Astrochemistry under high UV fields

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What is the limit for chemical complexity in the Insterstellar and Circumstellar media ?

Gas phase chemistry : Ion –Neutral, Neutral-Neutral,
radical-neutral. Radical-radical

Dust surface Chemistry :
Too many unknown parameters but per
to explain the formation of some comple
organic molecules (COMs)!!

TOPICS around CHEMICAL COMPLEXITY

- Dark Clouds (Pure gas-phase chemistry)
- Protostellar cores (Hot corinos)
- Warm Molecular Clouds
- Clouds surrounding O stars
- AGB stars (Thermod. Equilibrium Chemistry +
  UV dominated chemistry)
- Protoplanetary Nebula (UV dominated chemistry)
- Protoplanetary and Planetary disks (Gas, dust, UV, X-rays,…)

How we proceed to study chemistry ?

- Observing molecules (radio, mm, submm, far, mid, near-IR, optical and UV domains)
- Looking for a given molecule if frequencies are known
- Unbiased lines surveys
- Chemical complexity limited by line confusion limit in some cases
- Lack of accurate frequencies for most potential candidates
- Chemistry is biased towards high polar molecules : very little information for symmetrical species (IR, optical and UV can provide a new view for chemistry : carbon clusters (C_n), polyacetylenic chains (HC_nH), other hydrocarbons,…)

DARK CLOUDS

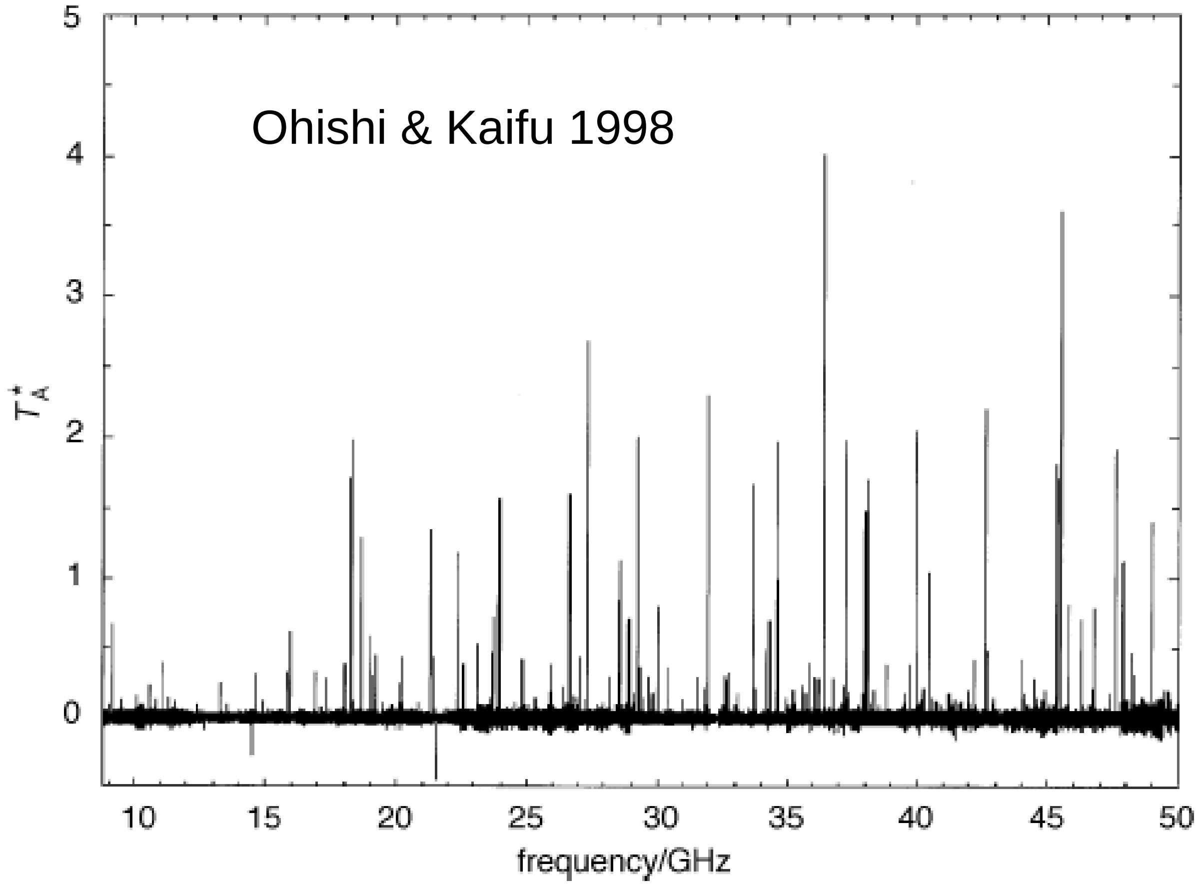


Fig. 1 Compressed spectrum from 8800 to 50 000 MHz toward TMC-1 (T_A^* is the antenna temperature corrected for atmospheric attenuation and ohmic loss of the antenna)

Gas phase chemistry is based on the following steps:

0) H2 formation on dust grains.

1) Ionization of H_2 and He by cosmic rays (no UV field)

2) $H_2^+ + H_2 \rightarrow H_3^+ + H$

3) Charge exchange between He^+ and all species

4) Reactions of H_3^+ with atoms and molecules

5) Molecular growth through reactions of molecular ions + Molecular Hydrogen ➔ larger molecular ion

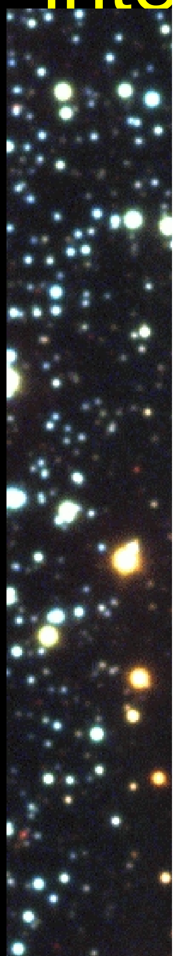
6) Dissociative electronic recombinatio

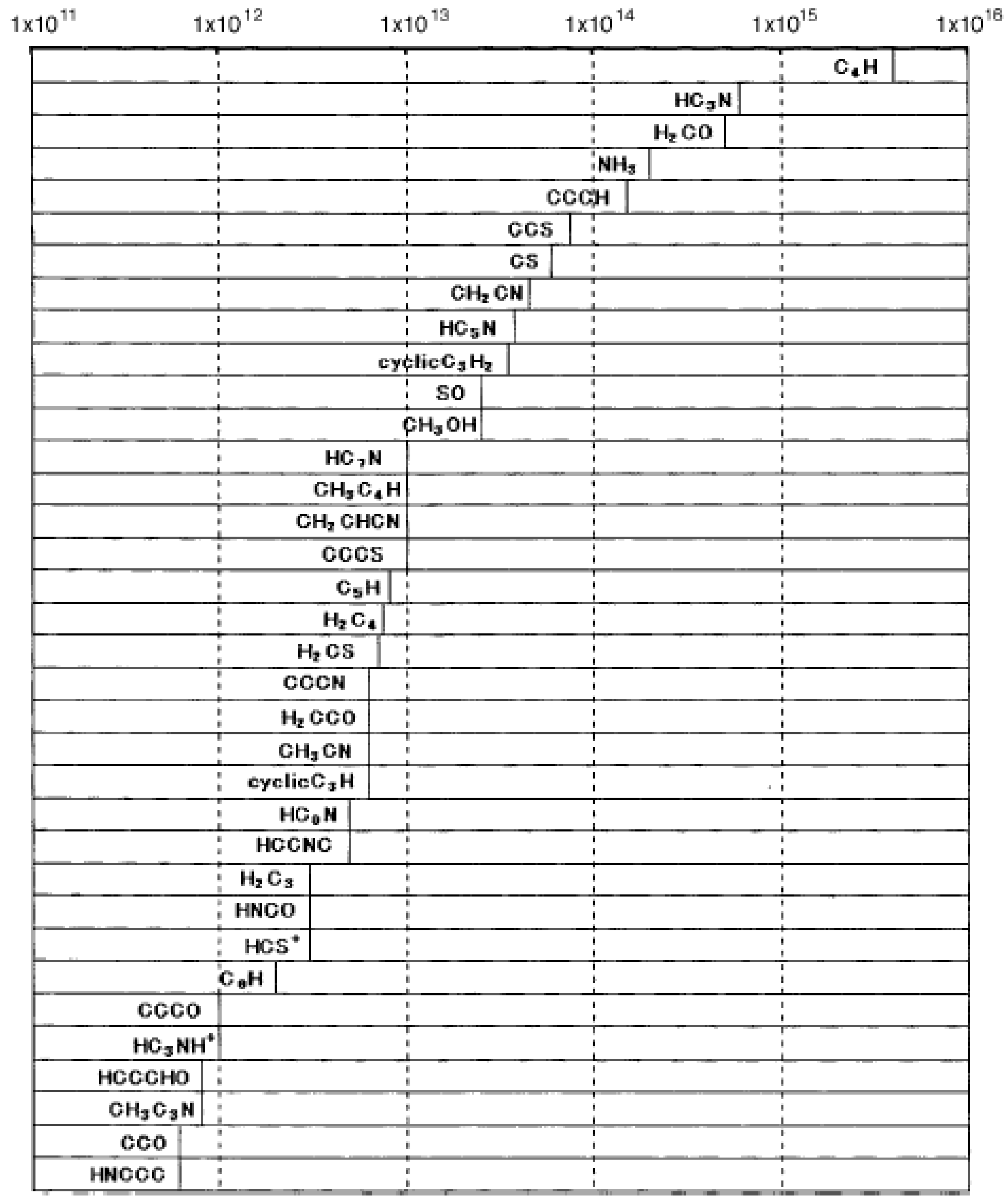
$$A^+ + e^- \rightarrow B + C$$

7) PHOTODISSOCIATION (UV)

8) Neutral-neutral reactions (high T_K)

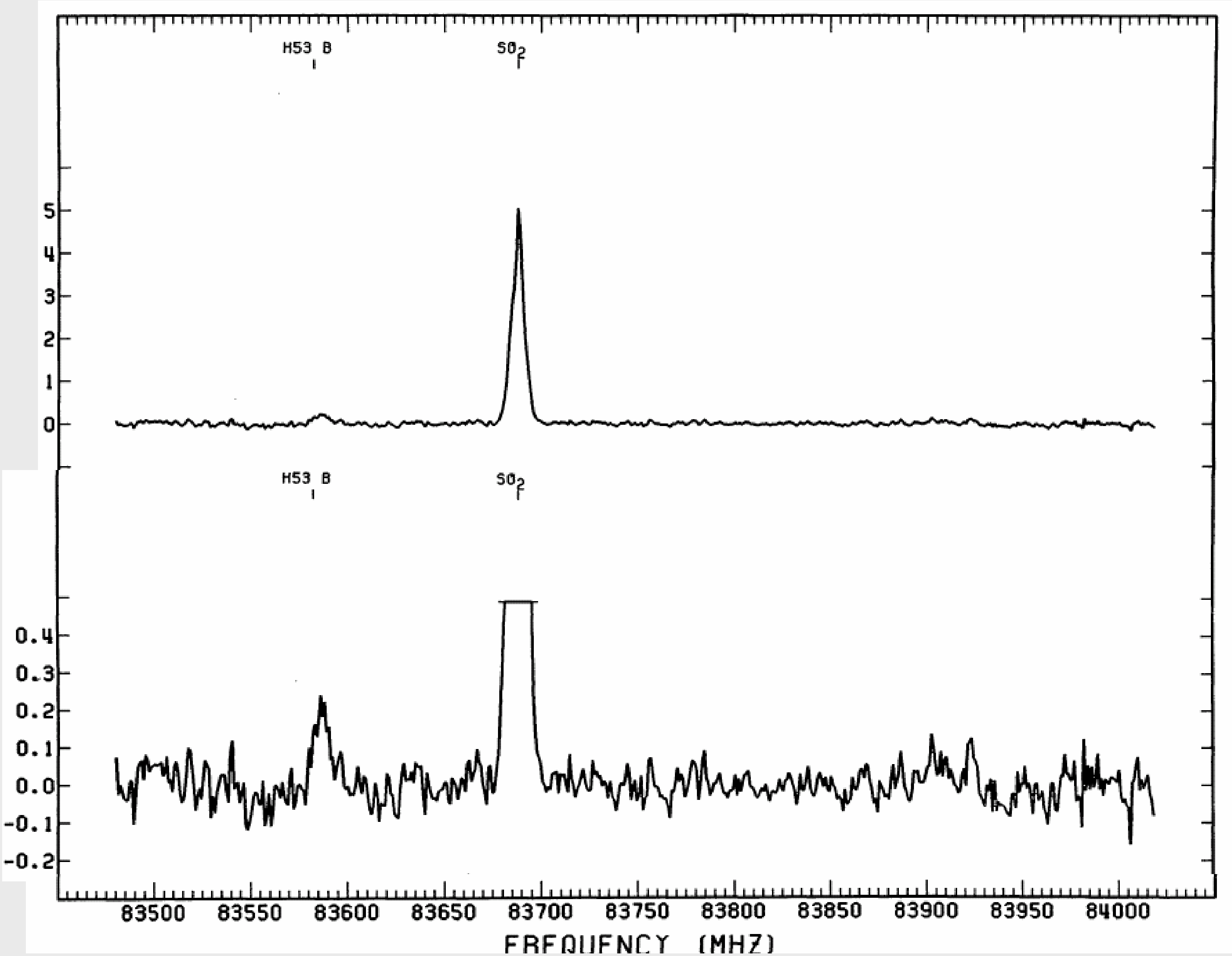
in ... sual
abs ... ects
the ... UV
inte





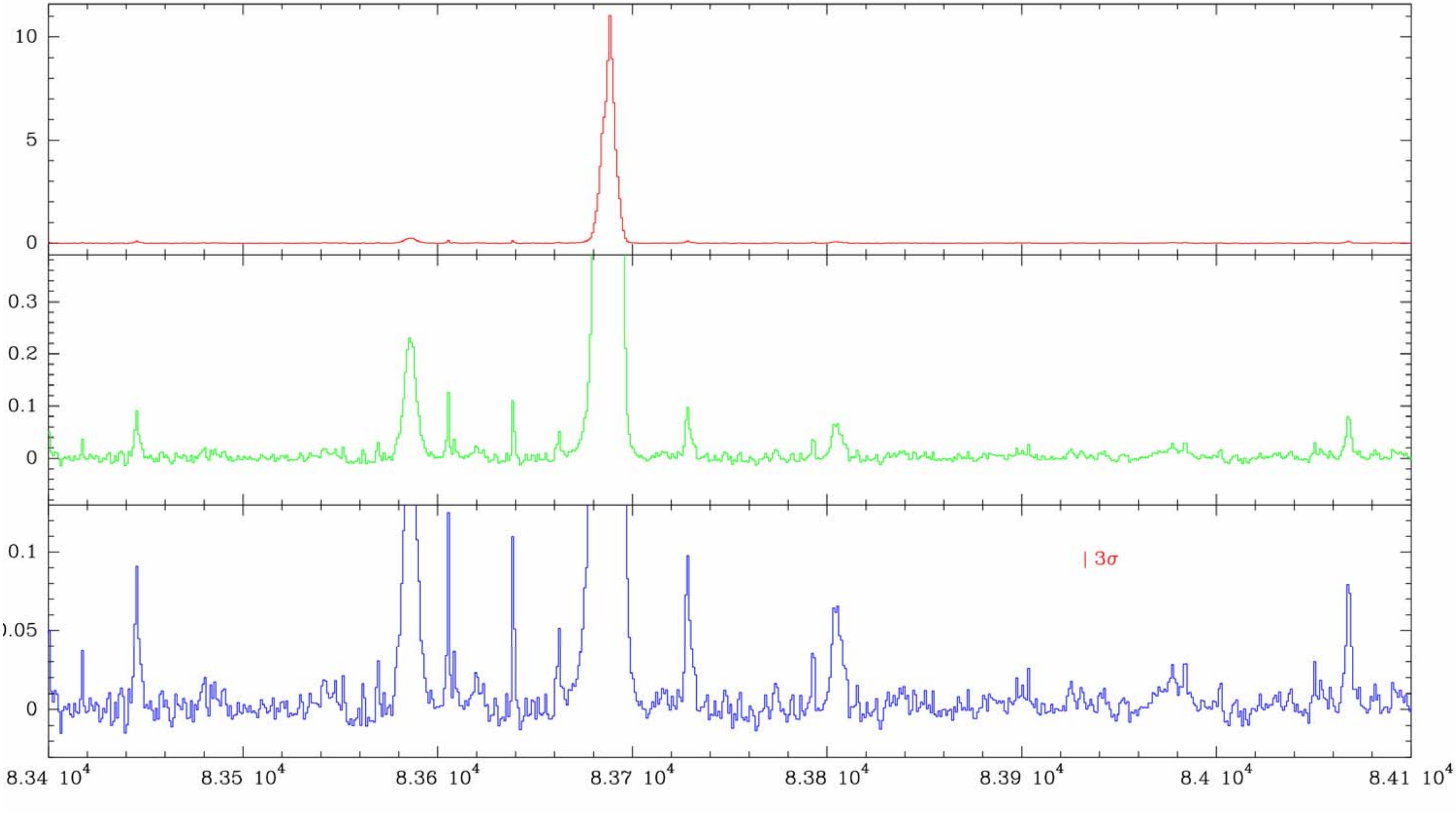
Warm Molecular Clouds

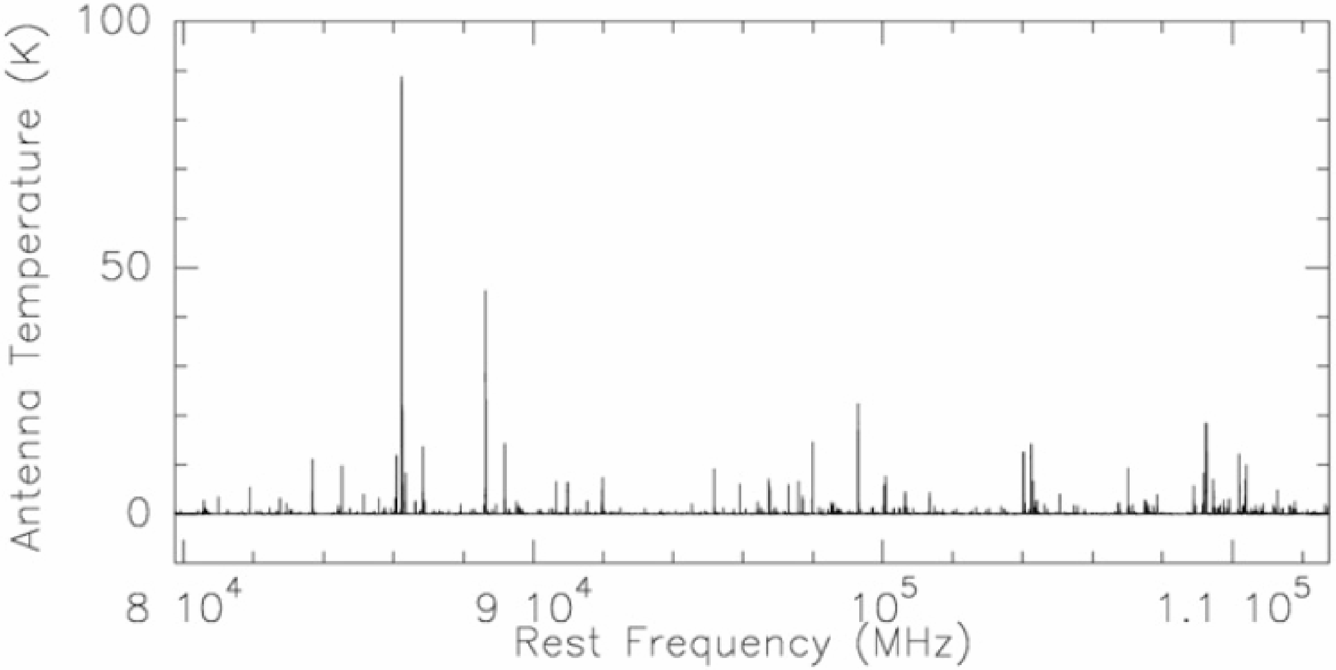
- The role of dust
- The line confusion limit
- Complex organic molecules
- How all these species are formed ?
- How big molecules can be under extreme conditions
- Increasing sensitivity or opening new windows of the electromagnetic spectrum : more complexity and unexpected results
- Two examples : Orion and the Trifid



