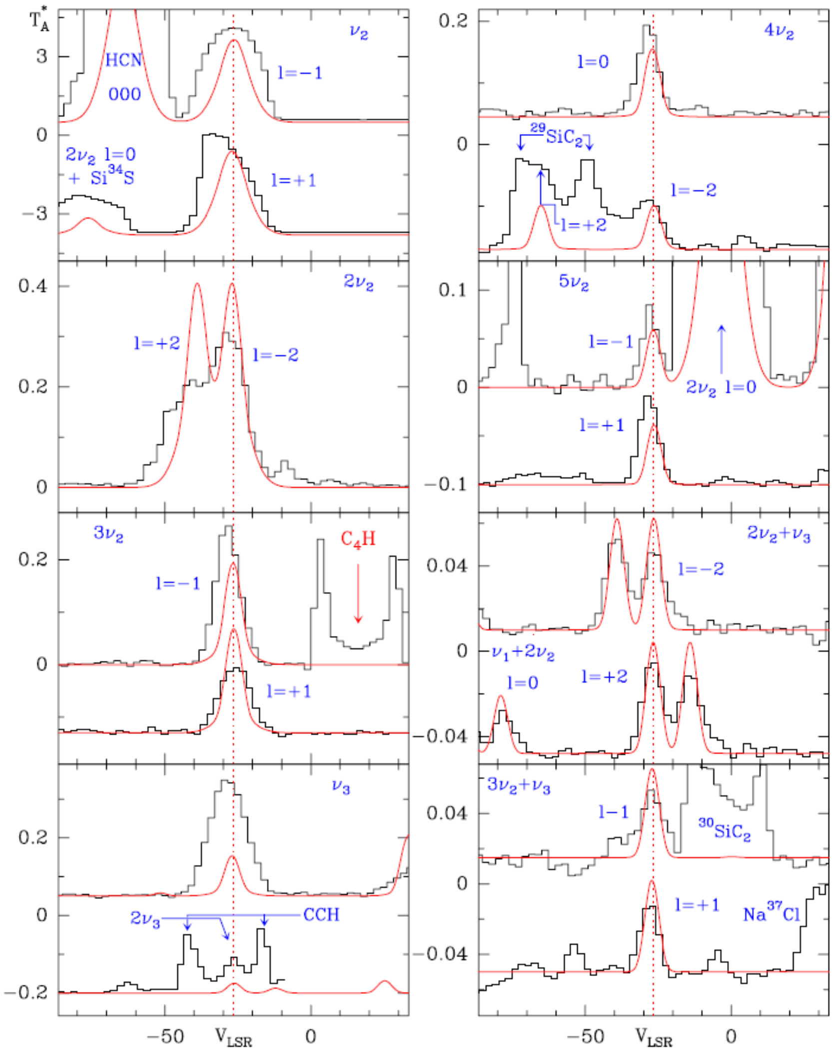


Fig. 1. Selected J = 3–2 lines of HCN in various vibrational states (blue labels). The spectra observed with the IRAM 30-m telescope are indicated by black histograms. The line profiles calculated from our model (see text) are plotted in red. The line parameters are given in Table 1. Intensity scale is antenna temperature. Main beam antenna temperatures can be obtained by dividing the T_A* scale of the 270 GHz data by a factor of 0.4. Velocity resolution is 2.3 km s^{-1}.

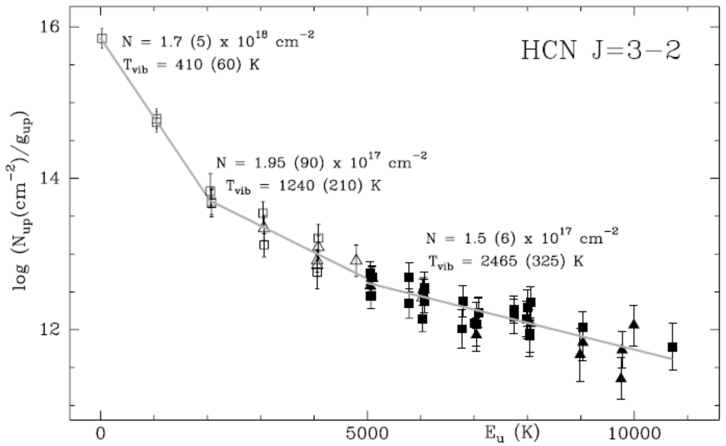
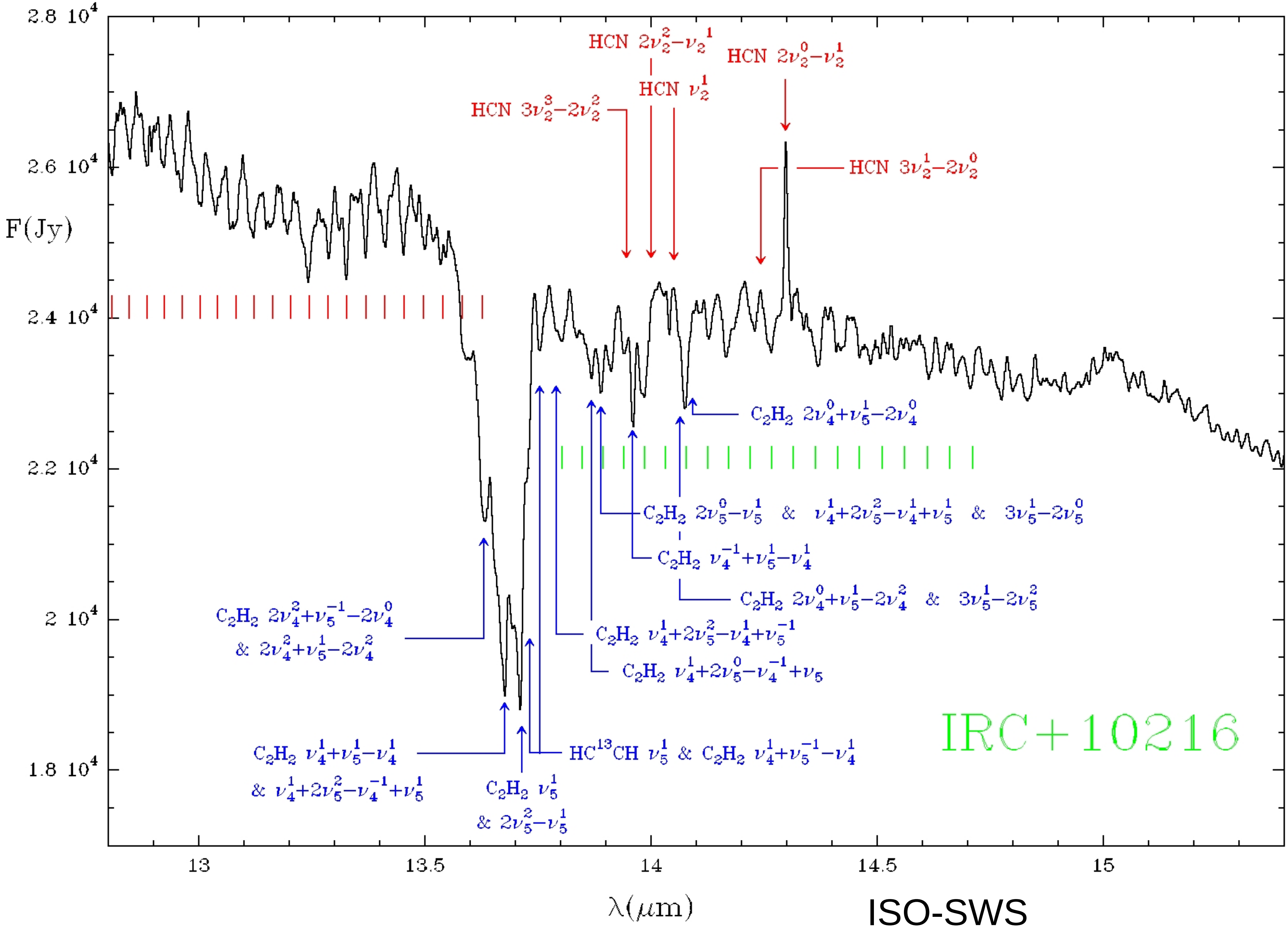
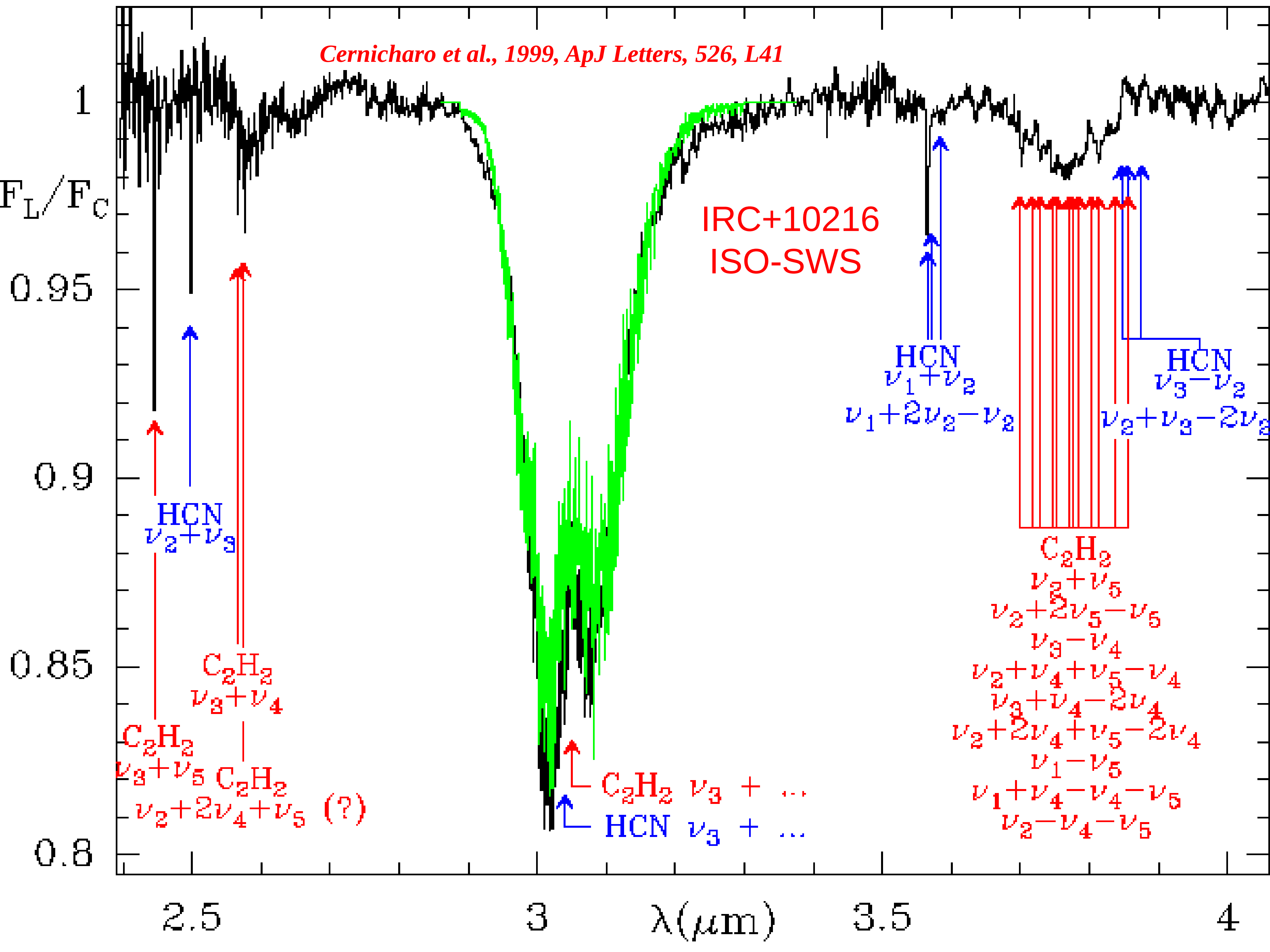


Fig. 2. Vibrational temperature diagram derived from the HCN J = 3–2 lines given in Table 1. Upper level population vs. its energy above the ground state. The data is fitted by 3 line segments corresponding to regions with temperatures T_{vib} ∼ 400 K, 1200 K, and 2400 K, respectively. HCN column densities are averaged over a source size of 1″ diameter. A conservative calibration error of 30% has been applied to all intensities. Values in parentheses correspond to 3σ errors on the derived vibrational temperatures and column densities. Filled triangles correspond to lines with half-power widths $\Delta v < 7$ km s^{-1}, filled squares correspond to lines with $7 < \Delta v < 9$ km s^{-1}, empty triangles correspond to lines with $9 < \Delta v < 12$ km s^{-1}, and empty squares to lines with $\Delta v > 12$ km s^{-1}.

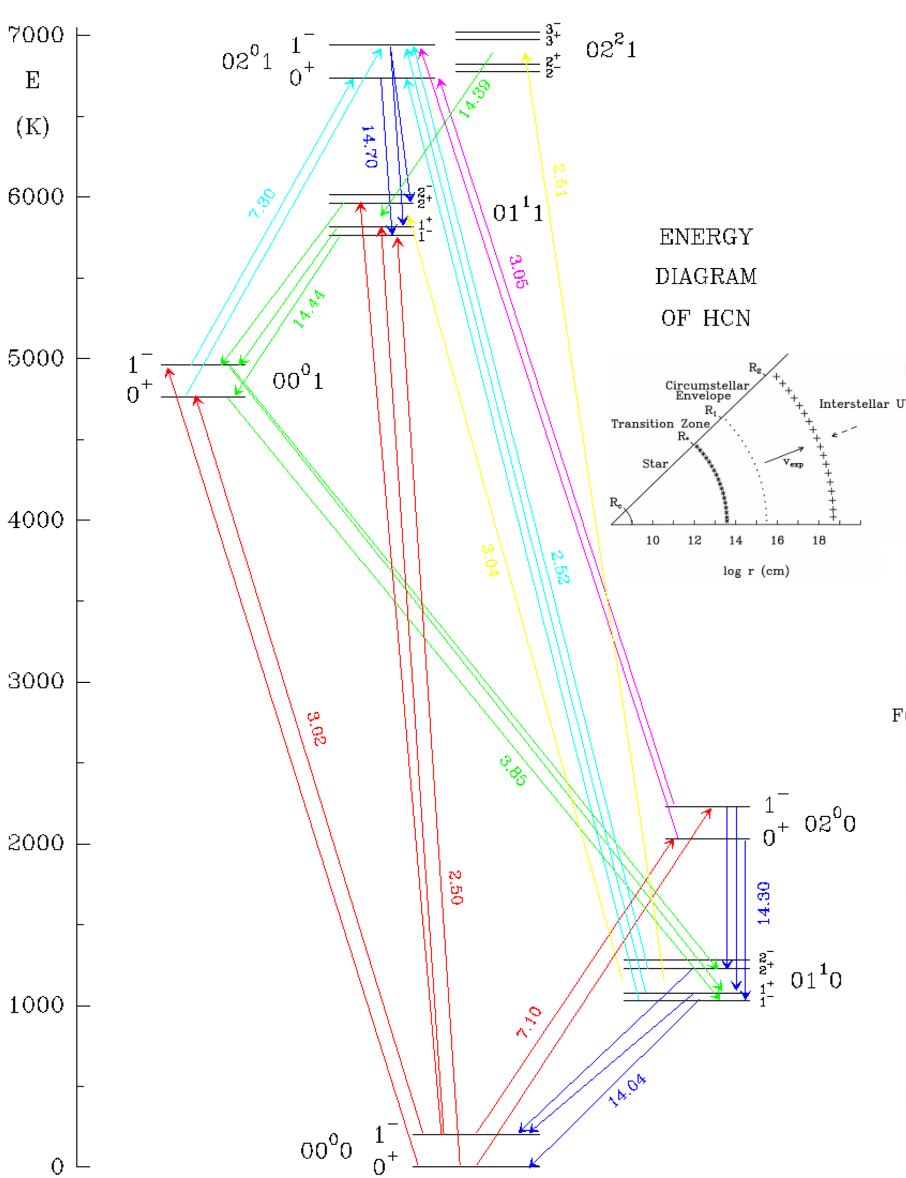


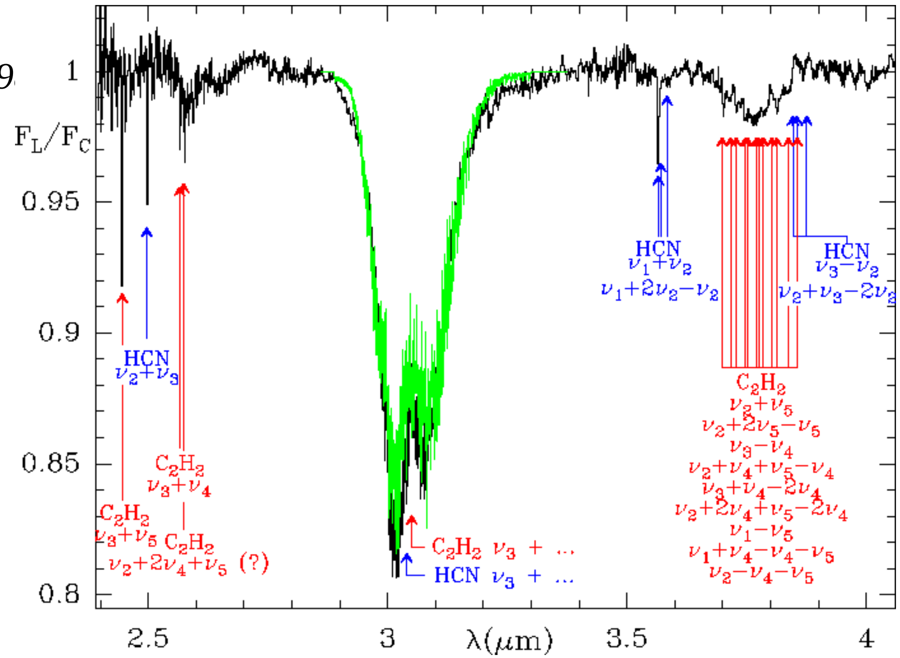
Cernicharo et al., 1999, ApJ Letters, 526, L41

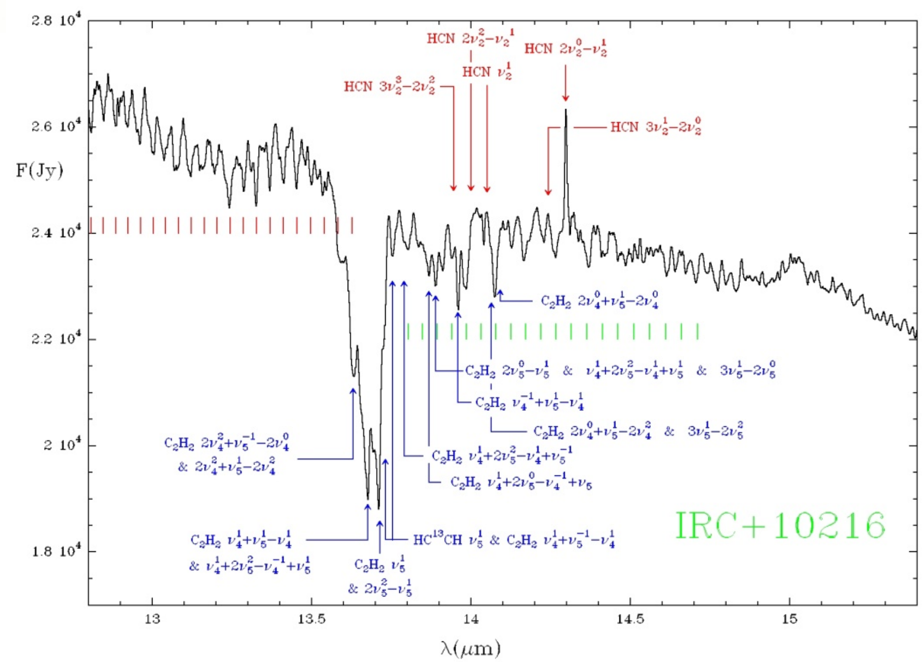


Cernicharo et al., 1999, ApJ Letters, 526, L41
IRC+10216
ISO-SWS
F_L/F_C
1
0.95
0.9
0.85
0.8
2.5
3
3.5
4
$\lambda(\mu m)$
HCN $\nu_2+\nu_3$
C_2H_2 $\nu_3+\nu_5$
C_2H_2 $\nu_3+\nu_4$
C_2H_2 $\nu_2+2\nu_4+\nu_5$ (?)
C_2H_2 ν_3 + ...
HCN ν_3 + ...
HCN $\nu_1+\nu_2$
$\nu_1+2\nu_2-\nu_2$
HCN $\nu_3-\nu_2$
$\nu_2+\nu_3-2\nu_2$
C_2H_2
$\nu_2+\nu_5$
$\nu_2+2\nu_5-\nu_5$
$\nu_3-\nu_4$
$\nu_2+\nu_4+\nu_5-\nu_4$
$\nu_3+\nu_4-2\nu_4$
$\nu_2+2\nu_4+\nu_5-2\nu_4$
$\nu_1-\nu_5$
$\nu_1+\nu_4-\nu_4-\nu_5$
$\nu_2-\nu_4-\nu_5$

González-Alfonso & Cernicharo 199







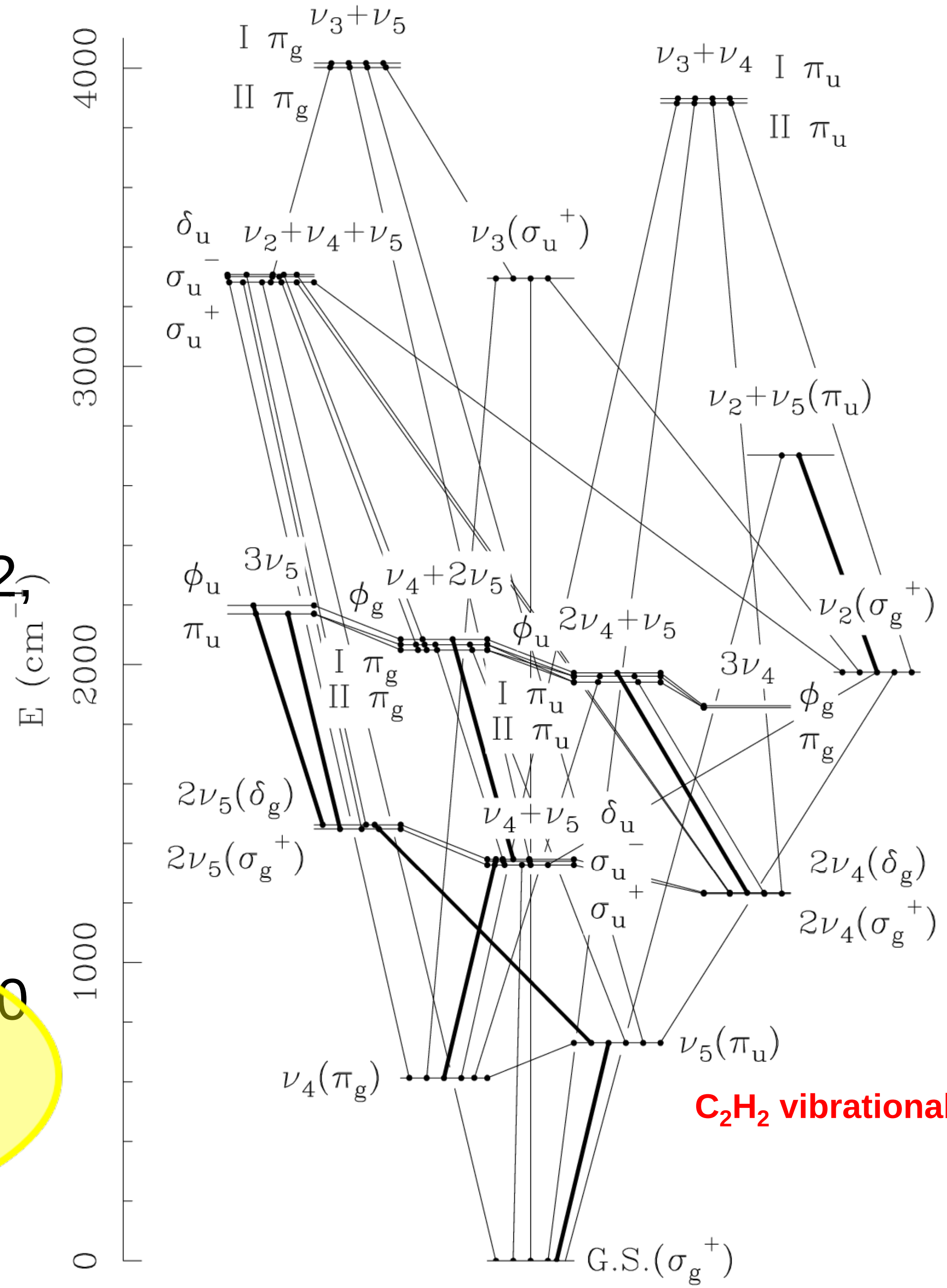
Observations of C_2H_2 and HCN observations with TEXES at the IRTF

PhD of J.Pablo Fonfría
(Fonfría et al., 2008, ApJ)