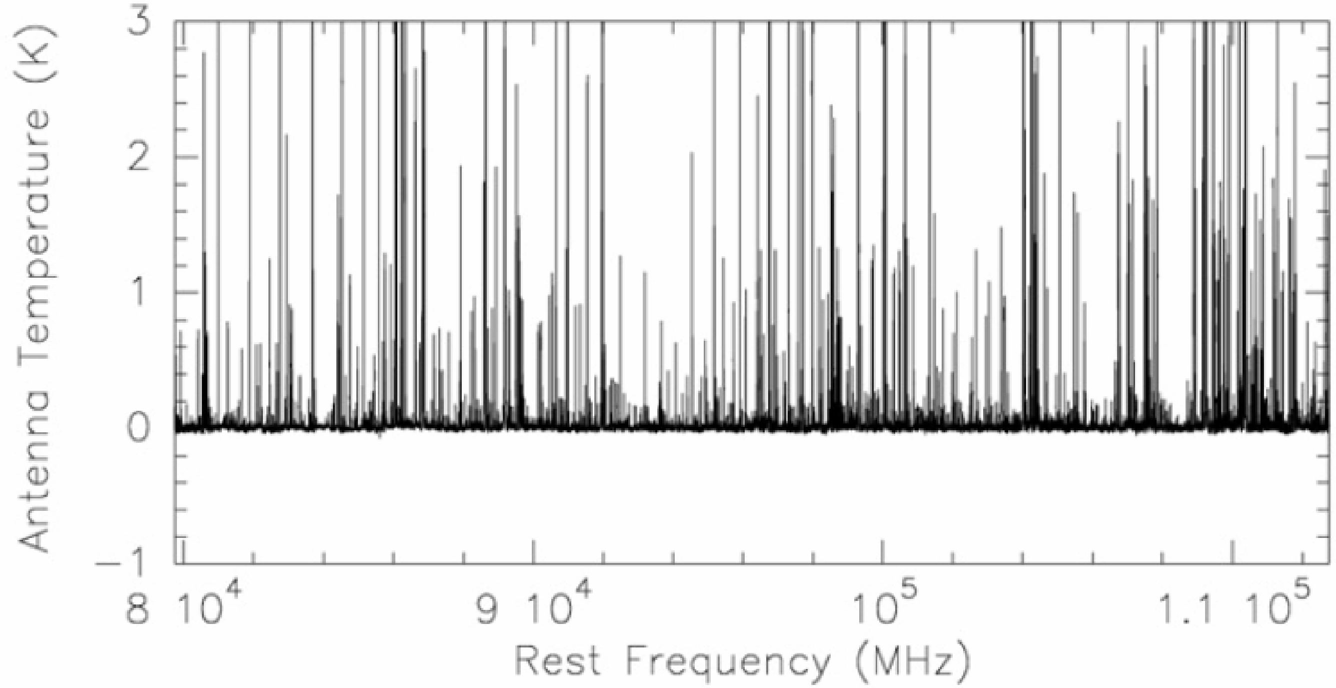
Onsala line survey of Orion. State of the art in the 8
Chemistry evolves with telescope sensitivities !!!

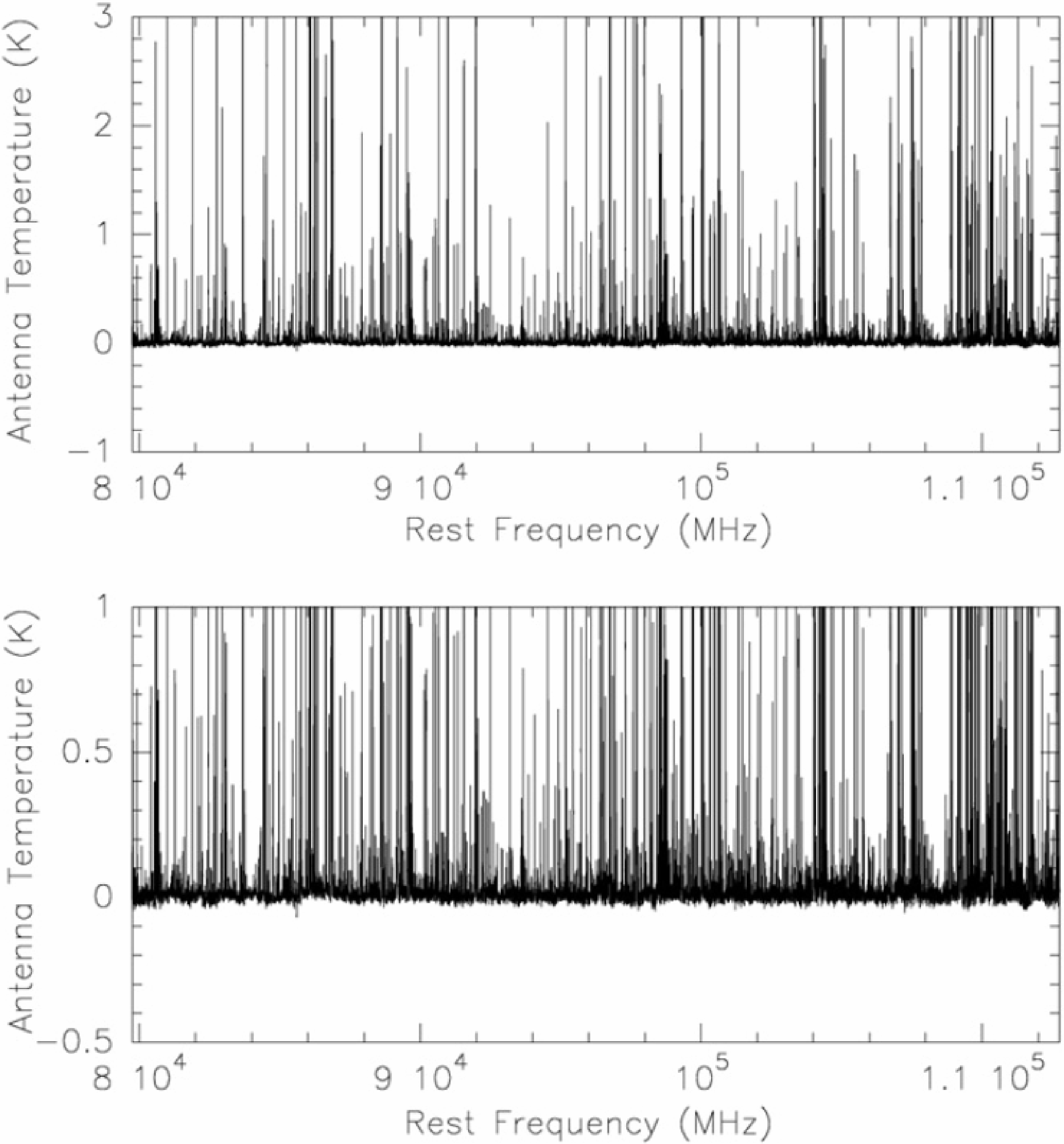
IRAM 30m spectrum; 40 min integration; Tsys=



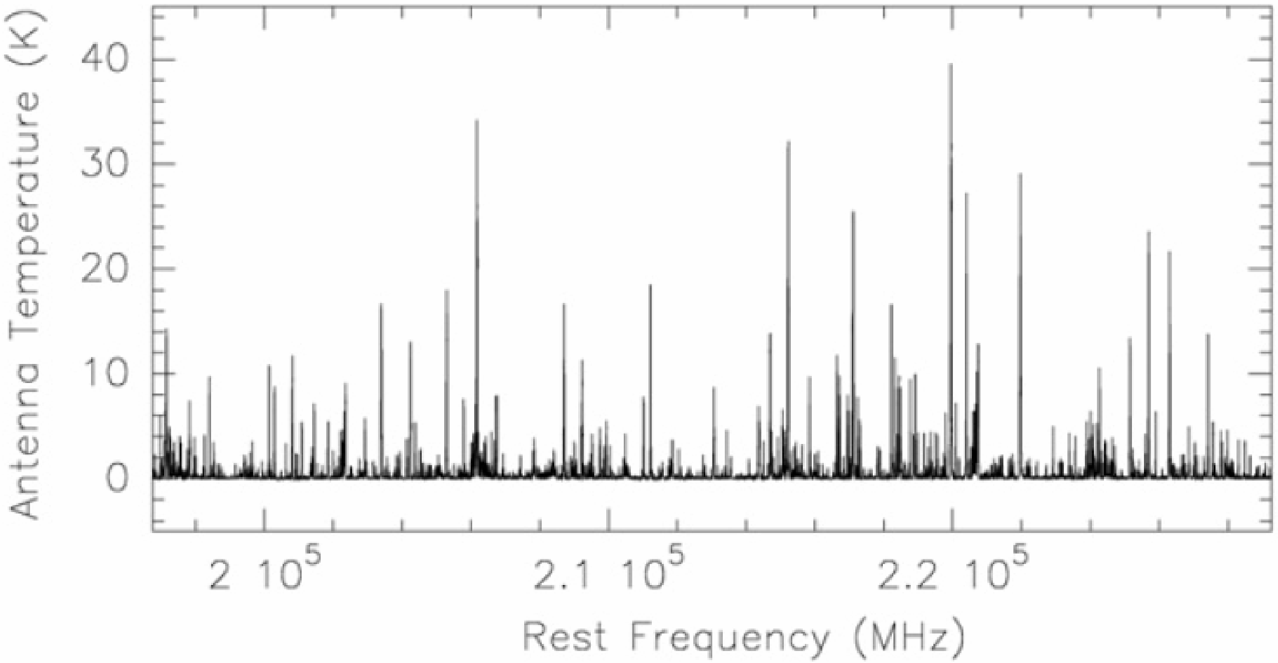


Belen Tercero, PhD, DAMIR





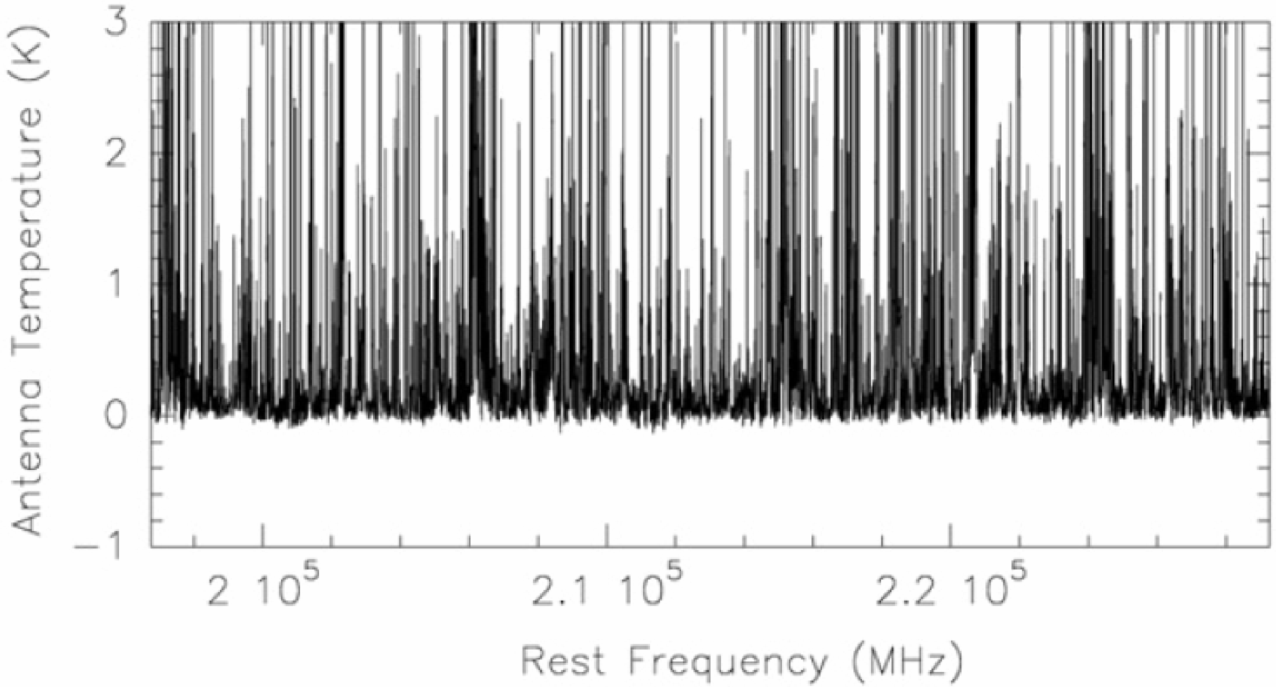
Antenna Temperature (K)
3
2
1
0
−1
8 10^4
9 10^4
10^5
1.1 10^5
Rest Frequency (MHz)
Antenna Temperature (K)
1
0.5
0
−0.5
8 10^4
9 10^4
10^5
1.1 10^5
Rest Frequency (MHz)

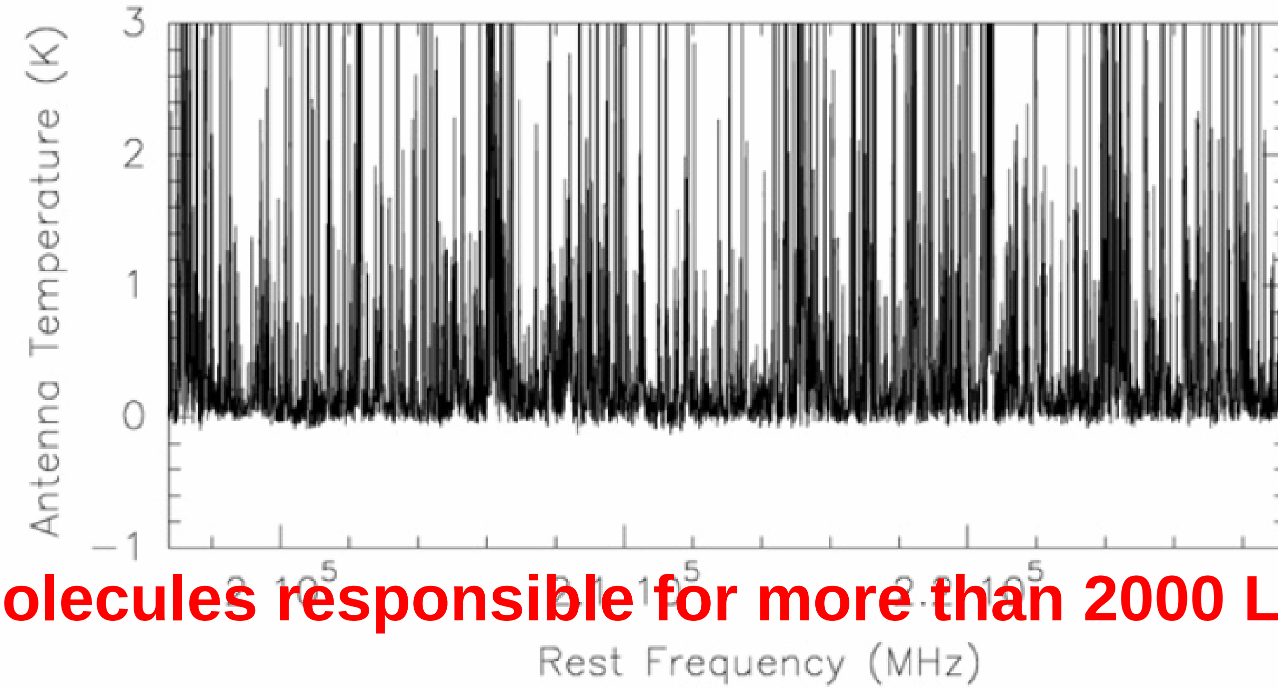


Orion as seen with the 30-m IRAM Telescope.
10 min observing time/GHz

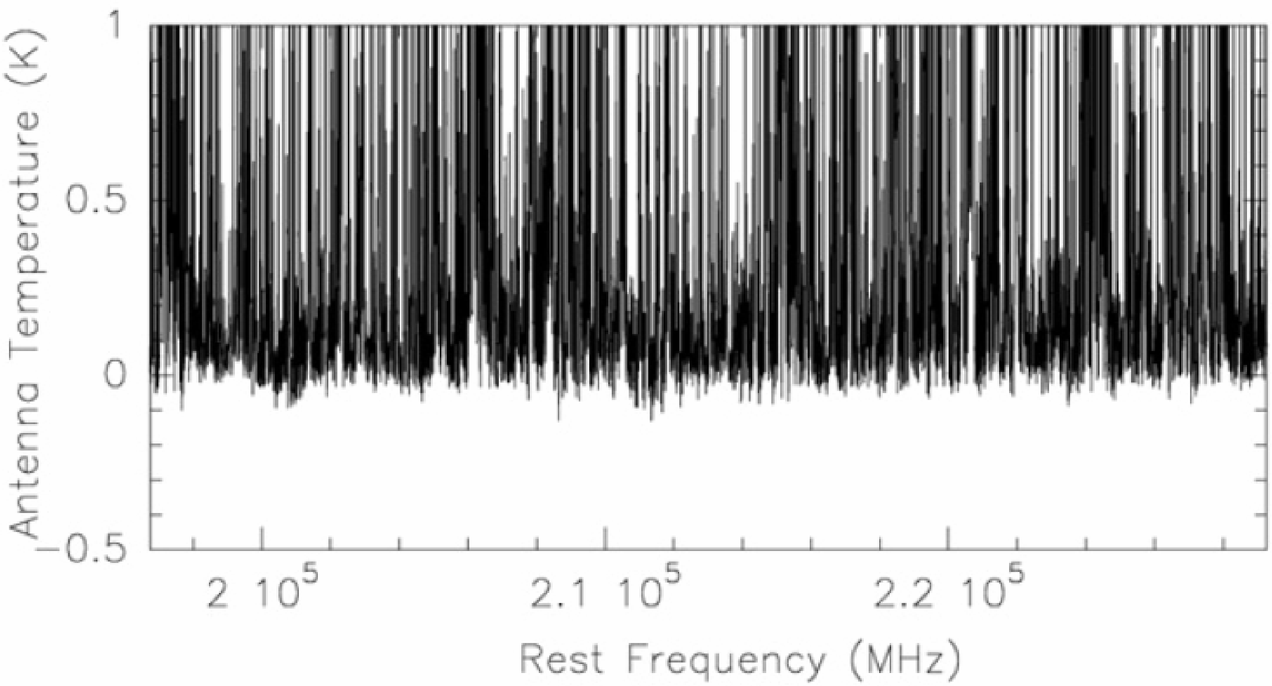
35 hours observing time

B. Tercero & Cernicharo



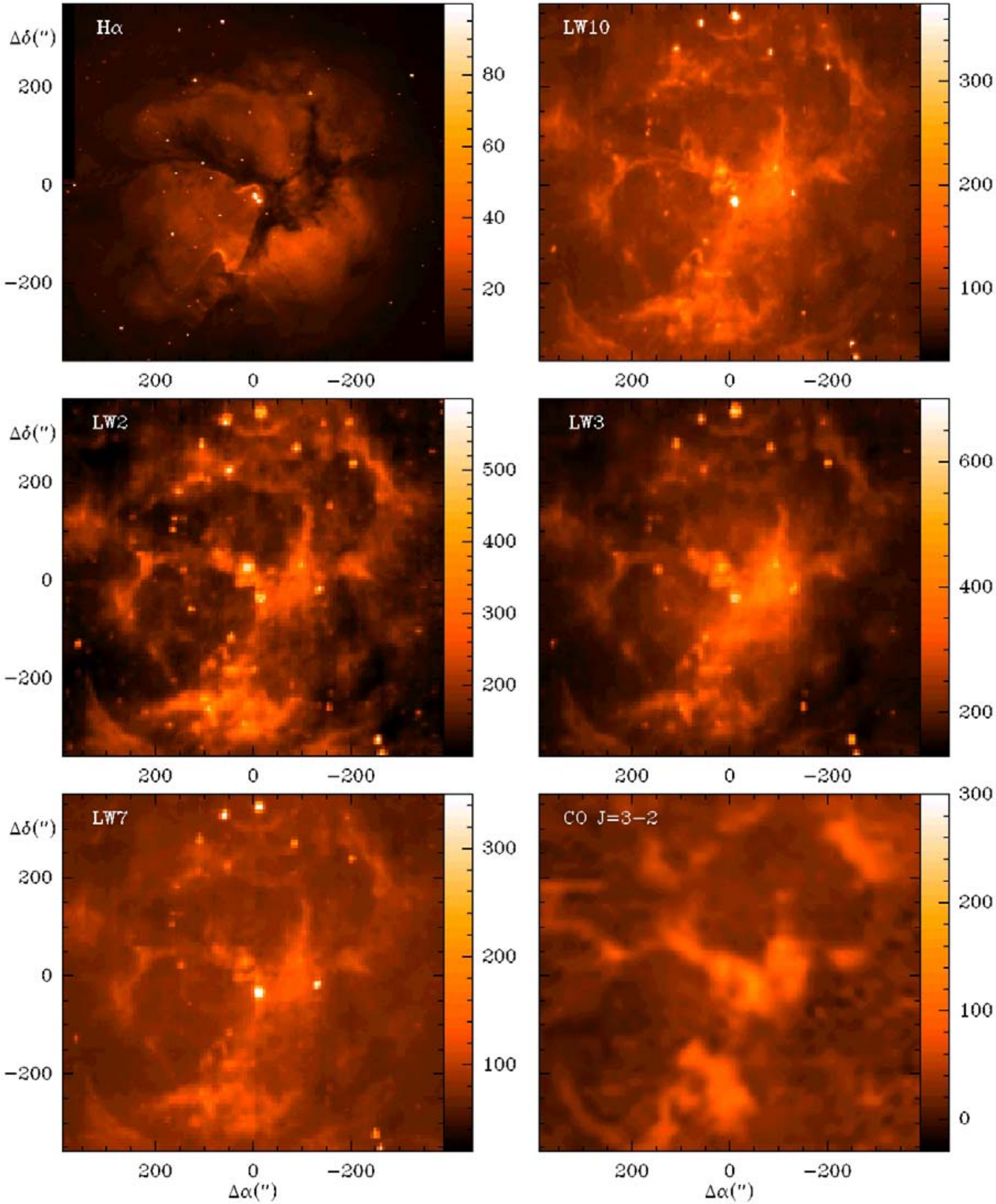


Some Molecules responsible for more than 2000 LINES !!!!!