TEXES::Lacy et al., 2002, PASP, 114, 153

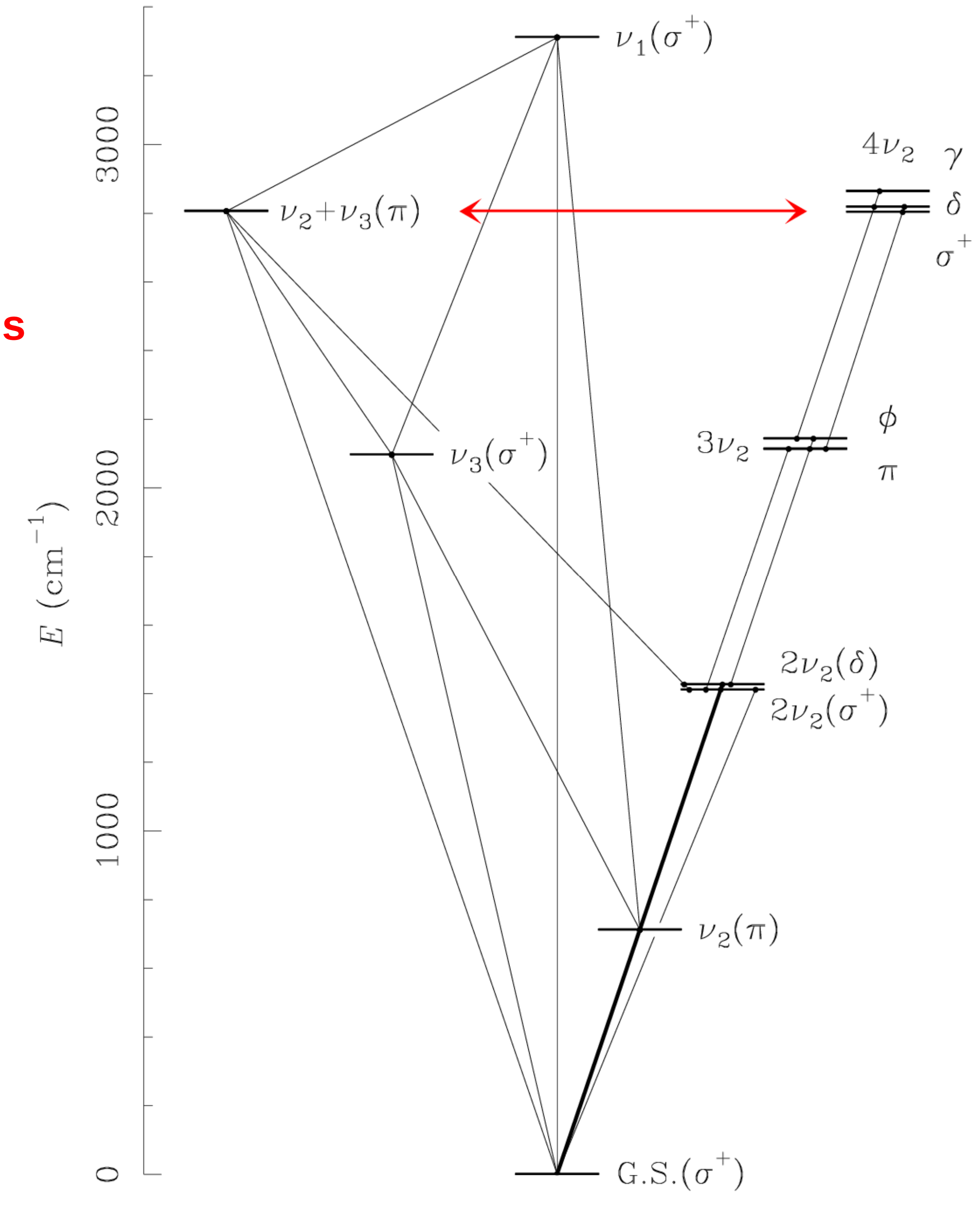
720-900 cm^{-1}
11.1-13.9 μm

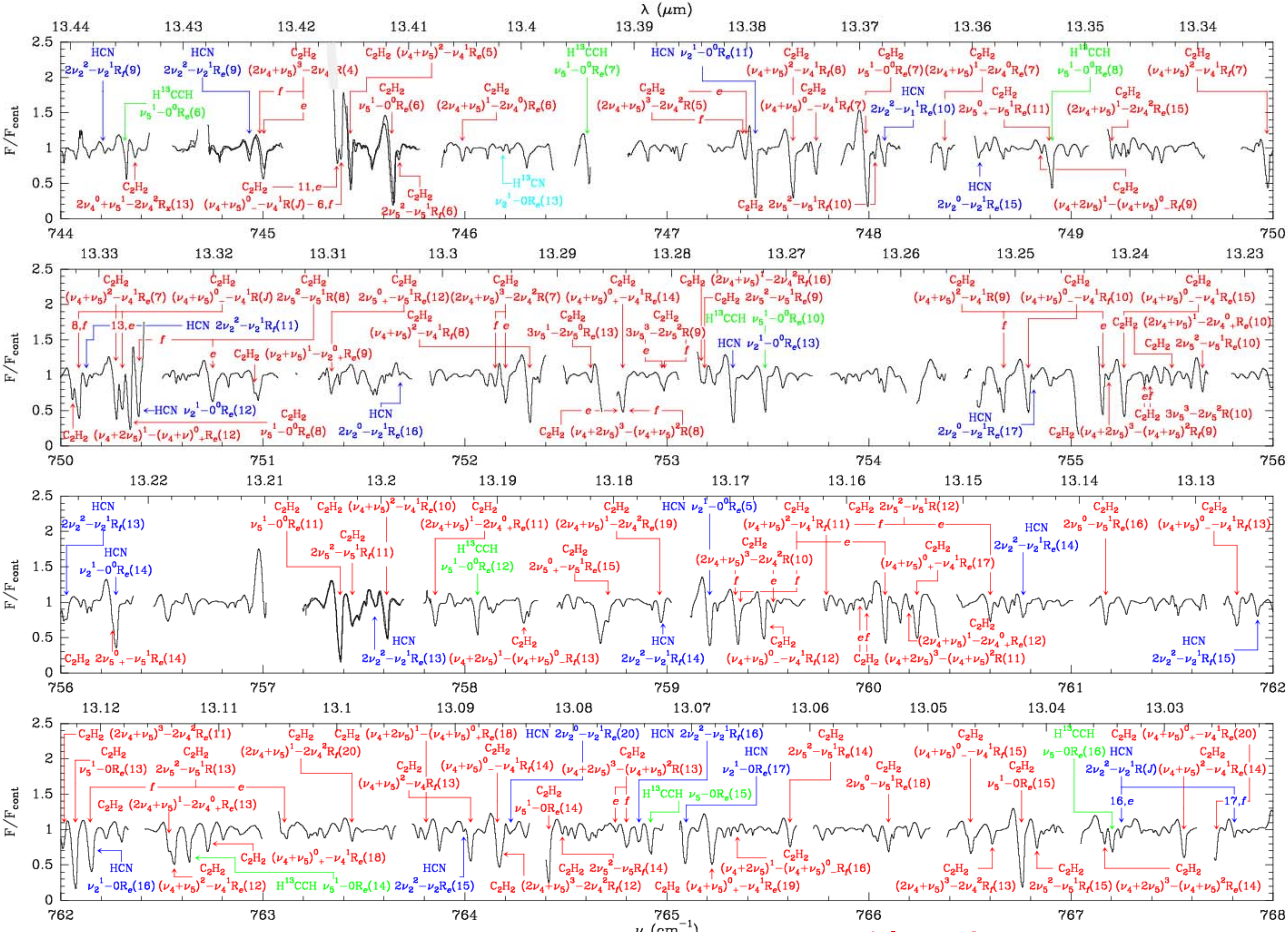
Spectral resolution 75000
4 km/s



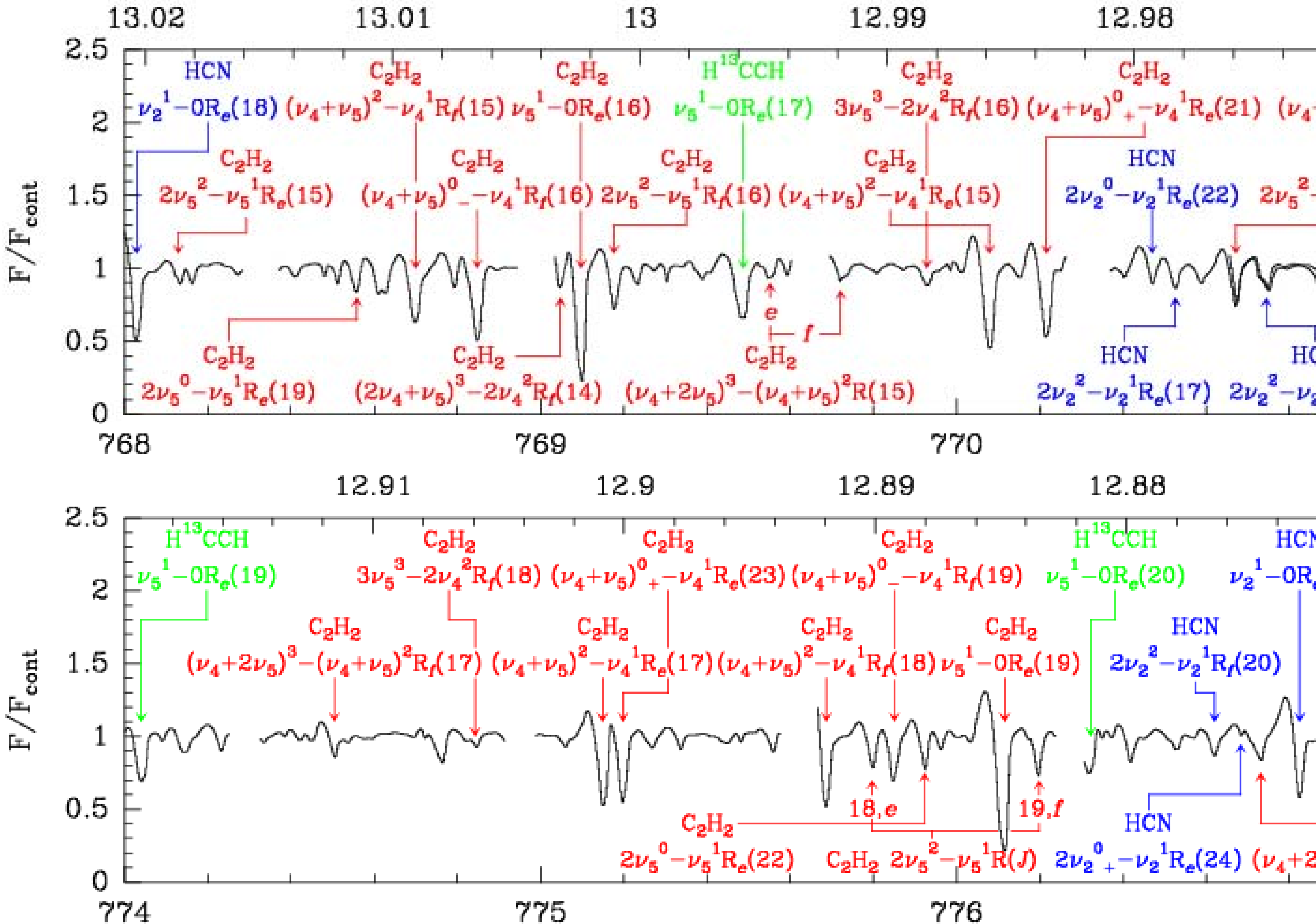
C_2H_2 vibrational levels

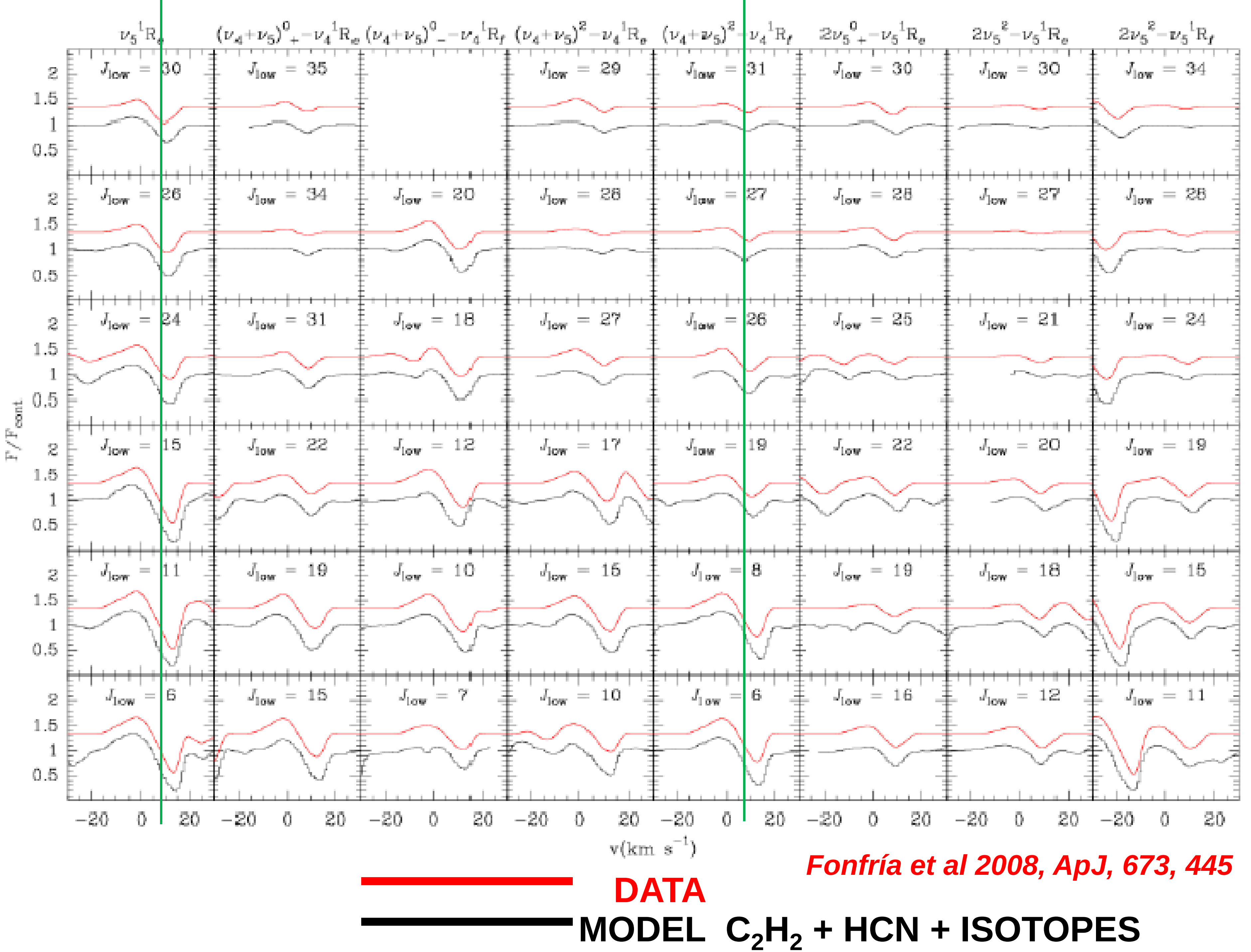
HCN vibrational levels





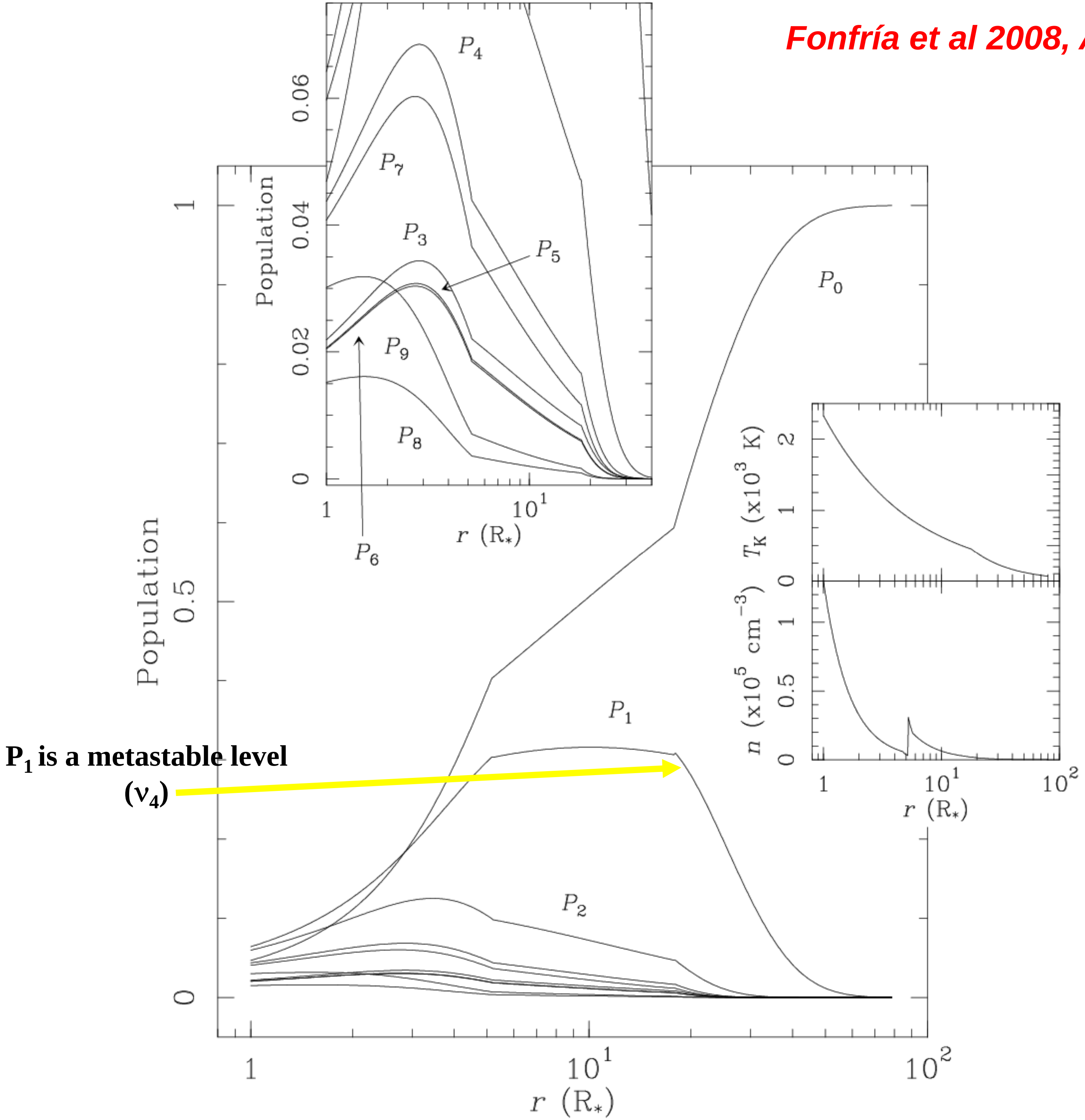
Fonfría et al 2008, ApJ, 673, 445


13.02
13.01
13
12.99
12.98
2.5
2
1.5
1
0.5
0
F/Fcont
HCN
ν2 1−0Re(18)
C2H2
(ν4+ν5)2−ν4 1Rf(15)
C2H2
ν5 1−0Re(16)
H13CCH
ν5 1−0Re(17)
C2H2
3ν5 3−2ν4 2Rf(16)
C2H2
(ν4+ν5)0+−ν4 1Re(21)
C2H2
2ν5 2−ν5 1Re(15)
C2H2
(ν4+ν5)0−−ν4 1Rf(16)
C2H2
2ν5 2−ν5 1Rf(16)
C2H2
(ν4+ν5)2−ν4 1Re(15)
HCN
2ν2 0−ν2 1Re(22)
e
f
C2H2
2ν5 0−ν5 1Re(19)
C2H2
(2ν4+ν5)3−2ν4 2Rf(14)
C2H2
(ν4+2ν5)3−(ν4+ν5)2R(15)
HCN
2ν2 2−ν2 1Re(17)
768
769
770
12.91
12.9
12.89
12.88
H13CCH
ν5 1−0Re(19)
C2H2
3ν5 3−2ν4 2Rf(18)
C2H2
(ν4+ν5)0+−ν4 1Re(23)
C2H2
(ν4+ν5)0−−ν4 1Rf(19)
H13CCH
ν5 1−0Re(20)
C2H2
(ν4+2ν5)3−(ν4+ν5)2Rf(17)
C2H2
(ν4+ν5)2−ν4 1Re(17)
C2H2
(ν4+ν5)2−ν4 1Rf(18)
C2H2
ν5 1−0Re(19)
HCN
2ν2 2−ν2 1Rf(20)
18,e
19,f
C2H2
2ν5 0−ν5 1Re(22)
C2H2 2ν5 2−ν5 1R(J)
HCN
2ν2 0+−ν2 1Re(24)
774
775
776



$\nu_5{}^1R_e$
$(\nu_4+\nu_5)^0{}_+-\nu_4{}^1R_e$
$(\nu_4+\nu_5)^0{}_--\nu_4{}^1R_f$
$(\nu_4+\nu_5)^2-\nu_4{}^1R_e$
$(\nu_4+\nu_5)^2-\nu_4{}^1R_f$
$2\nu_5{}^0{}_+-\nu_5{}^1R_e$
$2\nu_5{}^2-\nu_5{}^1R_e$
$2\nu_5{}^2-\nu_5{}^1R_f$
F/F_{cont}
$v(km\ s^{-1})$
Fonfría et al 2008, ApJ, 673, 445
DATA
MODEL C_2H_2 + HCN + ISOTOPES

Fonfría et al 2008, ApJ, 673, 445



RESULTS

x(C_2H_2)

Z I 7.5 10^{-6}

Z II 8.0 10^{-5}

ZIII 8.0 10^{-5}

x(HCN)

Z I 2.5 10^{-5}

Z II 5.0 10^{-5}

ZIII 5.0 10^{-5}

$^{12}C/^{13}C$=41

Z I 1- 5 R_*

Z II 5-20 R_*

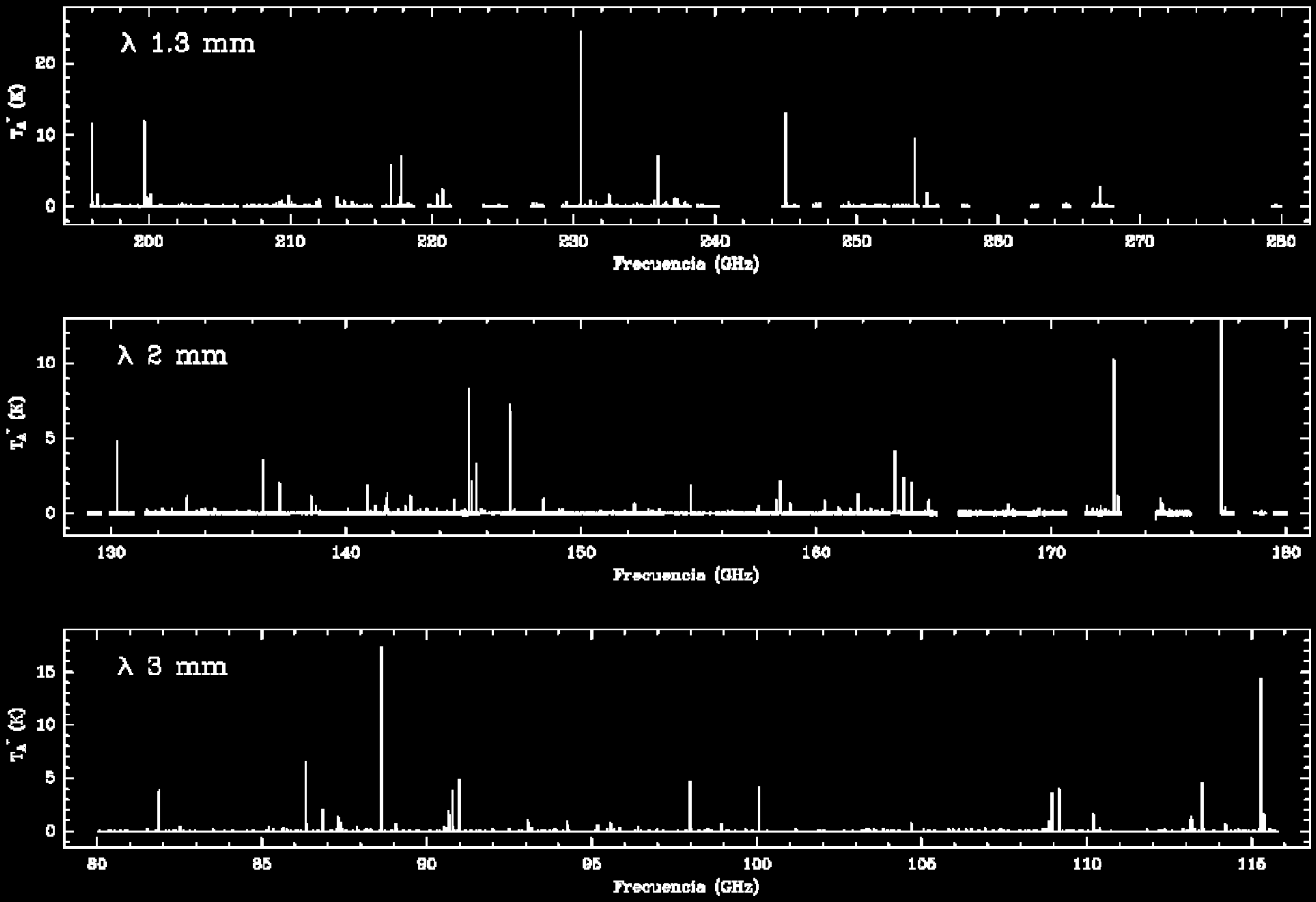
ZIII > 20 R_*

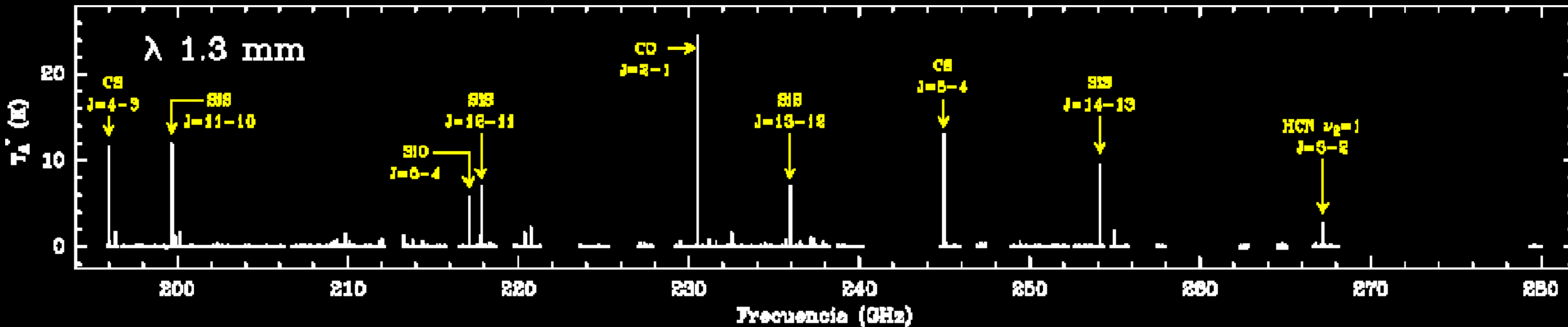
The radio data
The external shell (radicals and other exotic molecules)

Chemical Modelling : PhD of Marcelino Agúndez

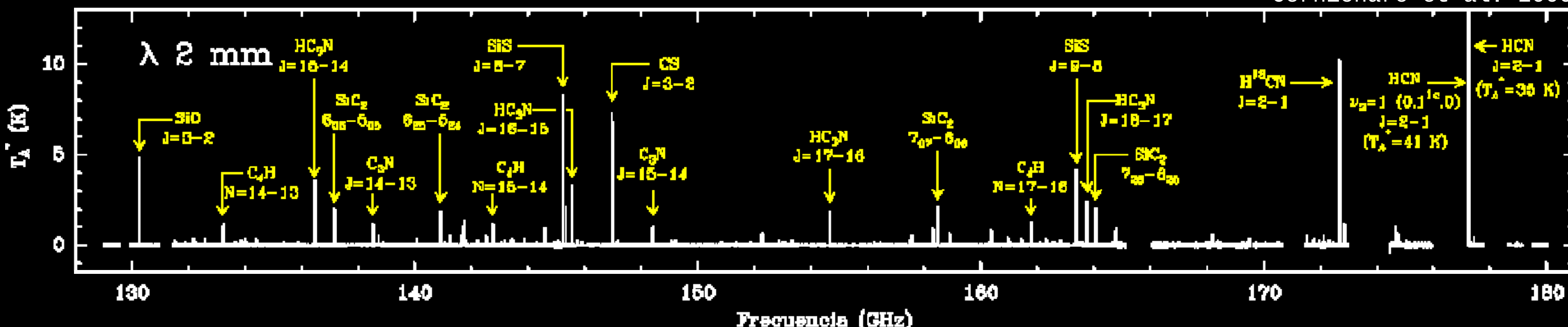
Input for chemistry : C_2H_2 & HCN in the inner shell
PhD of J.Pablo Fonfría

LINE SURVEYS

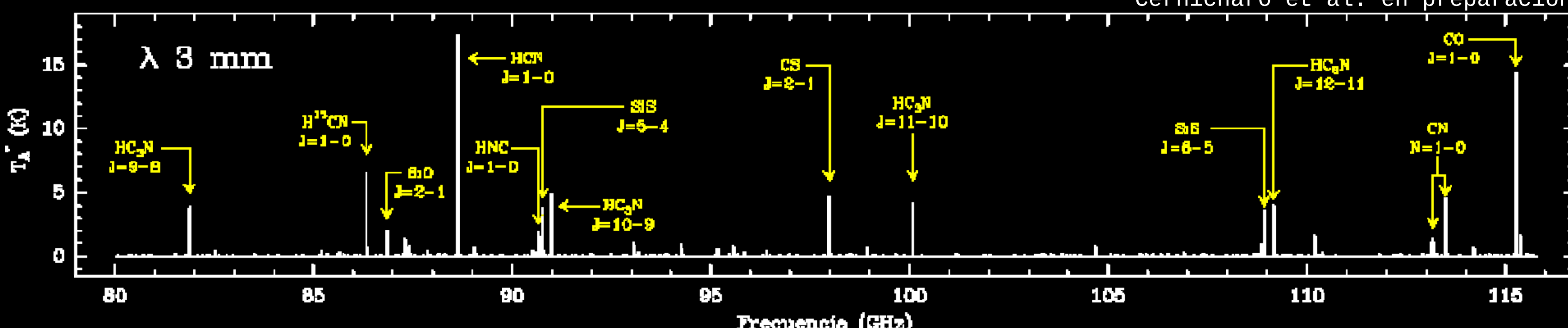




Cernicharo et al. 2000



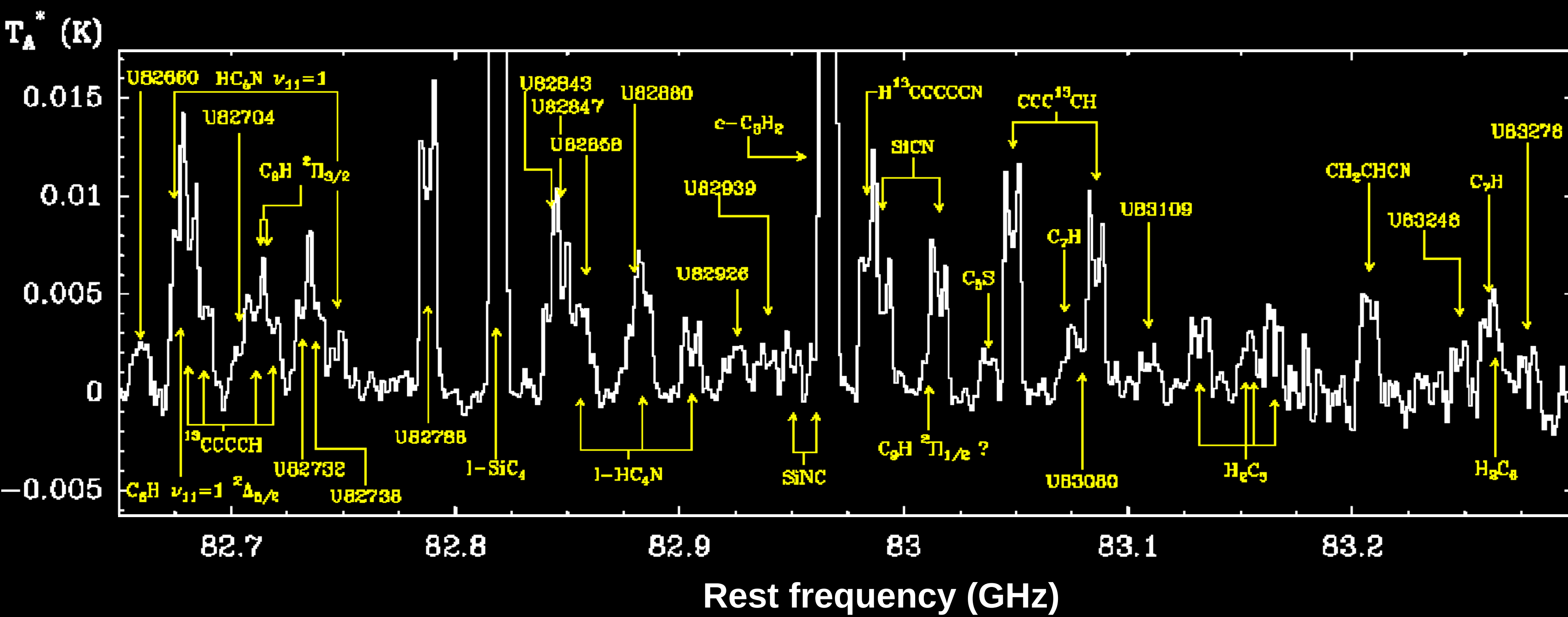
Cernicharo et al. en preparación



METHODS: Radio astronomical observations

Line survey at λ = 3 mm carried out with the IRAM 30-m radio telescope:

- 80.05-115.75 GHz
- 1339 emission lines (~37 lines/GHz)
- 886 assigned to rotational transitions of 60 molecules (+ different isotopoloques and vibrationally excited states)
- 453 unassigned lines (only 31 with $T_A^* > 10$ mK)
- high sensitivity: rms(T_A^*) < 1 mK for most frequencies



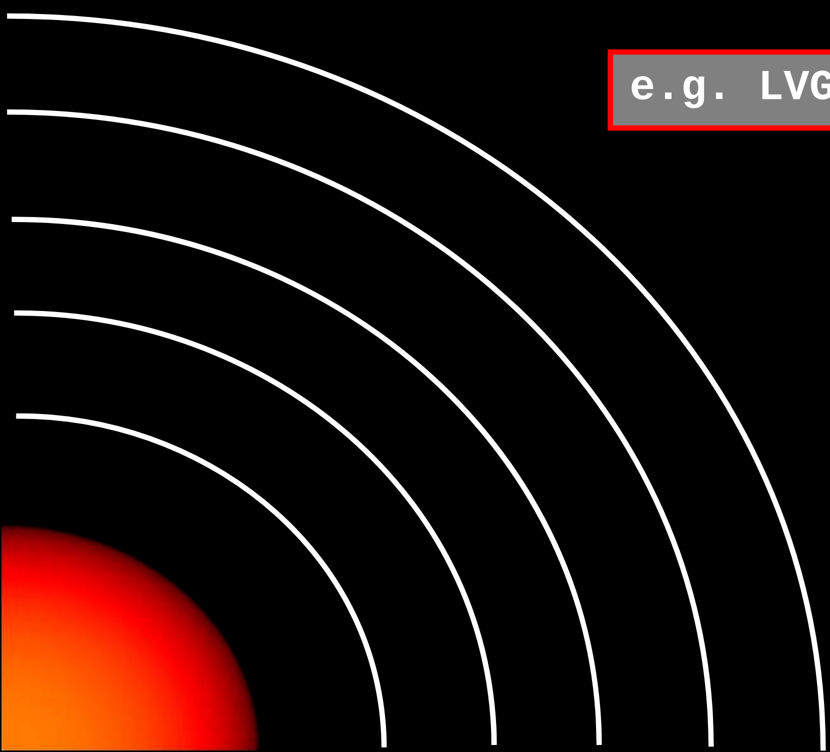
MODELING ASTROPHYSICAL DATA

Lines arise from a region where temperature and density vary very fast

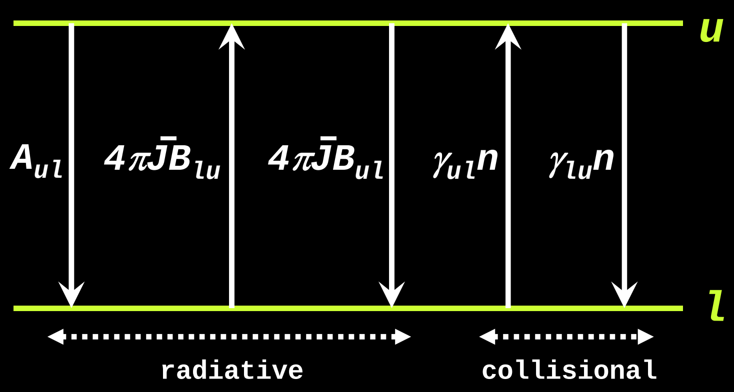
The medium is not homogeneous

It is necessary to use more sophisticated methods

e.g. LVG multishell or non-local codes

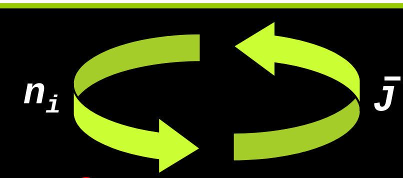


METHODS: Non LTE radiative transfer (LVG and non Local Codes)



Statistical Equilibrium

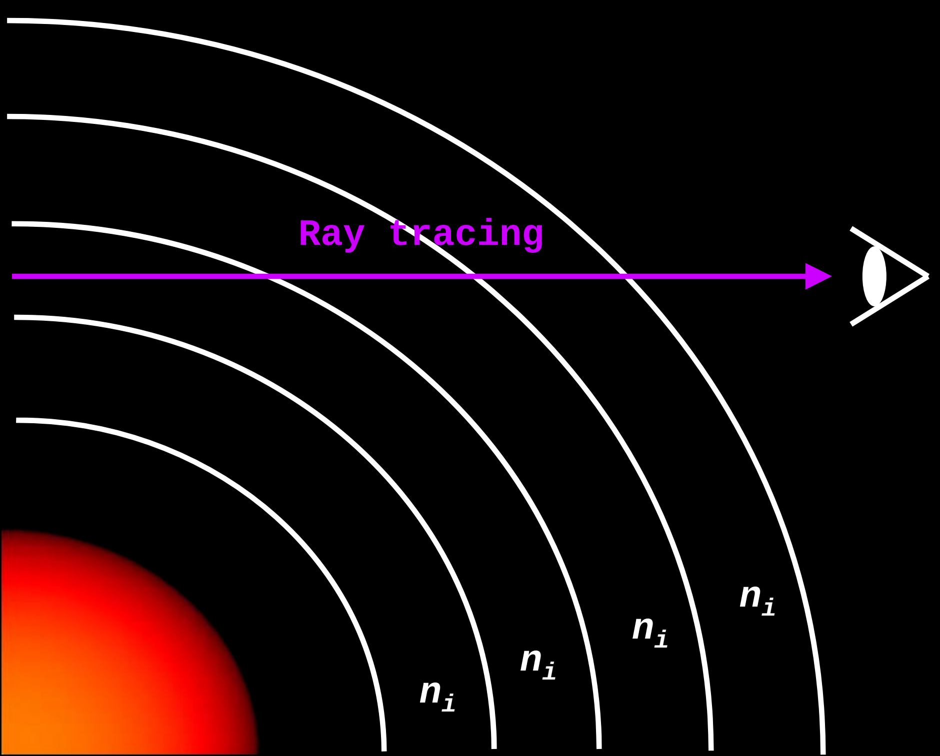
$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j(4\pi\bar{J}B_{ji} + \gamma_{ji}n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i}(4\pi\bar{J}B_{ij} + \gamma_{ij}n) - n_i \sum_{j<i} A_{ij}$$