How complex these molecules are ?

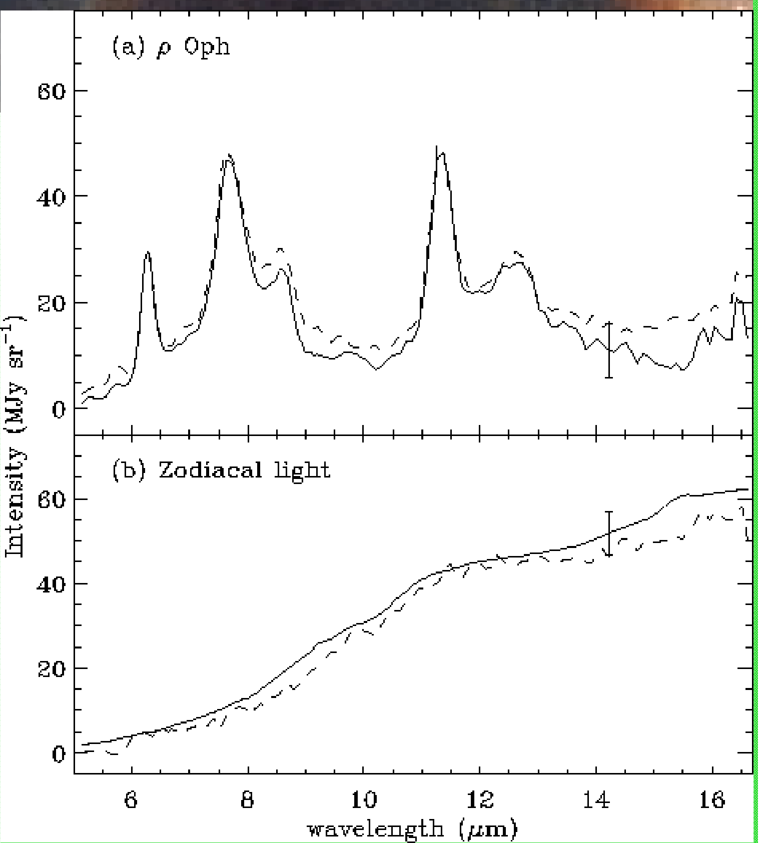
- All molecules typical of interstellar clouds are present in warm molecular clouds
- CH_3OH, CH_3CH_2OH, CH_2CHCN, CH_3CH_2CN, CH_3OCOH, CH_3OCH_3, CH_3COCH_3, $OHCH_2CH_2OH$,….
- Hot CORINOS show the same molecules (much weaker lines)
- Some of these molecules are also detected in cold dark clouds (HCOOH, HCO,…) but their abundances are much lower than in warm molecular clouds.
- Dust surface chemistry. Evaporation of ice mantles.
- PAHs ? YES at the cloud surface. Detected in regions exposed to strong UV fields

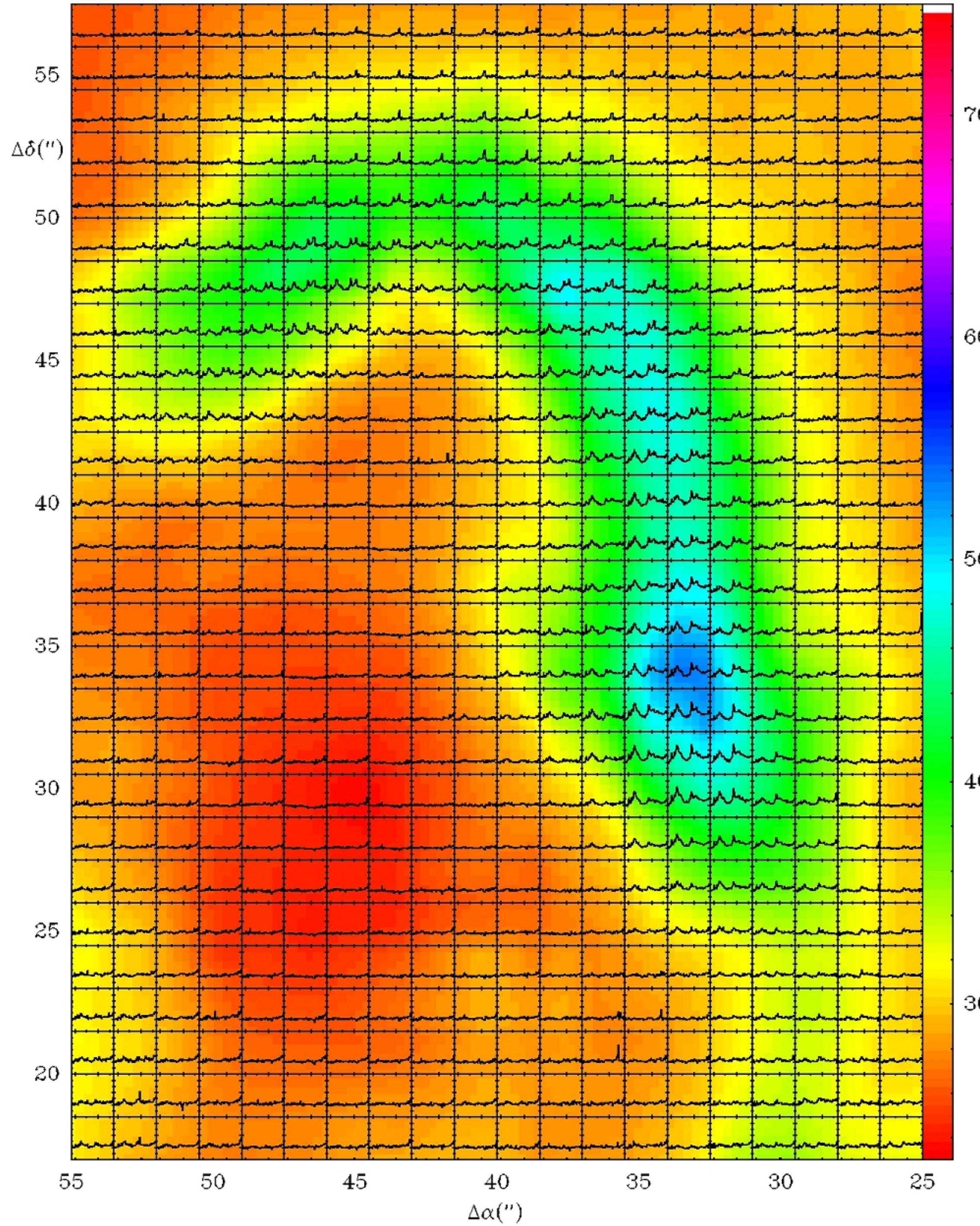


The Trifid Nebula in the visible (upper left) and in the mid-infrared as observed by ISO. The central object is a bright O7 star.

The molecular gas is shown in the bottom right panel (CO J=3-2 emission as observed with the CSO).

Cernicharo et al. 1998,Science 282, 462


(a) ρ Oph
(b) Zodiacal light
Intensity (MJy sr^{-1})
wavelength (μm)
0
20
40
60
6
8
10
12
14
16


Δδ('')
Δα('')
55
50
45
40
35
30
25
20
70
60
50
40
30

Evolved stars : The space factories of complex organic molecules

During the red giant or super-giant phase most stars produce an enormous amount of dust grains and gas phase molecules.

These objects are characterized by a low photospheric temperature surrounded by an envelope of cold dust and gas. These circumste-llar envelopes extend over 10^3-10^4 stellar radii.

The physical conditions of circumstellar envelopes are very different from those of the interstellar medium.

Molecules are formed inside the circunstellar envelope and outside, in a shell were UV photons start to penetrate the envelope and photodissociate CO, C_2H_2, HCN.…

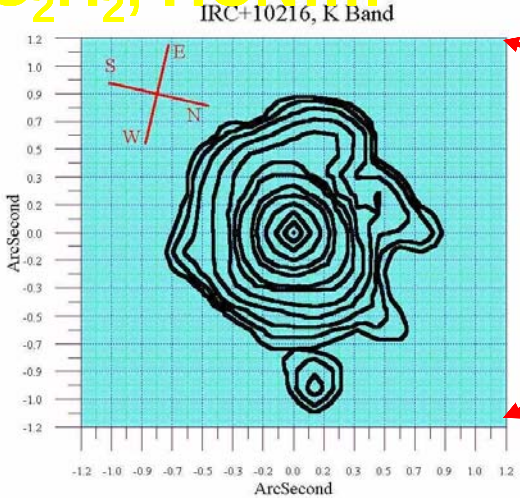
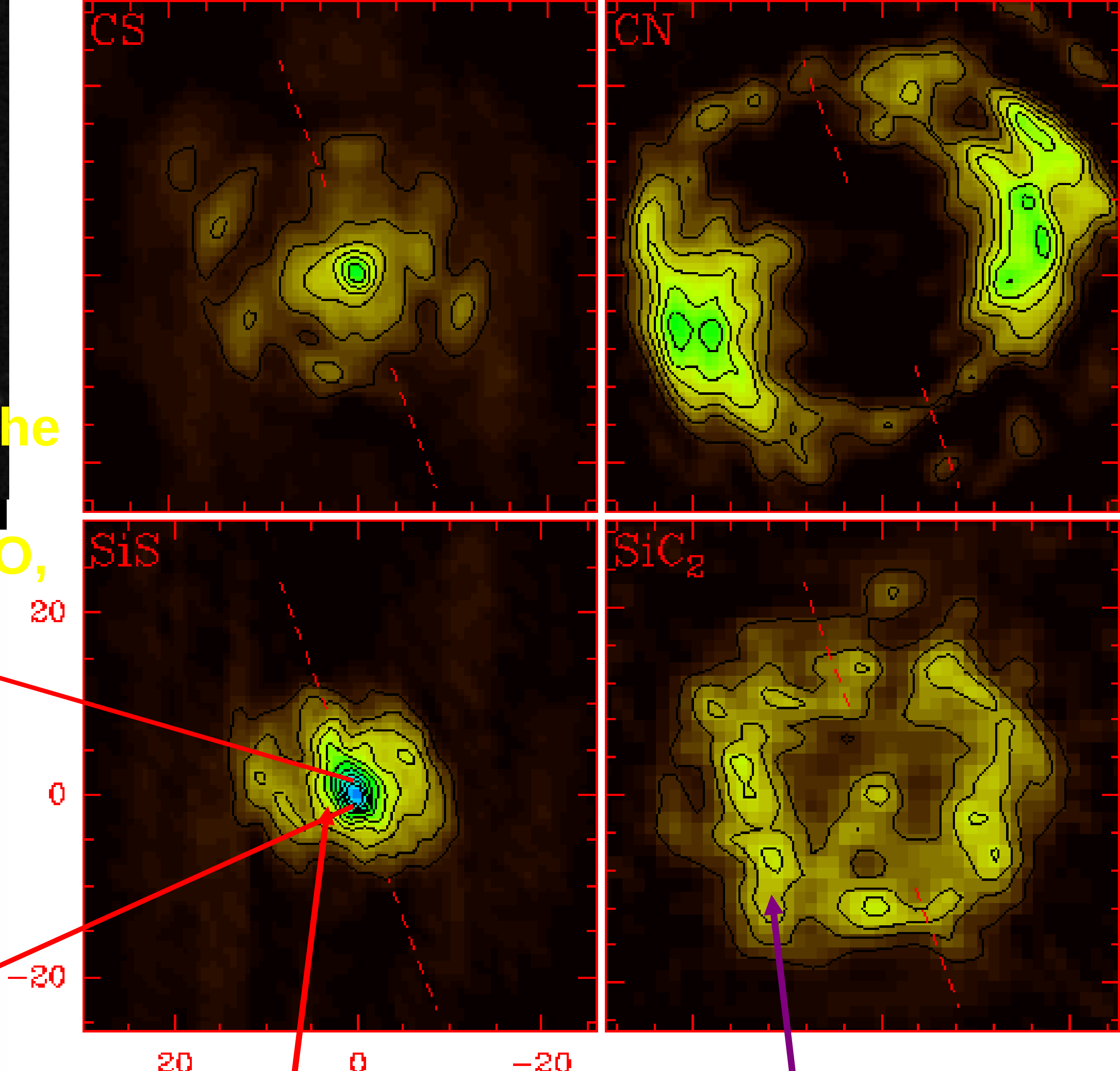


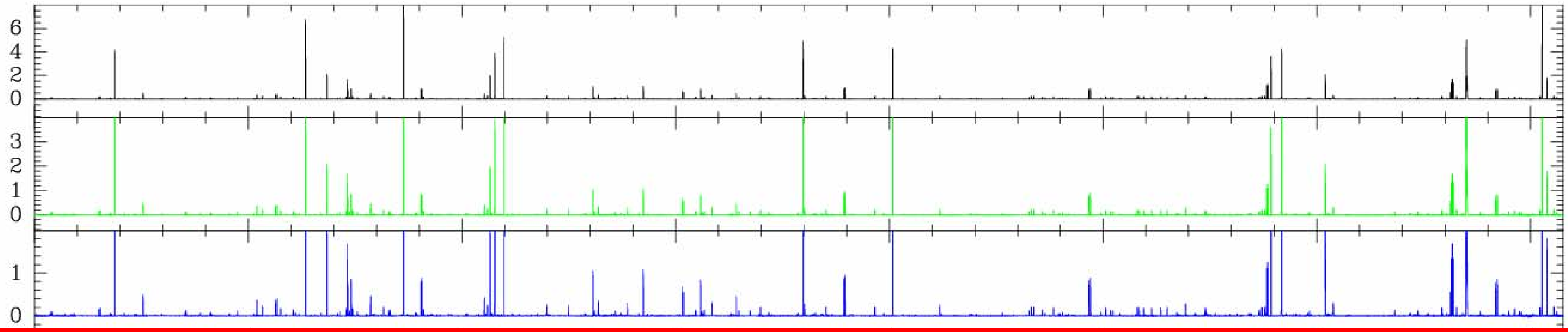
Figure 3: Contour plot of the carbon rich star IRC+10216.



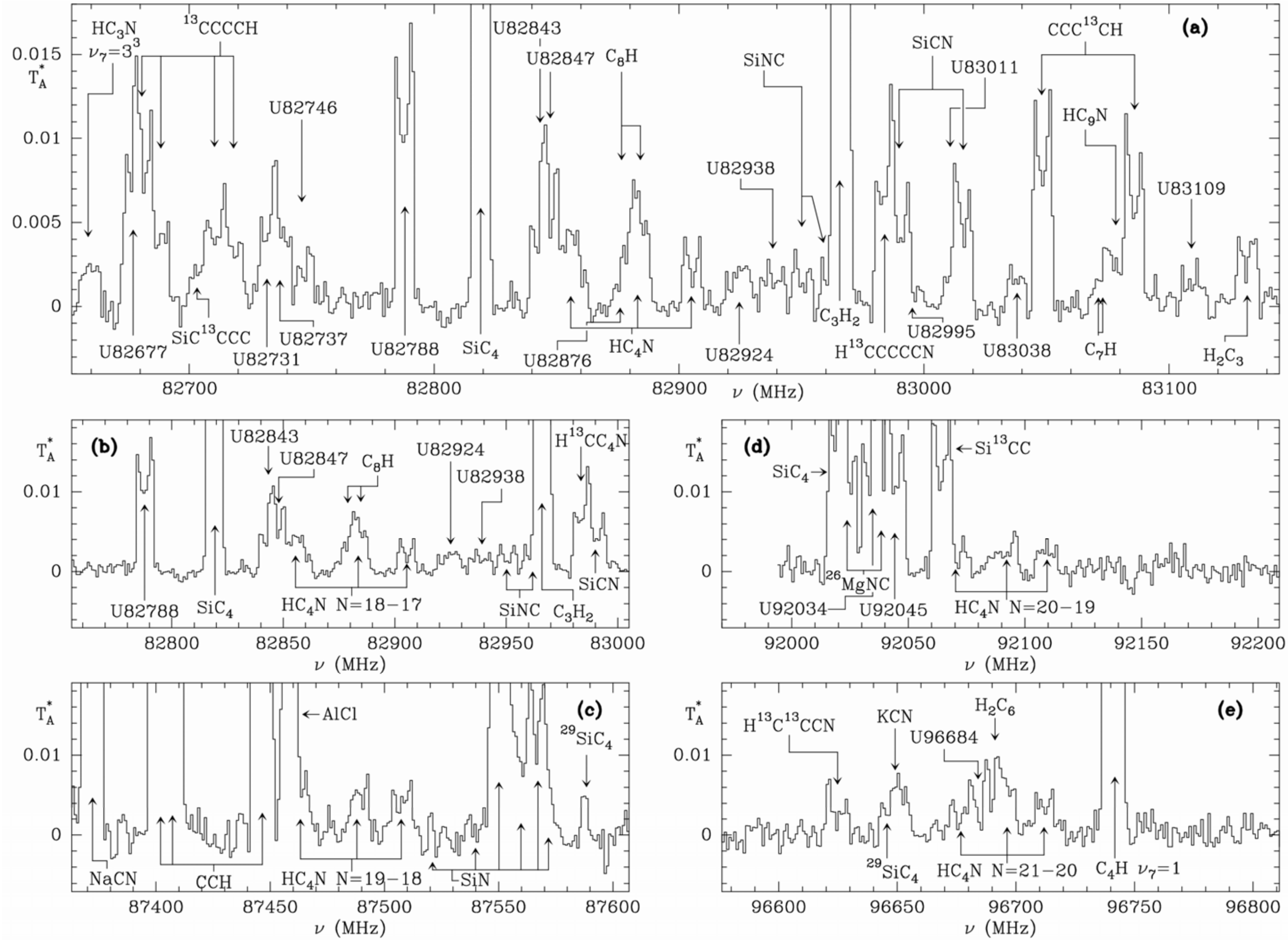
Therm. Equil. Chemistry

UV dominated chemistry

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

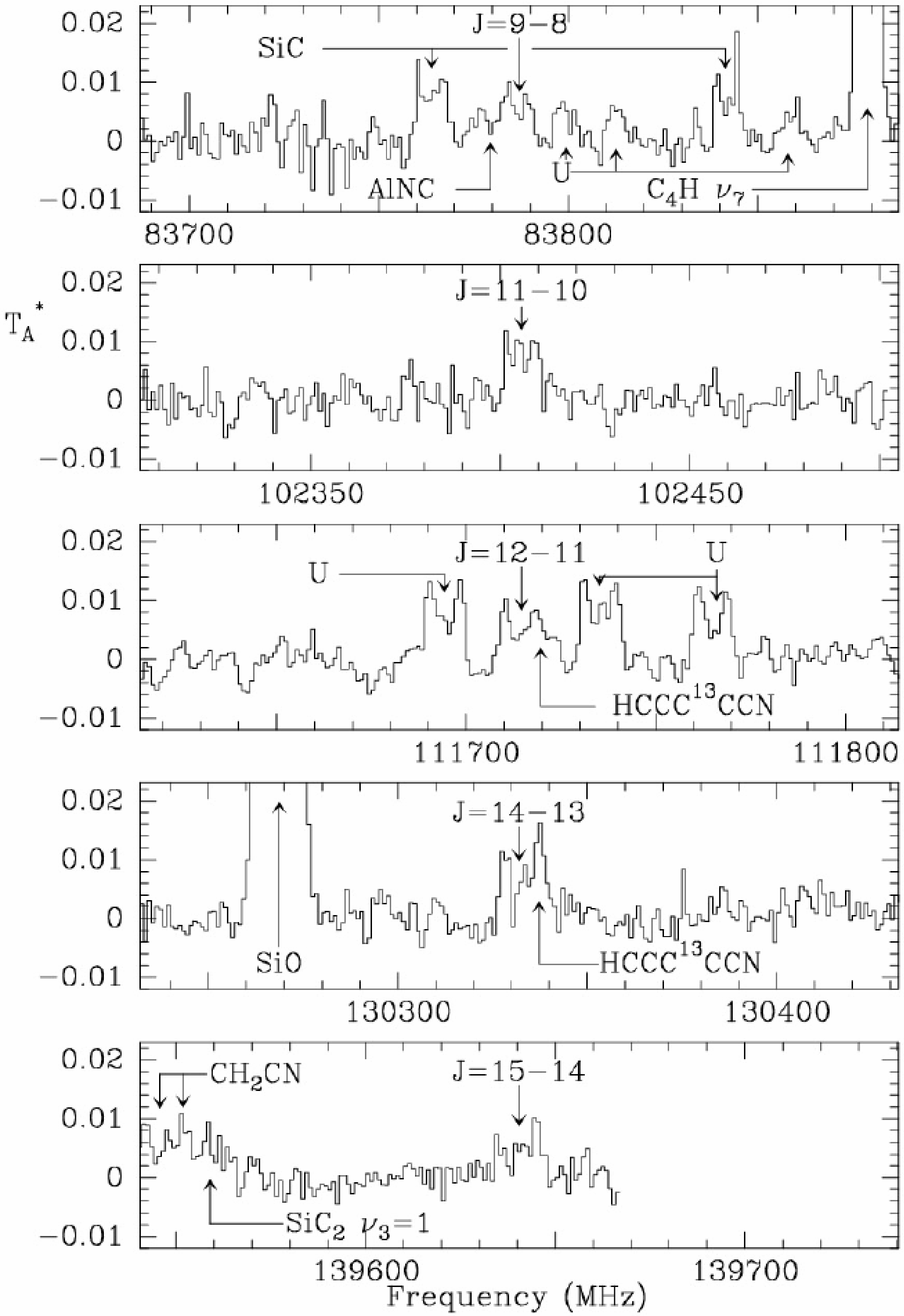


What we could expect from line surveys ?
Why we want to carry out ine surveys ?
What we need to interpret ALMA & Herschel line surveys ?

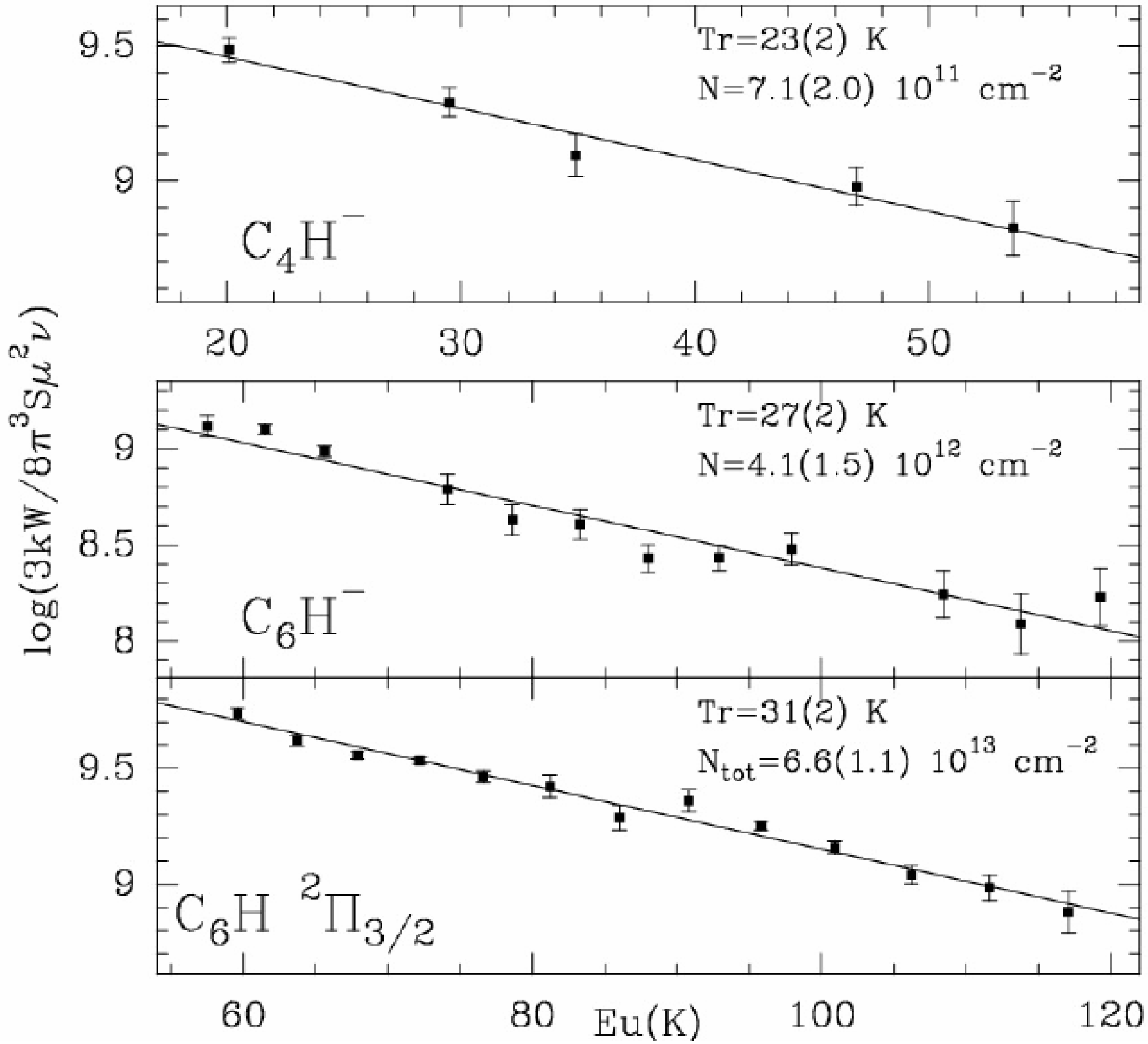


22/05/2008 10:35

HC_4N :: Cernicharo et al., 2004, ApJLetters   SiNC: Guélin et al., 2004, A&A



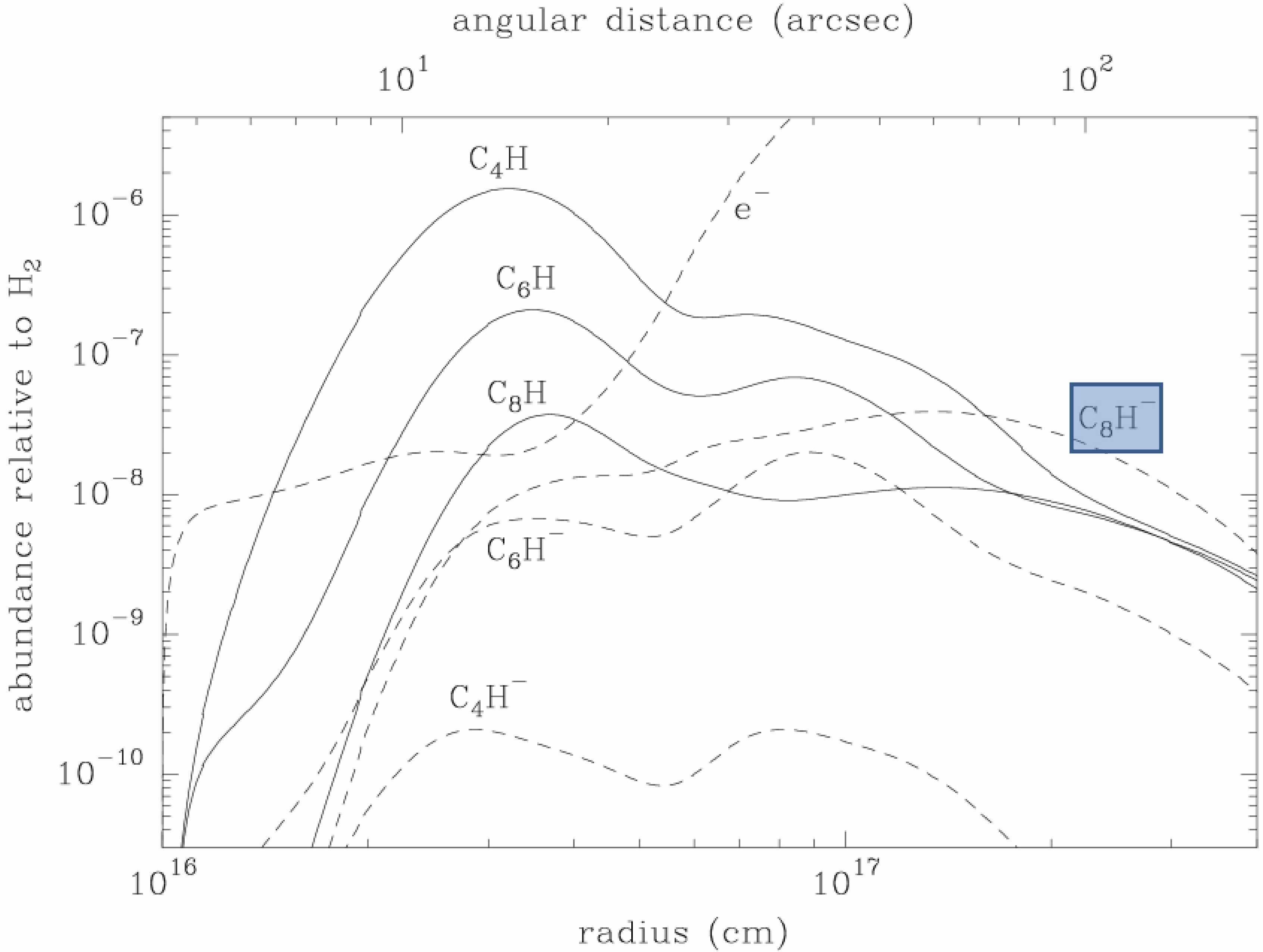
Detection of C_4H^-
Cernicharo et al., 2007
Astronomy & Astrophysics



$C_4H/C_4H^- = 5000$

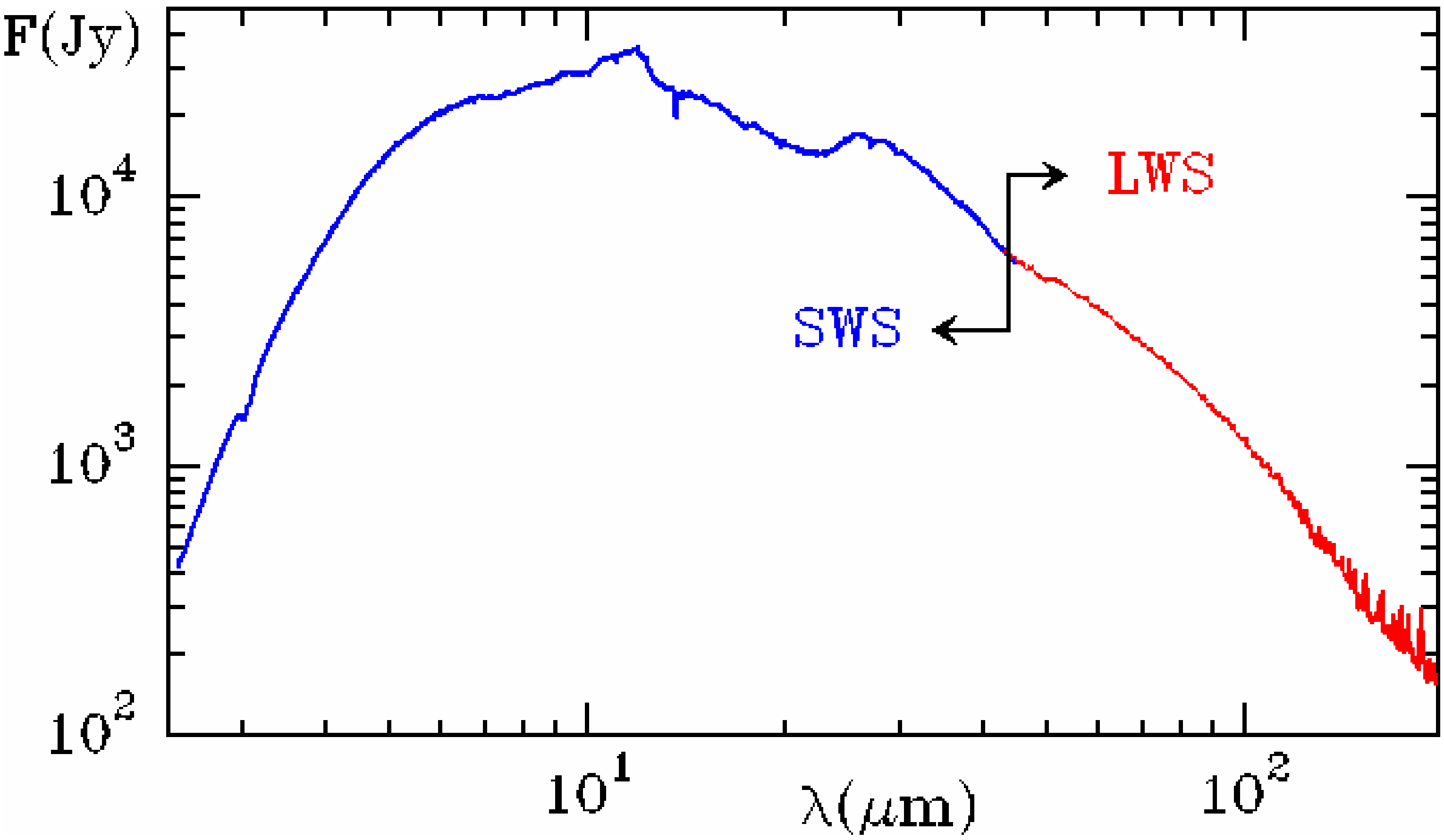
$C_6H/C_6H^- = 16$

$C_8H/C_8H^- \approx 1$?