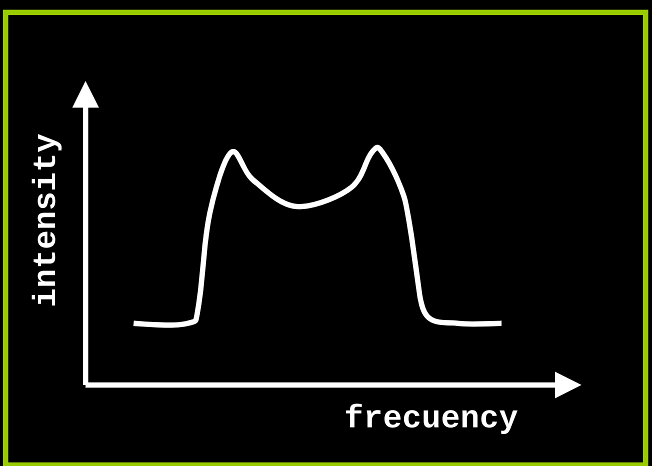


$$\bar{J} = (1-\beta)S_\nu + \beta I_\nu^{bg}$$

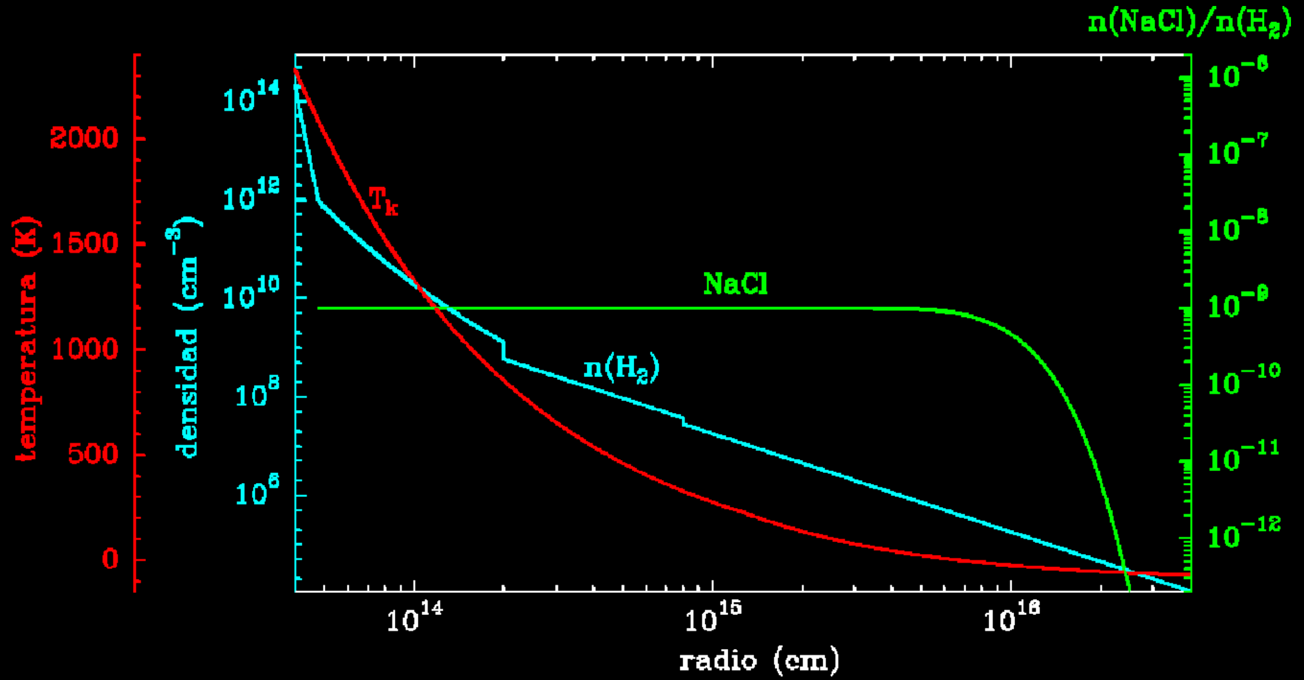
LVG codes

n_i population

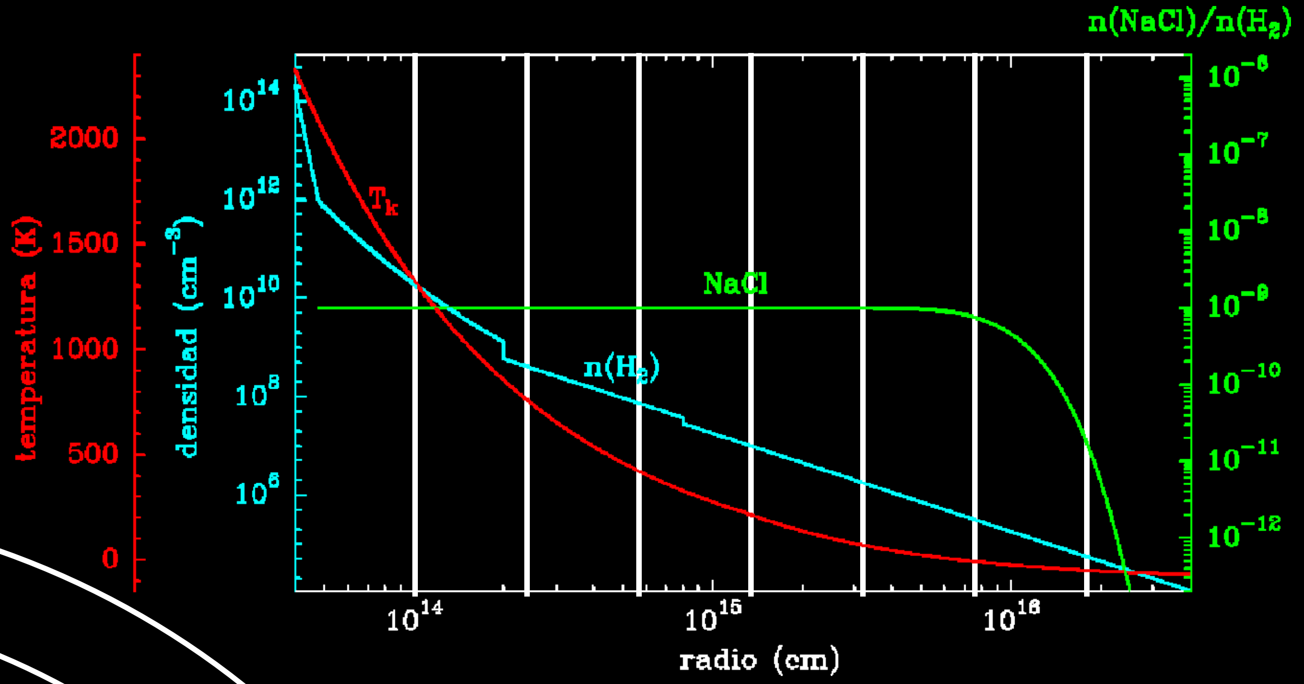


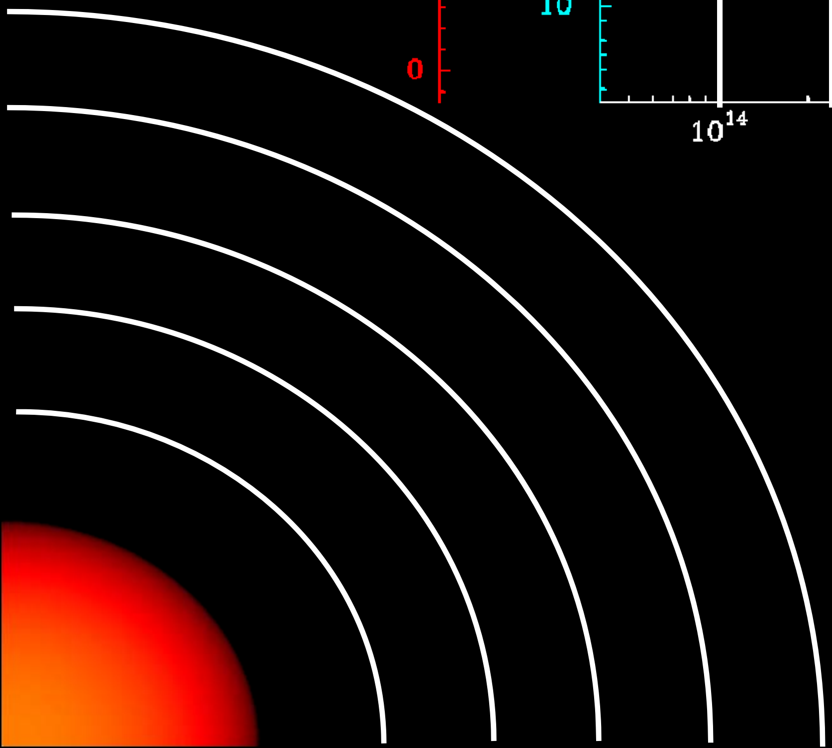


LVG multishell models

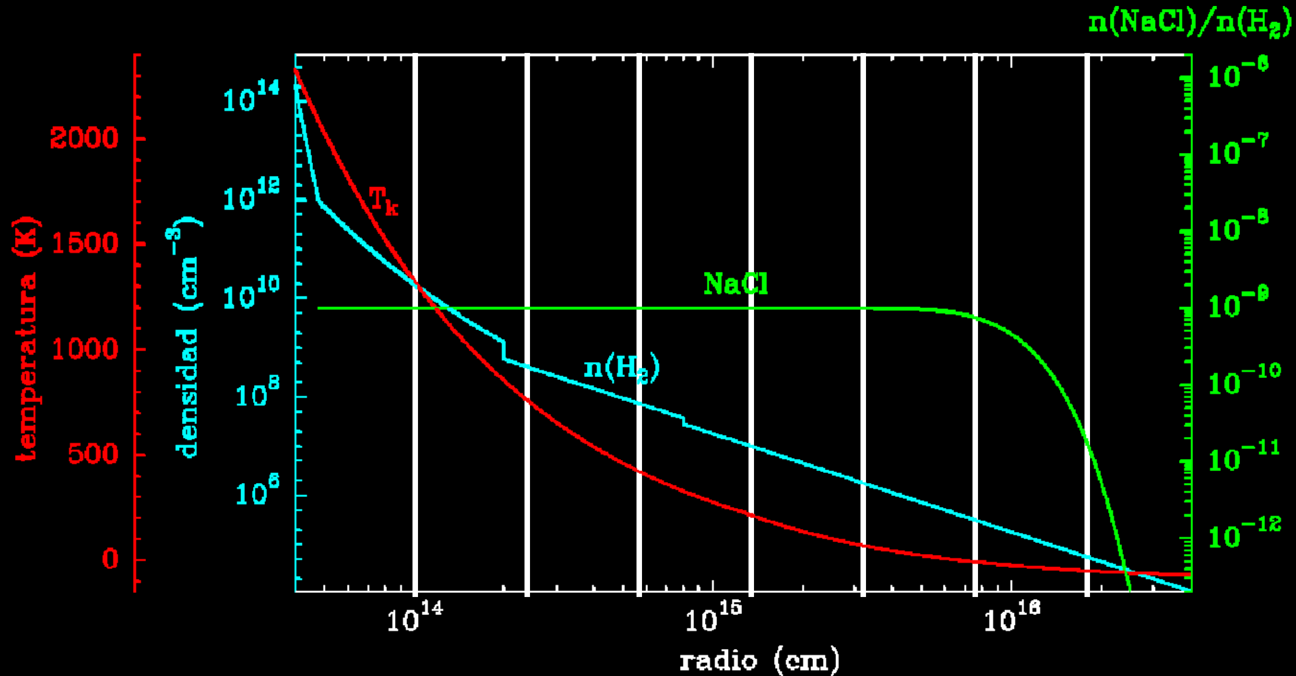


LVG multishell models

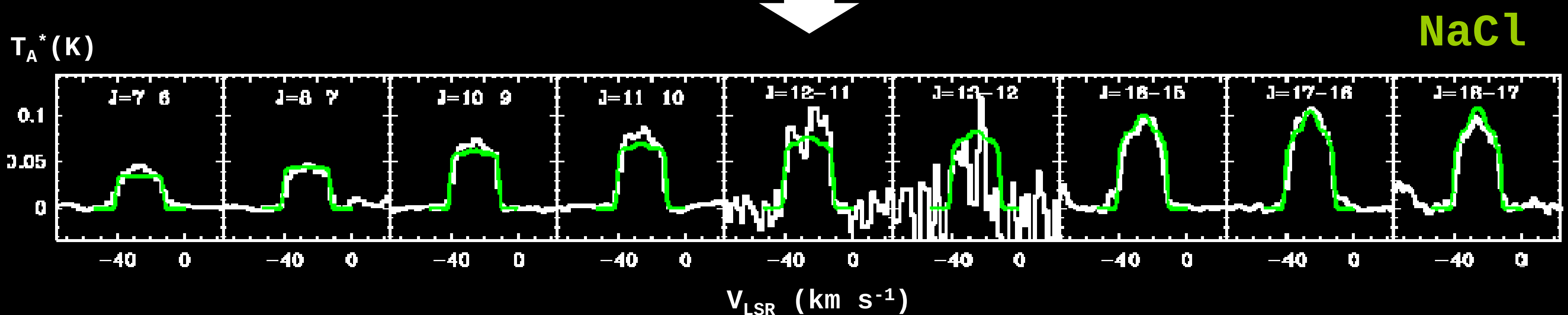




LVG multishell models

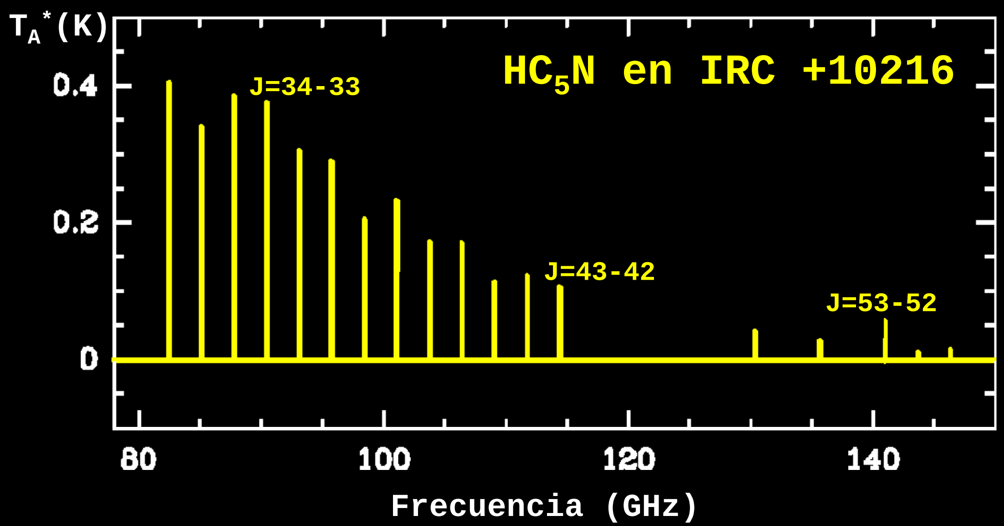


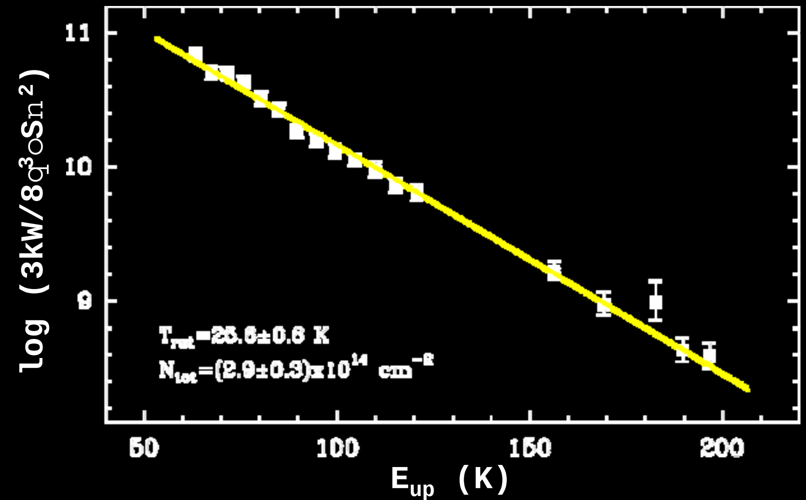
Results



Rotational temperature Diagram

$$\log\left(\frac{3kW}{8\pi^3 \nu S \mu^2}\right) = \log\left(\frac{N}{Z_{rot}}\right) - \frac{\log e}{kT_{rot}} E_{up}$$





Integrated intensity of the lines

Rotational temperature (T_{rot}) and column density (N)

Very crude approach for most species!

1) rotational levels in LTE at some Trot
2) the medium has to be homogeneous
3) optically thin lines
4) no infrared pumping
5) $T_{rot} >> T_{CMB}$

10^{-3}	CO 1(-3)						
10^{-4}							
		C_2H_2 8(-5)					
			HCN 2(-5)				
10^{-5}							
		CH_4 3.5(-6)					
		C_2H 3(-6)	NH_3 2(-6)				
		C_4H 2.5(-6)	CN 1.7(-6)				
		C_2 1(-6)	HC_3N 1.4(-6)		SiC_2 1.2(-6)		
10^{-6}		C_3 1(-6)			SiS 1(-6)		
			C_3N 4(-7)	CS 5(-7)			
					SiH_4 2.2(-7)		
			HC_5N 2(-7)		SiO 1.2(-7)		
10^{-7}	H_2O 1(-7)	C_5 1(-7)	HNC 1(-7)				
		l-C_3H 5(-8)					
	OH 4(-8)	C_6H 4(-8)			SiC 4(-8)		
		C_5H 3(-8)	CH_3CN 3(-8)	C_2S 3(-8)			$AlCl$ 3.5(-8)
		c-C_3H_2 3(-8)					
		CH_3C_2H 3(-8)					
		c-C_3H 2(-8)	HC_7N 2(-8)			HCP 2.5(-8)	
		C_2H_4 2(-8)					$NaCN$
	H_2CO 1.3(-8)	H_2C_4 1.4(-8)		C_3S 1.2(-8)			
10^{-8}						CP 1(-8)	
		C_8H 8(-9)	HC_9N 8(-9)	H_2CS 7(-9)	SiN 8(-9)	PH_3 8(-9)	$MgNC$ 8(-9)
			CH_2CN 7(-9)				AlF 7.5(-9)
			HC_2N 6(-9)				
			C_5N 4(-9)				
		C_7H 3(-9)	$HCCNC$ 4(-9)				
		H_2C_6 3(-9)	C_2H_3CN 4(-9)	H_2S 4(-9)	c-SiC_3 4(-9)		
		C_6H^- 3(-9)	C_5N^- 2.3(-9)		SiC_4 3(-9)		
	C_3O 2(-9)	C_8H^- 1.5(-9)	HC_4N 2(-9)		$SiCN$ 2(-9)		
		H_2C_3 1.5(-9)	C_3N^- 1.1(-9)	C_5S 1.2(-9)	$SiNC$ 1.1(-9)	PN 1(-9)	$NaCl$ 1(-9)
10^{-9}						C_2P 1(-9)	$AlNC$ 1(-9)
	HCO^+ 7(-10)		$HNCCC$ 5(-10)				$MgCN$ 5(-10)
		C_4H^- 3(-10)					KCl 2.5(-10)
10^{-10}							

Thermodynamical Chemical Equilibrium : Dissociation energies and partition functions are needed

T
P
ε_i
$K_{p,n}$

$$\varepsilon_i kT = p_i + \sum_{n=1}^{N_i} \frac{(p_i)^{h_n} (p_j)^{c_n} (p_k)^{o_n} \ldots}{K_{p,n}}$$

...

...

Set of non-lineal algebraic equations

Newton-Raphson

x_n

Chemical Kinetics: Reaction rates are required

$T(t)$
$n(t)$
x_i^0
k_j

$$\frac{dn_i}{dt} = \underbrace{\sum_{j=1}^{N_f} k_j \prod_{l=1}^{N_{reac}^{j}} n_{j,l}}_{\text{formation of i}} - \underbrace{\sum_{m=1}^{N_d} k_m n_i \prod_{s=1}^{N_{reac}^{m}} n_{m,s}}_{\text{Destruction og i}}$$

...

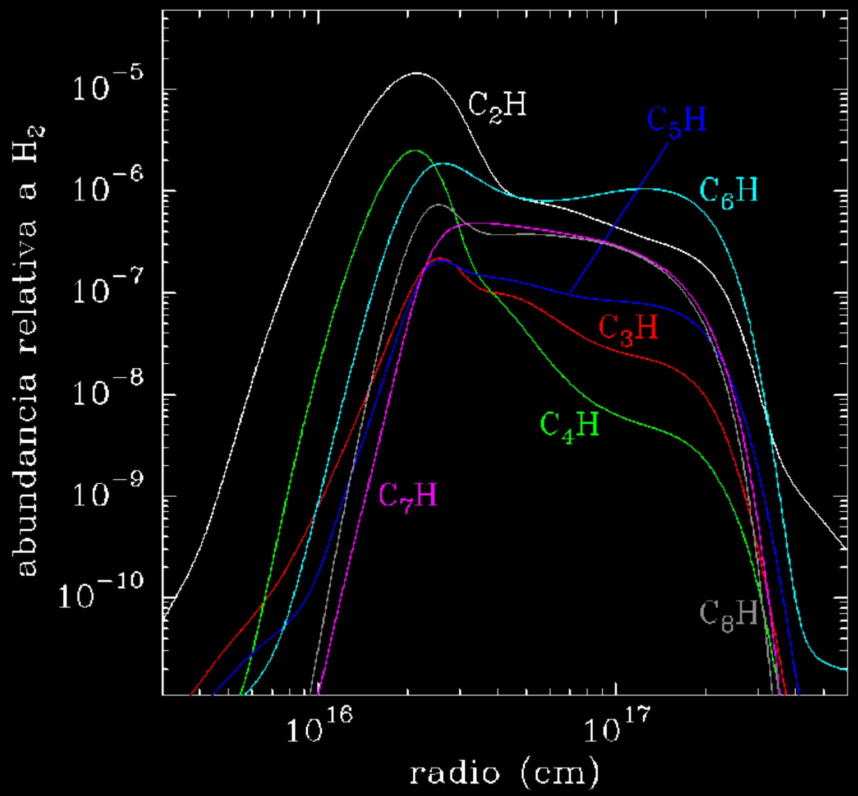
...

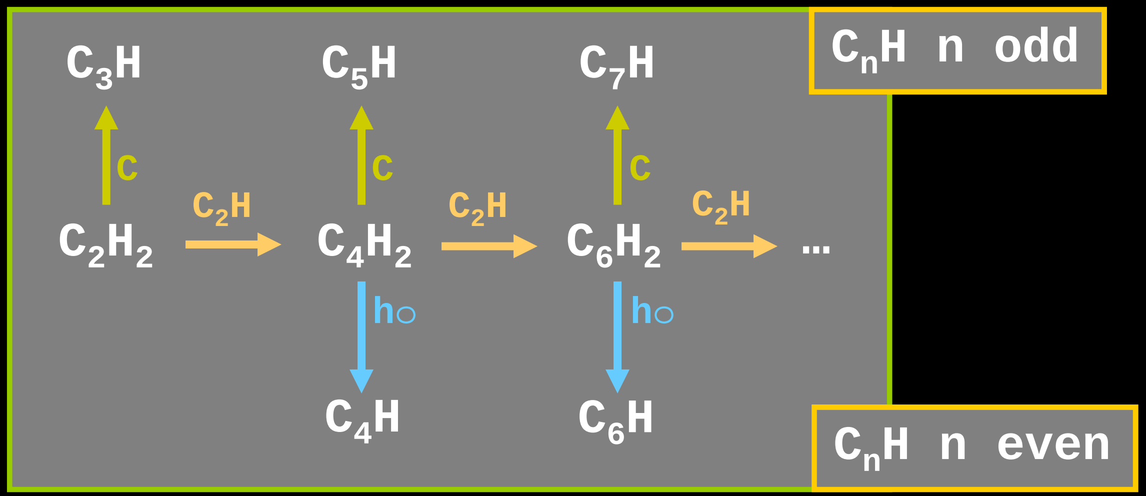
Set of differential ordinary non-lineal equations (Stiff and ill conditioned)

Runge-Kutta

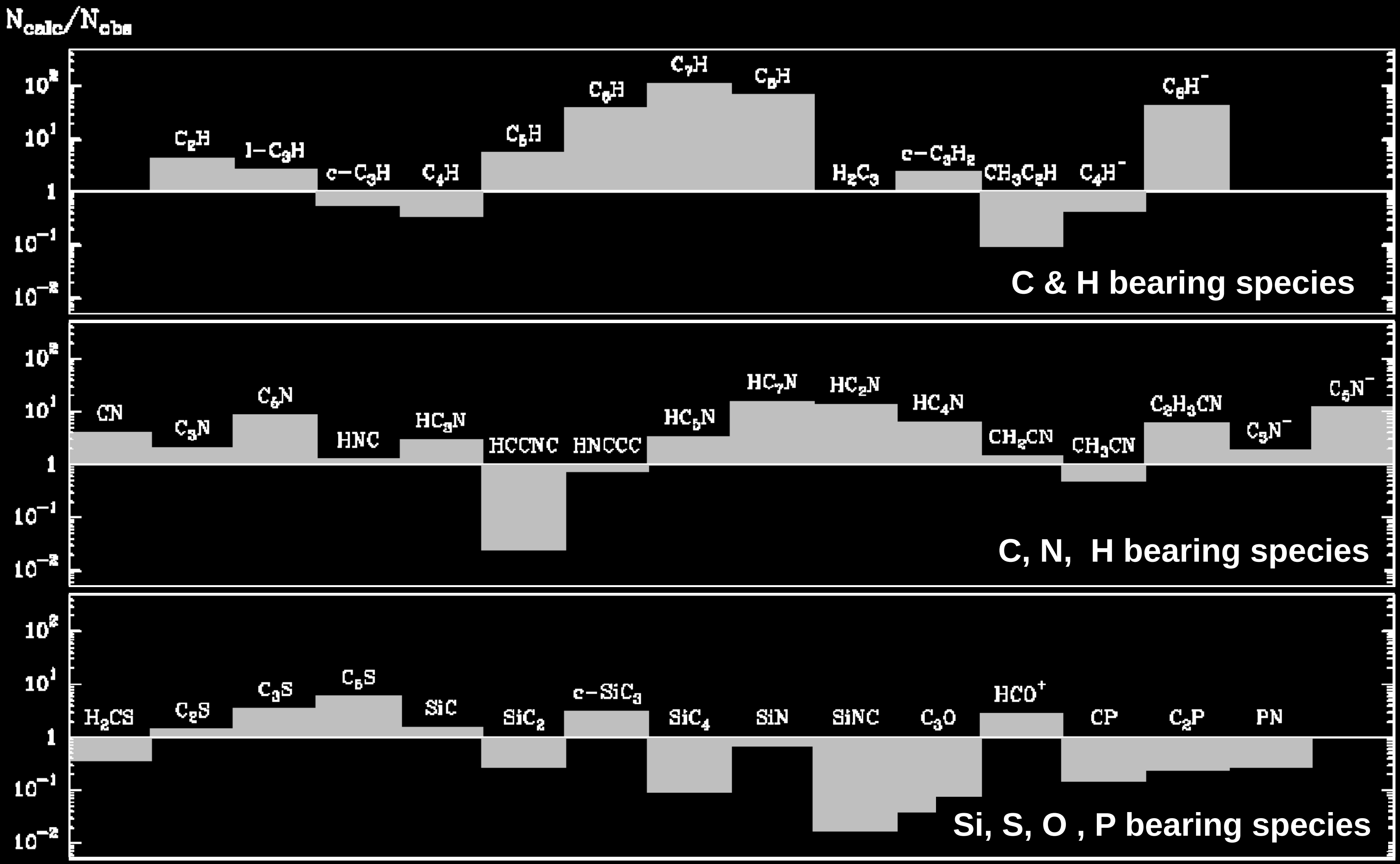
$x_i(t)$

RESULTS: THE OUTER ENVELOPE --- Chemical kinetic models

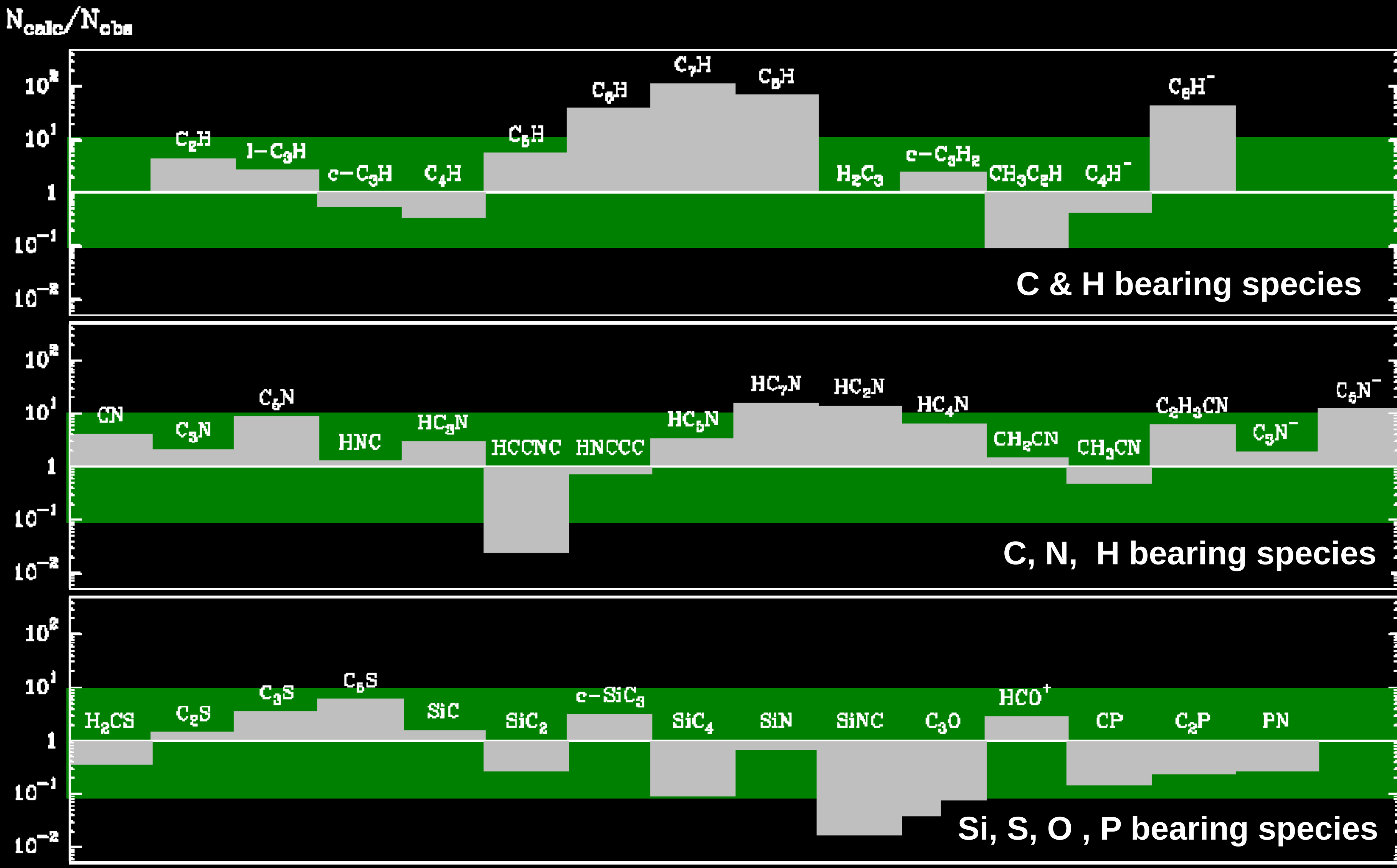




RESULTS: THE OUTER ENVELOPE --- Chemical kinetic models



RESULTS: THE OUTER ENVELOPE --- Chemical kinetic models

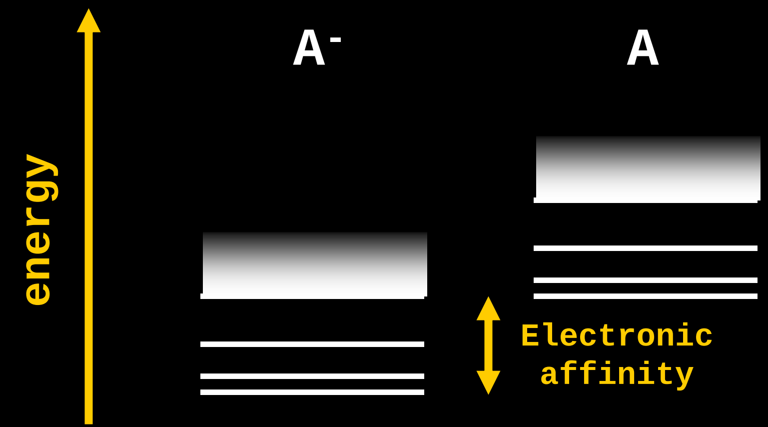


RESULTA: SPECIFIC RESULTS : ANIONS

¡ First detection of molecular anions in IRC+10216

C_6H^-, C_4H^-, C_8H^-, C_3N^-, C_5N^-

Thermodynamics — The formation of the anion is favoured



Kinetics — The formation of the anion is NOT favoured

$$A + e^- \Leftrightarrow A^- + h\nu$$

Except for species with a high electronic affinity and a large size

e.g. C_4H, C_6H, C_8H, C_3N, C_5N, …

Nature Vol. 289 19 February 1981

Can negative molecular ions be detected in dense interstellar clouds?

Eric Herbst

Department of Physics, Duke University, Durham,
North Carolina 27706

The recent laboratory measurement[1–3] of rapid radiative electron attachment processes

$$A + e \rightarrow A^- h\nu$$

where A is a molecular species has renewed speculation on whether negative molecular ions can be synthesized efficiently in dense interstellar clouds. We argue here that for certain interstellar species A, the abundance ratio [A⁻]/[A] may be as high as 0.01–0.1 in commonly assumed physical conditions. If this abundance ratio were correct, negative molecular ions might be detectable in dense interstellar clouds if their microwave spectral frequencies had been determined in the laboratory. It will be shown, however, that this is currently an unlikely prospect.

History:

2006 C_6H^- in IRC +10216 and TMC-1 (McCarthy et al.)

History:

2006 C_6H^- in IRC +10216 & TMC-1 (McCarthy et al.)

2007 C_4H^- in IRC +10216 (Cernicharo et al.)

2007 C_8H^- in IRC +10216 & TMC-1 (Remijan et al.; Brünken et al.)

2008 C_3N^- in IRC +10216 (Thaddeus et al.)

2008 C_5N^- in IRC +10216 (Cernicharo et al.)

History:

2006 C_6H^- in IRC +10216 & TMC-1 (McCarthy et al.)

2007 C_4H^- in IRC +10216 (Cernicharo et al.)

2007 C_8H^- in IRC +10216 & TMC-1 (Remijan et al.; Brünken et al.)

2008 C_3N^- in IRC +10216 (Thaddeus et al.)

2008 C_5N^- in IRC +10216 (Cernicharo et al.)

2010 CN- in IRC+10216 (Agúndez et al.)

Additional detections:

C_6H^- in L1527 (Sakai et al. 2007)

C_4H^- in L1527 (Agúndez et al. 2008)

C_6H^- in L1544 y L1521F (Gupta et al. 2009)

History:

2006 C_6H^- in IRC +10216 & TMC-1 (McCarthy et al.)

2007 C_4H^- in IRC +10216 (Cernicharo et al.)

2007 C_8H^- in IRC +10216 & TMC-1 (Remijan [illegible] .)

2008 C_3N^- in IRC +10216 (Tha [illegible]

2008 C_5N^- in IR [illegible]

[illegible])

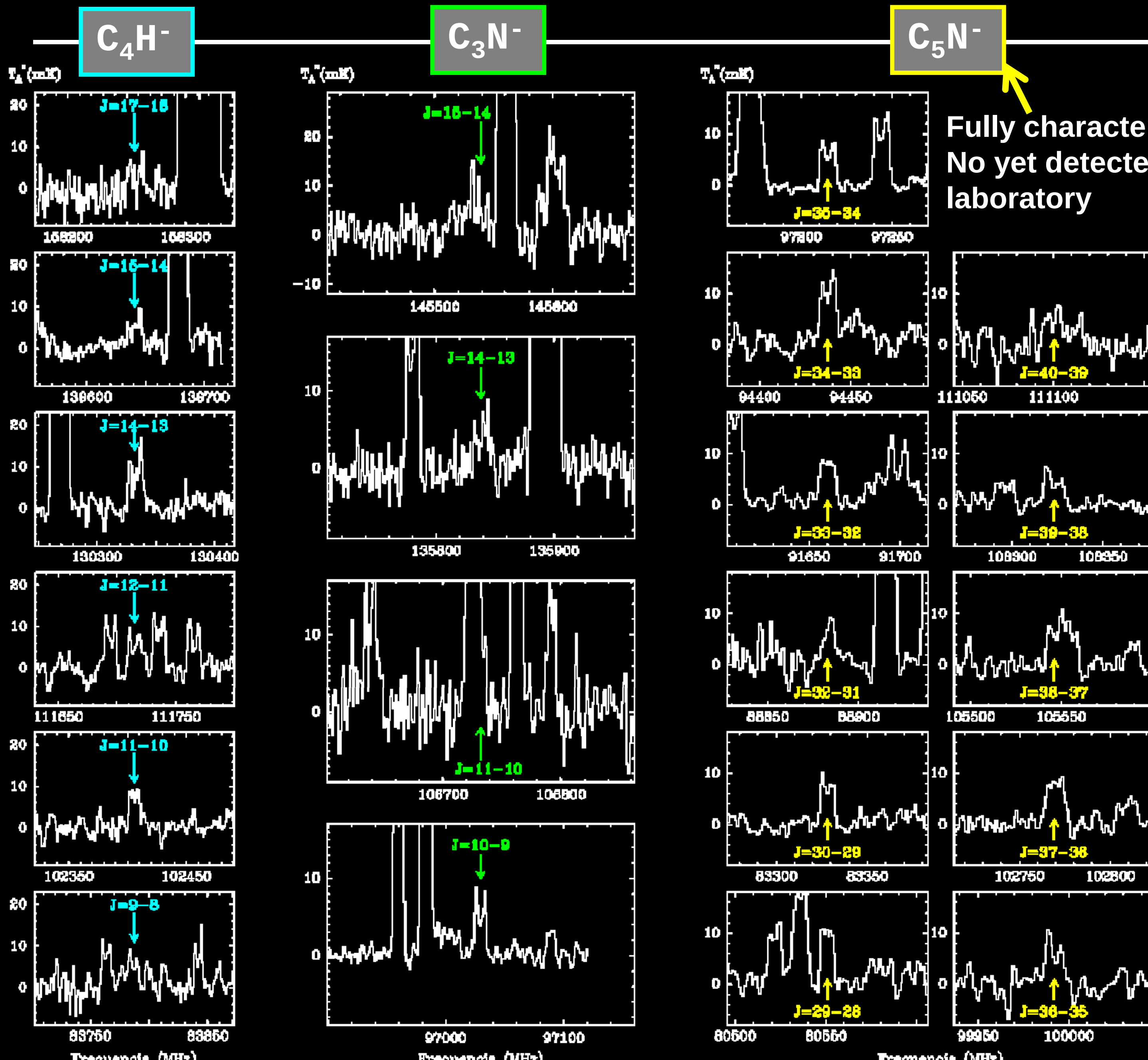
[illegible] (Sakai et al. 2007)

C_4H^- in L1527 (Agúndez et al. 2008)

C_6H^- in L1544 & L1521F (Gupta et al. 2009)

IRC +10216
Is the only source where all anions have been observed
CN^-, C_4H^-, C_6H^-, C_8H^-, C_3N^-, C_5N^-

RESULTS: SPECIFIC RESULTS : ANIONS



Fully characterized in space
No yet detected in the laboratory

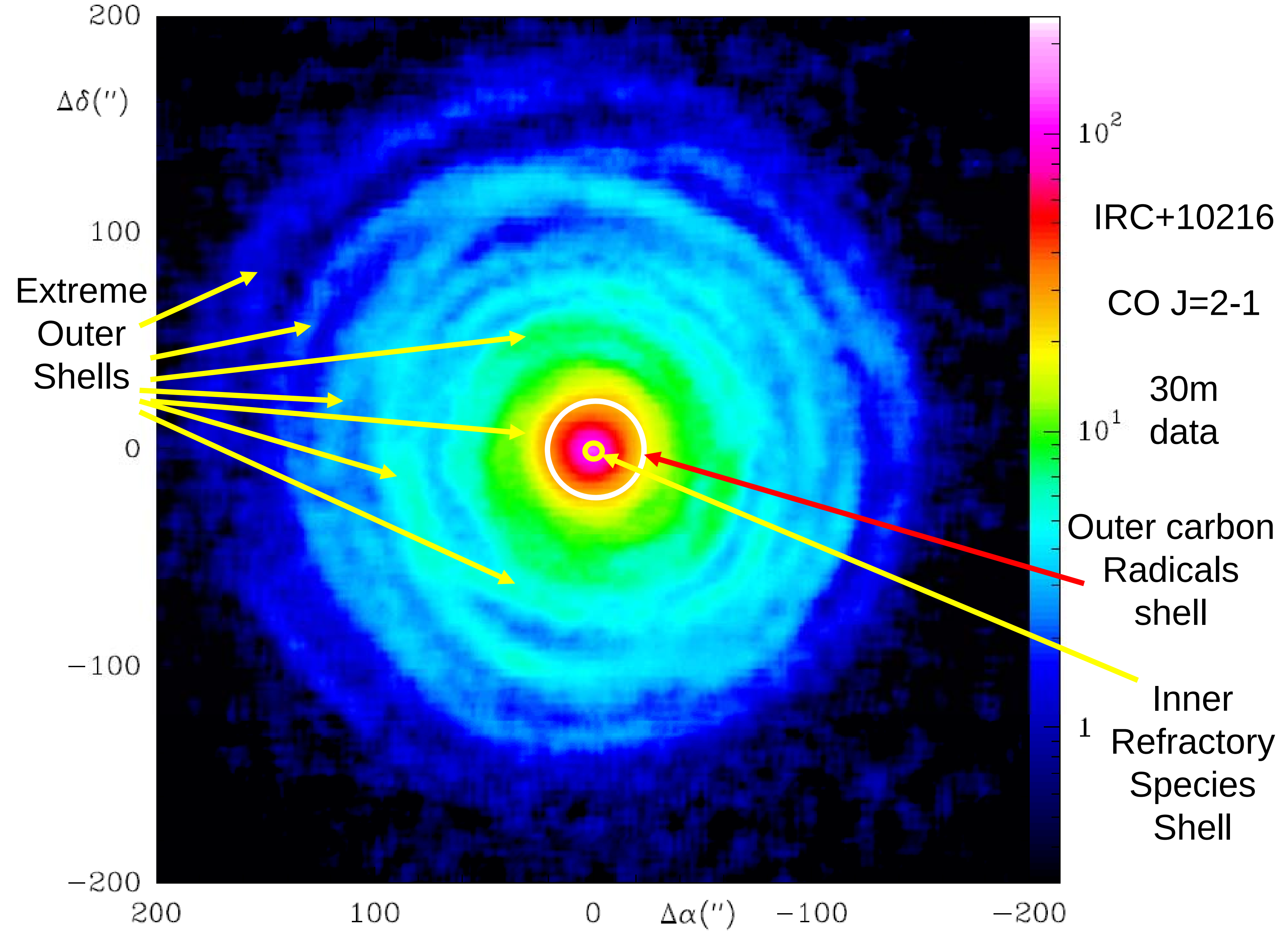
RESULTS : ANIONS

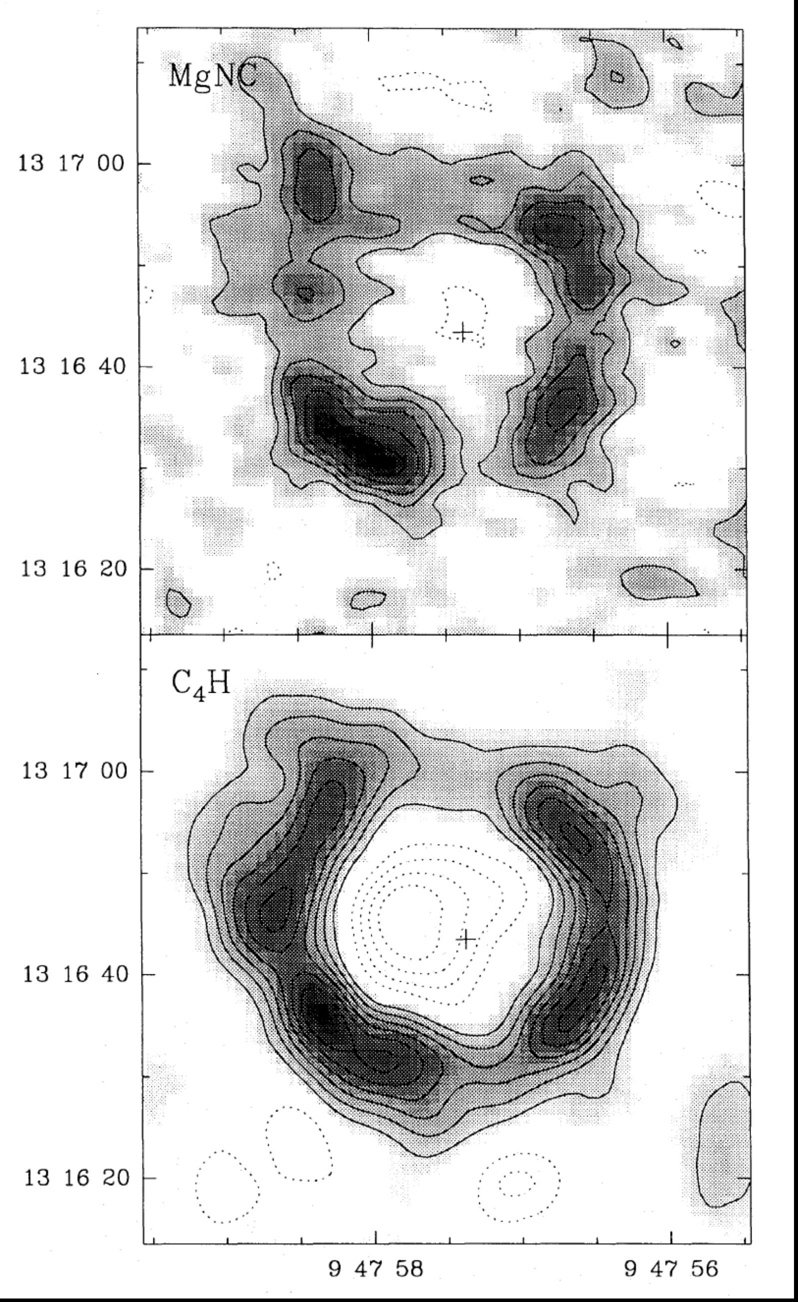
reaction	k_{ra}(300 K) IRC +10216	k_{ra}(300 K) theory[(a)]
$C_4H + e^- \Leftrightarrow C_4H^- + h\nu$	2-7x10^{-11}	1.1x10^{-8}
$C_6H + e^- \Leftrightarrow C_6H^- + h\nu$	3.0x10^{-8}	6.2x10^{-8}
$C_8H + e^- \Leftrightarrow C_8H^- + h\nu$	1.5x10^{-7}	6.2x10^{-8}
$C_3N + e^- \Leftrightarrow C_3N^- + h\nu$	2-5x10^{-9}	2.0x10^{-10}
$C_5N + e^- \Leftrightarrow C_5N^- + h\nu$	5.0x10^{-7}	-

k_{ra} with units of $cm^3\ s^{-1}$
(a) Herbst & Osamura 2008; Petrie & Herbst 1997.

THE FINAL PRODUCT OF A DETAILED STUDY

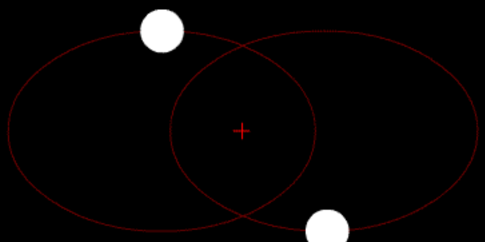
- New Molecules
- Abundances for all species
- Isotopic abundances (nuclear evolution)
- Clear differentation of the different layers of the CSE
- Chemistry of exotic species (anions)
- A fine study of the missing reactions of the actual chemical networks

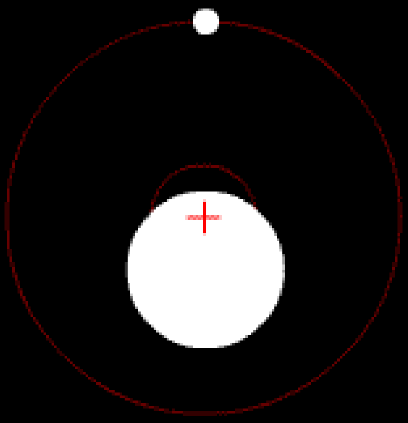

200
Δδ('')
100
0
−100
−200
200
100
0
Δα('')
−100
−200
10^2
10^1
1
Extreme Outer Shells
IRC+10216
CO J=2-1
30m data
Outer carbon Radicals shell
Inner Refractory Species Shell



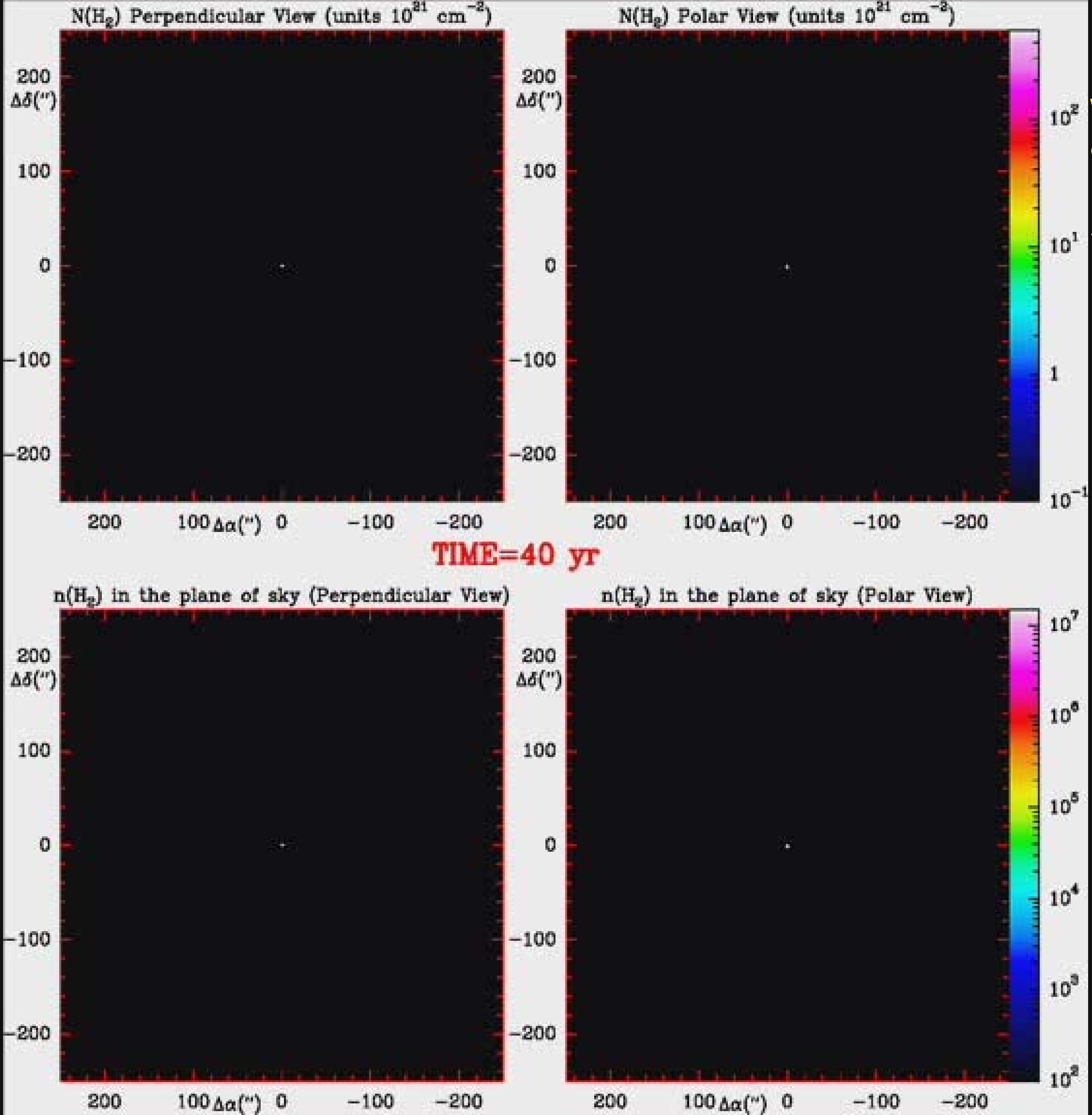
What structure could we expect for the circumstellar envelope of an AGB binary star ?

Is the AGB loosing mass uniformely with time or it is having episodic events of high mass loss ?





Guélin, Lucas, Cernicharo, 1993, A&A, 280, L19



Mass loss increased when the stars are at the closest distance.

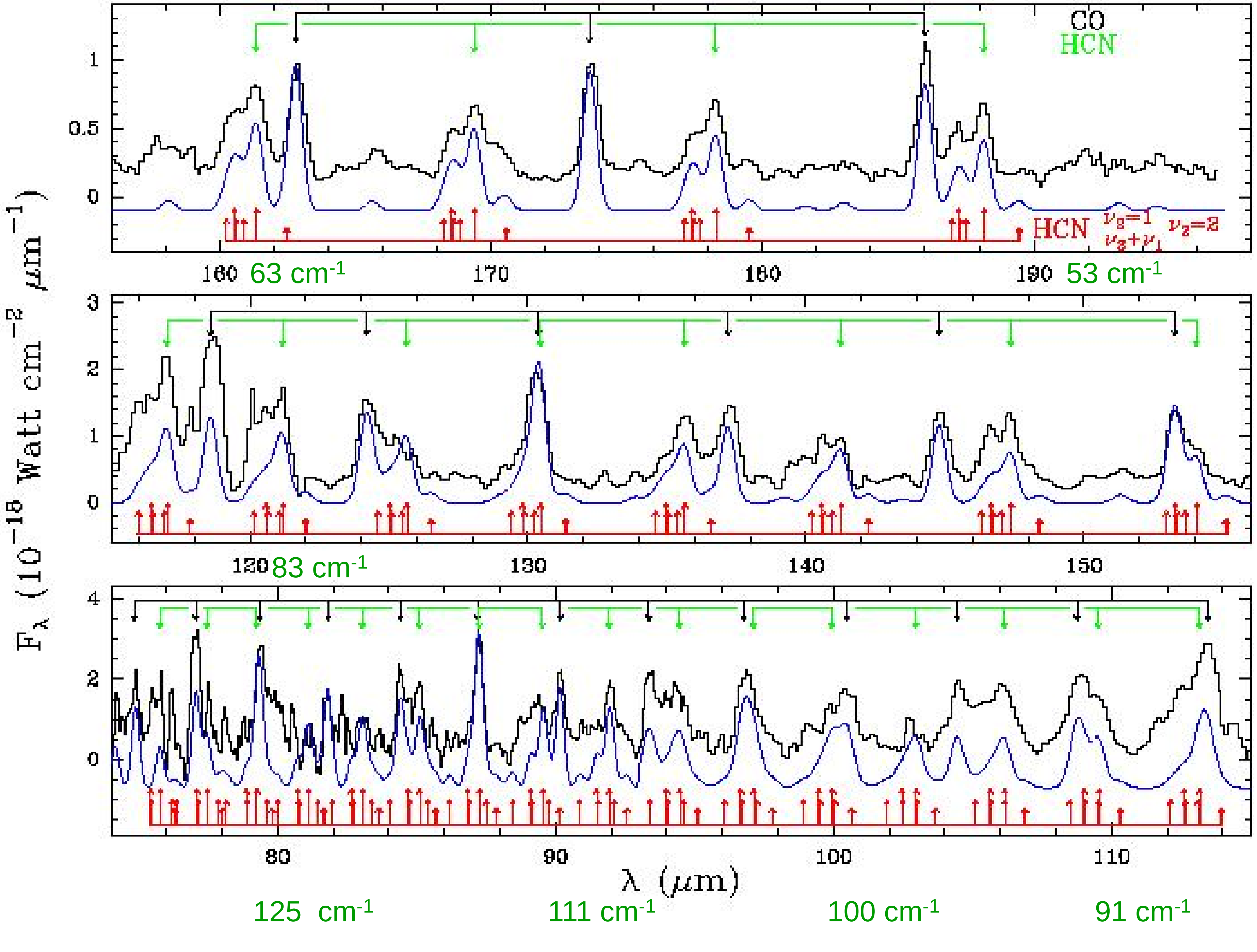
Ad hoc mass loss rate increased by a factor 10

WATER IN C-rich and O-rich AGBs

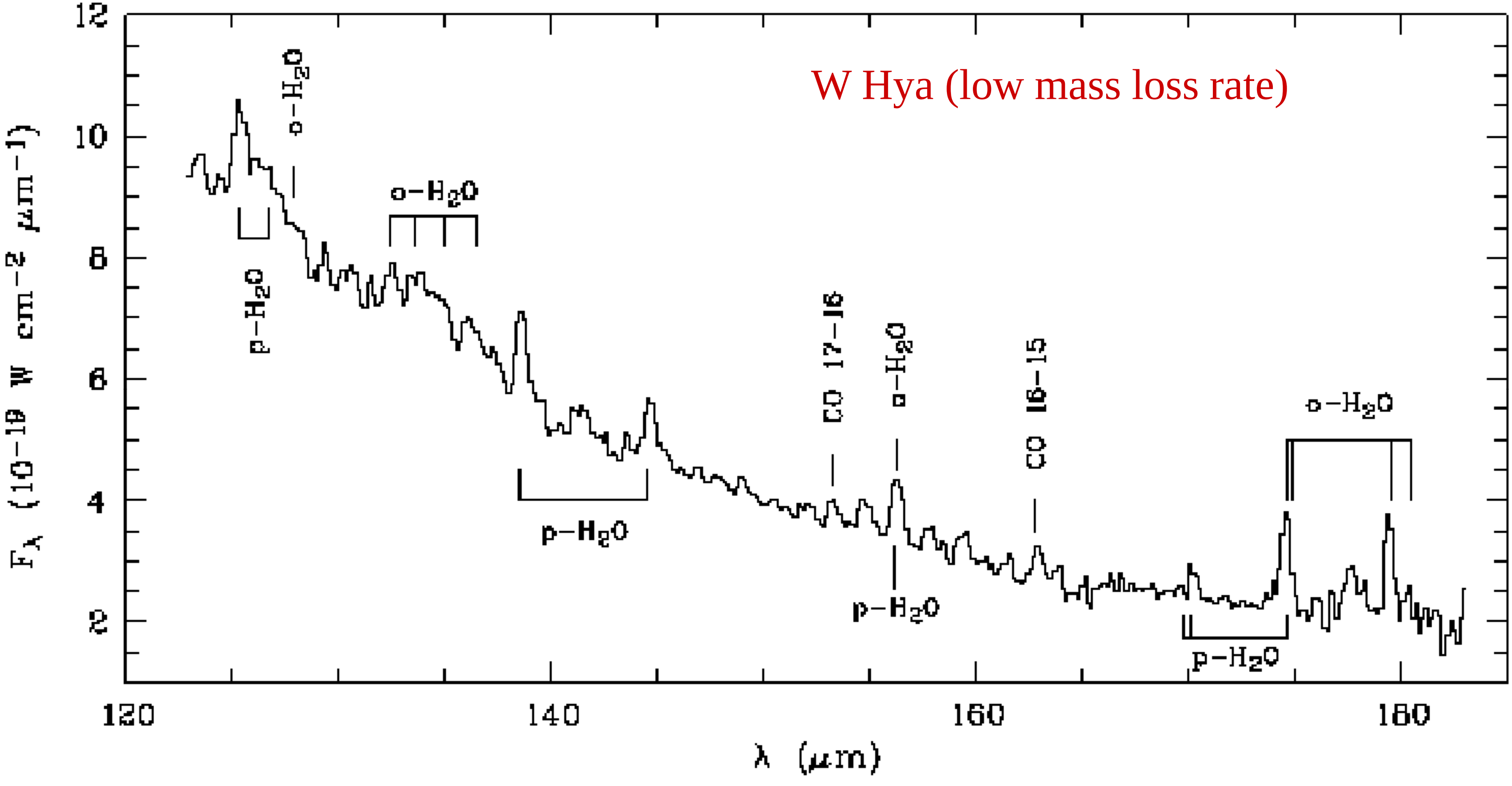
ALMA can do it !

Cernicharo et al., 1996, A.&A., 315, 201

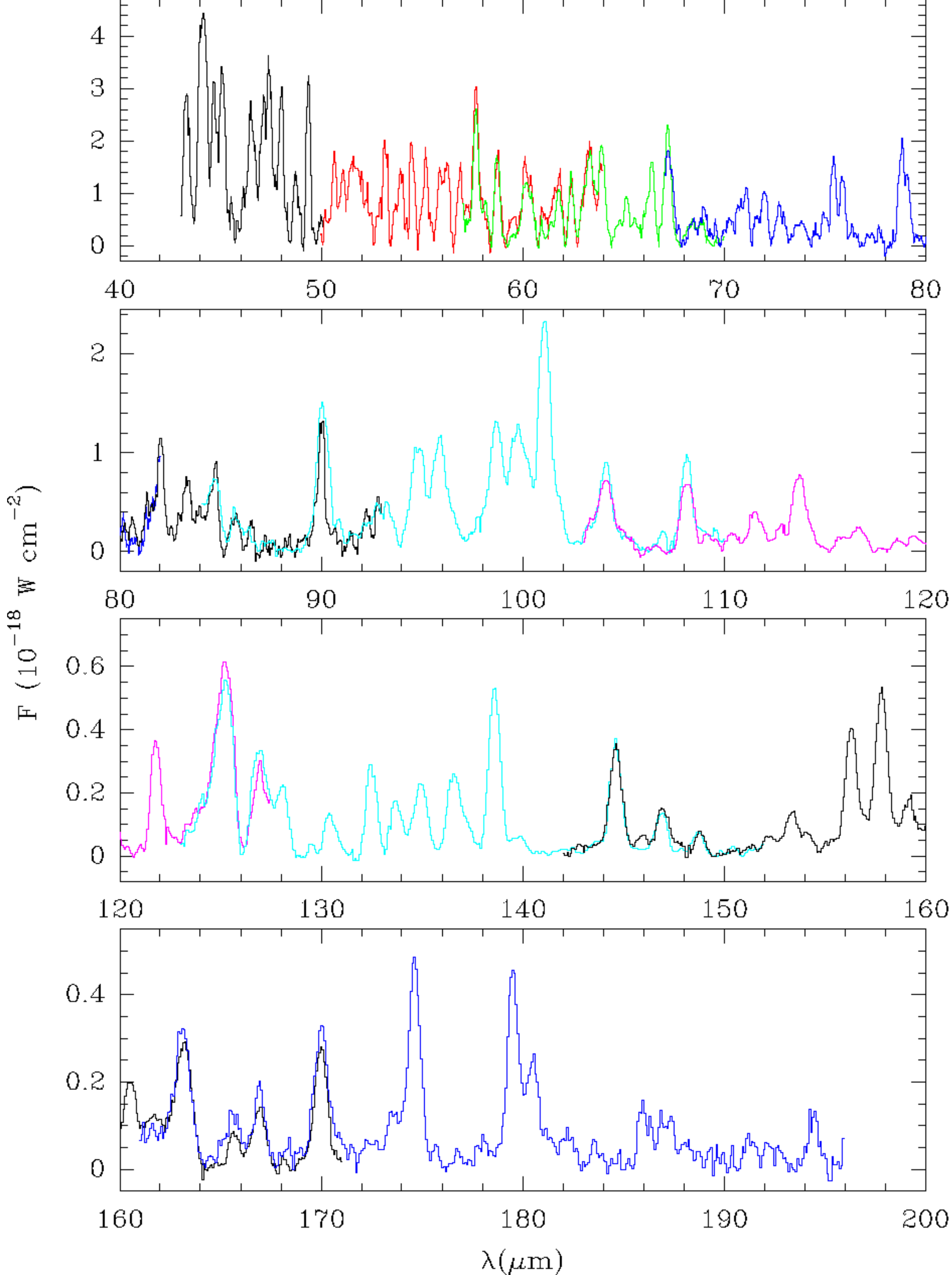
IRC+10216 => HCN (in all ν) + CO; λ/Δλ~300



Water in O-rich AGB stars



Barlow et al., 1996; Neufeld et al., 1996



VY CMa

All features are real and belong (95%) to H_2O (5% from CO)

All pure rotational lines of water wapour with λ>43 um detected

Some lines from the v_2=1 bending level also detected

Modelling requires collisional rates for T_k=20-2000 K including ro-vibrational collisions

ISO DATA 1998

VyCMa is a high mass loss rate object

PACS/Herschel data for VyCMa from Decin et al

If C-rich : CO, C_2H_2, HCN, SiO, SiS and a lot of species including H_2O.

When AGBs move towards the PPN phase => warm photochemistry using the UV photons from the central star. Significant amounts of water, and other O-bearing species are produced

If O-rich: CO, H_2O, OH, SiO, SiS, HCN, …

GROUND BASED OBSERVATIONS OF WATER

The problem of the observation of water vapor :

Our atmosphere is full of water vapor.

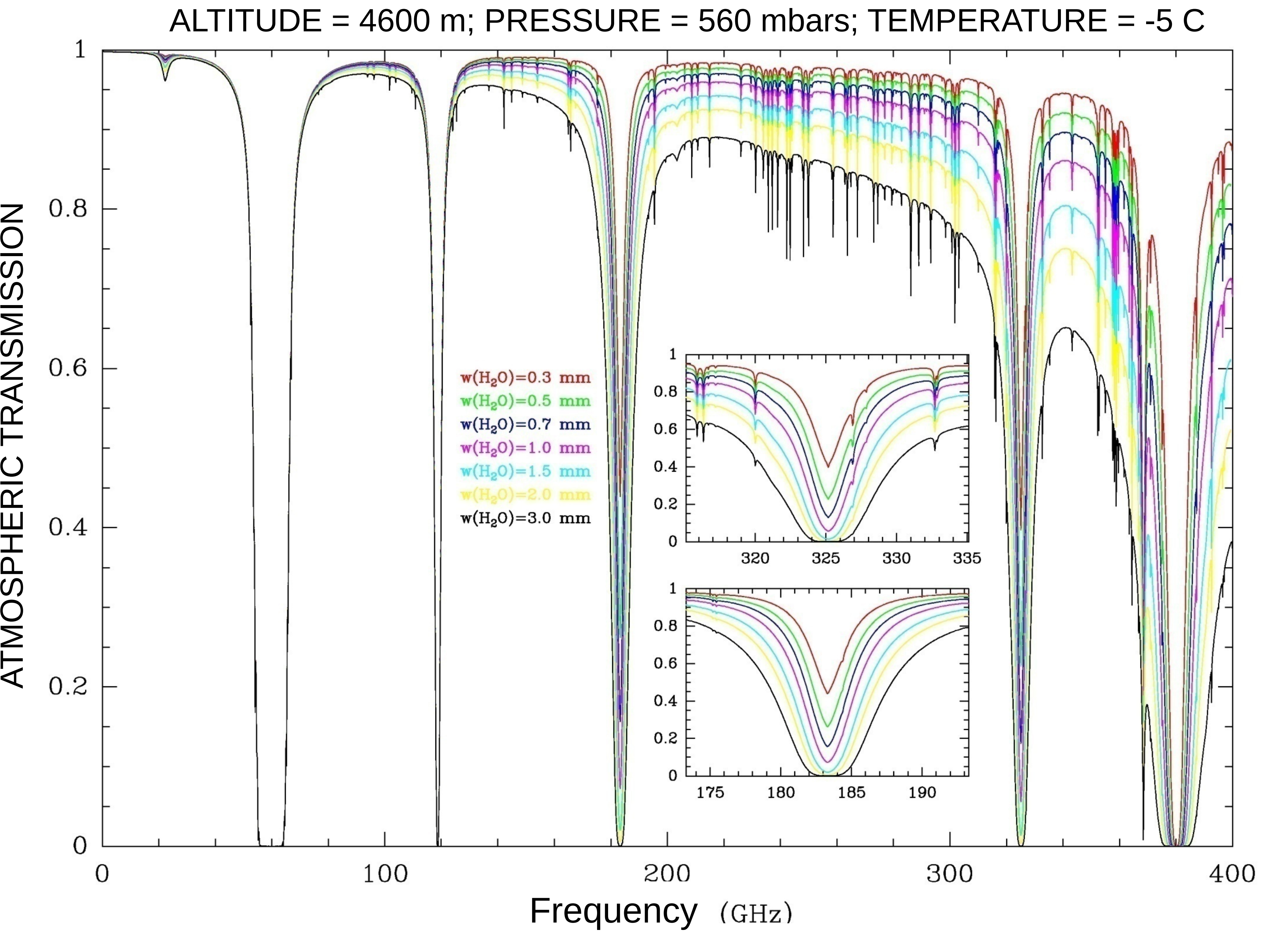
Water vapor was detected in the ISM and CSM in 1969 from observations at a 22 GHz (Cheung et al.).

Our atmosphere is transparent at this frequency as the transition involves two levels around 700 K and the line strength is rather low.

Water detected only in small regions of the ISM and CSM

To observe H_2O we have to go to space !!!

But this is not completely true !!!!!!



ALTITUDE = 4600 m; PRESSURE = 560 mbars; TEMPERATURE = -5 C
ATMOSPHERIC TRANSMISSION
Frequency (GHz)
w(H2O)=0.3 mm
w(H2O)=0.5 mm
w(H2O)=0.7 mm
w(H2O)=1.0 mm
w(H2O)=1.5 mm
w(H2O)=2.0 mm
w(H2O)=3.0 mm
0
0.2
0.4
0.6
0.8
1
0
100
200
300
400
320
325
330
335
175
180
185
190

Astron. Astrophys. 231, L 15–L 18 (1990)

ASTRONOMY AND ASTROPHYSICS

Letter to the Editor

Detection of 183 GHz water vapor maser emission from interstellar and circumstellar sources

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[2] IRAM, Av. Divina Pastora N7 NC, E-18012 Granada, Spain
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Received January 12, accepted February 13, 1990

SUMMARY: We have observed, with the IRAM 30-m telescope, the emission of the 183 GHz 3_{13}-2_{20} rotational transition of water from a selected sample of giant molecular clouds, low mass star forming regions and evolved stars. The zenith atmospheric transmission was 25-30% during our observations. The water emission shows strong and narrow masing lines (flux ≈ 1000-15000 Jy) toward the hot molecular clouds with strong 22 GHz water masers. Broad line emission, perhaps of thermal origin, is found in the sources associated with molecular outflows. Double peaked profiles, corresponding to masing lines (flux ≈ 100-600 Jy), are observed toward the evolved stars. Finally, 183 GHz maser emission is also observed in the more quiescent clouds, but at velocities different from those of the associated 22 GHz masers.

Keywords: *Interstellar medium : molecules : clouds. Masers. Radio lines : molecular. Earth : atmosphere. Stars : Circumstellar matter.*

I) INTRODUCTION:

Chemical models predict water vapor to be one the most abundant molecules in the interstellar medium (ISM) and in the molecular envelopes of oxygen-rich stars. That H_2O is present in the ISM is known since the detection of maser emission from its 6_{16}-5_{23} 22 GHz line (Cheung et al., 1969). At this frequency the terrestrial atmosphere is fairly transparent and the 22 GHz maser emission has been detected toward a large number of star-forming regions, evolved stars, and extragalactic objects. In spite of the large amount of observations of the masing 6_{16}-5_{23} line, little is known about the abundance of this molecule and its spatial distribution in interstellar molecular clouds. The problems with observing other rotational transitions of this molecule arise from the terrestrial atmosphere, which absorbs the extraterrestrial radiation precluding any observation from low altitude sites.

Two submillimeter H_2O lines have been observed toward Ori-A (KL) with the Kuiper Airborne Observatory (KAO) : the 3_{13}-2_{20} line at 183 GHz (Waters et al. 1980, and Kuiper et al. 1984), and the 4_{14}-3_{21} line at 380 GHz (Phillips et al. 1980). These observations indicate a high H_2O

In this Letter we report the discovery of strong maser and thermal emission from the 3_{13}-2_{20} H_2O line toward molecular clouds, and discuss briefly its spatial distribution and origin. Further analysis of our data will be presented elsewhere (Cernicharo et al., 1990).

TABLE 1

ZENITH ATMOSPHERIC TRANSMISSION AT PICO VELETA FOR WATER LINES BELOW 500 GHz

LINE	FREQUENCY (GHz)	TRANSMISSION T=-5°C RH=30% W=2.6mm	T=-5°C RH=10% W=0.9mm	T=-15°C RH=10% W=0.4mm	T=-20°C RH=5% W=0.1mm
3_{13} -2_{20}	183.31012	4%	31%	52%	73%
	183.3±0.1	4%	34%	58%	80%
10_{29} -9_{36}	321.22564	50%	78%	88%	94%
5_{15} -4_{22}	325.15292	3%	27%	50%	72%
4_{14} -3_{21}	380.19737				5%
11_{210} -10_{37}	390.13674	29%	65%	78%	89%
7_{53} -6_{60}	437.34667	12%	47%	66%	80%
6_{43} -5_{50}	439.15081	1%	19%	43%	68%
7_{52} -6_{61}	443.01830	2%	25%	49%	73%
4_{23} -3_{30}	448.00108				3%
6_{42} -5_{51}	470.88895	8%	40%	61%	79%
5_{33} -4_{40}	474.68913		11%	32%	59%
6_{24} -7_{17}	488.49113	3%	12%	15%	17%

In all calculations we have assumed a pressure of 704 mbar, and a water scale height of 2.5km. T is ambient temperature and RH is relative humidity. W is the amount of water vapor above the observatory site. Frequencies are from De Lucia (1972).

GROUND BASED OBSERVATIONS of H_2O:

Maser lines at 22, 183, 321 and 325 GHz + some observations of ν_2=1

INFRARED SPACE OBSERVATORY (ISO) :

Observation of a large number of pure rotational and ro-vibrational lines. Most observations with reduced spectral resolution.