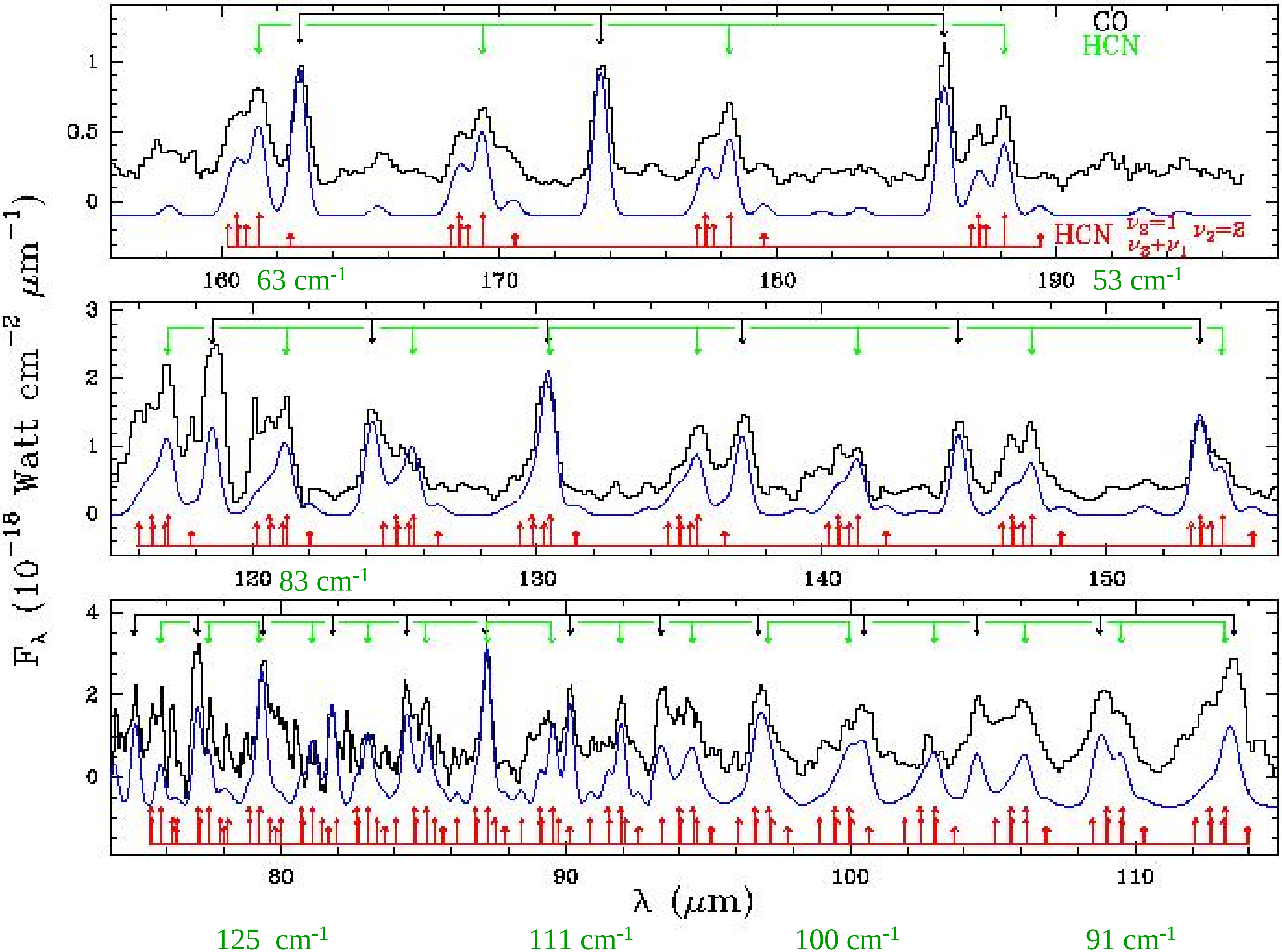


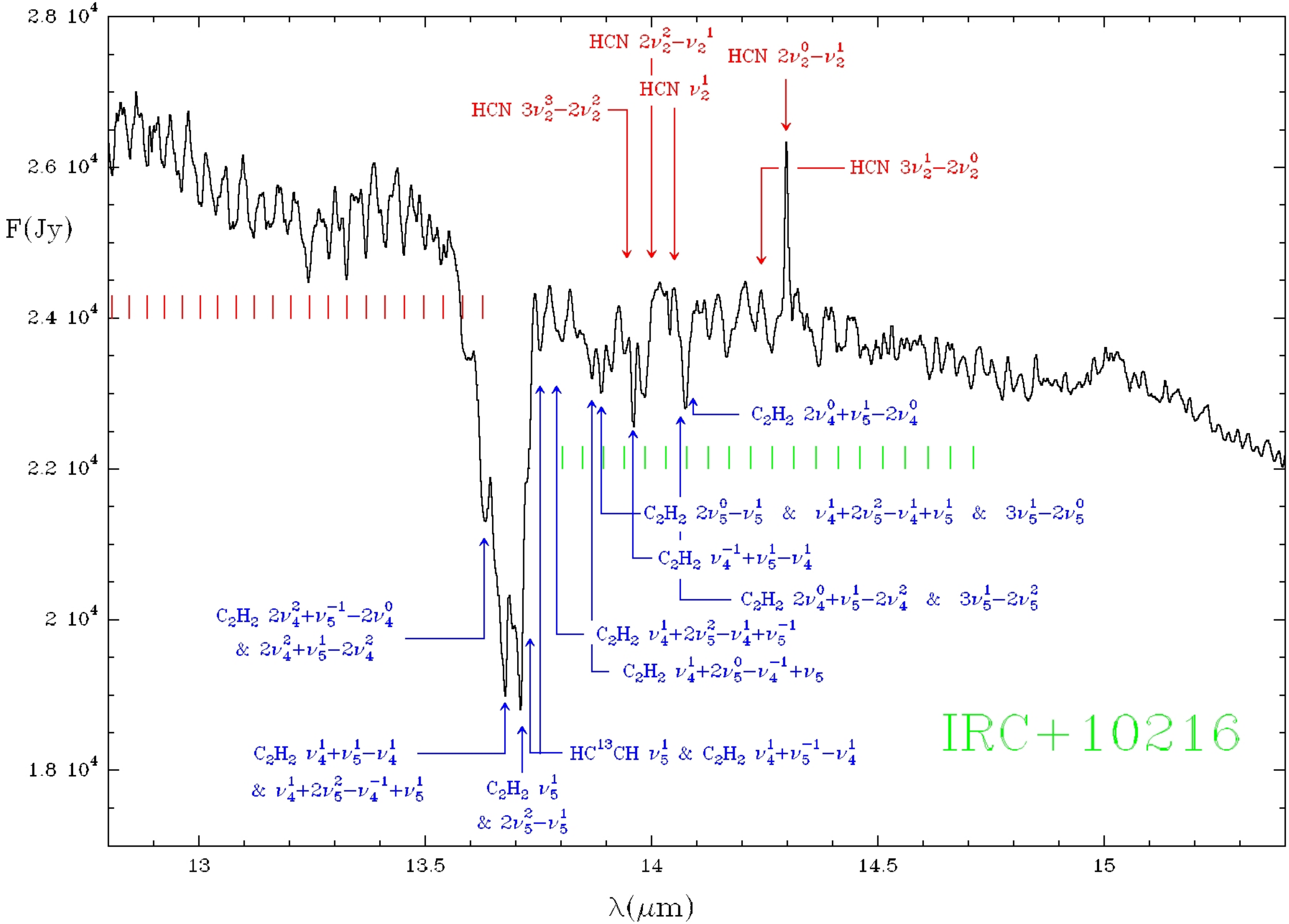
Cernicharo et al., 2007, A&A

EVOLVED STARS : IRC+10216, The Prototype of C-rich Red Giant
and our main target for new molecular species !!!

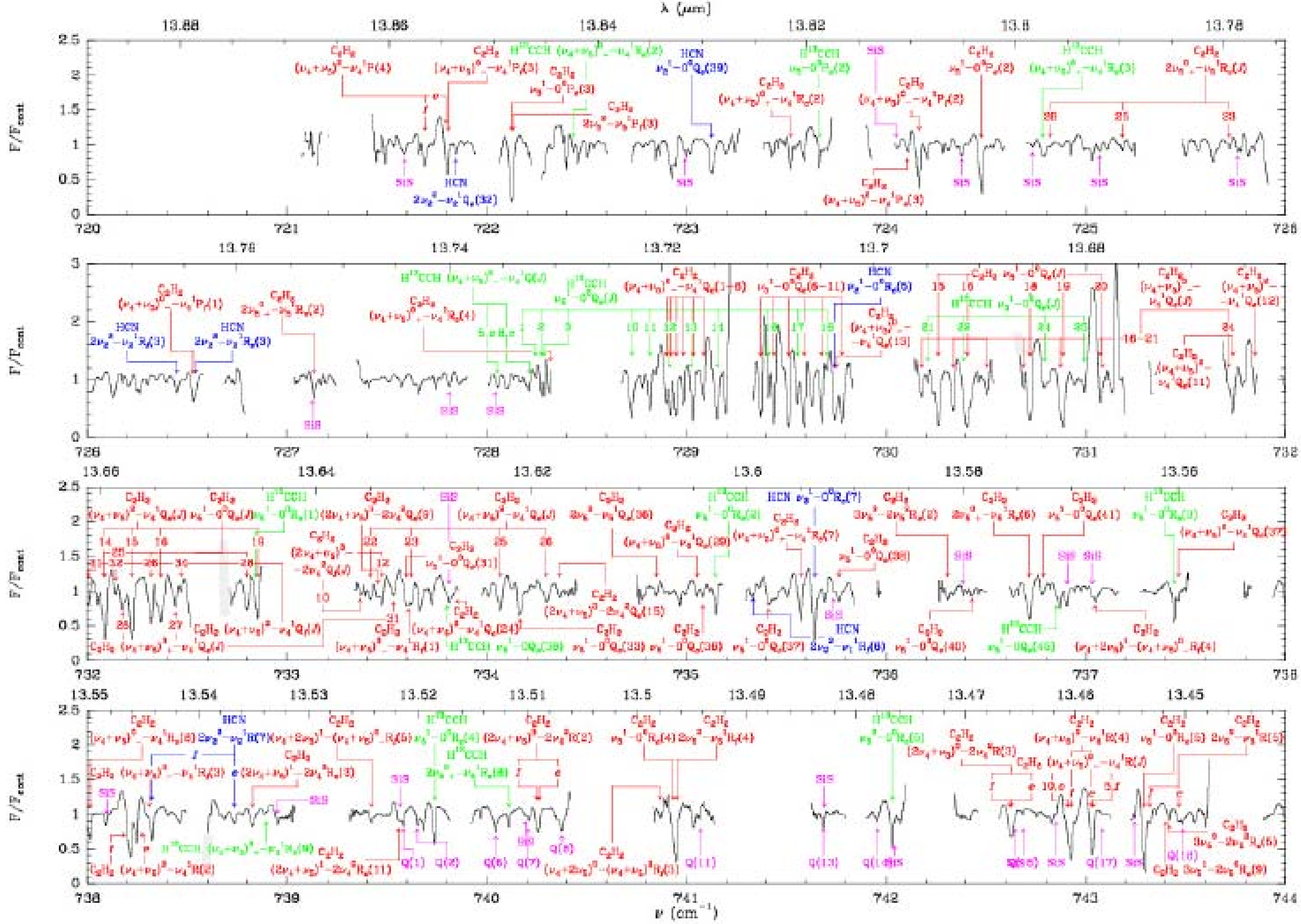


Cernicharo et al., 1996, A.&A., 315, 201

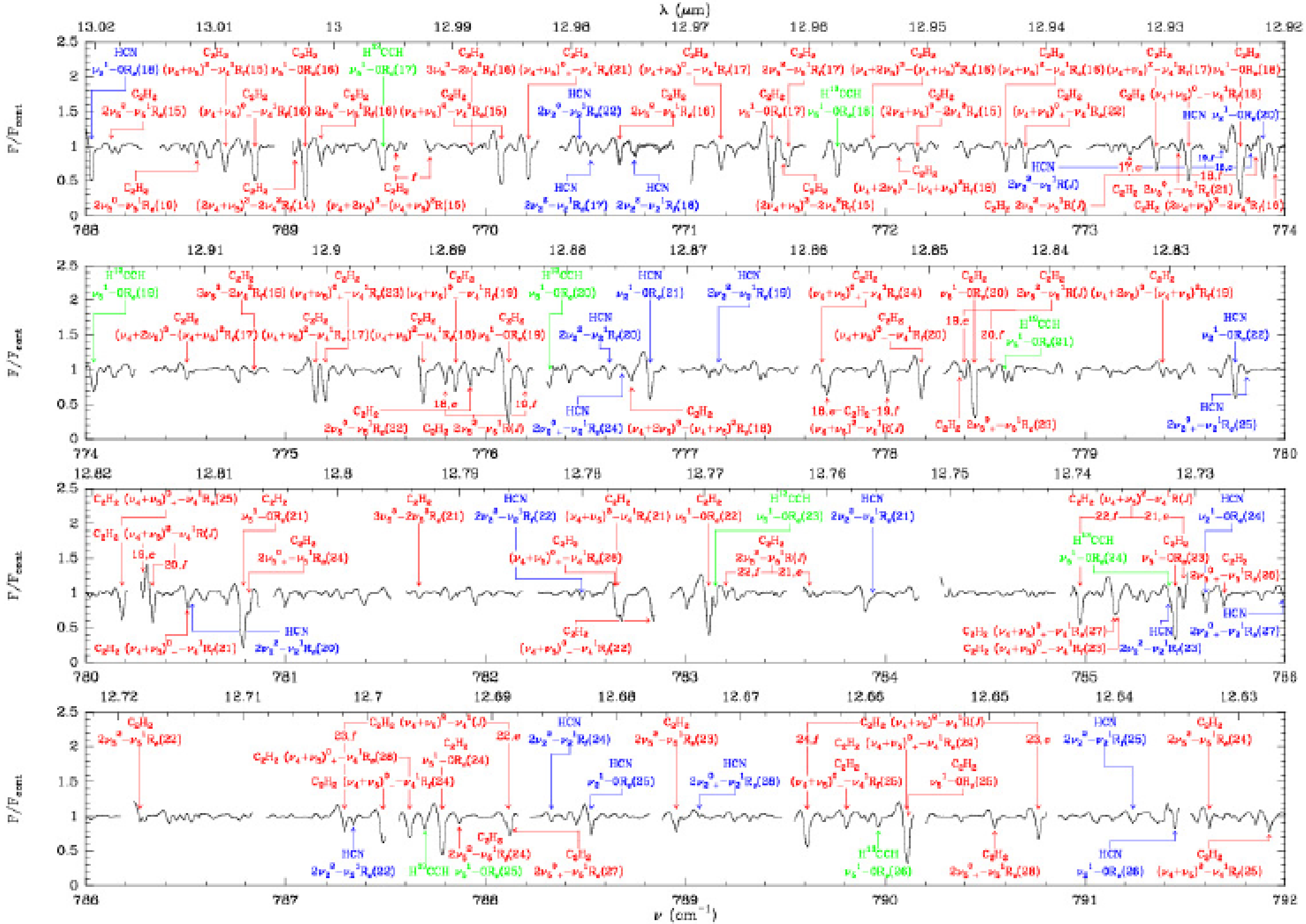




Cernicharo et al., 1999, ApJ Letters, 526, L41



Fonfría et al., 2007; IR high spectral resolution line survey of IRC+10216



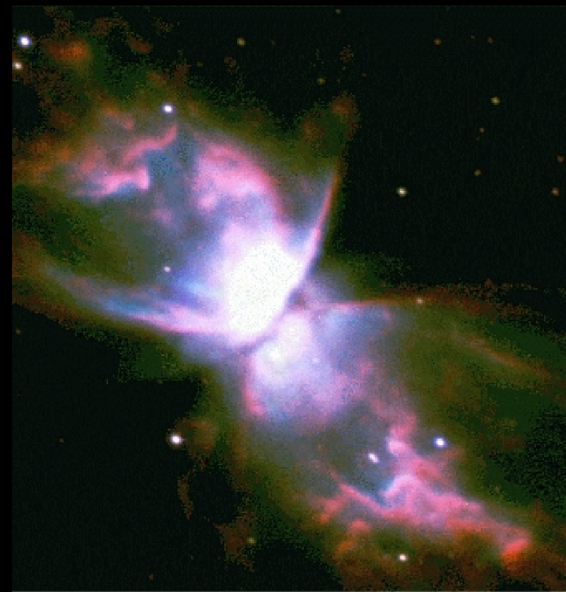
Infrared observations : only way to observe symmetrical molecules !!

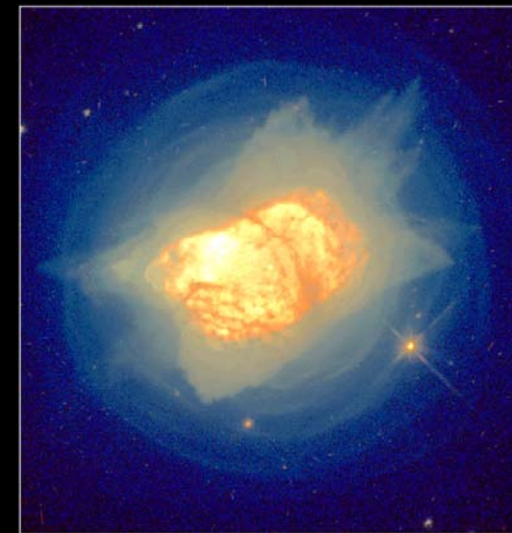
PLANETARY NEBULA:

When a red giant starts its evolution towards the white dwarf phase the UV photons scaping its photosphere ionize the circumstellar envelope created during the AGB phase. High velo-city winds are also produced disrupting the AGB envelope

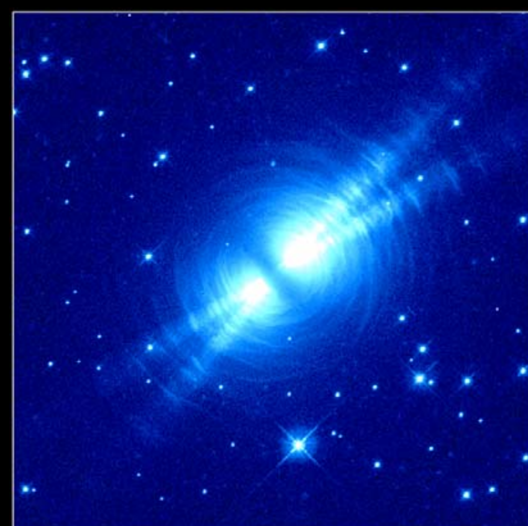
The physical and chemical conditions change again and new molecules are produced

They are, probably, the ni-cest objects in the sky.

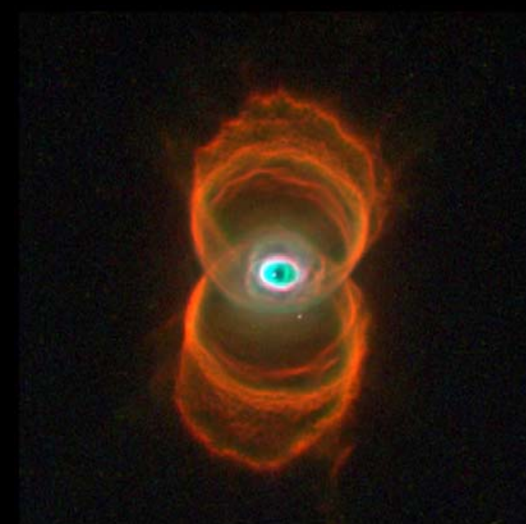




Planetary Nebula NGC 7027 HST • WFPC2
PRC96-05 • ST ScI OPO • January 16, 1996 • H. Bond (ST ScI) and NASA



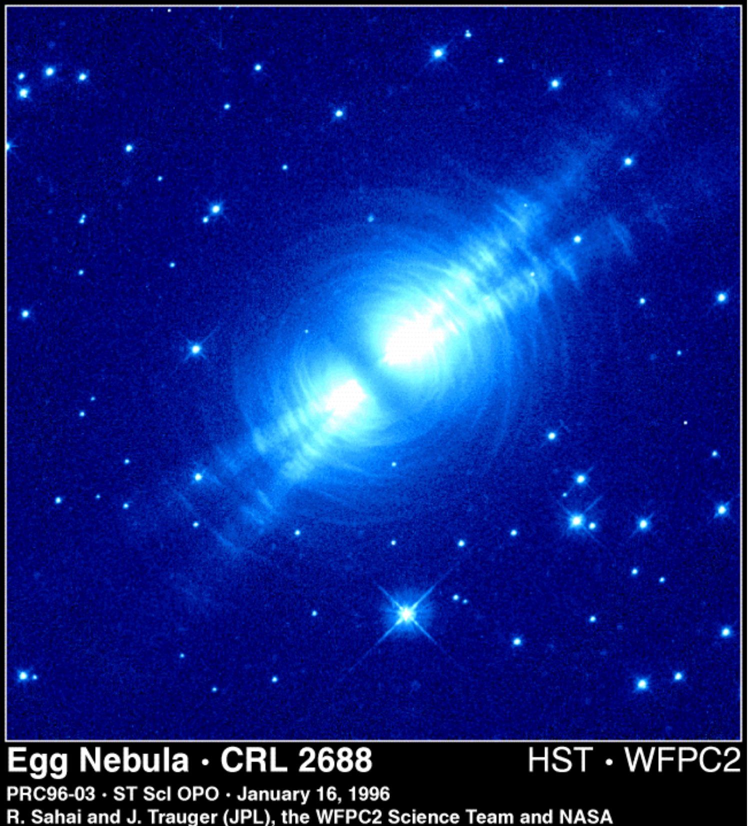
Egg Nebula • CRL 2688 HST • WFPC2
PRC96-03 • ST ScI OPO • January 16, 1996
R. Sahai and J. Trauger (JPL), the WFPC2 Science Team and NASA



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 inner part of the neutral envelope is quickly ionized by the UV photons from the hot central star. An HII region is created and in the frontier with the neutral envelope a photodissociation region is produced.

The increase of temperature and the presence of UV photons, together with the anisotropic winds arising from the star excavate the neutral envelope and an important fraction of ionizing photons escape the envelope.