SWAS :

Large scale maps with high spectral resolution of interstellar clouds. Pointed observations of evolved stars. Water in C-rich objects

Herschel (operating since May 2009):

Largest telescope in space (3.5 meters)

Three instruments :

SPIRE (15-52 cm^{-1}). Spectral resolution = 2.5 GHz (FTS)

PACS (52-190 cm^{-1}). Spectral resolution = 1500-4000 (grating)

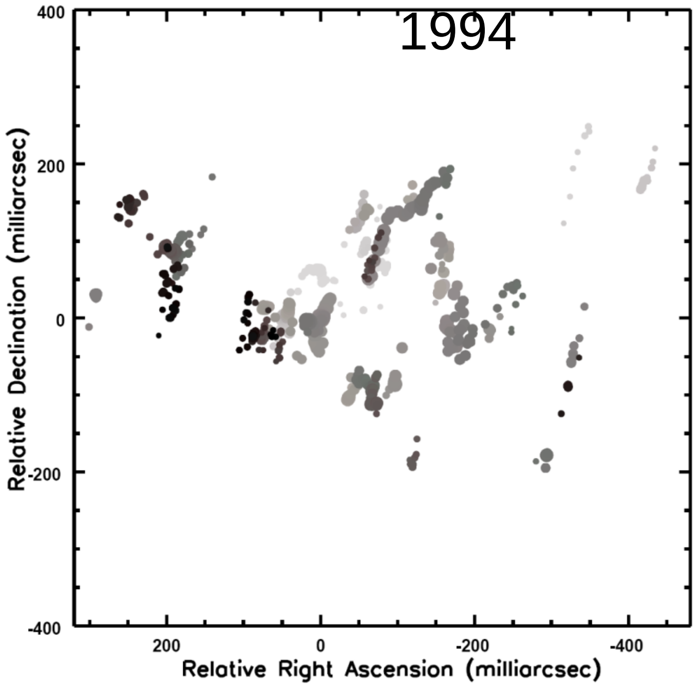
HIFI (15-65 cm^{-1}). Spectral resolution = 10^6 (Heterodyne)

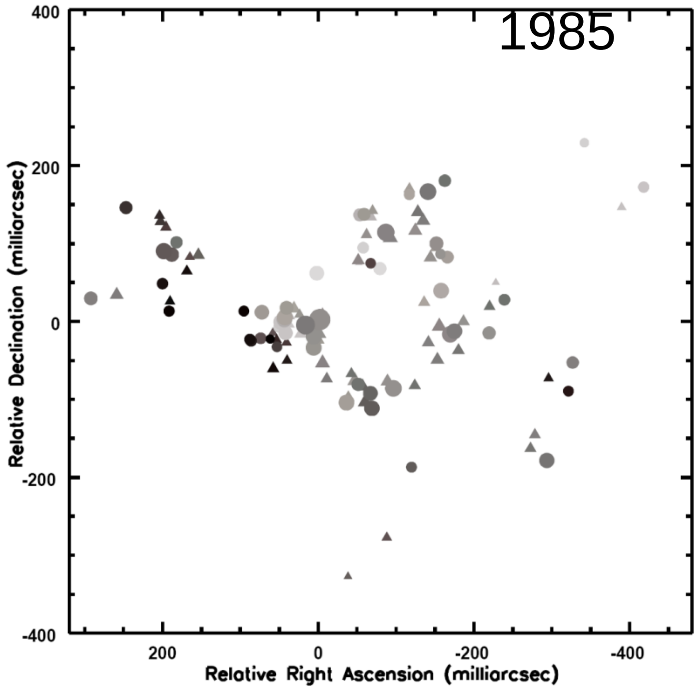
ALMA can observe at 325 GHz and in the next future at 183.3 GHz

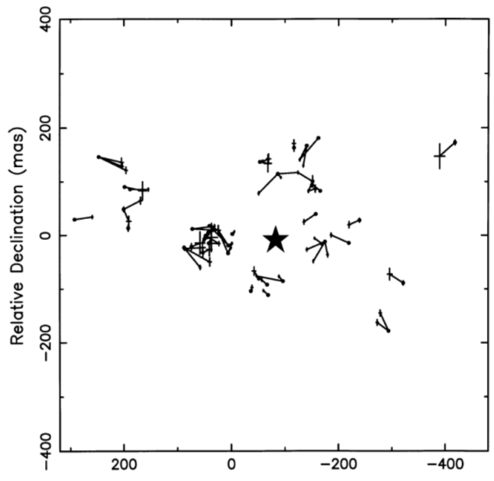
WHAT IS KNOWN ON WATER VAPOUR IN THE ISM & CSM ?

22 GHz observations of evolved stars (Vy CMa)

A. M. S. Richards, J. A. Yates and R. J. Cohen Mon. Not. R. Astron. Soc. **299,** 319–331 (1998)







Astron. Astrophys. 334, 1016–1027 (1998)

ASTRONOMY AND ASTROPHYSICS

Water vapour in circumstellar envelopes

E. González-Alfonso[1,2], J. Cernicharo[2,3], J. Alcolea[2], and M.A. Orlandi[3]

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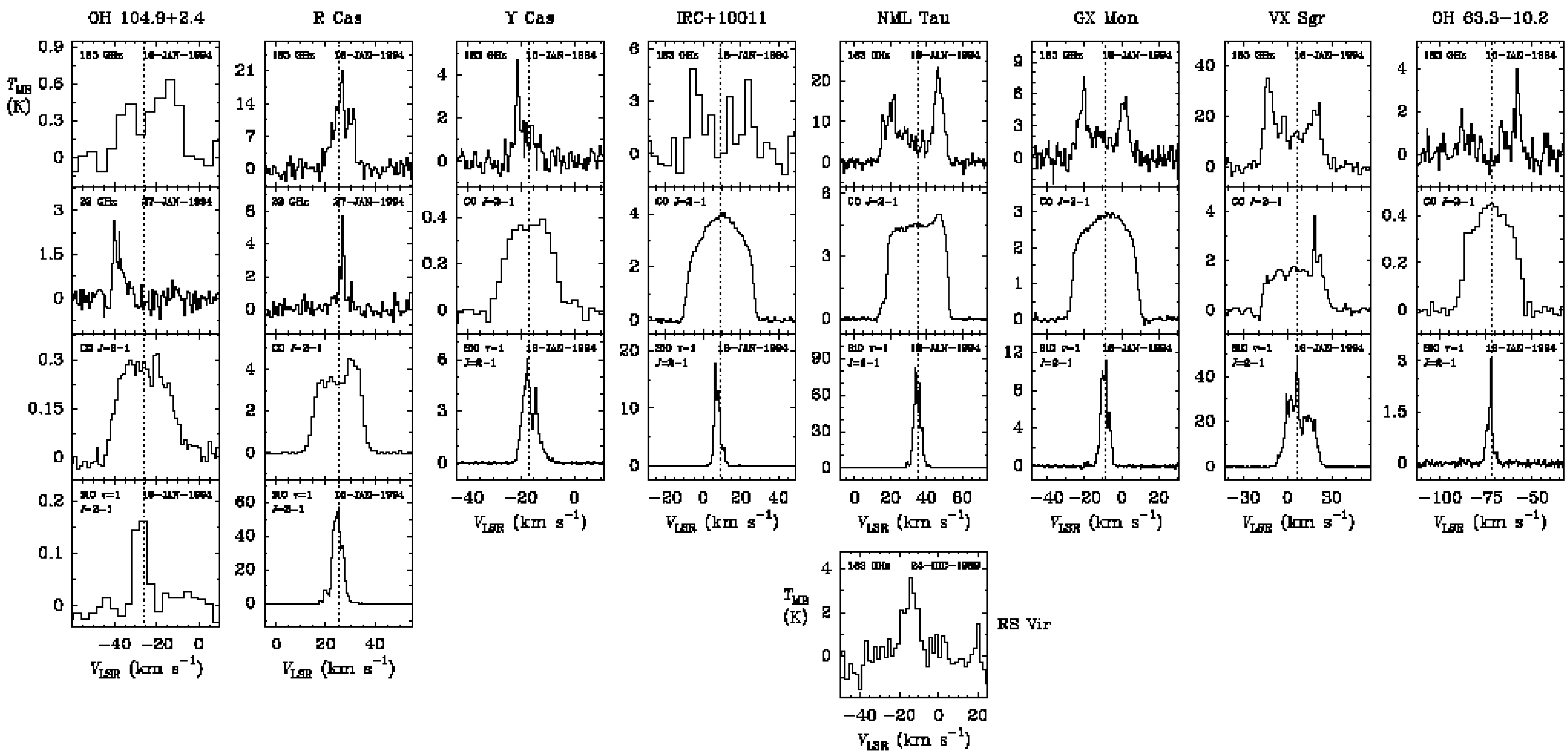


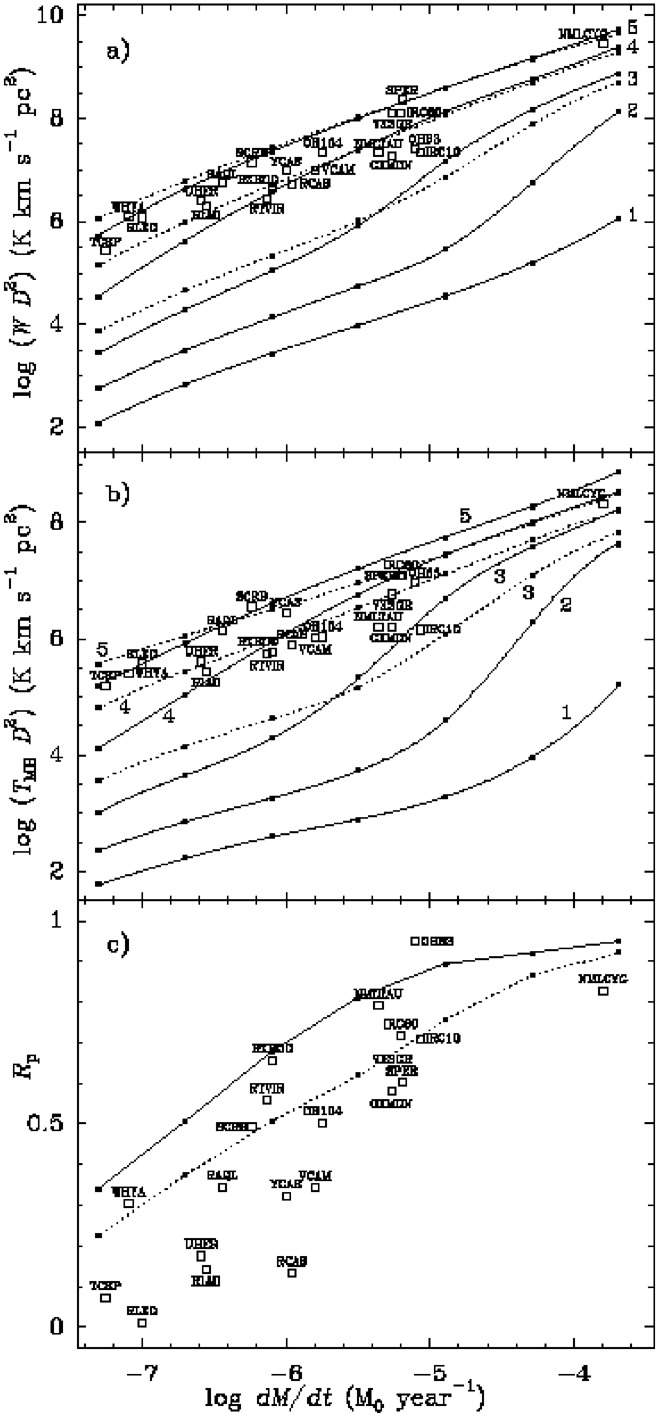
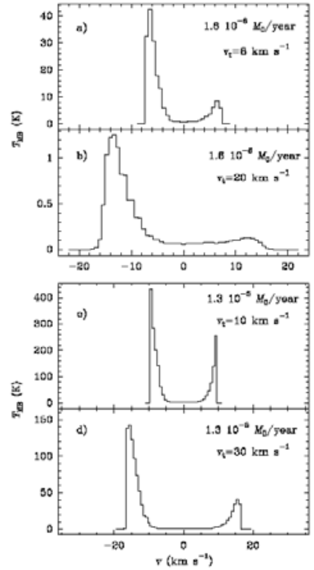
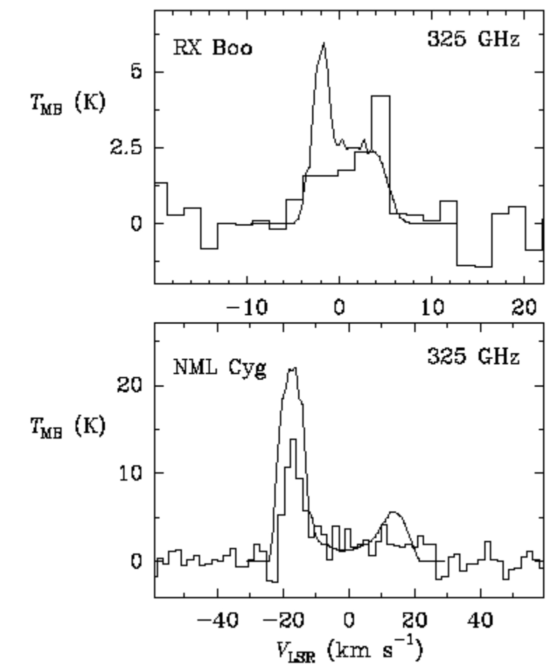


FIG. 12.—W_i, T_i, and R_p for models that differ in $\dot{M}$, x(p-H_2O) and v_t. Solid lines correspond to models with $F_t = 10$, while dashed lines show model results for $F_t = 20$. v_t is determined from $v_t = 1.9 \times 10^2 \dot{M}^{0.2}$ (Paper I). (*a* and *b*) Each curve corresponds to a given value of x(p-H_2O): (1) 10^{-6}; (2) 3.3×10^{-6}; (3) 10^{-5}; (4) 3.3×10^{-5}; (5) 10^{-4}. (*c*) Results of calculatior with x(p-H_2O) $= 3.3 \times 10^{-5}$ only. The observational values are als shown.





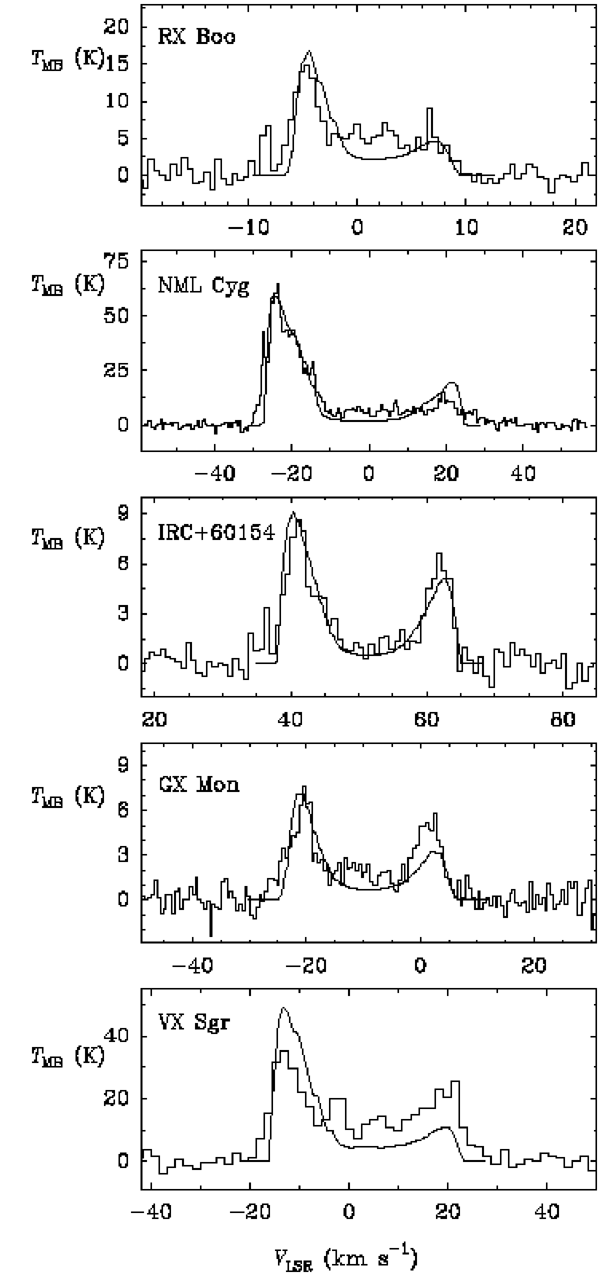
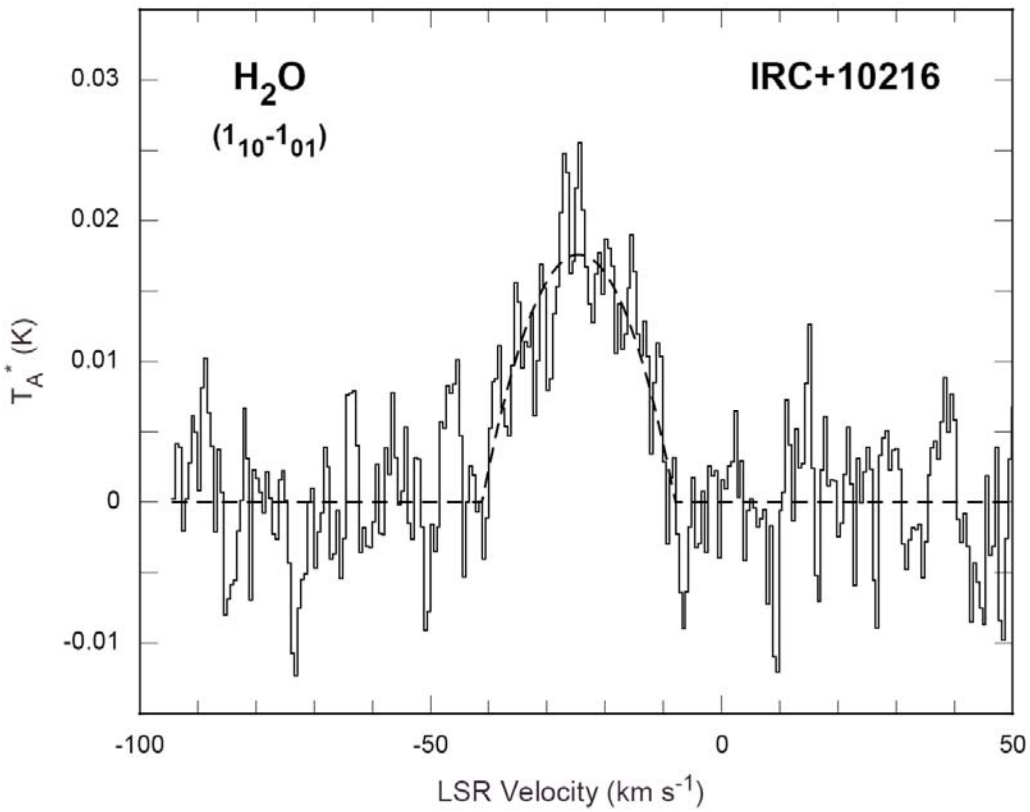


FIG. 13*a*

WATER in C-rich AGB STARS

WATER in Carbon rich AGBs stars



Melnick et al., 2001, Nature, 412, 160

Source of water : Comet evaporation

THE ASTROPHYSICAL JOURNAL, 650:374–393, 2006 October 10

OXYGEN CHEMISTRY IN THE CIRCUMSTELLAR ENVELOPE OF THE CARBON-RICH STAR IRC +

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Received 2006 March 21; accepted 2006 May 25

ABSTRACT

In this paper we study the oxygen chemistry in the C-rich circumstellar shells of IRC +10216. The recent discoveries of oxygen-bearing species (water, hydroxyl radical, and formaldehyde) toward this source challenge our current understanding of the chemistry in C-rich circumstellar envelopes. The presence of icy comets surrounding the star or catalysis on iron grain surfaces have been invoked to explain the presence of such unexpected species. This detailed study aims at evaluating the chances of producing O-bearing species in the C-rich circumstellar envelope only by gas-phase chemical reactions. For the hot inner envelope we show that although most of the oxygen is locked in CO near the photosphere (as expected for a C/O ratio greater than 1), for radial distances larger than ~15 stellar radii, species such as H_2O and CO_2 have a large abundance under the assumption of thermochemical equilibrium. It is also shown how non-LTE chemistry makes the CO → H_2O, CO_2 transformation predicted in LTE very difficult. Concerning the chemistry in the colder, outer envelope, we show that formaldehyde can be formed through gas-phase reactions. However, in order to form water vapor, it is necessary to include a radiative association between atomic oxygen and molecular hydrogen with quite a high rate constant. The chemical models explain the presence of HCO^+ and predict the existence of SO and H_2CS (which has been detected in a 3 mm line survey to be published). We have modeled the line profiles of H_2CO, H_2O, HCO^+, SO, and H_2CS using a nonlocal radiative transfer model and the abundance profiles predicted by our chemical model. The results have been compared to the observations and discussed.

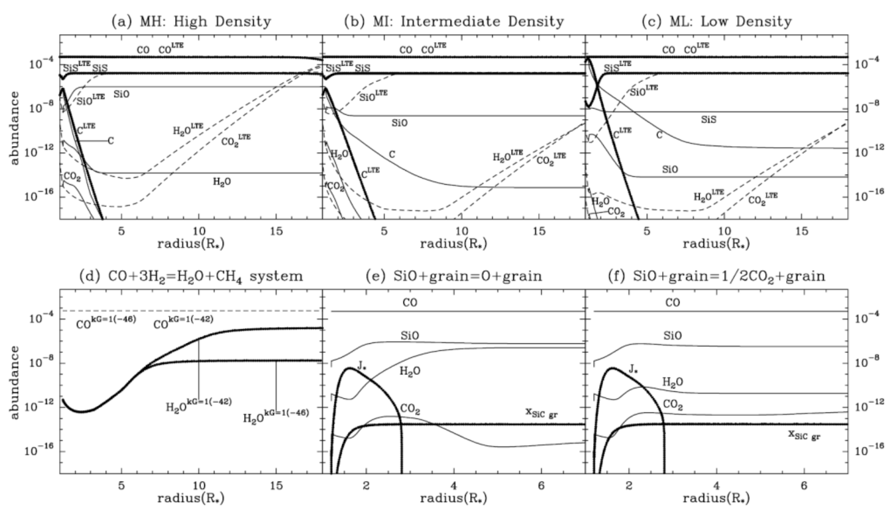

FIG. 3.—Abundances, relative to total number of hydrogen nuclei, of some O-bearing molecules. (*a*), (*b*), and (*c*) Abundances given by LTE (*dotted and dashed lines*) and by chemical kinetics (*solid lines*) assuming a constant velocity expansion of 1 km s^{-1} and the density profiles (*a*) MH, (*b*) MI, and (*c*) ML. (*d*) Abundances of CO and H_2O for a CO, H_2, CH_4, and H_2O system with k_G (see text) equal to 10^{-42} and 10^{-46} cm^9 s^{-1}. (*e*) and (*f*) Abundances given by chemical kinetics with the density profile MH when we consider that 90% of SiO gas is deposited onto SiC grains and that the corresponding oxygen is released to the gas phase either as (*e*) atomic oxygen or as (*f*) CO_2. The nucleation rate of SiC grains J_* (with units of nuclei cm^{-3} s^{-1}) and its abundance x_{SiCgr}, relative to total number of hydrogen nuclei, are also plotted as dotted lines. [*See the electronic edition of the Journal for a color version of this figure.*]

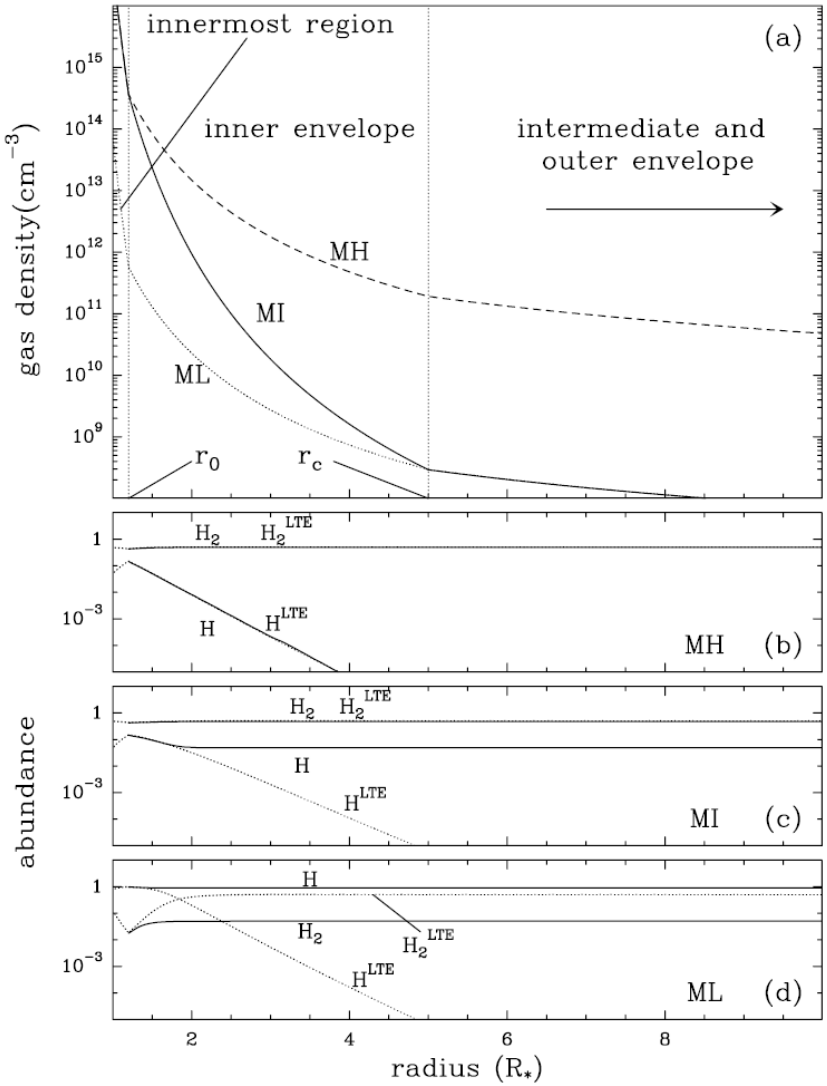

FIG. 1.—(*a*) Three different density profiles considered for the inner and innermost envelope: "MH" [$K_n = 1$, $n(r_0) = 3.7 \times 10^{14}$ cm^{-3}], "MI" [$K_n = 1.8565$, $n(r_0) = 3.7 \times 10^{14}$ cm^{-3}] and "ML" [$K_n = 1$, $n(r_0) = 1.2 \times 10^{12}$ cm^{-3}]. All profiles use a r^{-2} law for $r > r_c$. Panels (*b*), (*c*), and (*d*) show the abundances of H and H_2, relative to total number of hydrogen nuclei [$n(H) + 2n(H_2)$], as given by LTE (*dotted lines*) and by chemical kinetics (*solid lines*) for the three density profiles, (*b*) MH, (*c*) MI, and (*d*) ML. Note the strong dependence of the H/H_2 ratio on the densities considered.

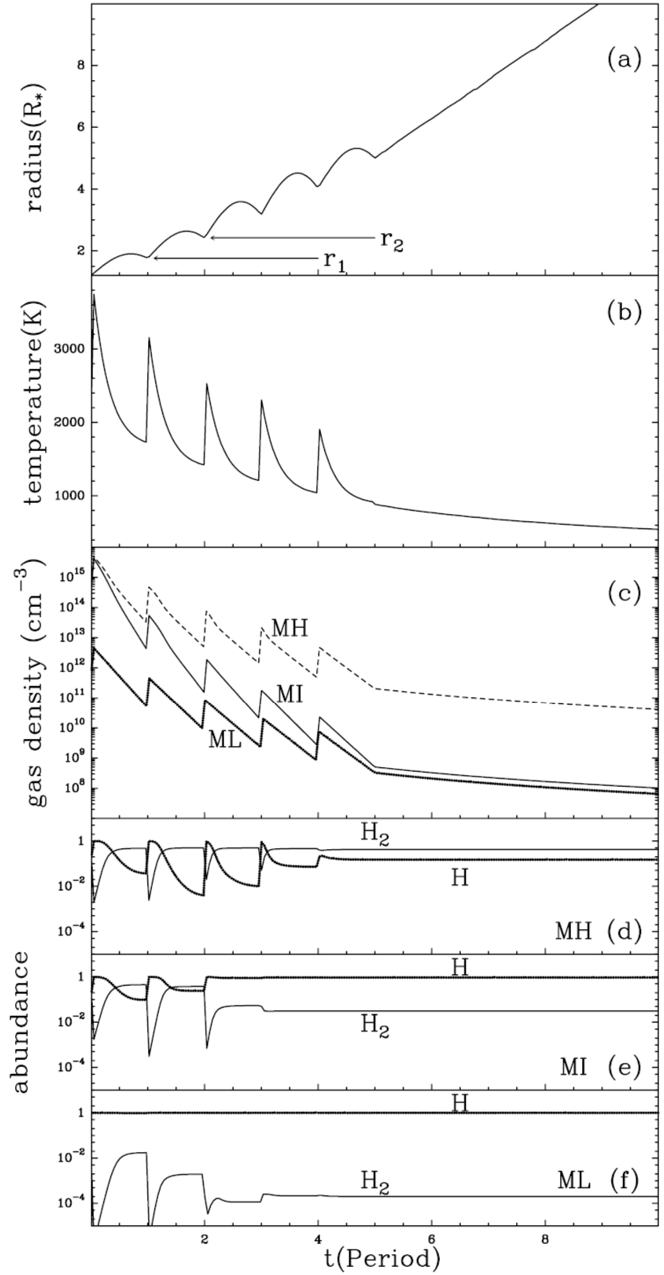

FIG. 2.—Parameters for a volume element of gas that suffers a history of five shocks: (*a*) trajectory; (*b*) temperature history; (*c*) density histories for models MH, MI, and ML. Panels (*d*), (*e*), and (*f*) show the H and H_2 abundances, relative to total number of hydrogen nuclei, calculated by chemical kinetics for the three density laws shown in (*c*).

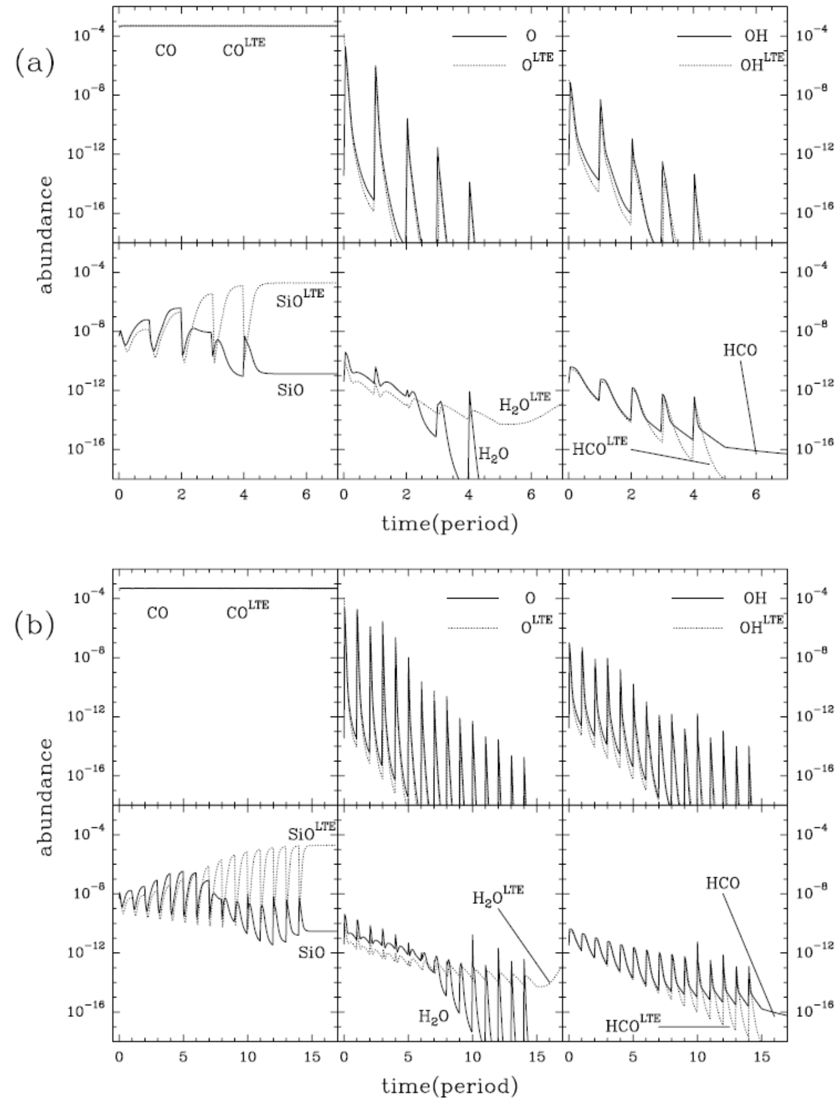

FIG. 4.—Evolution of the abundances, relative to total number of hydrogen nuclei, of some O-bearing molecules for a (*a*) 5 shock history ($N_{\rm shocks} = 5$) and (*b*) 15 shock history ($N_{\rm shocks} = 15$). The history starts at r_0 ($t = 0$) and reaches r_c at time $N_{\rm shocks} P$. The LTE abundances for the physical conditions of the gas at each instant are shown as dotted lines.

Results in agreement with previous models by Cherchneff

The role of infrared pumping

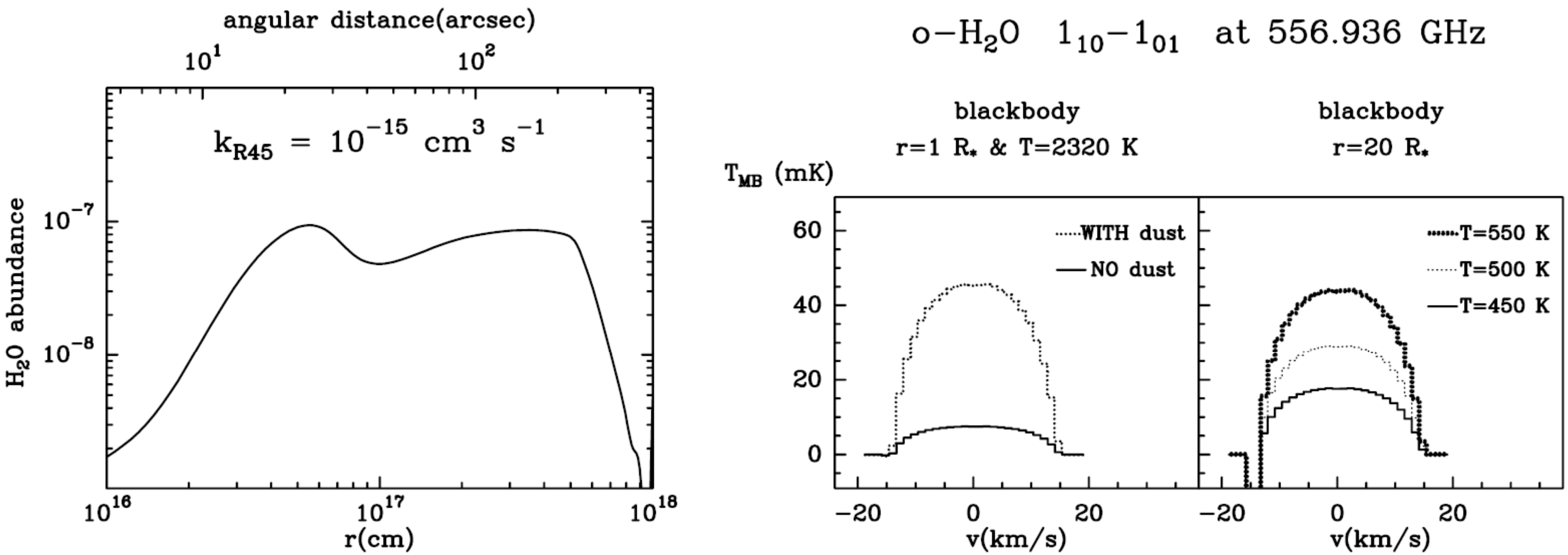

FIG. 7.—*Left:* Water vapor abundance, relative to total number of hydrogen nuclei, when assuming a rate constant for (R45) of 10^{-15} cm^3 s^{-1}. *Right:* Calculated line intensities and profiles for the $1_{1,0}-1_{0,1}$ transition of ortho-H_2O for different IR fluxes. The *Odin* beam size ($\sim 2'$) has been considered, and the lines have been smoothed to a resolution of 1.3 km s^{-1}.

A&A 526, L11 (2011)
DOI: 10.1051/0004-6361/201016035

Astronomy & Astrophysics

Letter to the Editor

Water in IRC+10216: a genuine formation process by shock-induced chemistry in the inner wind★

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Received 31 October 2010 / Accepted 22 December 2010

ABSTRACT

Context. The presence of water in the wind of the extreme carbon star IRC+10216 has been confirmed by the *Herschel* telescope. The regions where the high-J H_2O lines have been detected are close to the star at radii $r \leq 15\ R_\star$.
Aims. We investigate the formation of water and related molecules in the periodically-shocked inner layers of IRC+10216 where dust also forms and accelerates the wind.
Methods. We describe the molecular formation by a chemical kinetic network involving carbon-and oxygen-based molecules. We then apply this network to the physical conditions pertaining to the dust-formation zone which experiences the passage of pulsation-driven shocks between 1 and 5 $R_\star$. We solve for a system of stiff, coupled, ordinary, and differential equations.
Results. Non-equilibrium chemistry prevails in the dust-formation zone. H_2O forms quickly above the photosphere from the synthesis of hydroxyl OH induced by the thermal fragmentation of CO in the hot post-shock gas. The derived abundance with respect to H_2 at 5 $R_\star$ is 1.4×10^{-7}, which excellently agrees with the values derived from *Herschel* observations. The non-equilibrium formation process of water will be active whatever the stellar C/O ratio, and H_2O should then be present in the wind acceleration zone of all stars on the Asymptotic Giant Branch.

Key words. astrochemistry – molecular processes – stars: low-mass – stars: carbon – stars: AGB and post-AGB

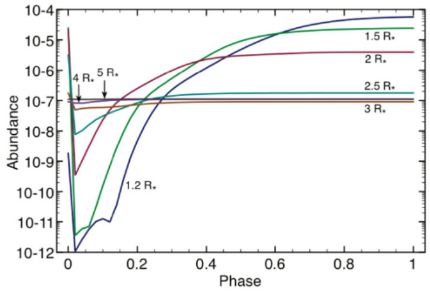


Fig. 1. H_2O abundances with respect to total gas as a function of pulsation phase θ and radius in the inner wind (shocks form at $\theta = 0$ and $\theta = 1$).

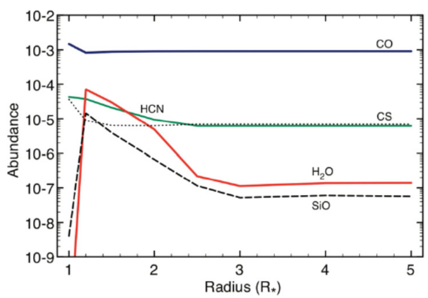
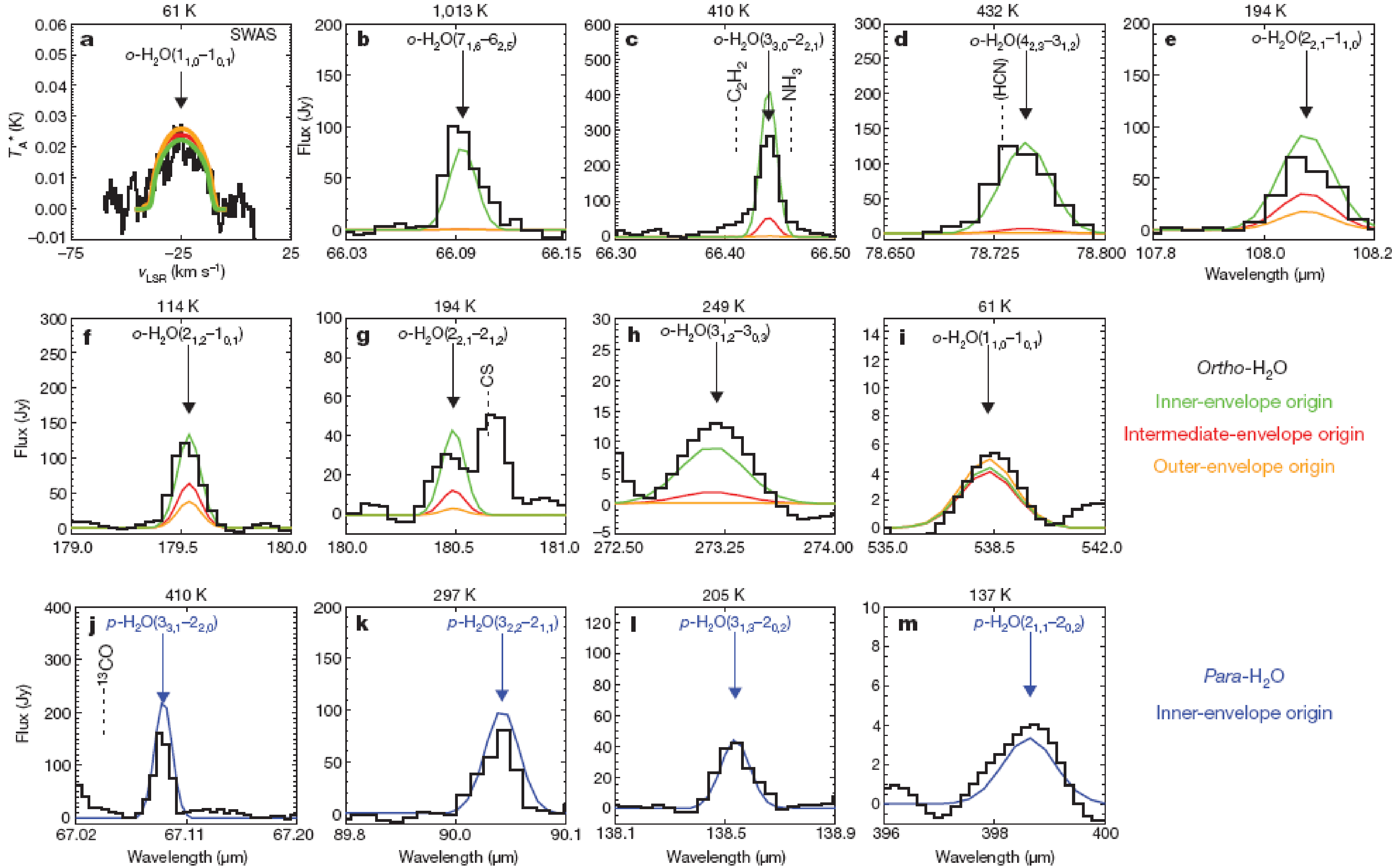


Fig. 2. Abundances with respect to H_2 of key molecules including H_2O taken at $\theta = 1$, as a function of radius. Values at $r = 1\ R_\star$ are derived from thermodynamical equilibrium calculations.

Far-IR data from PACS/Herschel



From Decin et al., 2010, Nature, 467, 64

D. A. Neufeld et al.: Water vapour in V Cygni

Herschel/HIFI
A&A, 521, L5

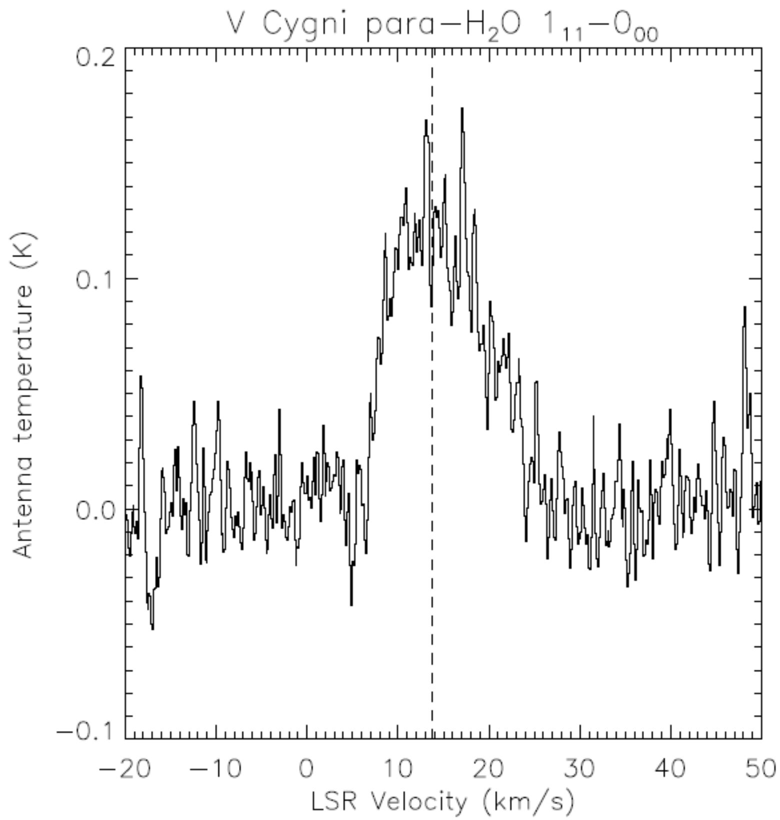
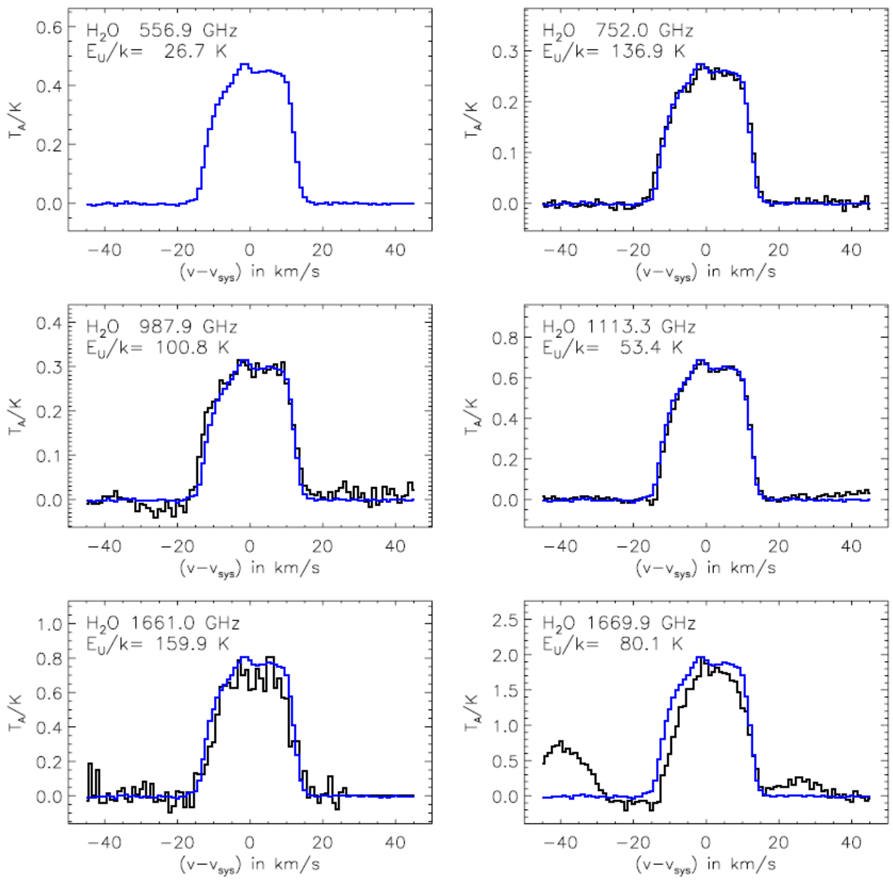
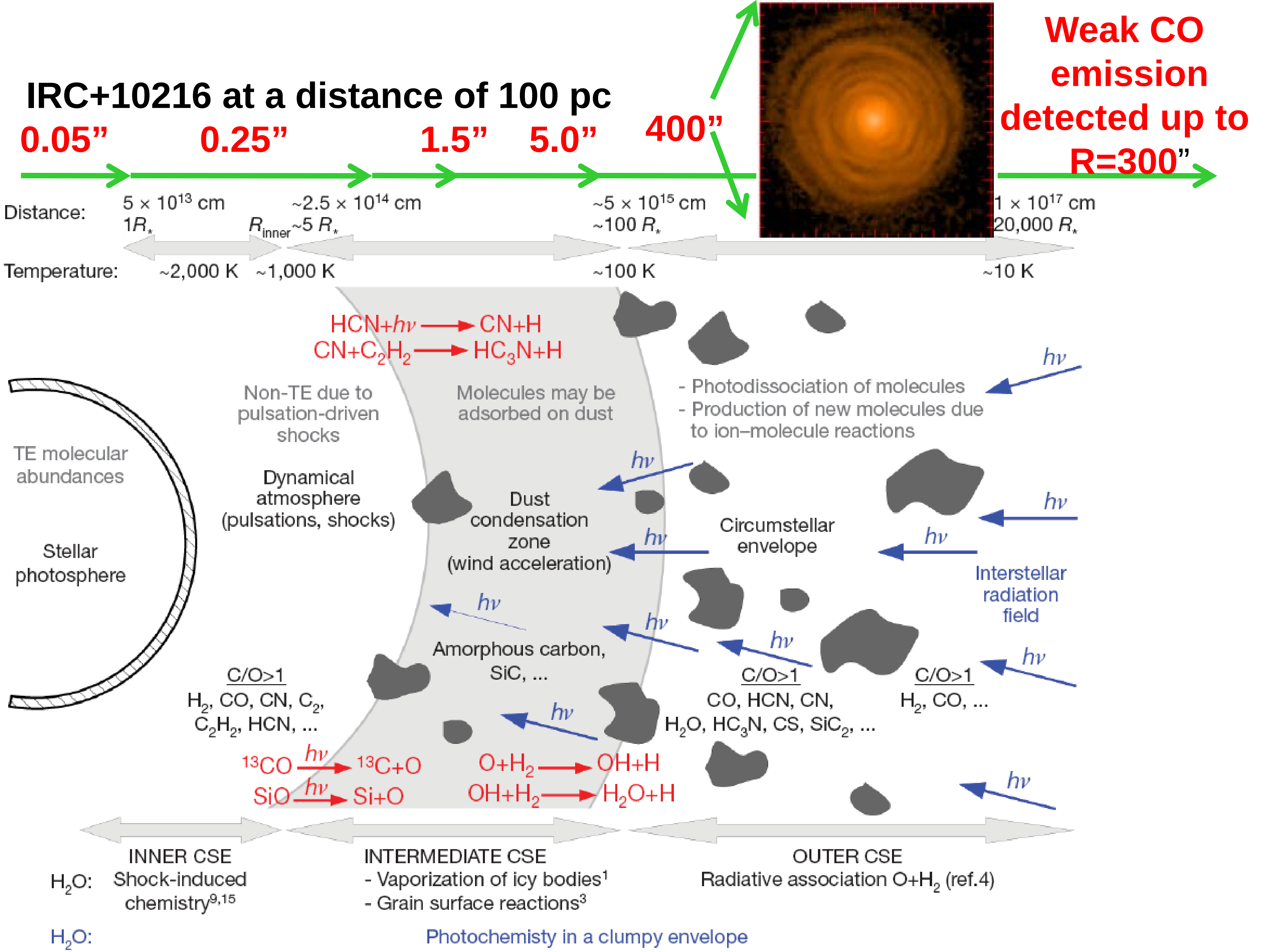


Fig. 1. Continuum-subtracted spectrum of para-H_2O $1_{11}-0_{00}$ obtained toward V Cygni. The vertical dashed line indicates the LSR velocity of the source, as determined by BW01 from observations of the CO J = 2–1 line.

Neufeld et al., Water in IRC+10216
ApJ, 2011, 727, L28





From Decin et al., 2010, Nature

I) Water produced in inner shocks (I. Cherchneff, 2011, A&A, 526, L11)

II) Oxygen atoms available from the photodissociation of ^{13}CO and SiO

Agúndez & Cernicharo 2006

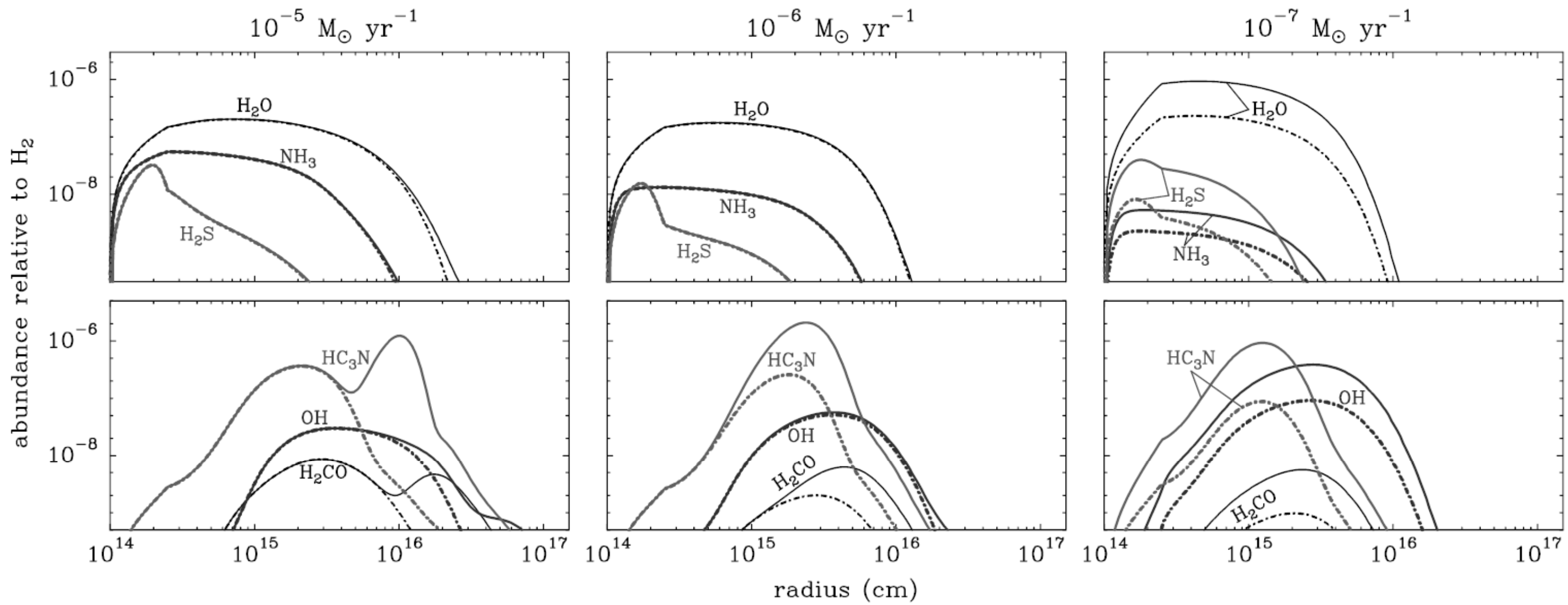


Fig. 2.— Calculated abundance of several molecules as a function of radius for carbon-rich CSEs with mass loss rates of 10^{-5}, 10^{-6}, and 10^{-7} $M_\odot$ yr^{-1}. Dashed-dotted lines correspond to the abundance of the minor UV exposed component and continuous lines to the abundance weighted-averaged over the minor and major components.

Detailed chemical modeling of clumpy envelopes : H_2O, OH and H_2CO could be abundant in C-rich AGBs. HC_3N abundance enhanced in the inner envelope.

Decin et al., 2010, Nature; Agúndez, Cernicharo & Guélin 2010, ApJ, 724, L133,

CRL618

Carbon Rich Protoplanetary Nebula

H_2O, HCO^+, OH and H_2CO

Herpin & Cernicharo 2000, 2001

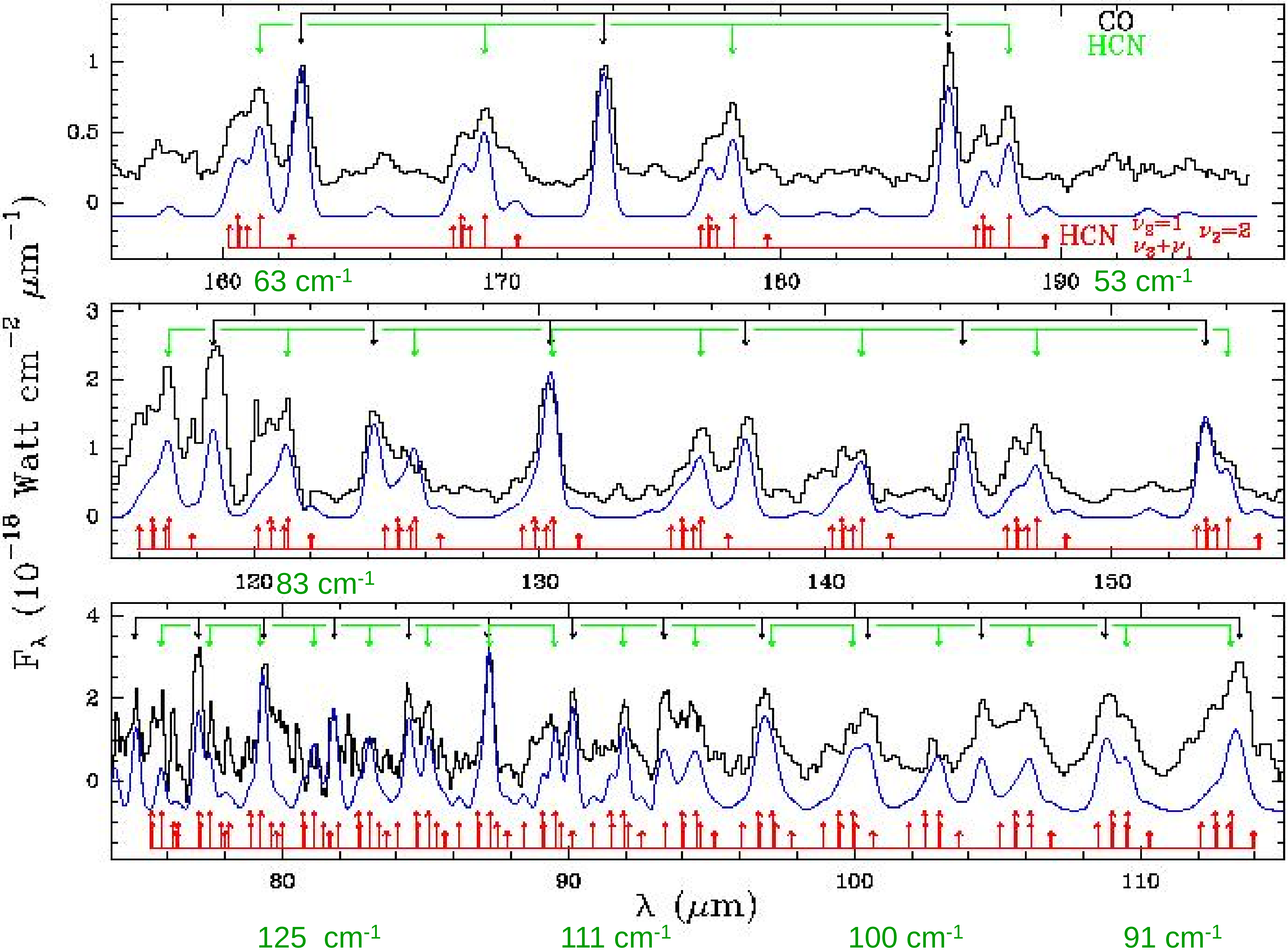
(why only these O-bearing species ?)

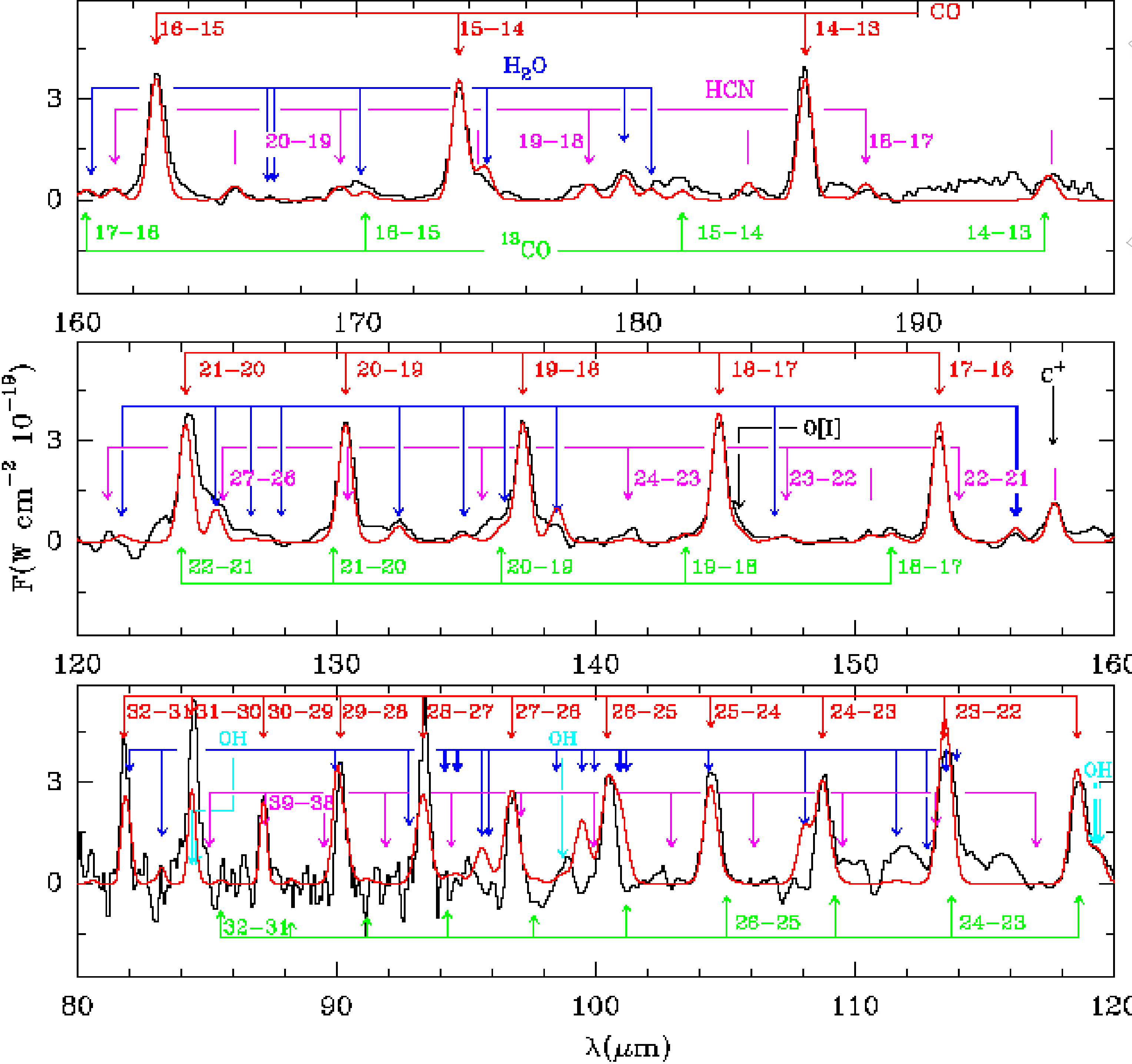
How to interpret a line survey close to the line confusion limit ?

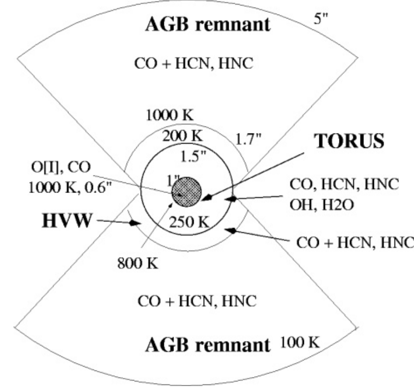
WORK DONE AT DAMIR (CSIC; MADRID) by Juan Ramón PARDO and collaborators (J. Cernicharo, J.R. Goicoechea, M. Guélin, A. Asensio)

Cernicharo et al., 1996, A.&A., 315, 201

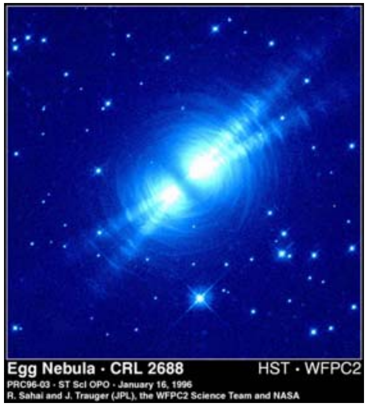
IRC+10216 => HCN (in all ν) + CO; λ/Δλ~300







In C-rich AGB stars

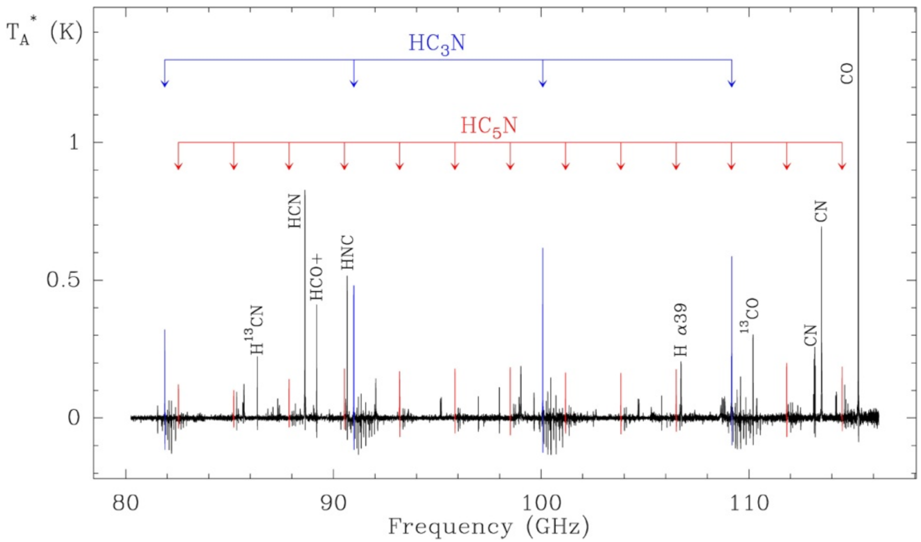


Herpin & Cernicharo, 2000, ApJ Letters, 530, L129

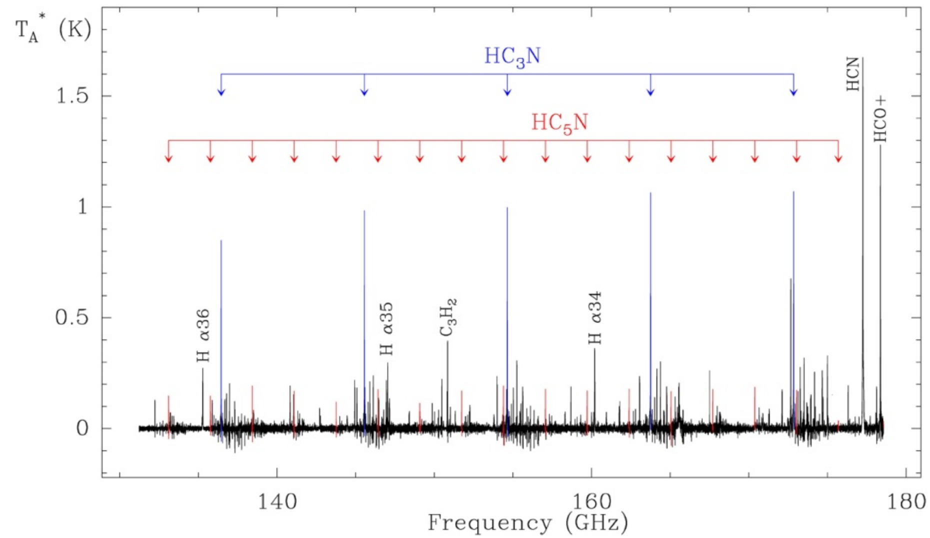
See Chemical Modelling by Cernicharo 2004, ApJ Lett.