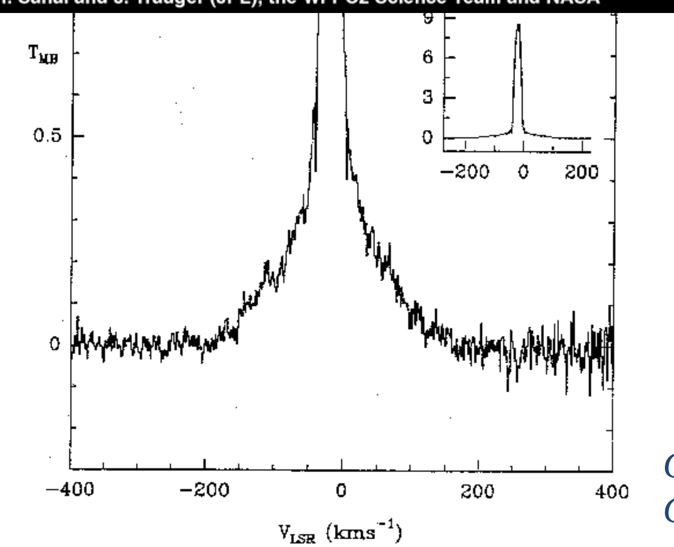
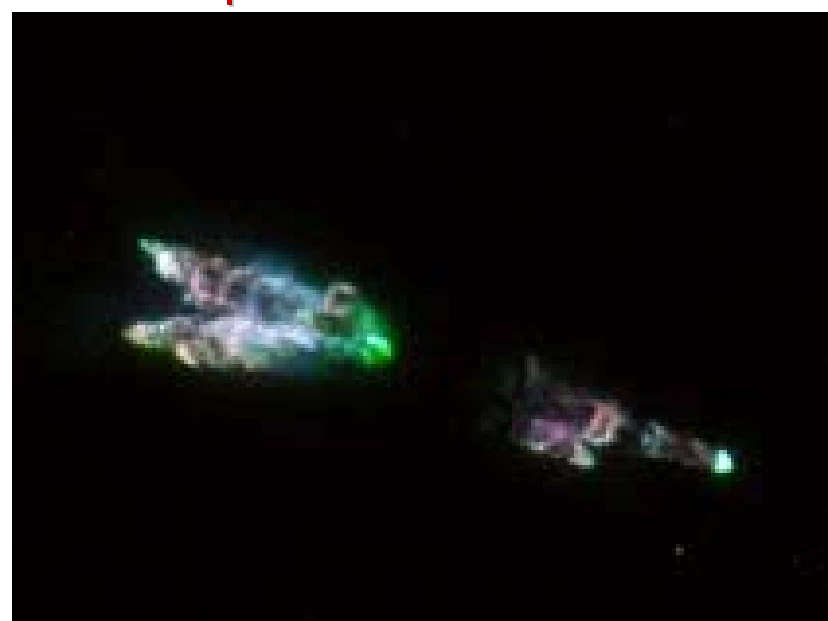
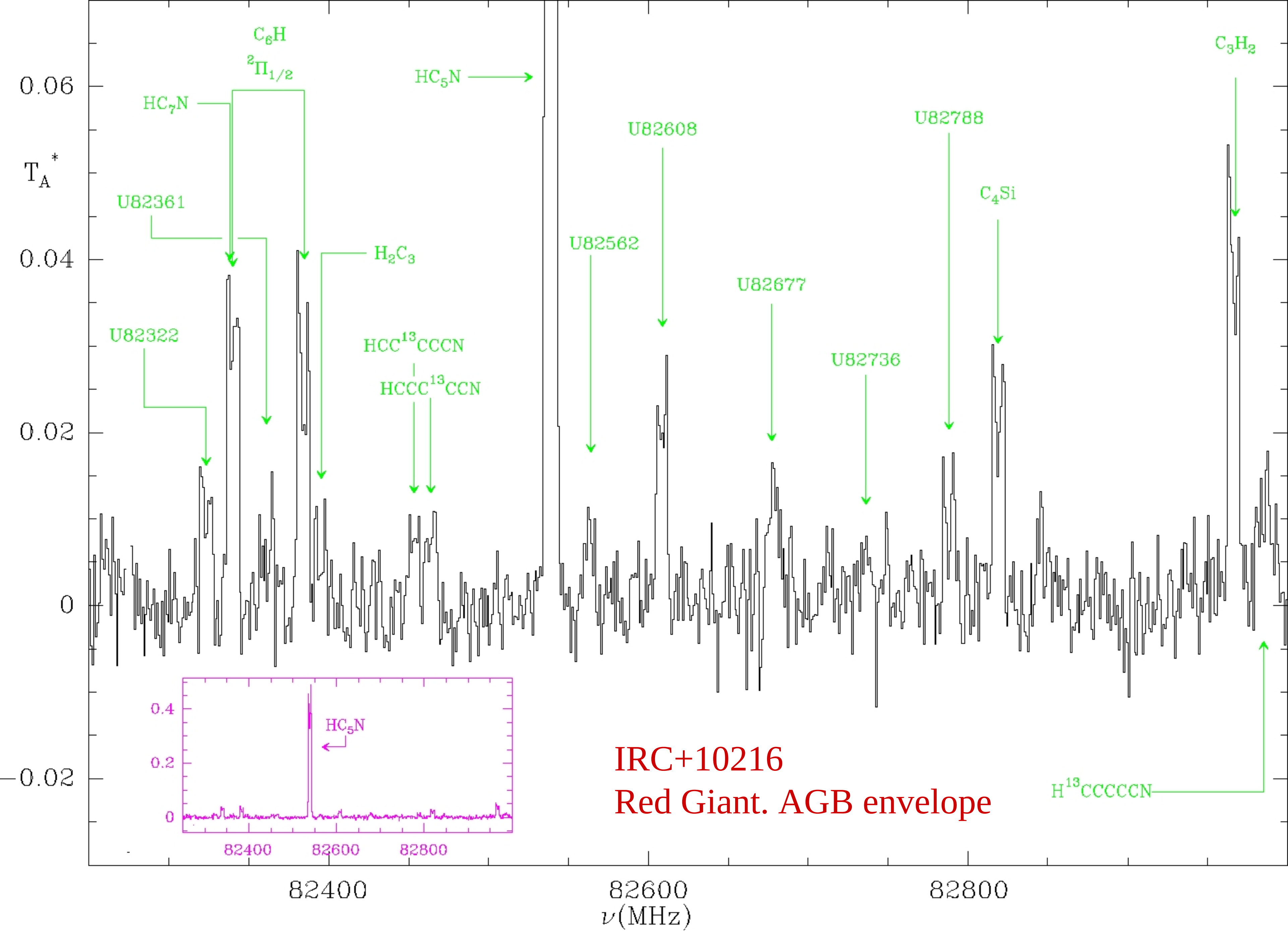


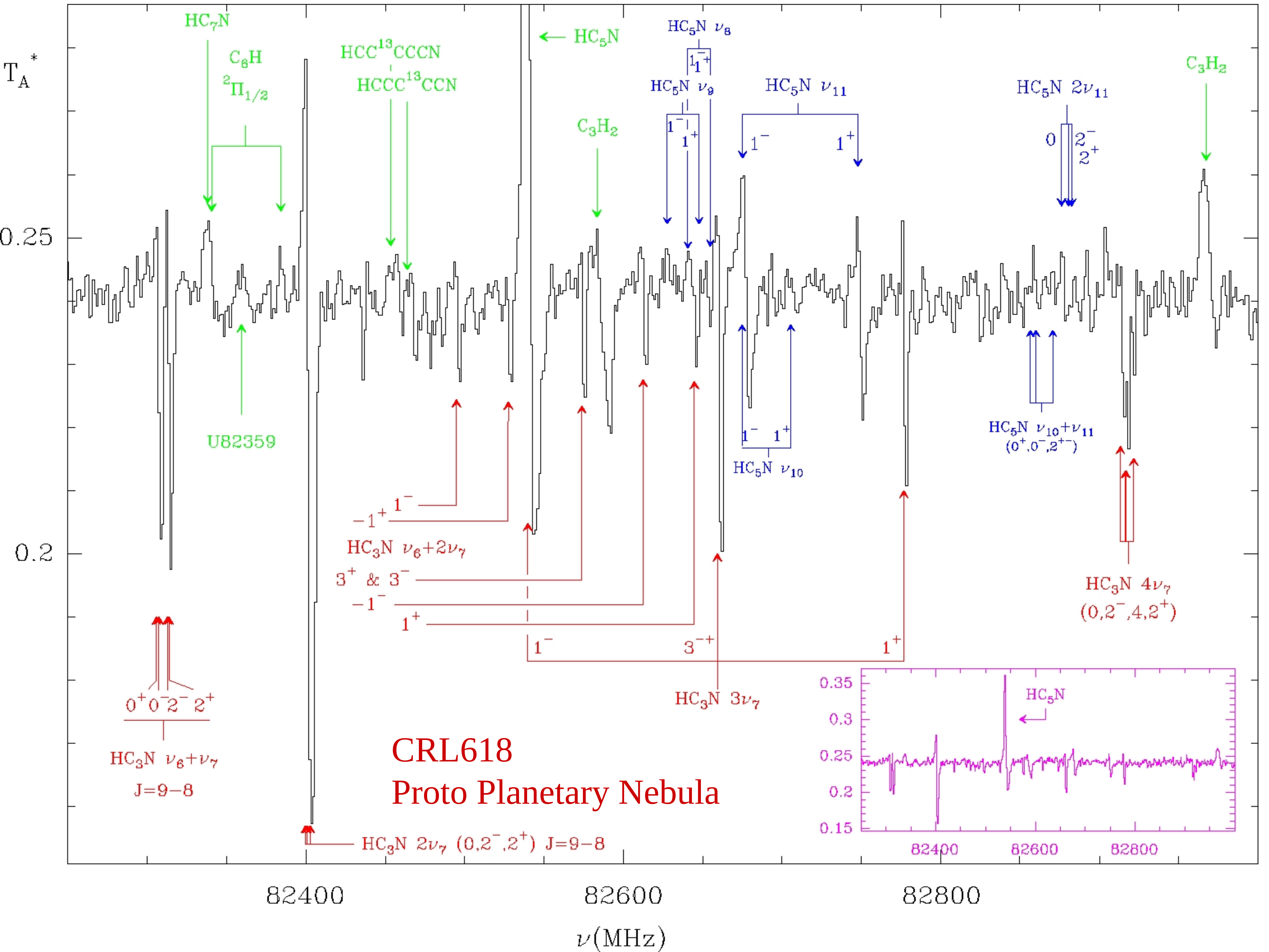
Fig. 1: CO J=2–1 line profile toward CRL 618. Ordinate is the main beam-averaged brightness temperature in kelvin.

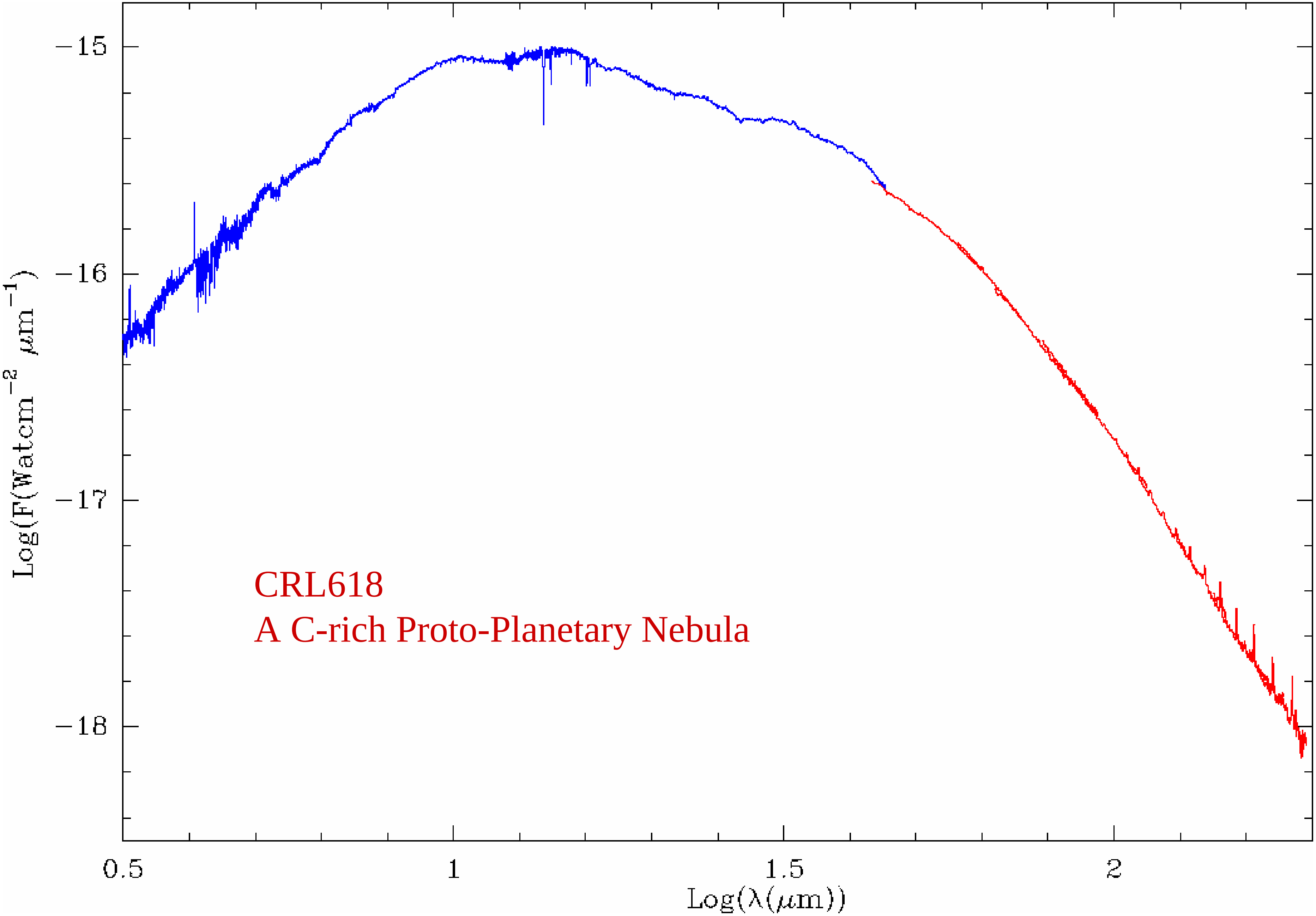
Cernicharo et al., 1989
Gammie et al., 1989



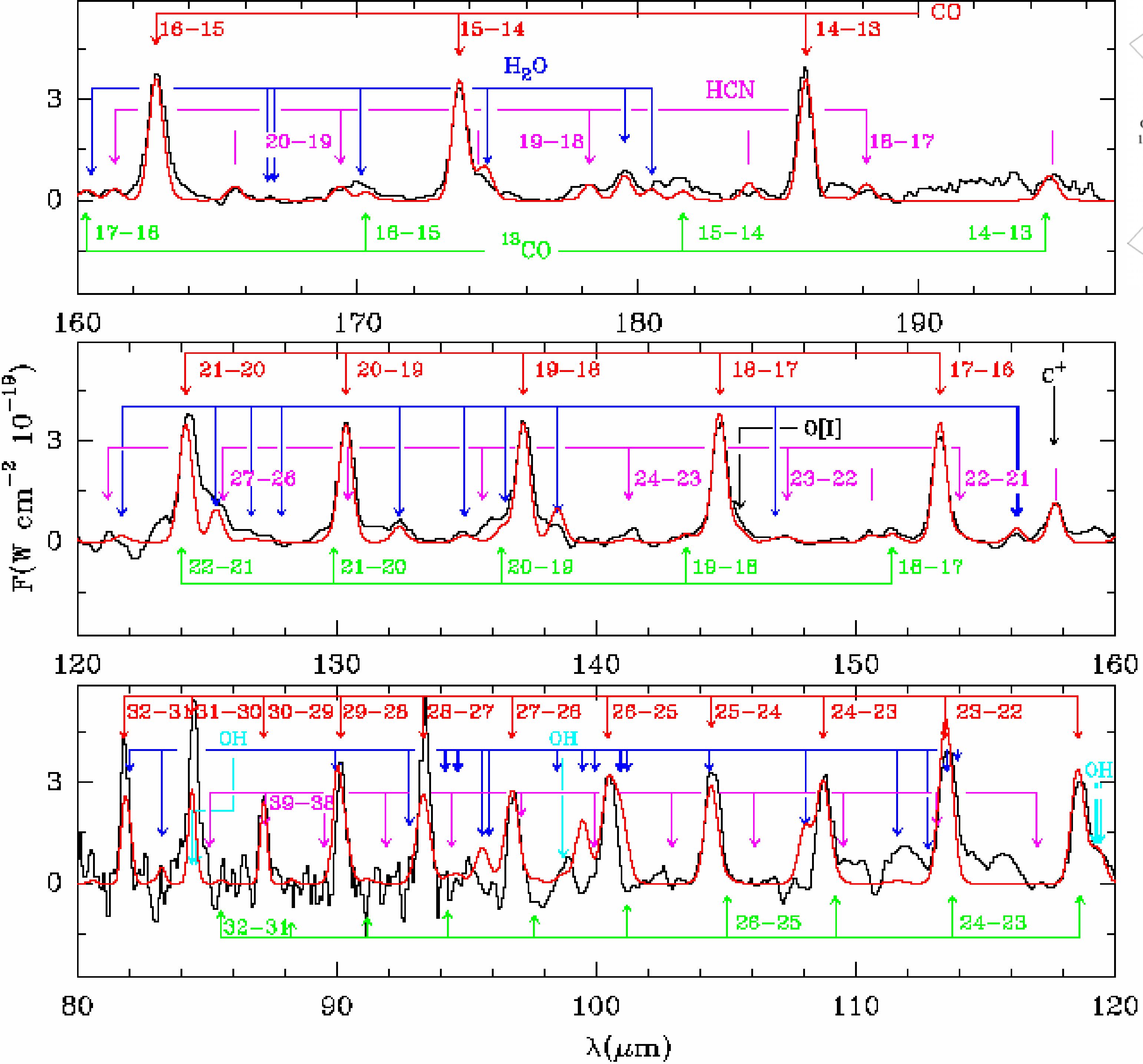


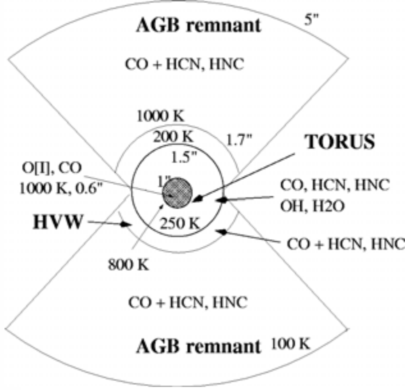
C6H
2Π1/2
HC5N
C3H2
0.06
HC7N
U82608
U82788
T_A*
C4Si
U82361
0.04
U82562
H2C3
U82677
U82322
HCC13CCCN
U82736
HCCC13CCN
0.02
0
0.4
HC5N
0.2
−0.02
IRC+10216
Red Giant. AGB envelope
H13CCCCCN
82400
82600
82800
82400
82600
82800
ν(MHz)


CRL618
Proto Planetary Nebula
T_A*
0.25
0.2
82400
82600
82800
ν(MHz)
HC7N
C6H
2Π1/2
U82359
HCC13CCCN
HCCC13CCN
HC5N
C3H2
HC5N ν8
1− 1+
HC5N ν9
1− 1+
HC5N ν11
1− 1+
HC5N 2ν11
0 2− 2+
C3H2
HC5N ν10
1− 1+
HC5N ν10+ν11
(0+,0−,2+−)
HC3N ν6+2ν7
1−
−1+
3+ & 3−
−1−
1+
1− 3−+ 1+
HC3N 3ν7
HC3N 4ν7
(0,2−,4,2+)
0+ 0− 2− 2+
HC3N ν6+ν7
J=9−8
HC3N 2ν7 (0,2−,2+) J=9−8
0.35
0.3
0.25
0.2
0.15
HC5N
82400
82600
82800

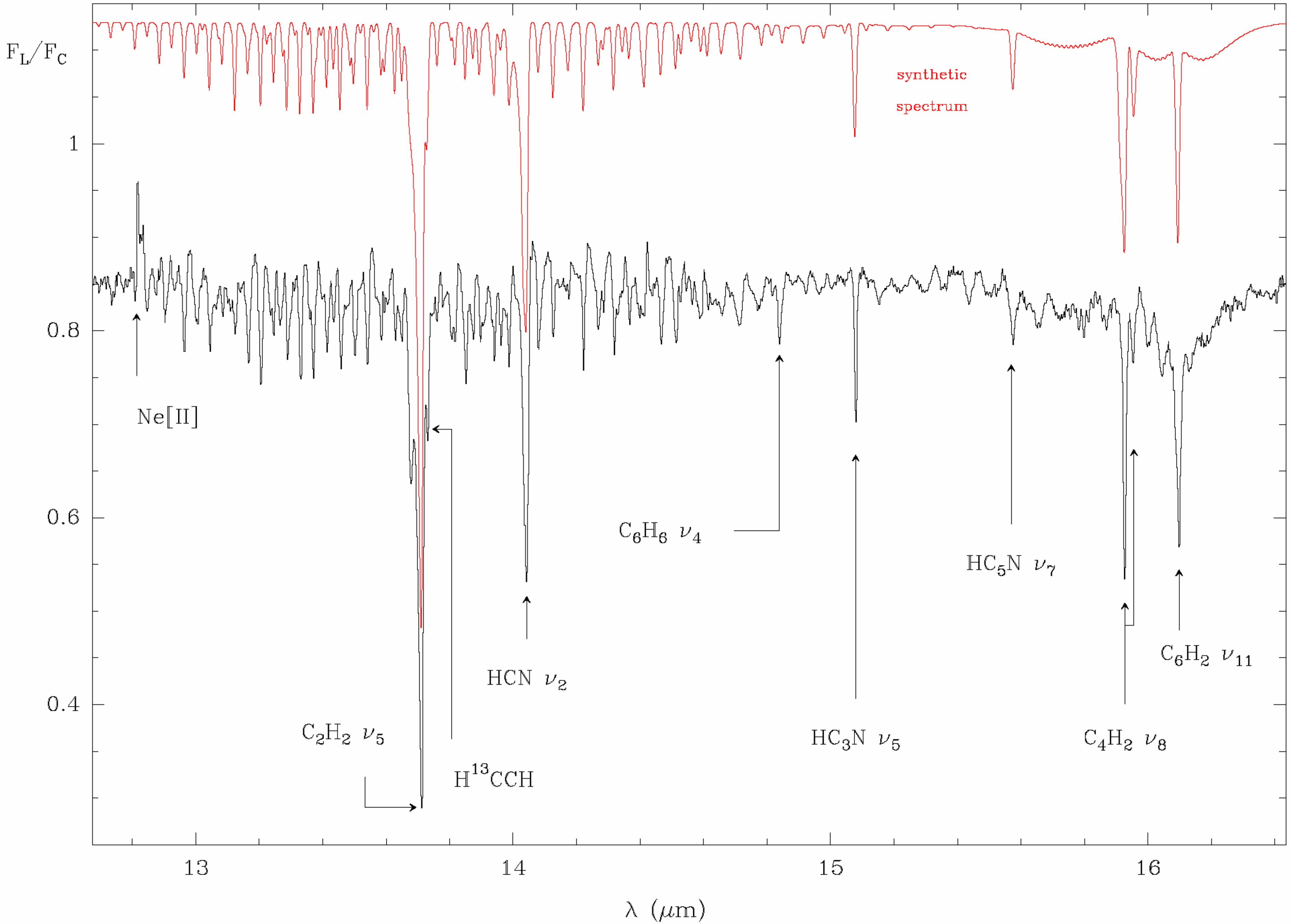


−15
−16
−17
−18
Log(F(Watcm^{-2} μm^{-1}))
0.5
1
1.5
2
Log(λ(μm))
CRL618
A C-rich Proto-Planetary Nebula

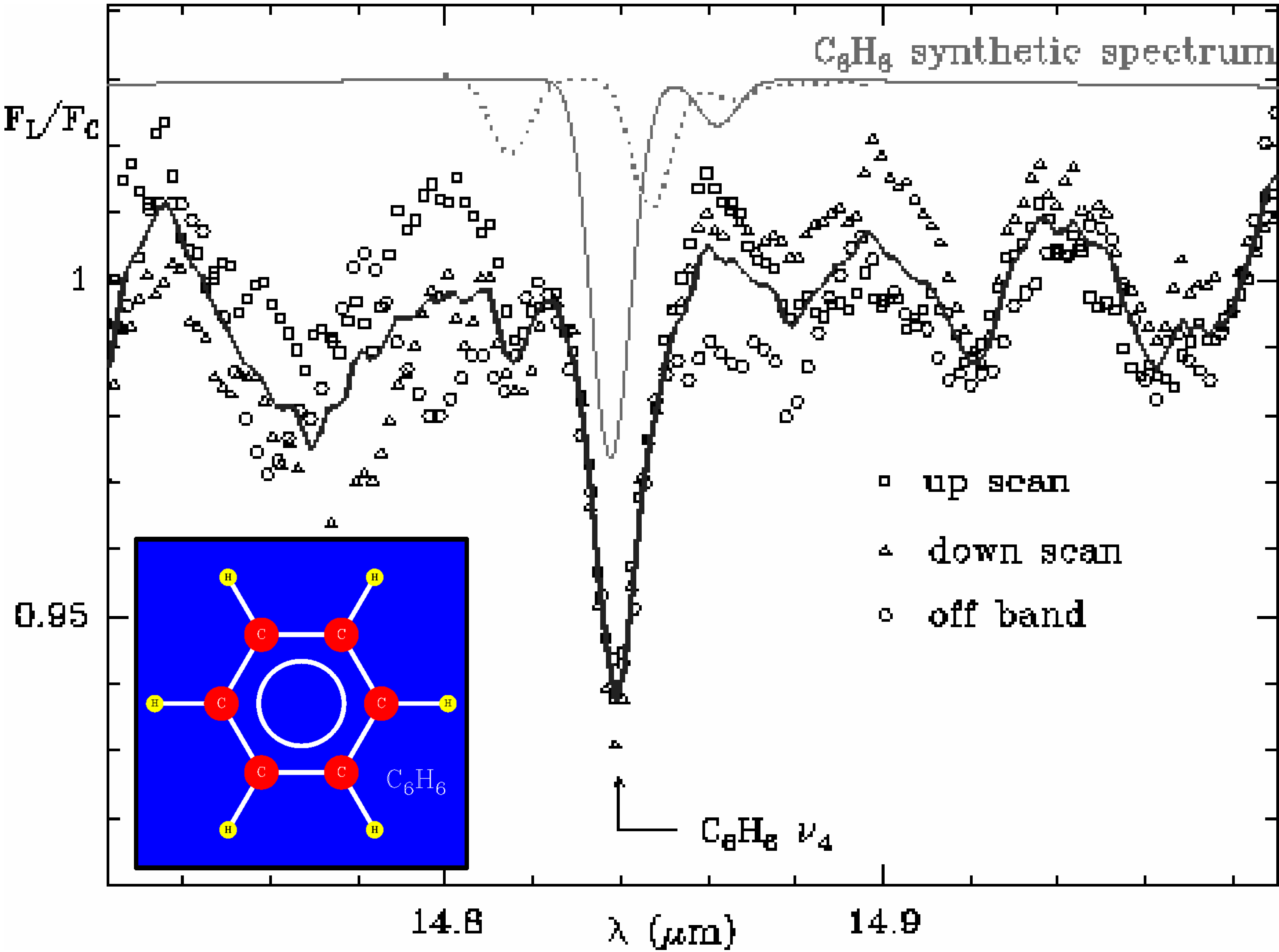




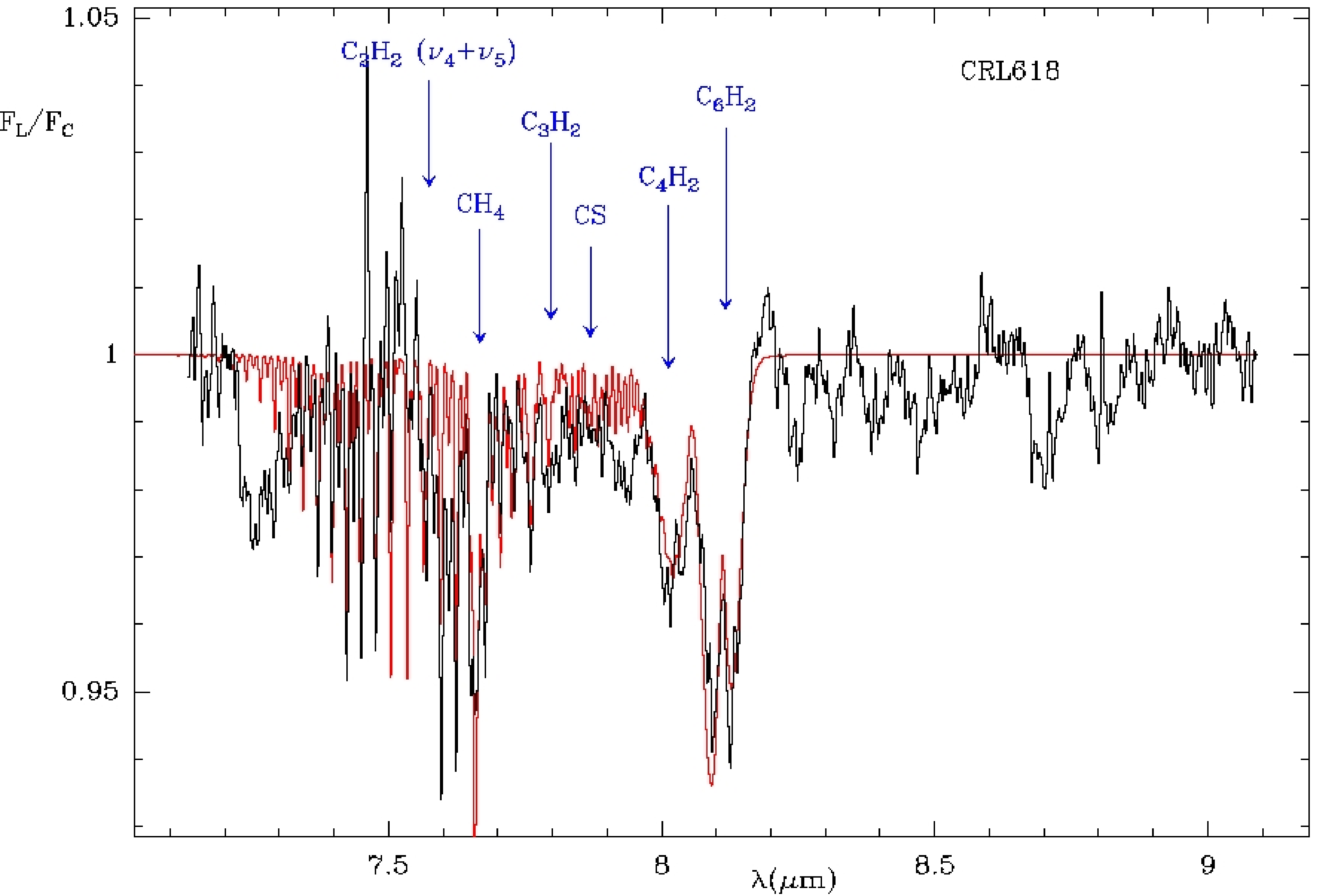
Herpin & Cernicharo, 2000, ApJ Letters, 530, L129



F_L/F_C
synthetic
spectrum
1
0.8
0.6
0.4
Ne[II]
C_2H_2 ν_5
$H^{13}CCH$
HCN ν_2
C_6H_6 ν_4
HC_3N ν_5
HC_5N ν_7
C_4H_2 ν_8
C_6H_2 ν_{11}
13
14
15
16
λ (μm)

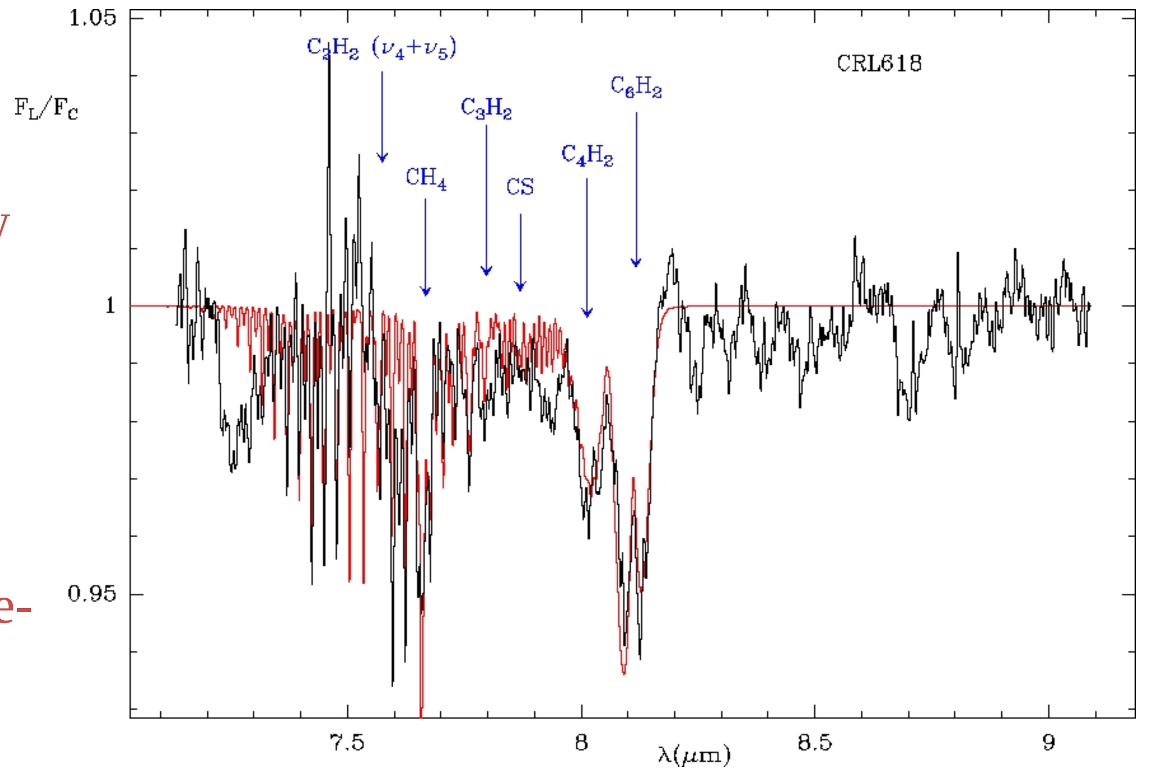


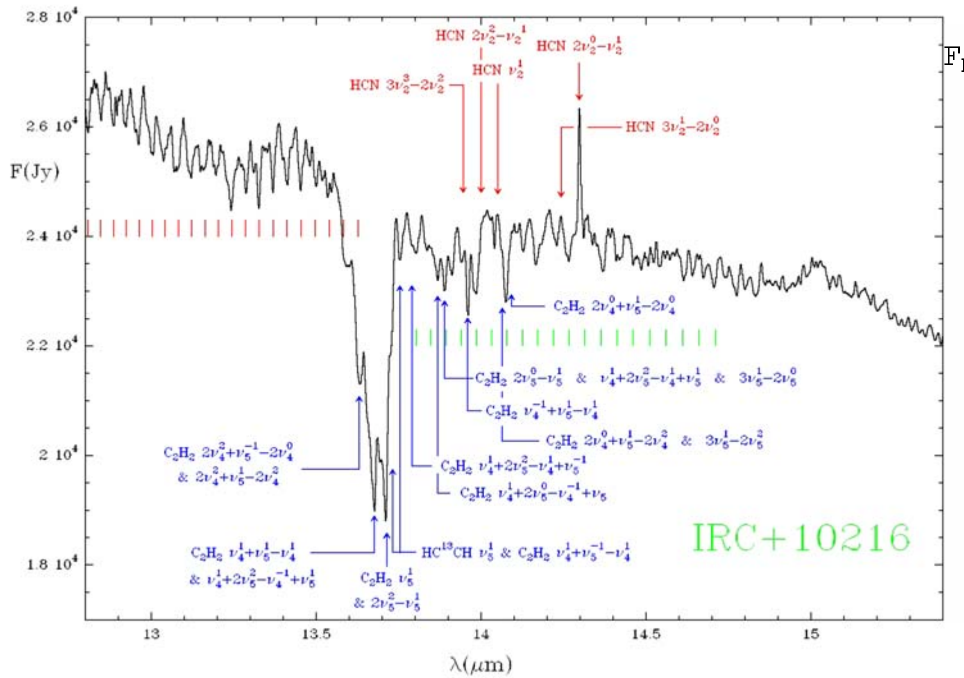
C6H6 synthetic spectrum
FL/Fc
1
0.95
up scan
down scan
off band
C6H6
C6H6 ν4
14.8
λ (μm)
14.9

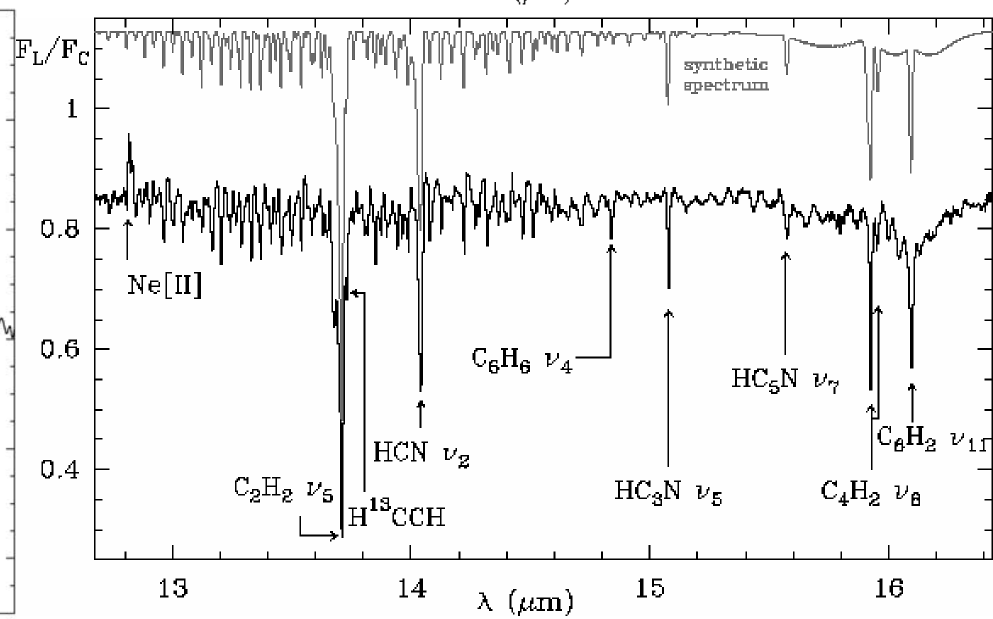


1.05
1
0.95
F_L/F_C
C_2H_2 ($\nu_4+\nu_5$)
CH_4
C_3H_2
CS
C_4H_2
C_6H_2
CRL618
7.5
8
8.5
9
$\lambda(\mu m)$

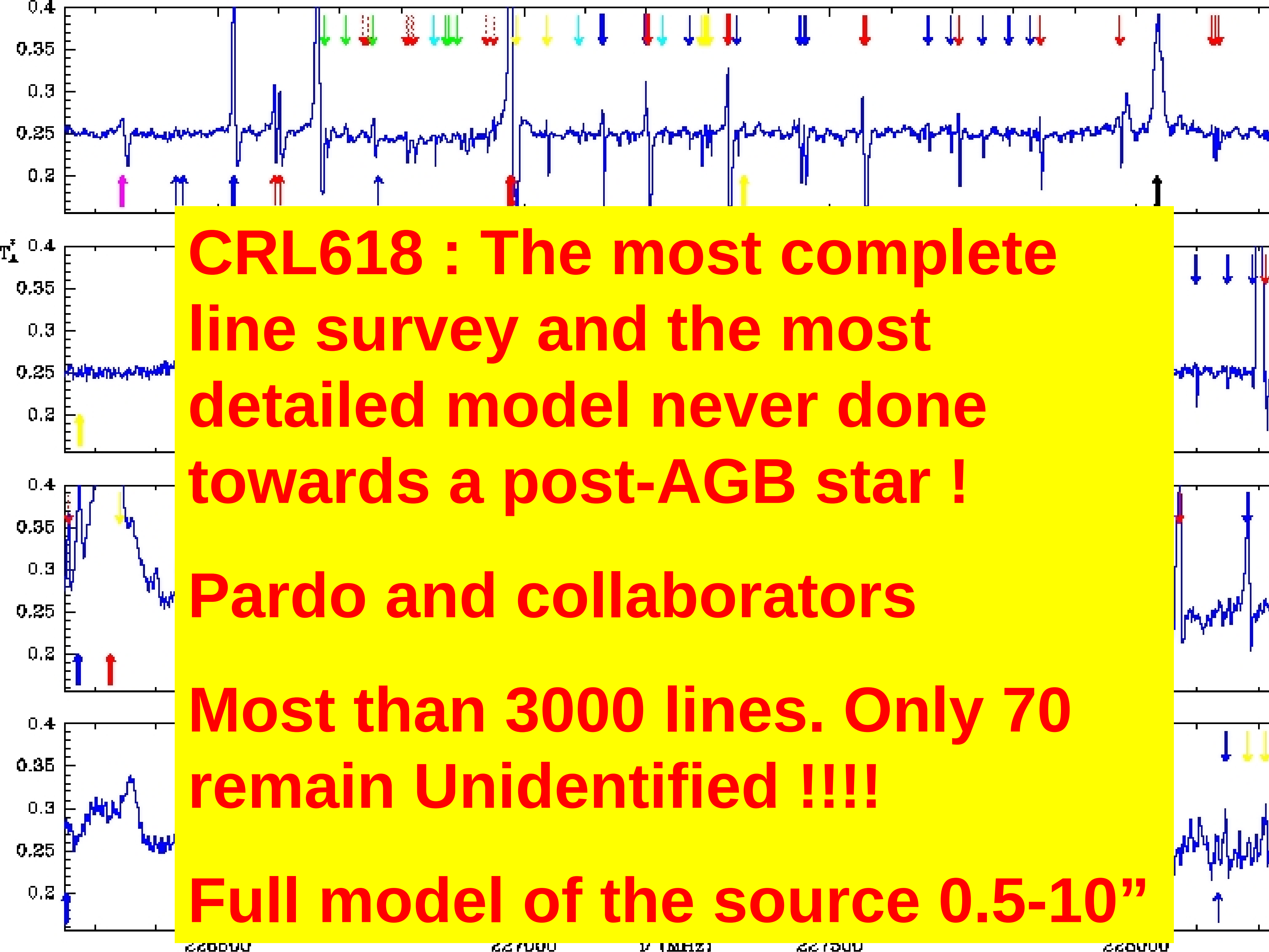
The UV photons from the central star of CRL618 photodissociated most molecules in the PDRs. New molecules are formed following a chemical network similar to that of molecular clouds. O-bearing species and small hydrocarbons are formed much more efficiently than in the AGB phase of the envelope