CRL618 Spectral Line Survey

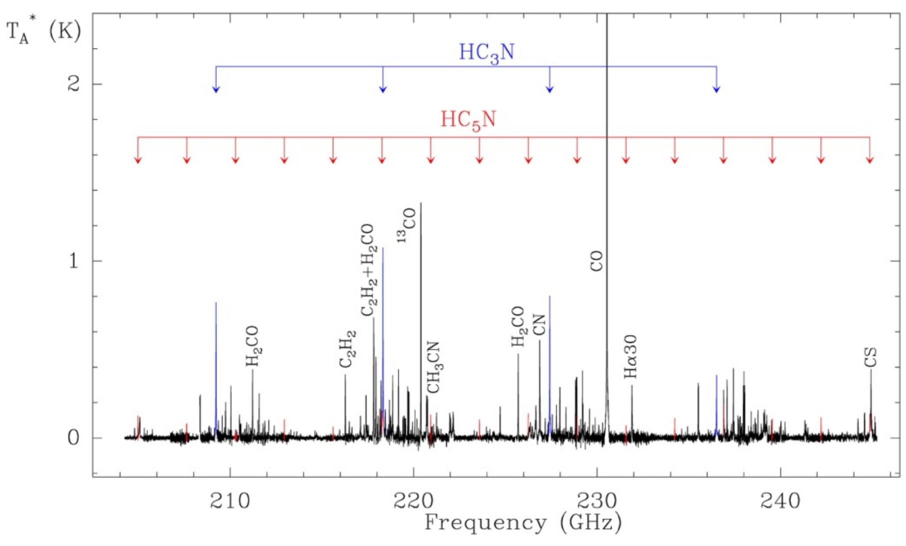
~ 3 mm



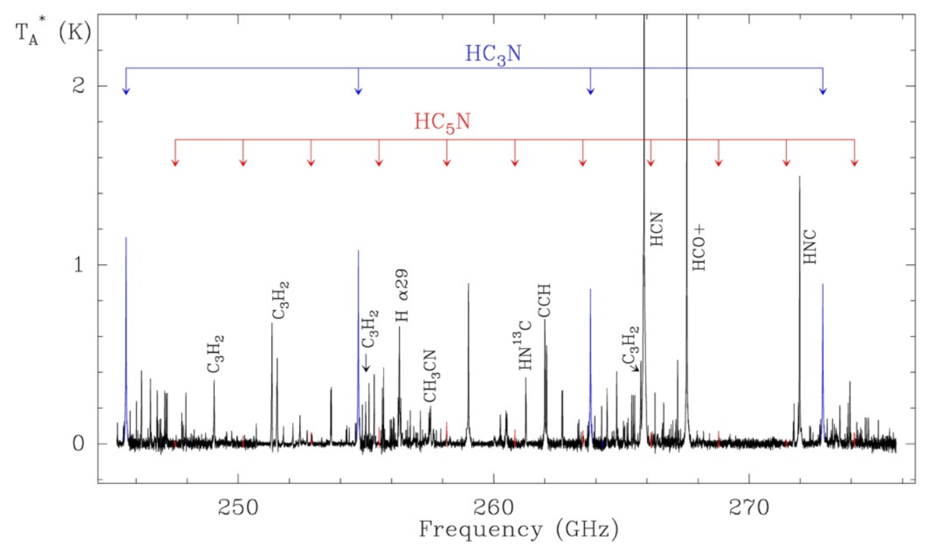
~ 2 mm



~ 1.3 mm



~ 1.0 mm



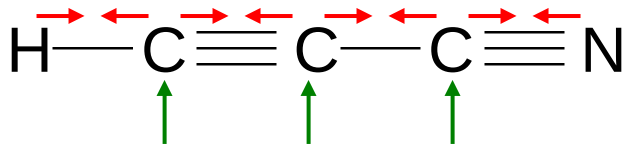
The line survey

- **Around 2500 líneas from 24 molecular species + recombination lines of H y He.**
- **Initially more than 80% of lines were U. Very soon we realized that the spectrum is dominated by HC_3N & HC_5N which are responsible for 85% of the total number of detected lines.**
- **Most lines have P-Cygni profiles. They transform into pure emission at high frequency. Some molecules do not show any absorption components, even at low freq.**
- **Abundant species show broad linewings (CO, HCN, HC_3N, HCO^+)**

The large number of transitions for each molecule allows to reconstruct the morphology of the object:

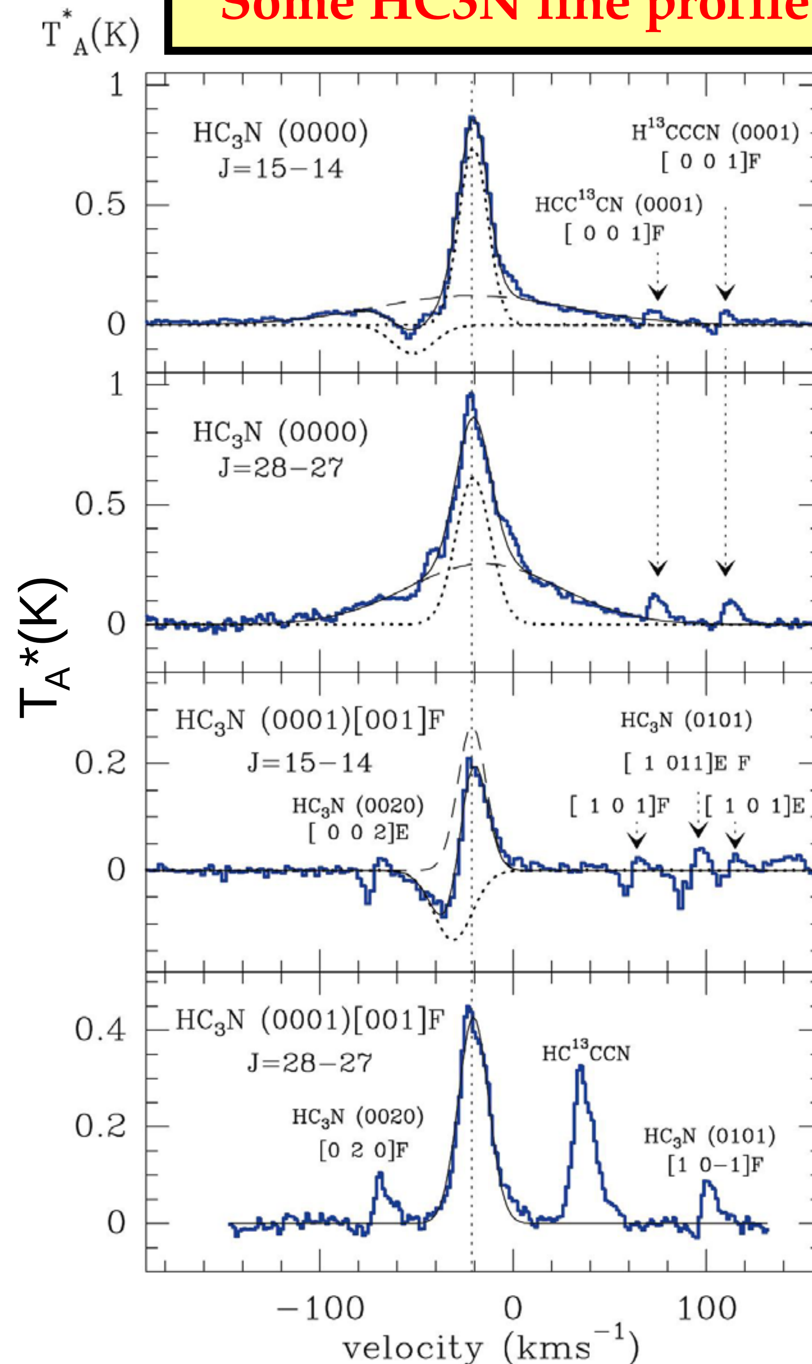
MORPHOLOGY – PHYSICAL CONDITIONS – CHEMICAL ABUNDANCES.

Spectroscopy of HC_3N



- 3 bending modes and four stretching modes.
- Bending modes: (○$_7$,○$_6$,○$_5$): Energies below 663 cm^{-1}
- Stretching mode ○$_4$ at 881 cm^{-1}. The other are above 2000 cm^{-1} (and not detected in CRL618).
- 14 vib states detected in CRL618 with energies up to 1100 cm^{-1}.
- The line profiles show : high velocity wind, low velocity expanding envelope, P-Cygni profiles decreasing when increases.

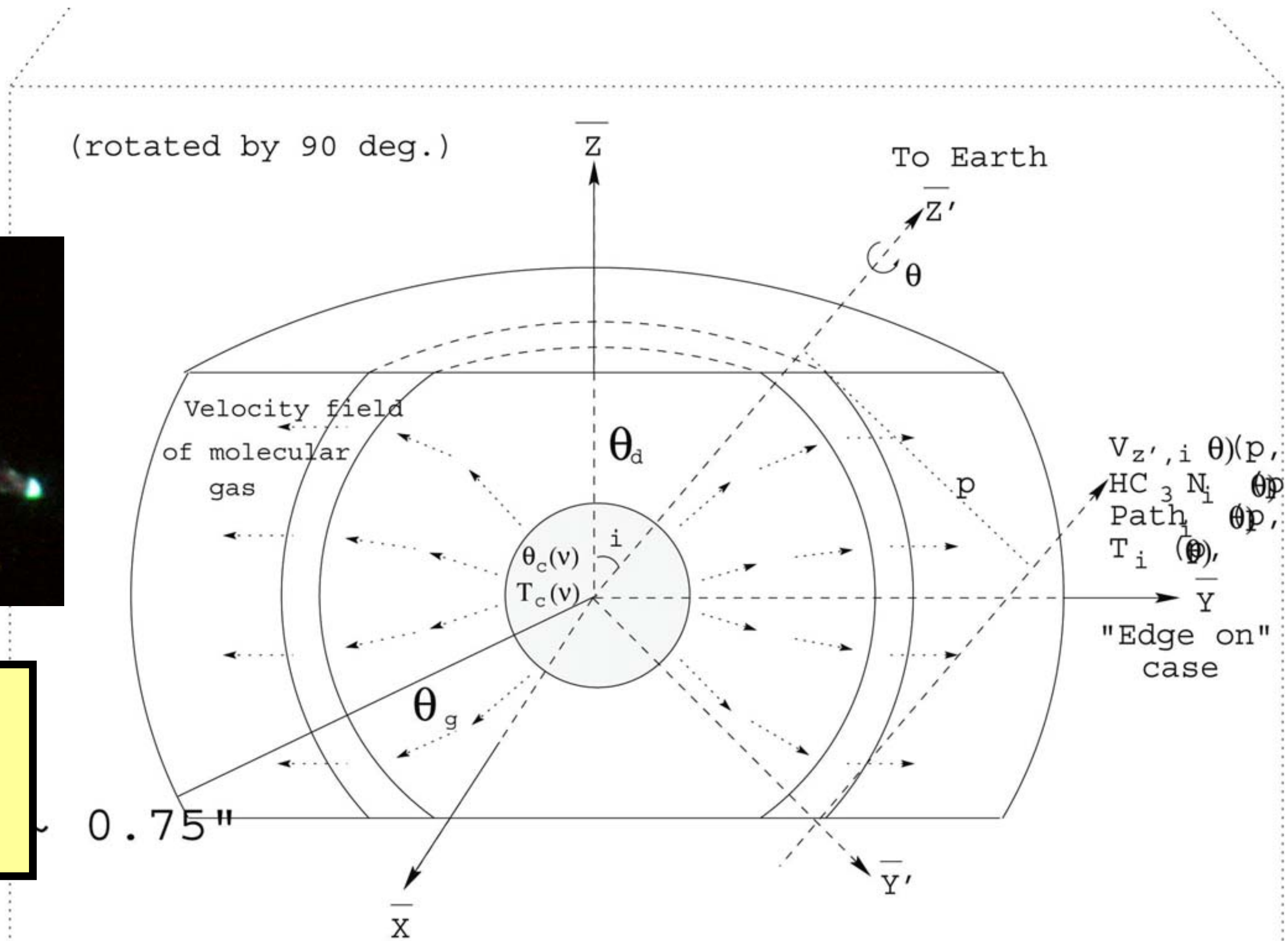
Some HC3N line profiles



Reconstructing CRL618 step by step

Region responsible for the P-Cygni (inner envelope)

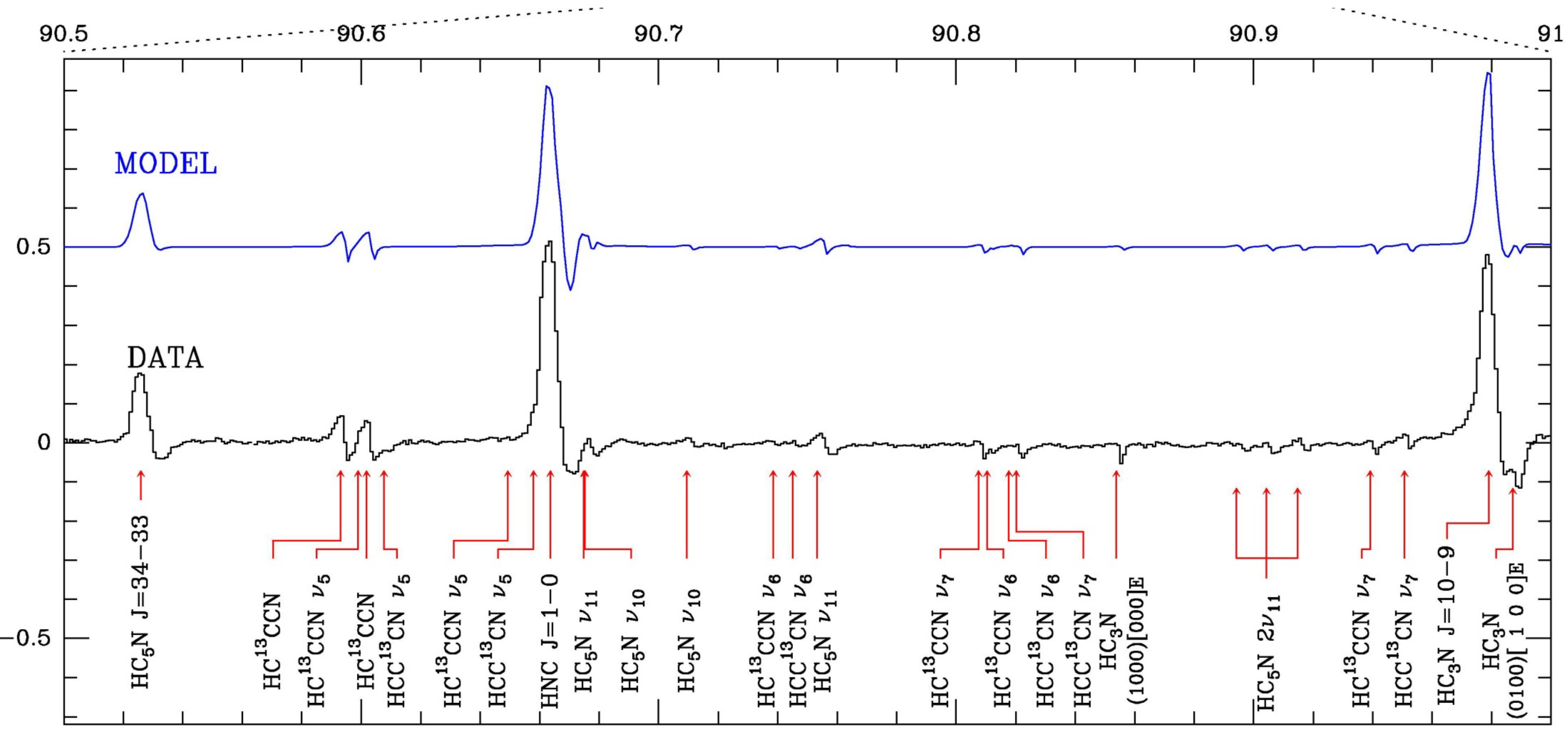
Tracer : code for HC_3N in vib excited states



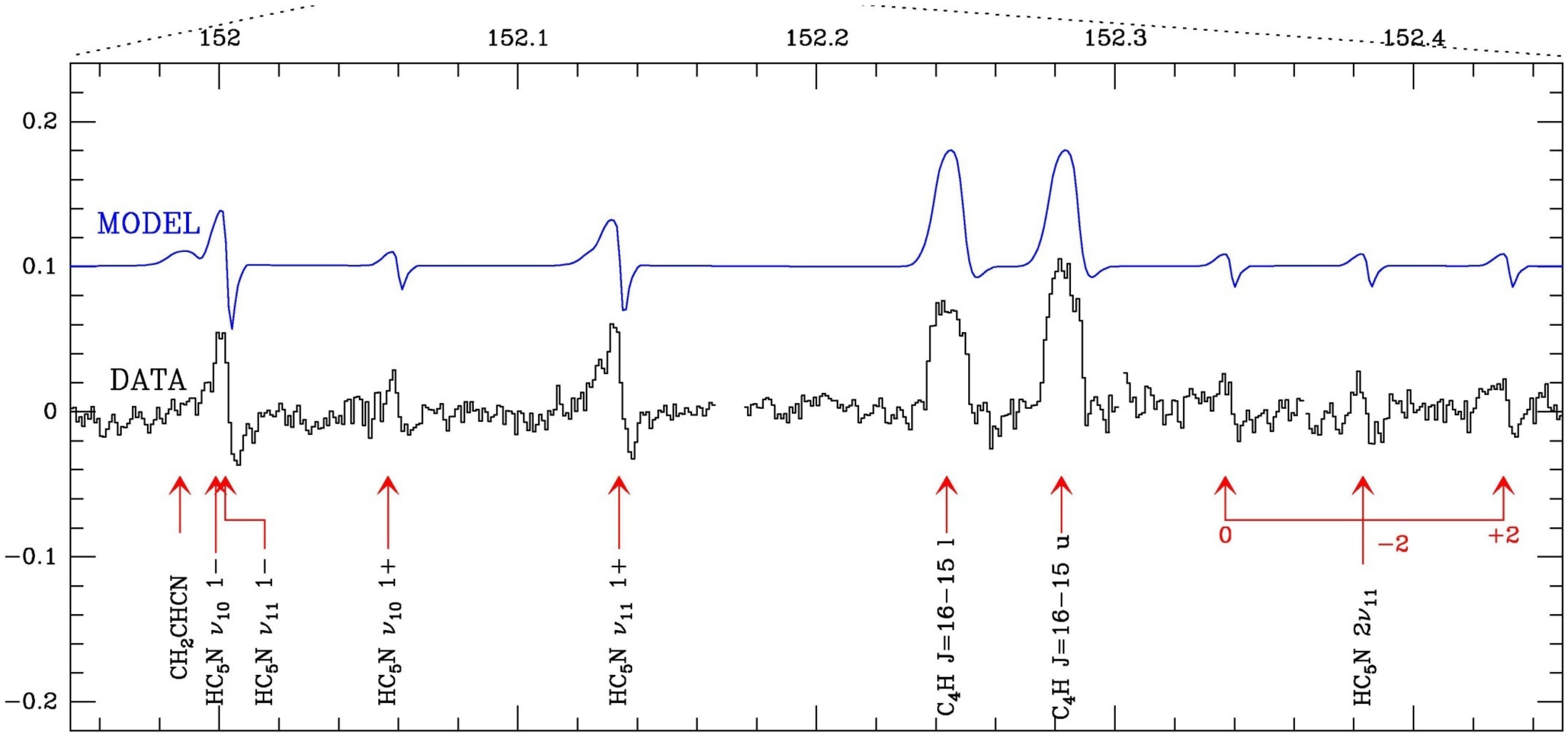
Help: Previous studies, continuum and lines

Pardo & Cernicharo 2007, ApJ 654; Pardo et al., 2004, ApJ, 615, 495 & 2005, ApJ, 628, 275;

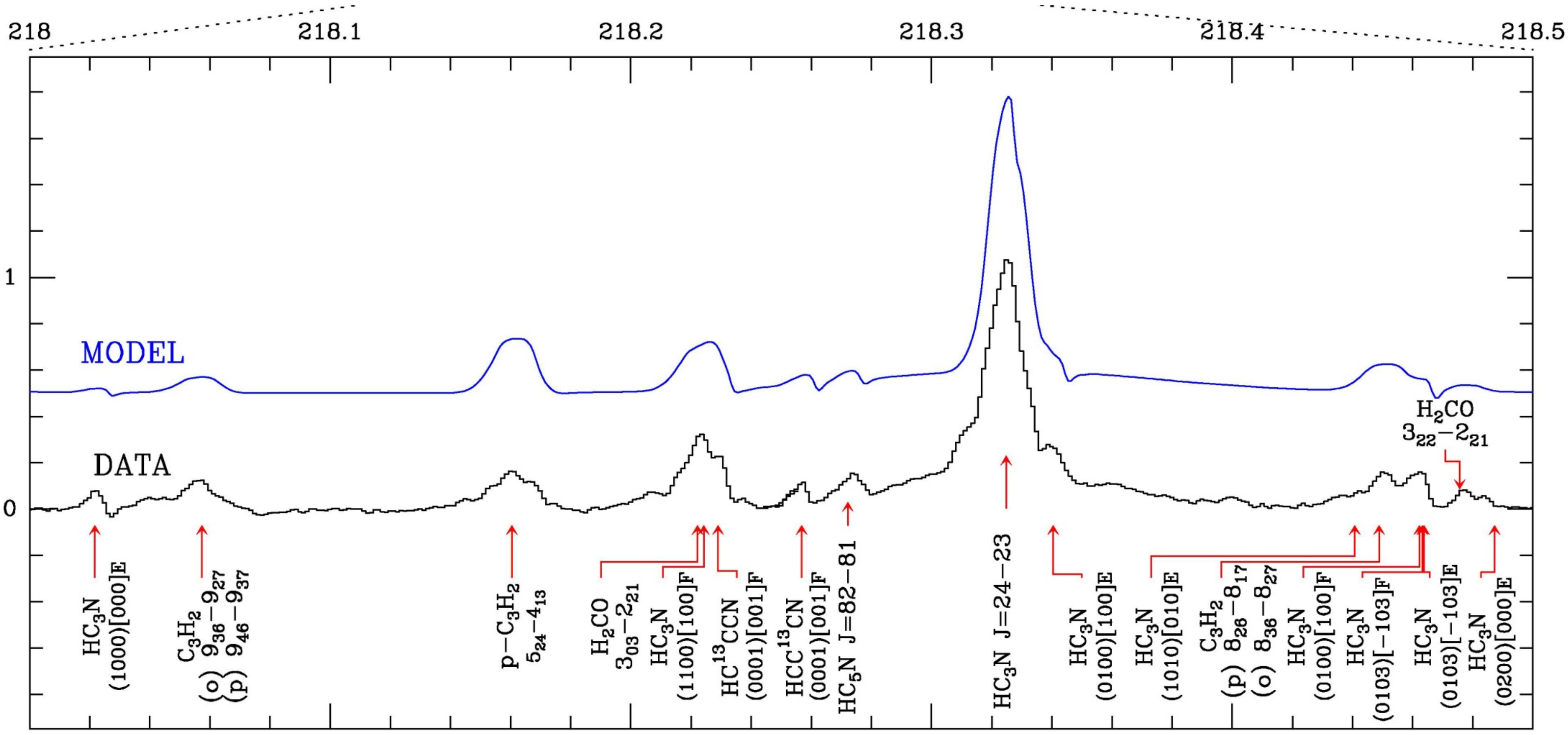
3 mm window : Data and final model



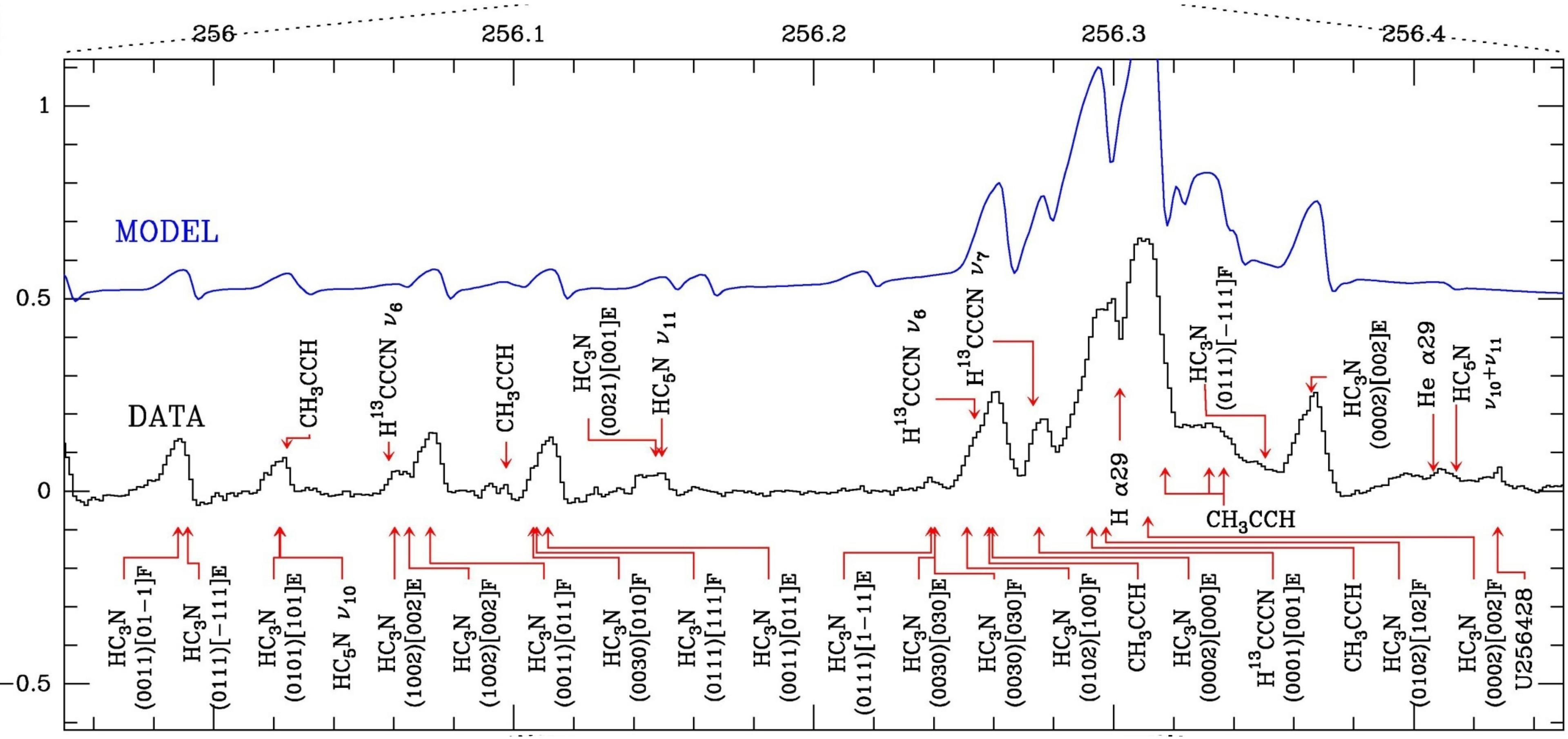
2 mm window : Data and final model



1.3 mm window : Data & final model

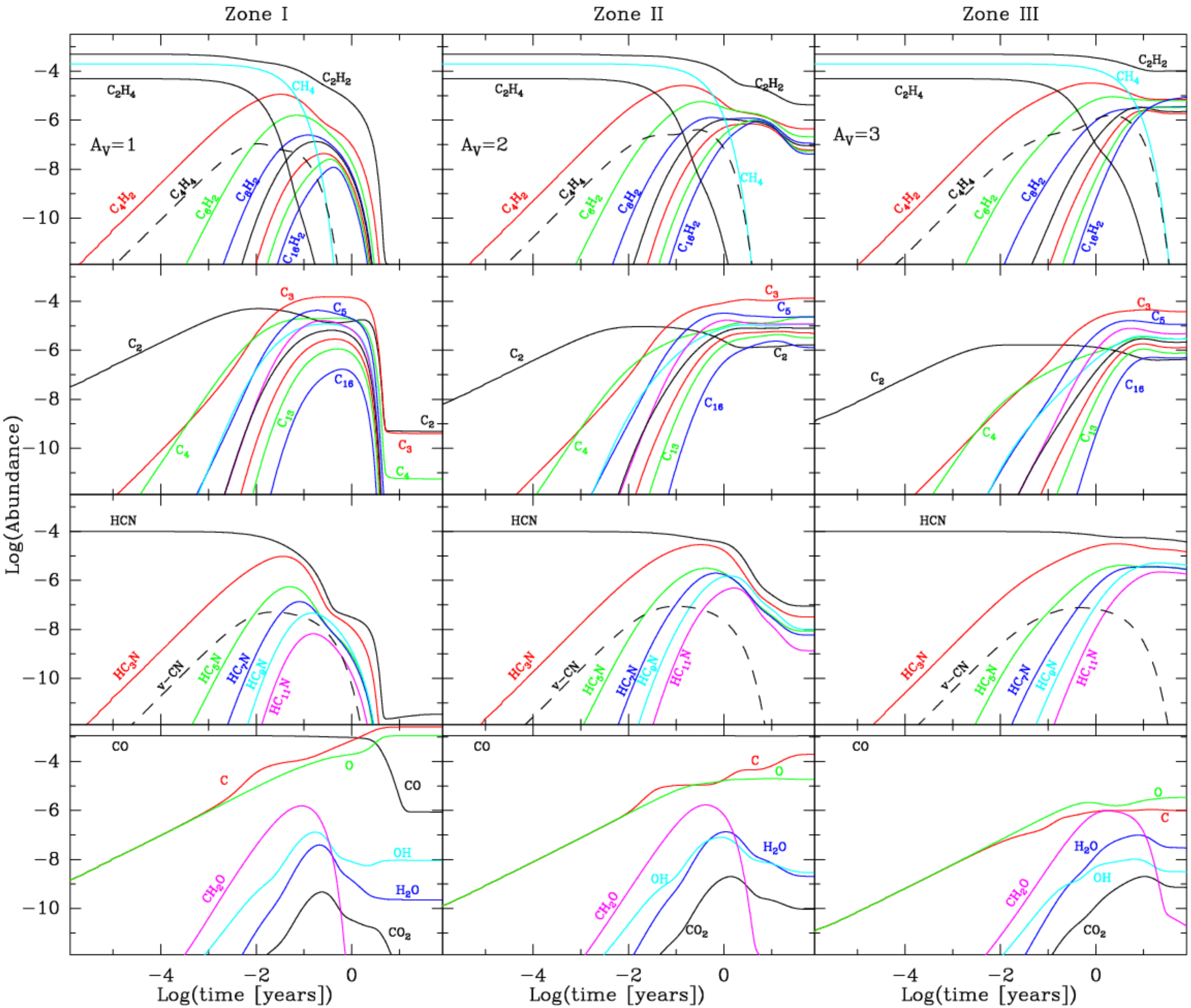


1 mm window : Data & final model

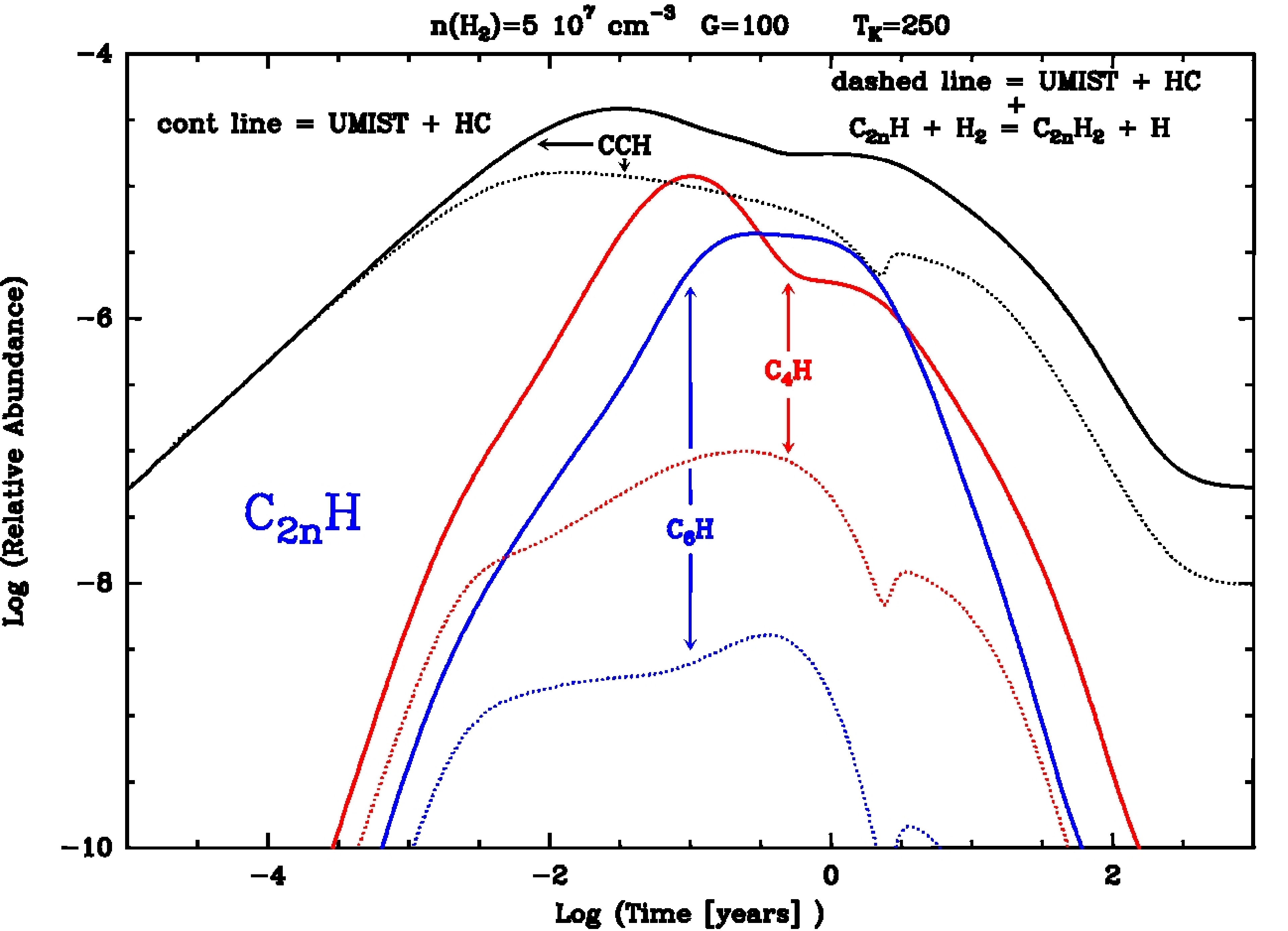


Looking for new molecules : Modelling

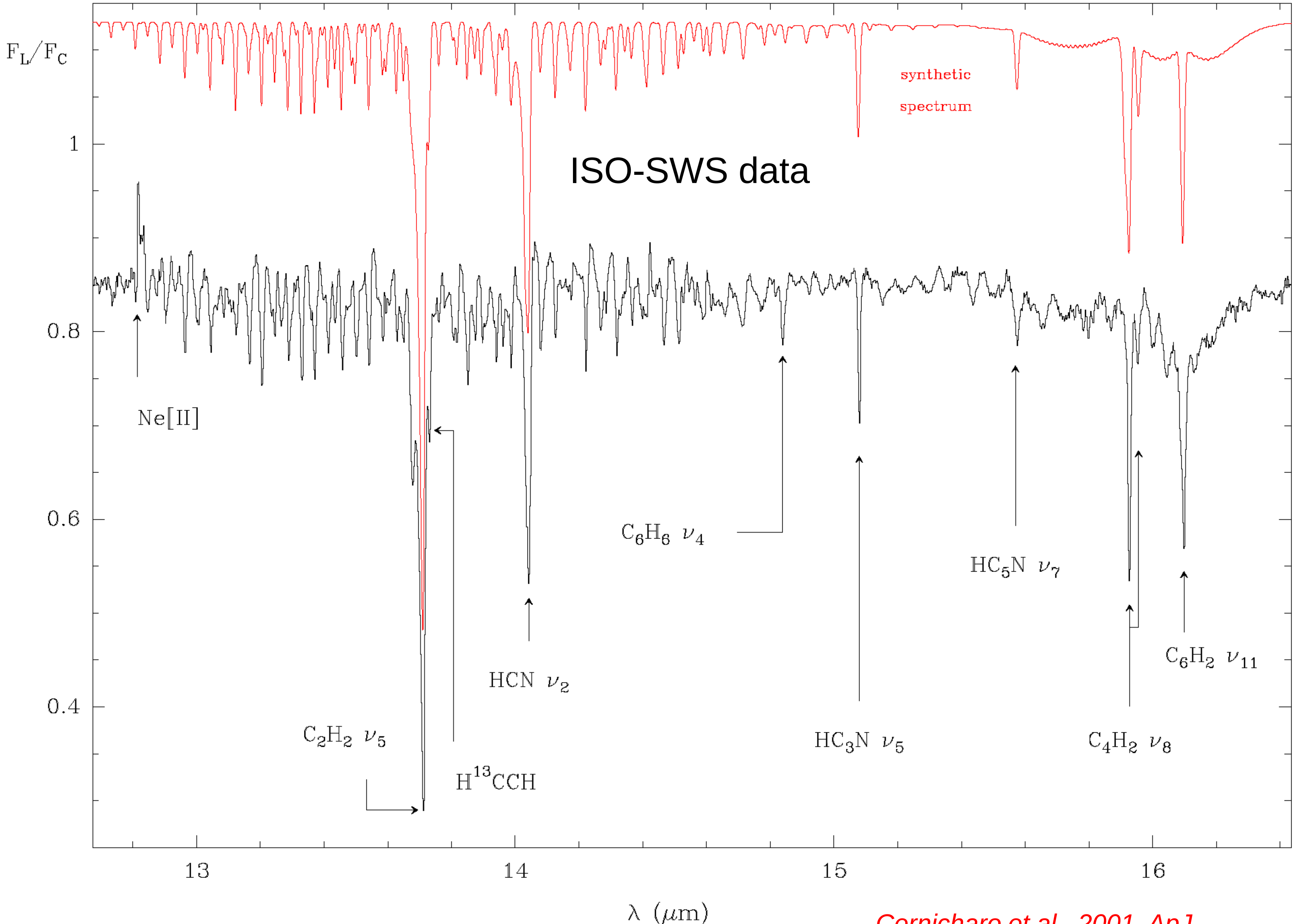
Chemical modelling specific to a C-rich PDR



Cernicharo 2004, ApJ, 608, L41



n(H2)=5 10^7 cm^-3 G=100 TK=250
dashed line = UMIST + HC + C2nH + H2 = C2nH2 + H
cont line = UMIST + HC
CCH
C4H
C6H
C2nH
Log (Relative Abundance)
Log (Time [years])
-4
-6
-8
-10
-4
-2
0
2



Cernicharo et al., 2001, ApJ

LINE SURVEYS : ASTROCHEMISTRY WITH ALMA

- **The need to know essential molecular parameters to interpret observations appear as a mandatory step in any observation of the Interstellar and Circumstellar media.**
- **Many molecules detected in space are exotic species difficult to be produced and observed in the Earth laboratories (C_nH, C_nN, C_nH^-, C_nN^-,…). Special physical conditions have to be reproduced. Spectroscopy is needed**
- **In most cases astrophysical environments are out of equilibrium (physical and chemical). Collisional rates between molecules and H_2/He/H/e^- are needed.**
- **Weeds to be identified before we can progress in the study of chemical complexity and improve our chemical models. Reaction rates are needed**

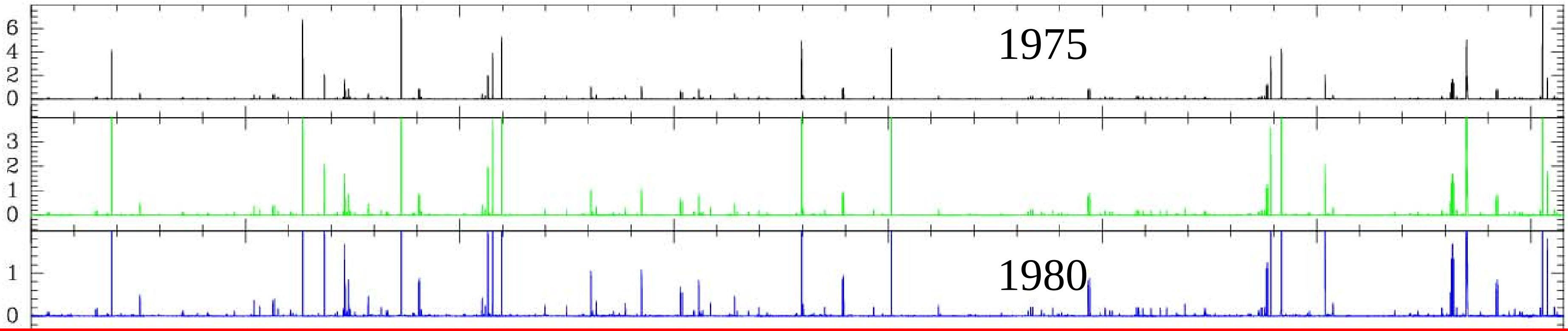
THE SPECTROSCOPY PROBLEM

- Weeds
- How to deal with future ALMA data ?
- What we need from laboratory groups ?
- Which direction have we to follow ?

=> high frequency (ALMA) => Physical processes

=> Low frequency (GBT, VLA, SKA) => Heavy species ?

3mm line survey of IRC+10216 -30m IRAM telescope-



• What we could expect from line surveys ?

• Why we want to carry out line surveys ?

•What we need to interpret ALMA & Herschel line surveys ?

2007

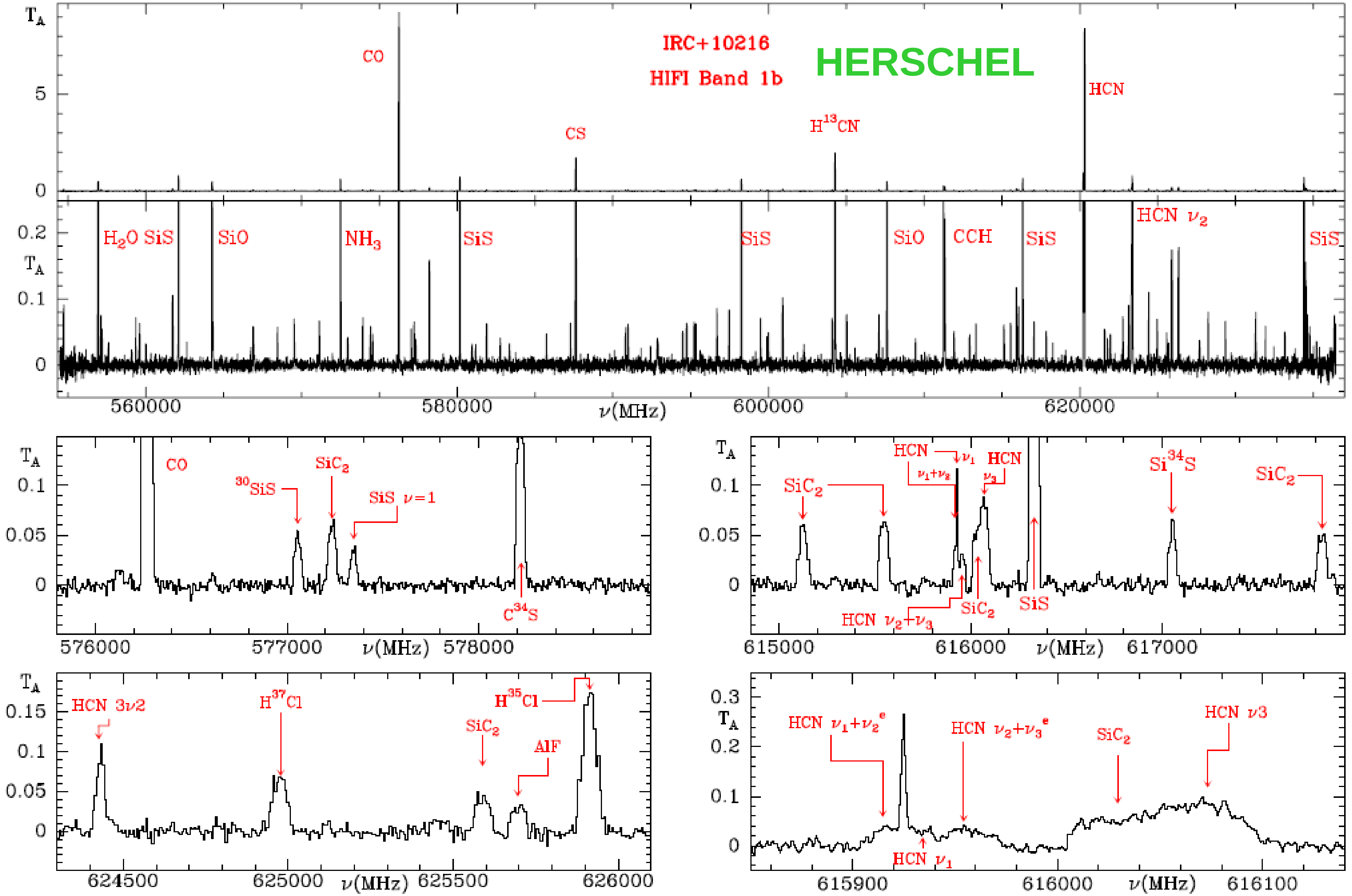


Fig. 1. Spectra of IRC +10216 observed with HIFI band 1b. The two upper panels present the complete spectrum on two different intensity scales. The panels below show different 3 GHz wide ranges of the survey. All data have been smoothed to a spectral resolution of 2.8 km s^{-1} except for the right bottom panel, which shows the spectrum around several vibrational lines of HCN with the nominal WBS resolution (1.1 MHz, ≃0.5 km s^{-1}).

Cernicharo et al., 2010, A&A, 521, L8. SiC_2 spectroscopy from space.

HCl has been detected with PACS/SPIRE (Cernicharo et al., 2010, A&A, 518, L136)

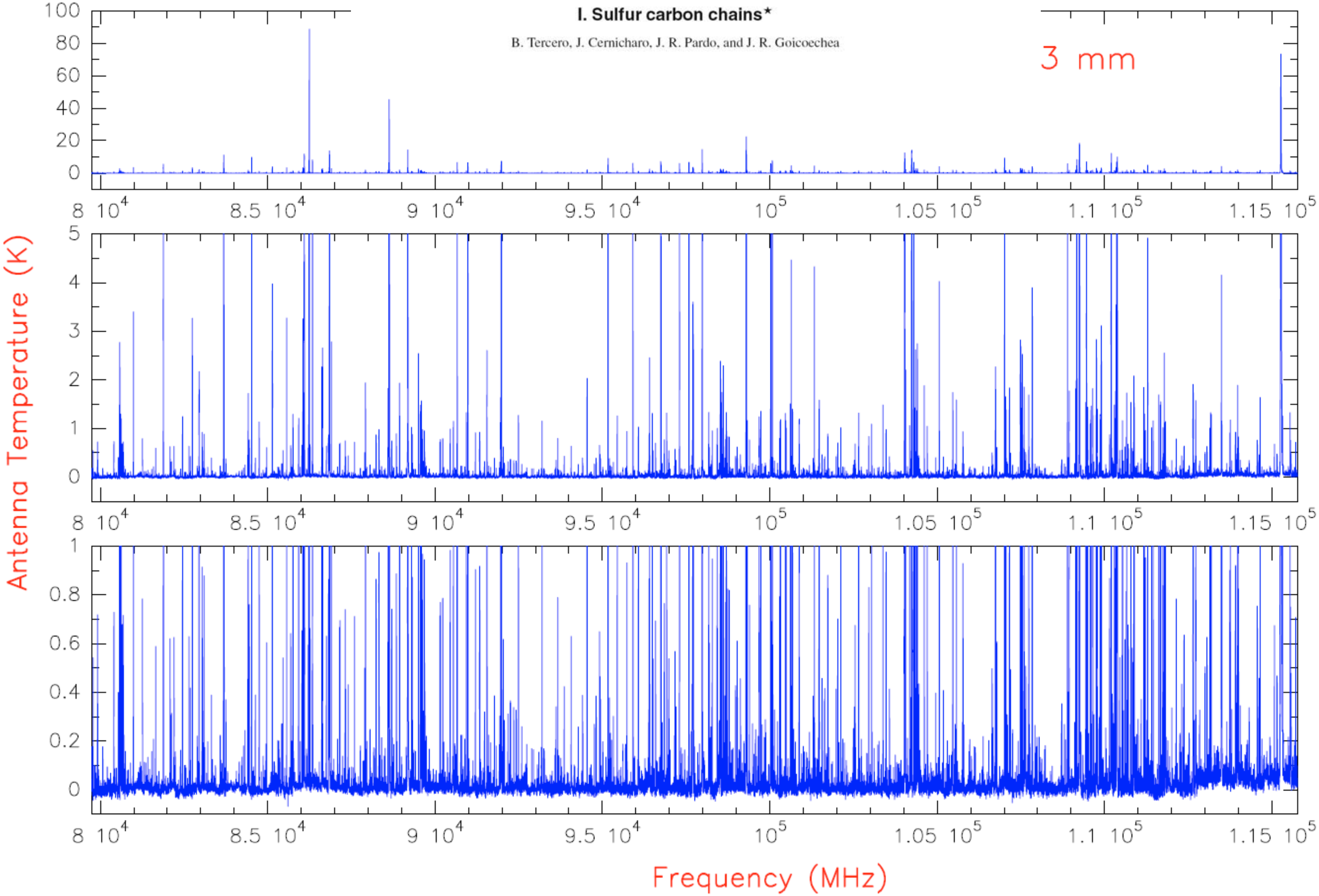
A&A 517, A96 (2010)
DOI: 10.1051/0004-6361/200913501

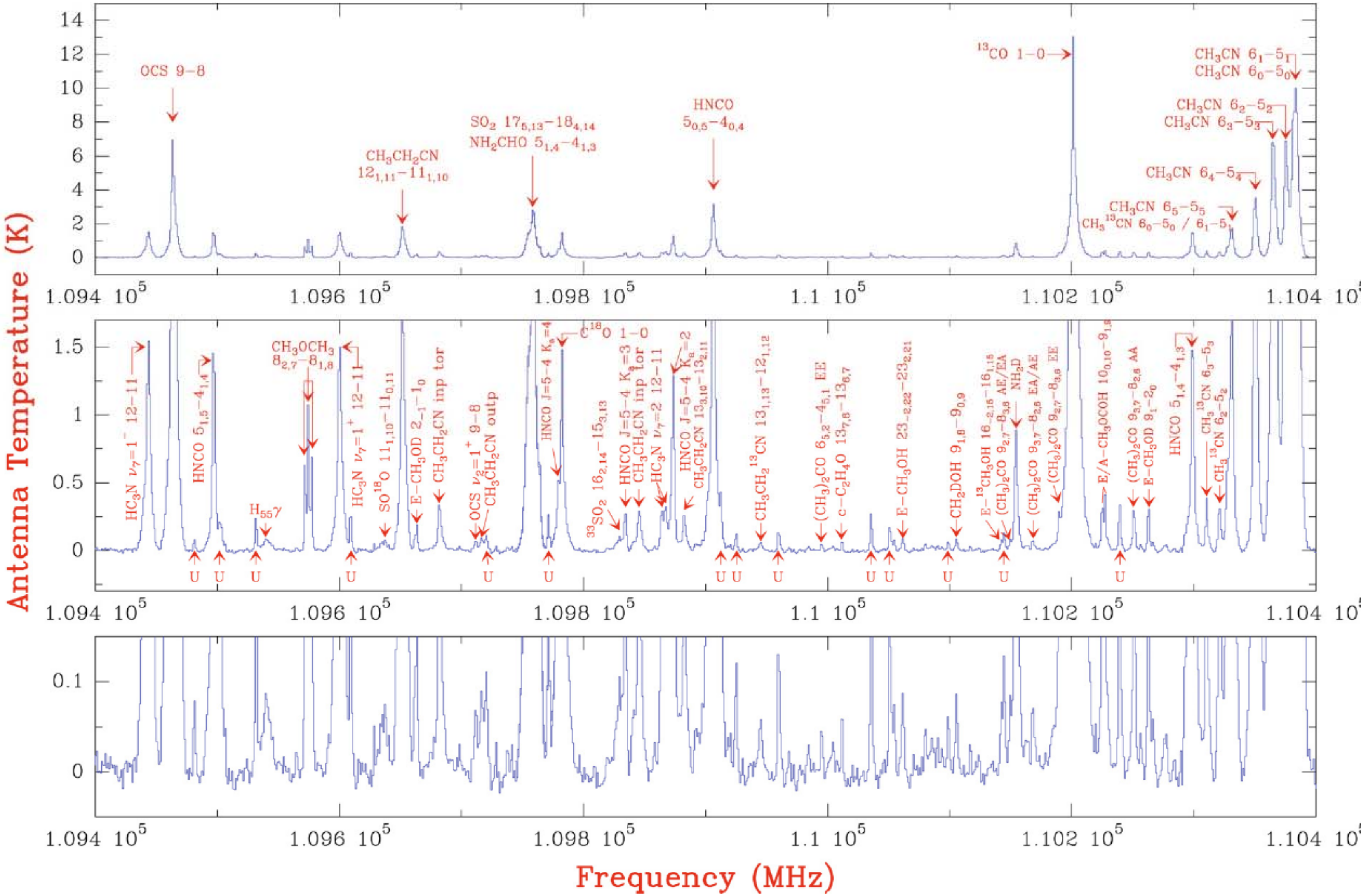
Astronomy & Astrophysics

A line confusion limited millimeter survey of Orion KL

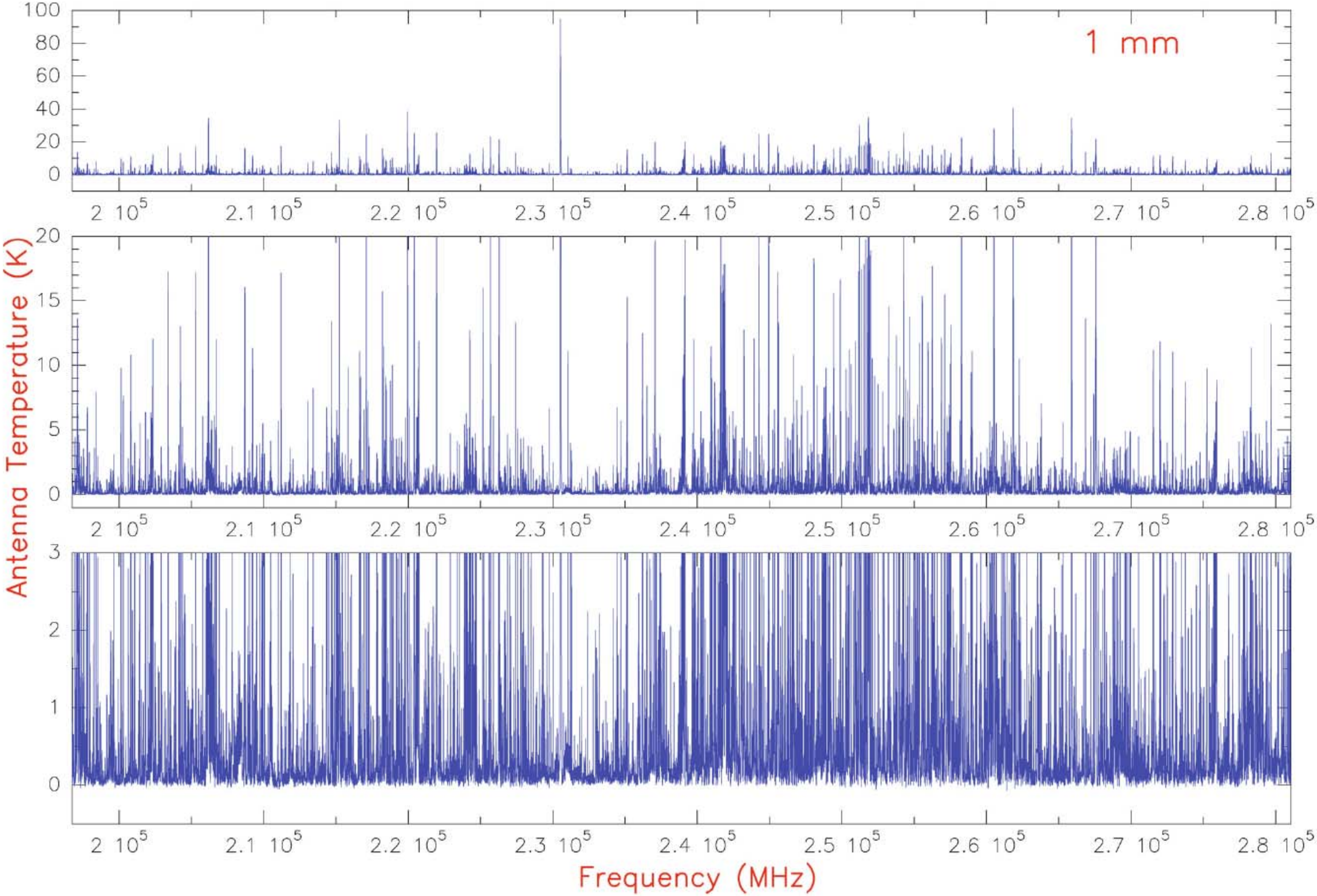
I. Sulfur carbon chains*

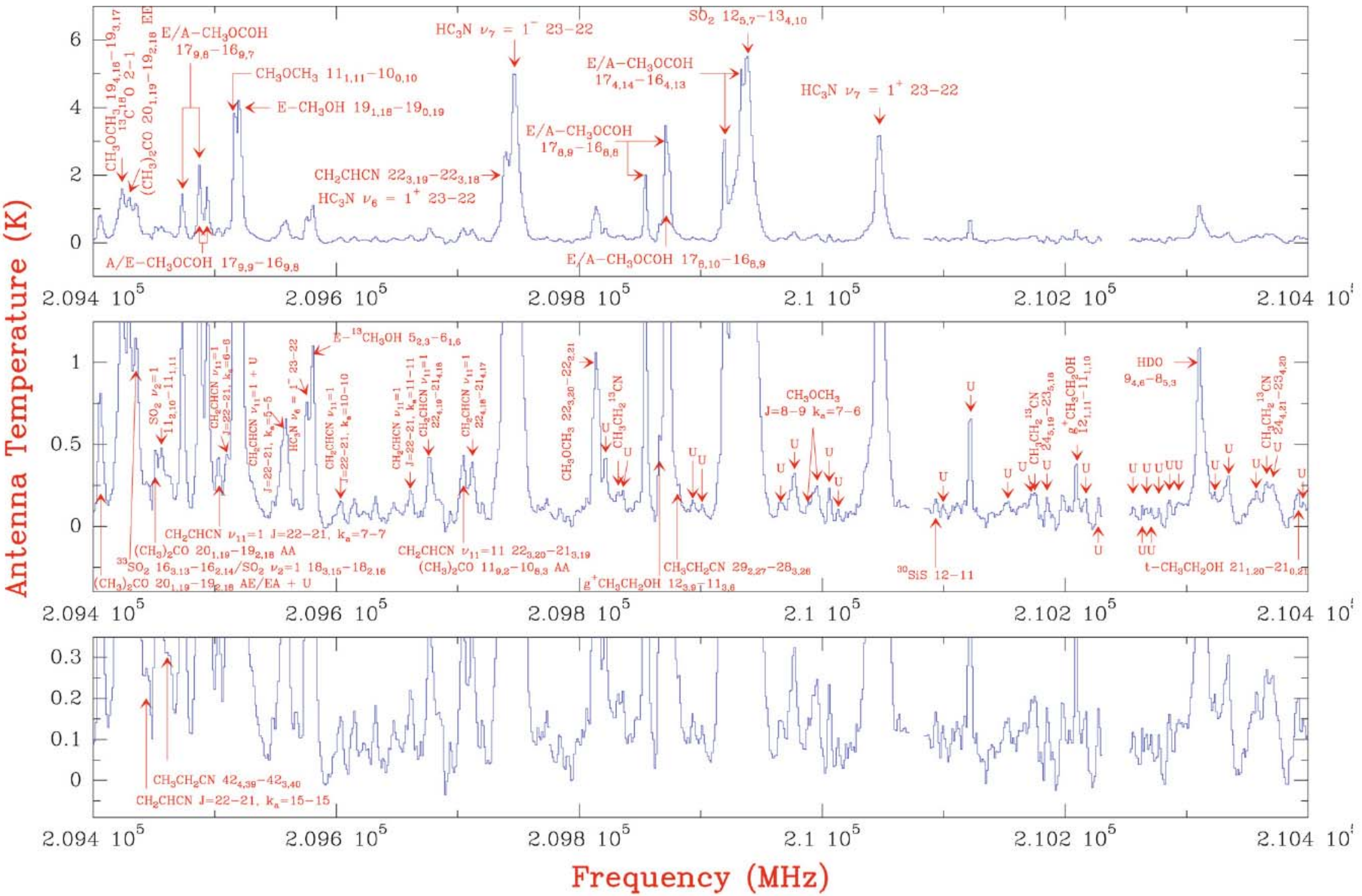
B. Tercero, J. Cernicharo, J. R. Pardo, and J. R. Goicoechea





Antenna Temperature (K)
Frequency (MHz)
OCS 9–8
CH_3CH_2CN $12_{1,11}-11_{1,10}$
SO_2 $17_{5,13}-18_{4,14}$
NH_2CHO $5_{1,4}-4_{1,3}$
HNCO $5_{0,5}-4_{0,4}$
^{13}CO 1–0
CH_3CN 6_1-5_1
CH_3CN 6_0-5_0
CH_3CN 6_2-5_2
CH_3CN 6_3-5_3
CH_3CN 6_4-5_4
CH_3CN 6_5-5_5
$CH_3{}^{13}CN$ 6_0-5_0 / 6_1-5_1
HC_3N $\nu_7=1^-$ 12–11
HNCO $5_{1,5}-4_{1,4}$
$H_{55}\gamma$
CH_3OCH_3 $8_{2,7}-8_{1,8}$
HC_3N $\nu_7=1^+$ 12–11
$SO^{18}O$ $11_{1,10}-11_{0,11}$
E–CH_3OD $2_{-1}-1_0$
CH_3CH_2CN inp tor
OCS $\nu_2=1^+$ 9–8
CH_3CH_2CN outp
HNCO J=5–4 K_a=4
$C^{18}O$ 1–0
$^{33}SO_2$ $16_{2,14}-15_{3,13}$
HNCO J=5–4 K_a=3
CH_3CH_2CN inp tor
HC_3N $\nu_7=2$ 12–11
HNCO J=5–4 K_a=2
CH_3CH_2CN $13_{3,10}-13_{2,11}$
$CH_3CH_2{}^{13}CN$ $13_{1,13}-12_{1,12}$
$(CH_3)_2CO$ $6_{5,2}-4_{5,1}$ EE
c–C_2H_4O $13_{7,6}-13_{6,7}$
E–CH_3OH $23_{-2,22}-23_{2,21}$
CH_2DOH $9_{1,8}-9_{0,9}$
E–$^{13}CH_3OH$ $16_{-2,15}-16_{1,15}$
$(CH_3)_2CO$ $9_{2,7}-8_{3,6}$ AE/EA
NH_2D
$(CH_3)_2CO$ $9_{3,7}-8_{2,6}$ EA/AE
$(CH_3)_2CO$ $9_{2,7}-8_{3,6}$ EE
E/A–CH_3OCOH $10_{0,10}-9_{1,9}$
$(CH_3)_2CO$ $9_{3,7}-8_{2,6}$ AA
E–CH_3OD 9_1-2_0
HNCO $5_{1,4}-4_{1,3}$
$CH_3{}^{13}CN$ 6_3-5_3
$CH_3{}^{13}CN$ 6_2-5_2
U
1.094 10^5
1.096 10^5
1.098 10^5
1.1 10^5
1.102 10^5
1.104 10^5


1 mm
Antenna Temperature (K)
Frequency (MHz)
100
80
60
40
20
0
15
10
5
3
2
1
2 10^5
2.1 10^5
2.2 10^5
2.3 10^5
2.4 10^5
2.5 10^5
2.6 10^5
2.7 10^5
2.8 10^5



LINE CONFUSION LIMIT REACHED. WHAT TO DO ?

ALMA WILL BE 7 times more sensitive than the 30-m telescope !!!

Orion as seen with 30-m IRAM Telescope.
10 min observing time/GHz

Vibrational states
Isotopes
CH_3OCH_3
CH_3CH_2CN
$HCOOCH_3$,….

ALMA will see hundreds of Orions

How to identify new species ?
(Chemical Complexity)

Isotopes for most known species will be more abundant than unknown species !!

New species :
Alcohols, X-CN,
Ethers, (X-O-Y)
Cetones (X-CO-Y)
Isomers, …

A real challenge !!!!

We need to maintain a very fruitful and close collaboration with chemists and physicists
(laboratory and ab initio)

A&A 466, 255–259 (2007)
DOI: 10.1051/0004-6361:20066955

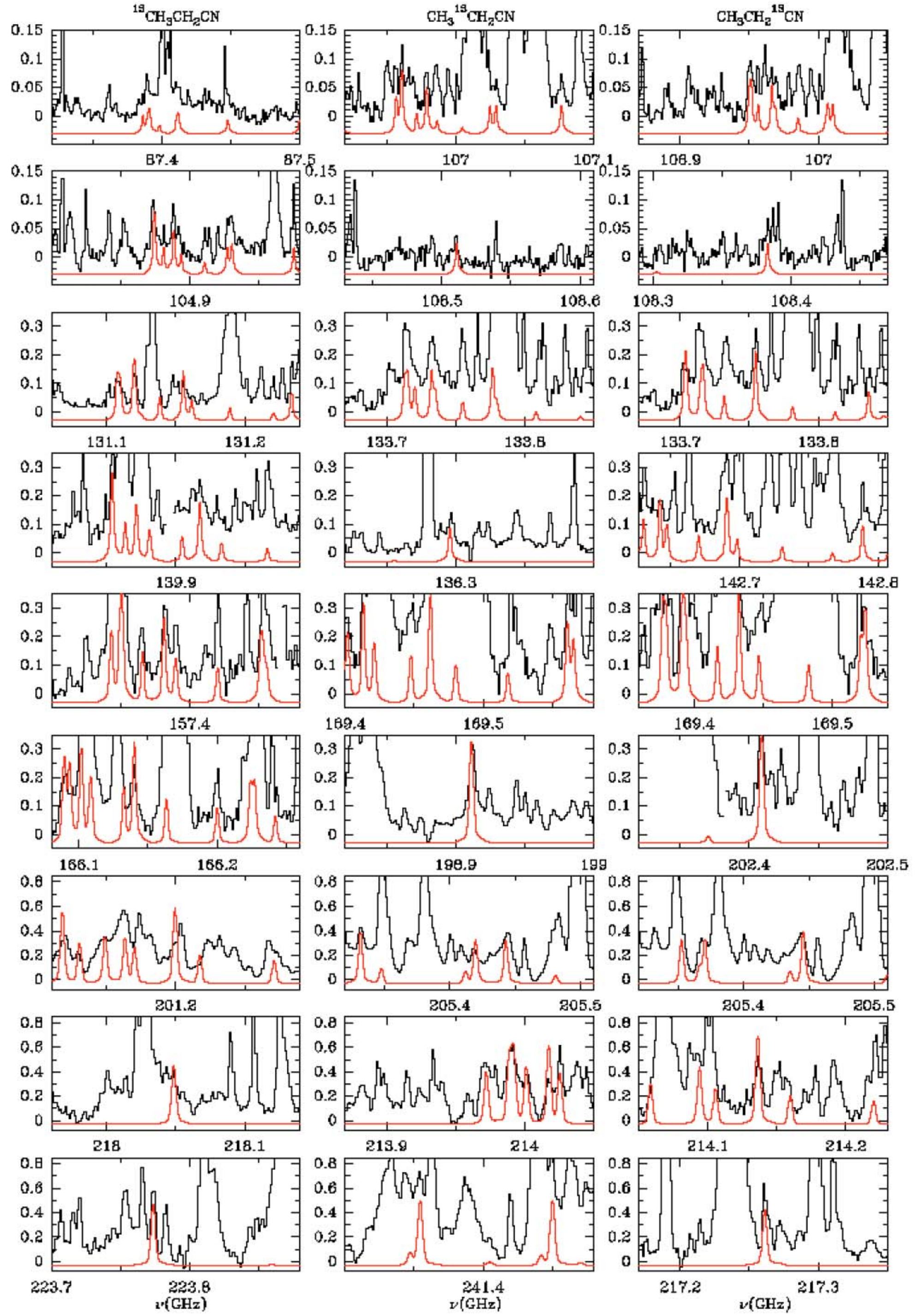
Astronomy & Astrophysics

Isotopic ethyl cyanide $^{13}CH_3CH_2CN$, $CH_3{}^{13}CH_2CN$, and $CH_3CH_2{}^{13}CN$: laboratory rotational spectrum and detection in Orion⋆,⋆⋆

K. Demyk[1], H. Mäder[2], B. Tercero[3], J. Cernicharo[3], J. Demaison[1], L. Margulès[1], M. Wegner[2], S. Keipert[2], and M. Sheng[2]

Table 2. Spectroscopic constants of the ground vibrational state of ^{13}C-CH_3CH_2CN, A-reduction.

	$^{13}CH_3CH_2CN^{(a)}$		$CH_3^{13}CH_2CN^{(b)}$		$CH_3CH_2^{13}CN^{(c)}$	
	Value	Uncertainty	Value	Uncertainty	Value	Uncertainty
A/MHz	27 342.6503	(20)	27 045.8630	(18)	27 635.4303	(19)
B/MHz	4598.06 735	(39)	4697.96 236	(40)	4689.91 341	(31)
C/MHz	4133.74 505	(37)	4207.10 003	(35)	4214.77 921	(29)
Δ_J/kHz	2.99 463	(31)	2.99 599	(45)	3.03 369	(25)
Δ_{JK}/kHz	–48.3778	(23)	–45.0189	(17)	–47.8322	(20)
Δ_K/kHz	546.335	(13)	525.801	(17)	553.930	(45)
δ_J/kHz	0.66 2503	(56)	0.68 4149	(84)	0.67 6665	(36)
δ_K/kHz	12.097	(14)	12.749	(14)	12.5104	(59)
Φ_J/Hz	0.010157	(90)	0.01169	(18)	0.009812	(68)
Φ_{JK}/Hz	–0.06061	(89)	0.03828	(13)	–0.0852	(35)
Φ_{KJ}/Hz	–1.7894	(28)	–1.827	(39)	–1.637	(12)
Φ_K/Hz	30.558	(44)	27.880	(64)	29.95	(30)
ϕ_J/Hz	0.003662	(18)	0.003886	(52)	0.003647	(17)
ϕ_{JK}/Hz	0.0798	(83)	0.143	(10)	0.1329	(36)
ϕ_K/Hz	4.7551	(fixed)	4.7551	(fixed)	2.77	(23)



More than 800 lines from the isotopes of CH_3CH_2CN

Around 600 lines from the vibrational excited states of ethyl cyanide

More than 400 lines from those of CH_3OCOH

Around 800-1000 lines identified every 2 years in Orion. All lines above confusion limit could be identified around 2020 !!!

Belen started her PhD based on this line survey in 2006.

When combined with HEXOS data=> Work for a long period (several Nigel's units)

ALMA ?

Astrochemistry : the problem of collisional rates

Getting physical and chemical conditions from data requires a detailed study of the radiative transfer through the observed source.

Only a few molecules (see, e.g., BASECOL) have been studied in detail and in most cases in collisions with He.

When collisional rates are not available astronomers do a lot of poor assumptions : This molecule is isoelectronic to this one, then let us use the same collisional rates !!

For example HNC and HCN. A rather simple case but HNC/HCN>1 in cold dark clouds. Chemical models have problems to explain this result. However,…

Detailed comparisons between species are only possible if collisional rates are available for both species

Even for an isotopologue and its mother molecule the rates can be very different (H_2O and HDO; CH_3OH, CH_2DOH and CH_3OD,…)

Source structure and isotopic shifts in the frequencies of vibrational and electronic transitions can affect the excitation of the molecule and even its chemistry (UV selfshielding).

The calculation of a the collisional rates for a complex molecule can take a long time, even with the faster and cheaper computers we have nowadays

We rely 100% on chemical-physics groups accepting to do the job in close collaboration with astronomers.

(When quoting databases, please, quote also the sources !!)