Cernicharo et al., 2001, ApJ 546, L123 & L127



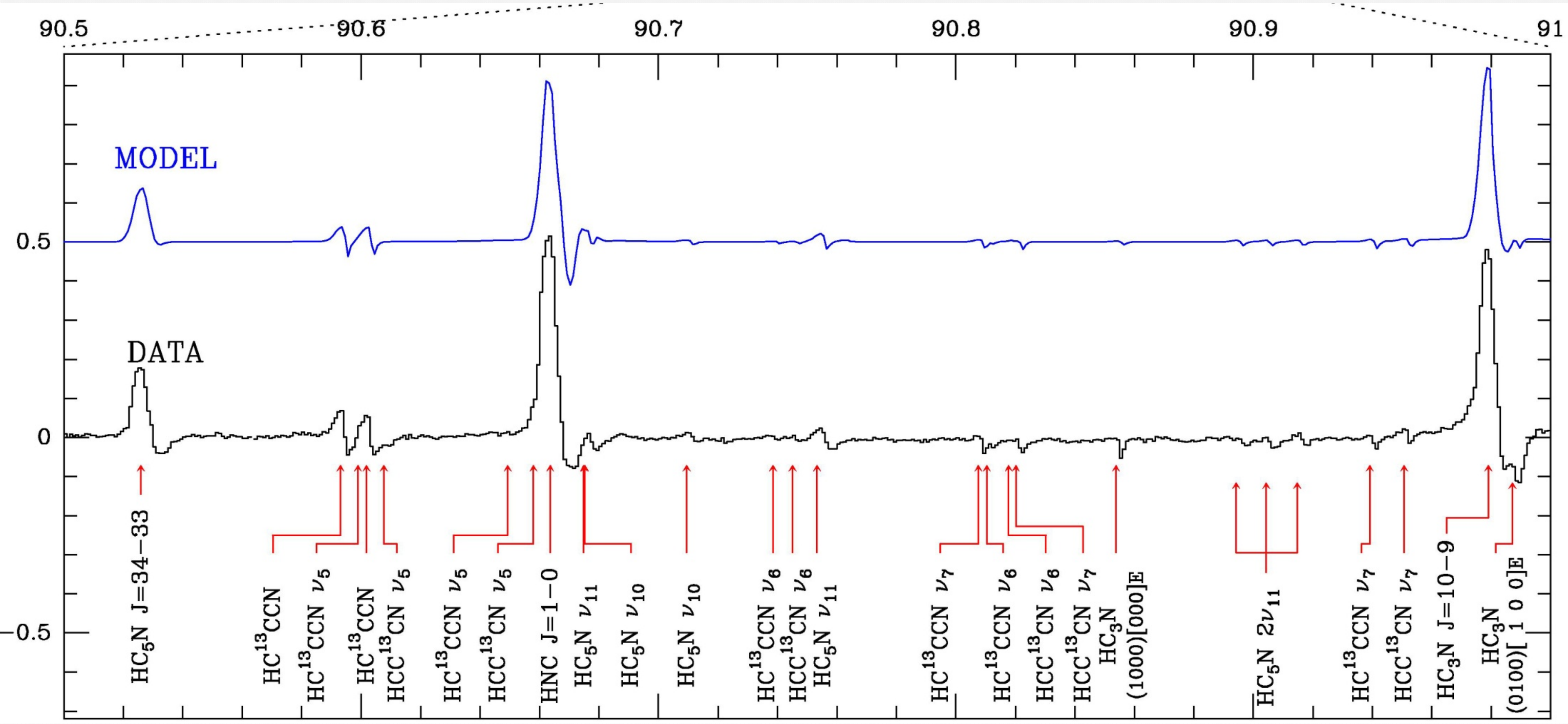
CRL618 : The most complete line survey and the most detailed model never done towards a post-AGB star !

Pardo and collaborators

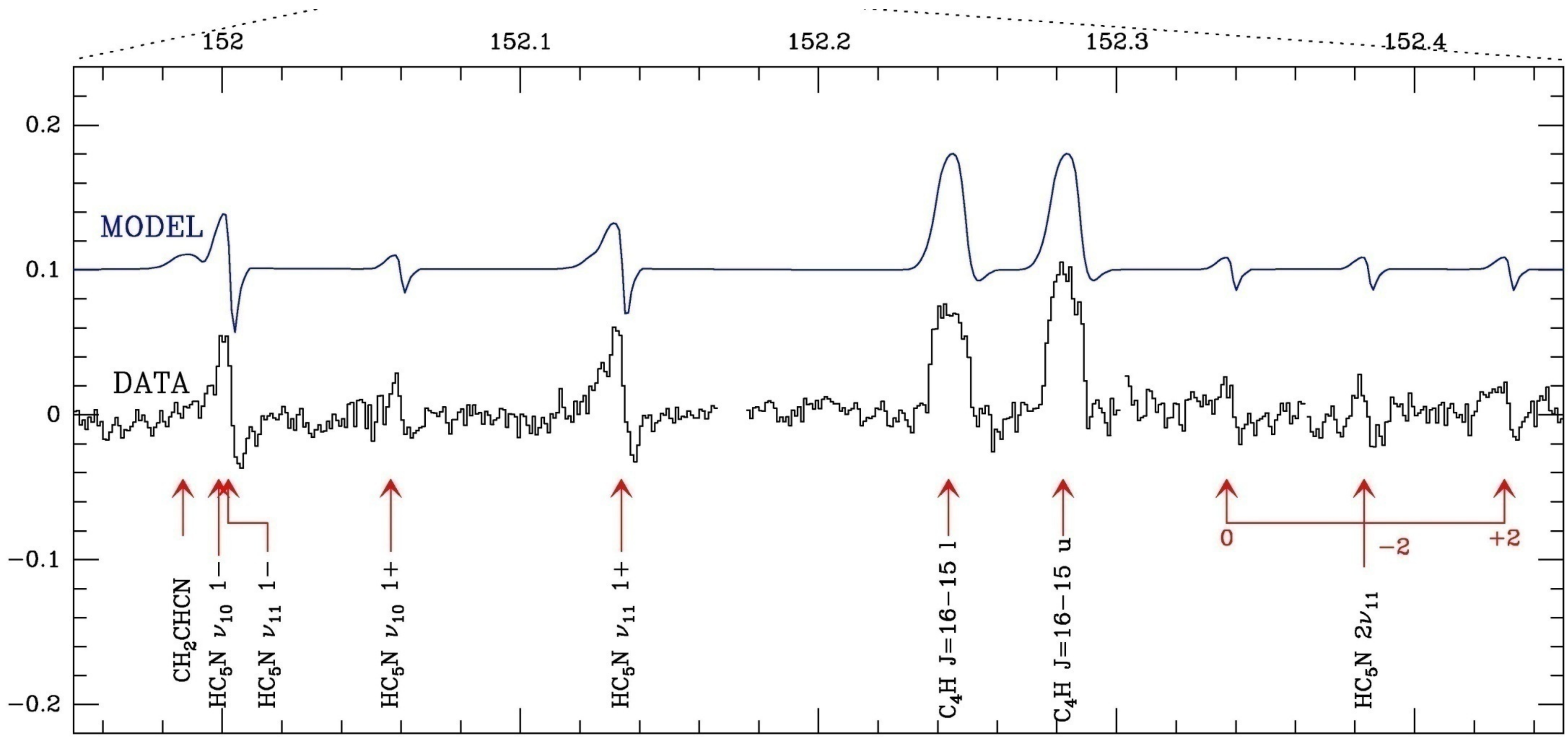
Most than 3000 lines. Only 70 remain Unidentified !!!!

Full model of the source 0.5-10”

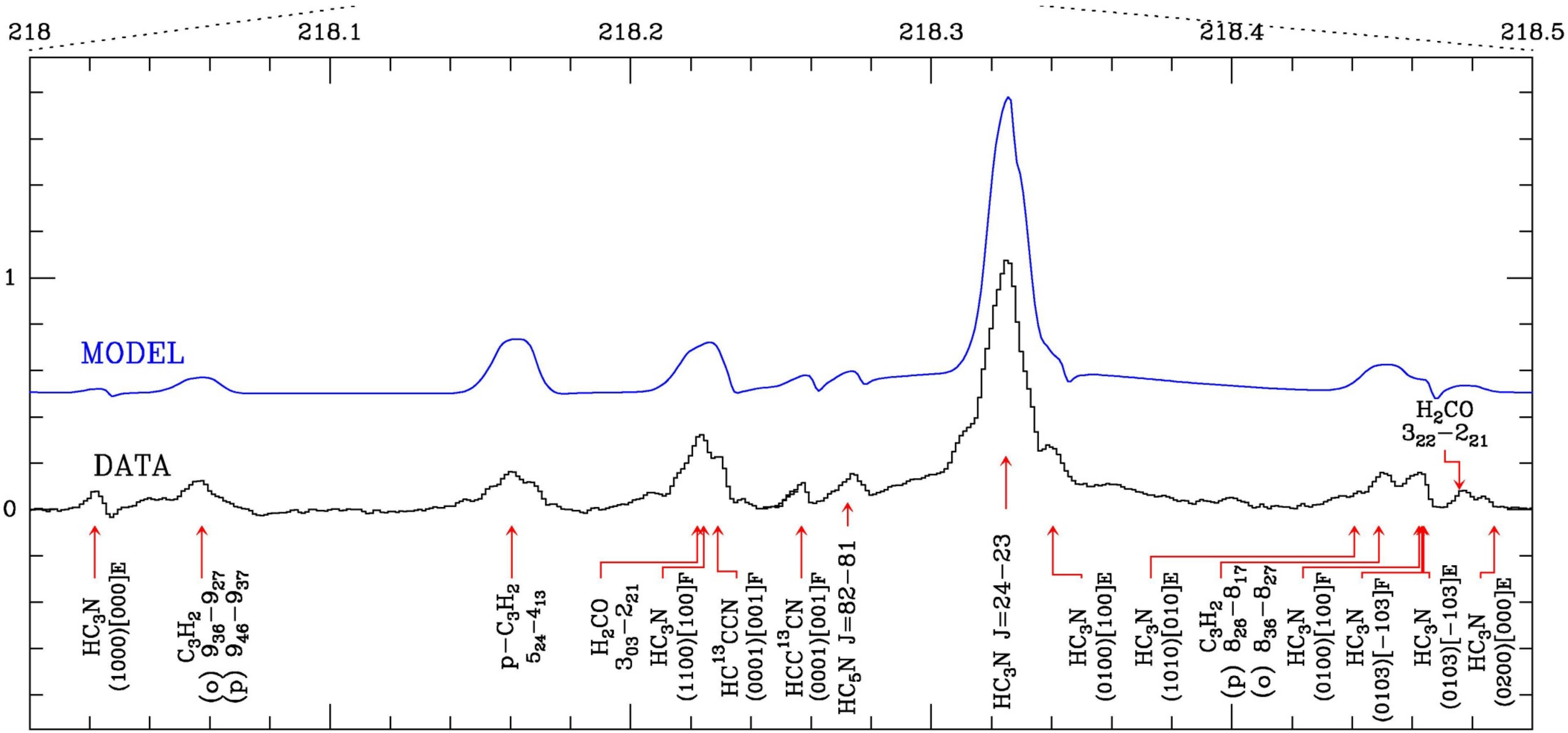
3 mm window : Data and final model



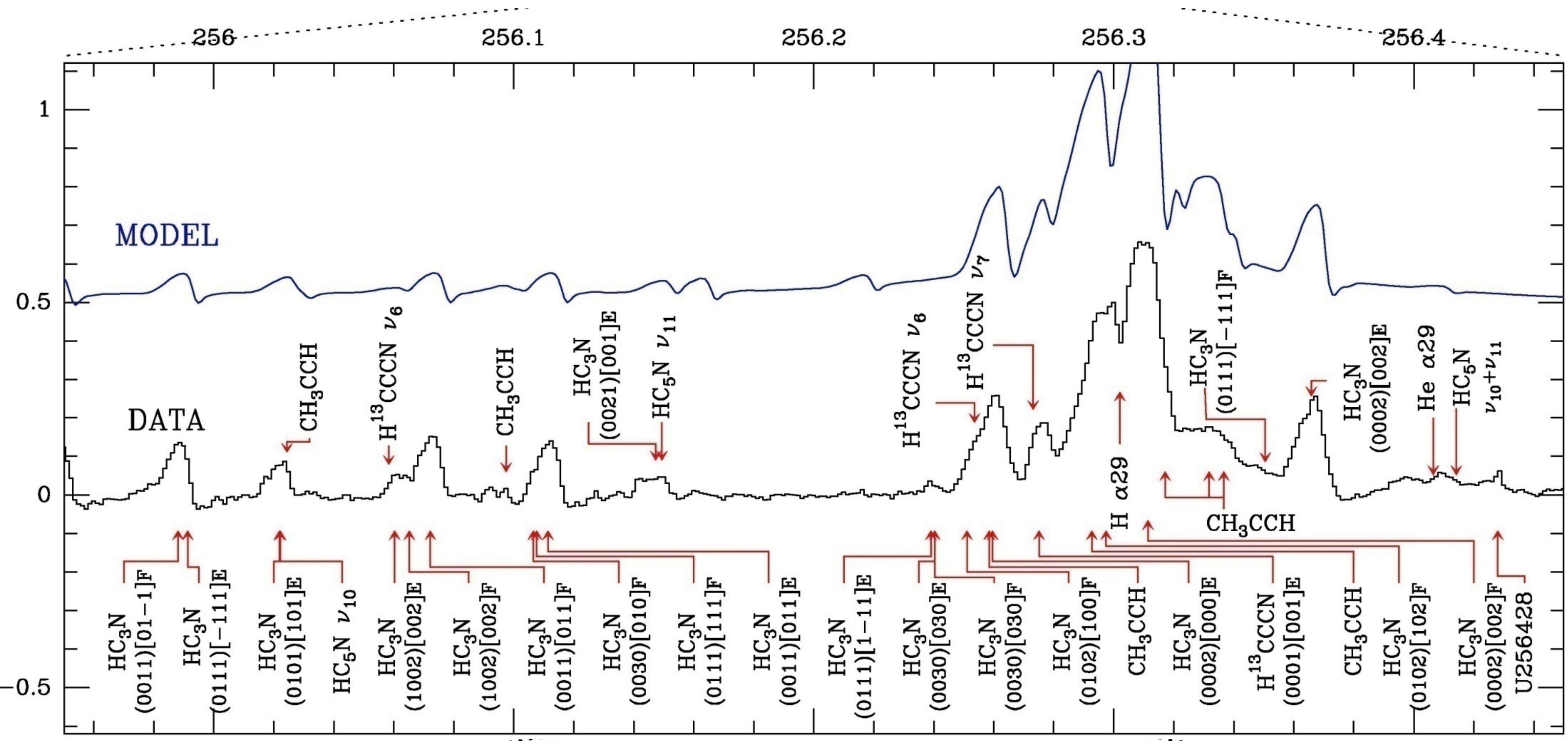
2 mm window : Data and final model

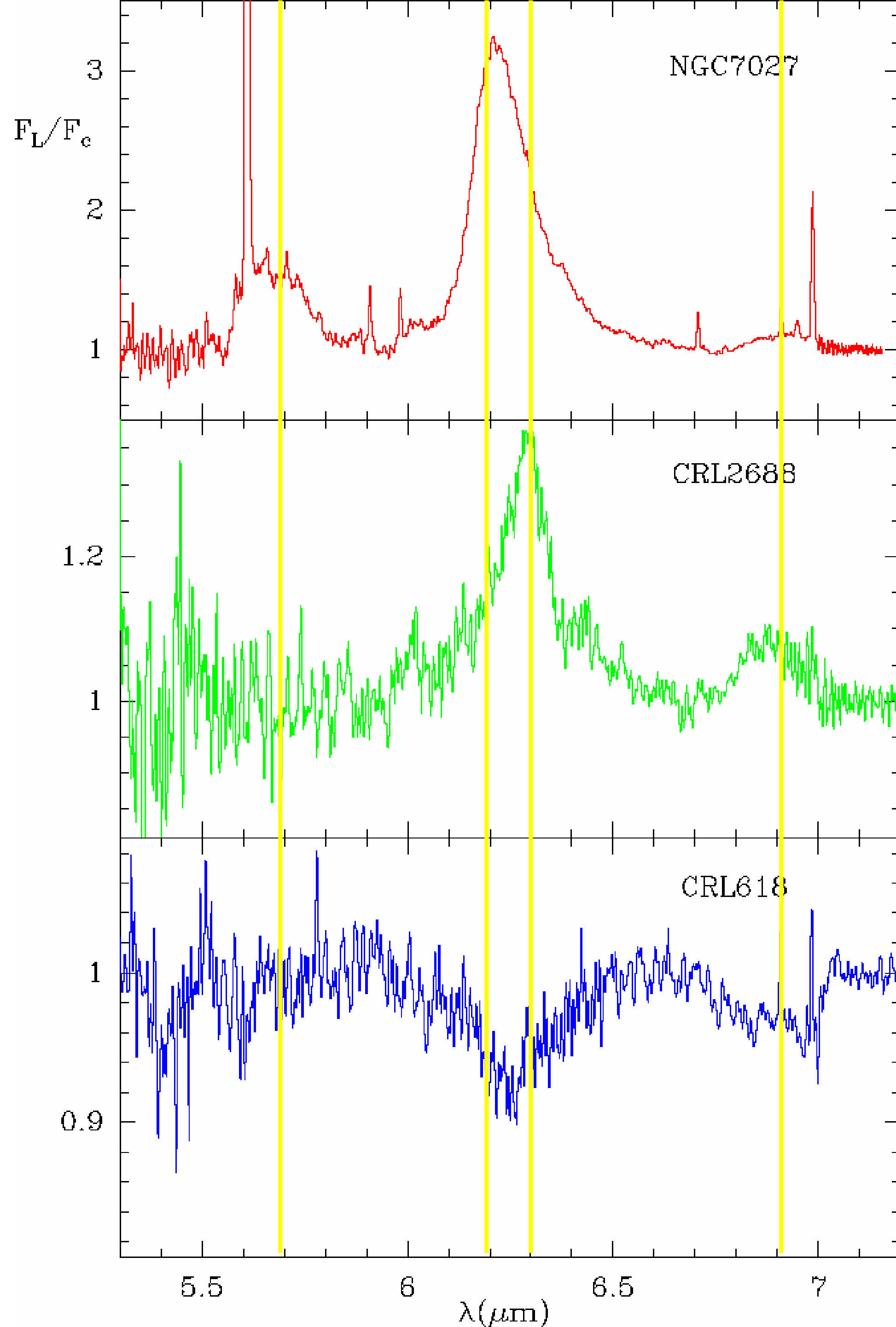


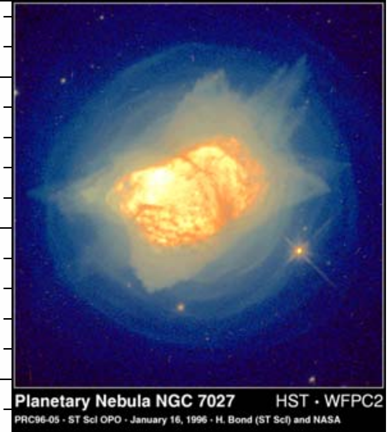
1.3 mm window : Data & final model

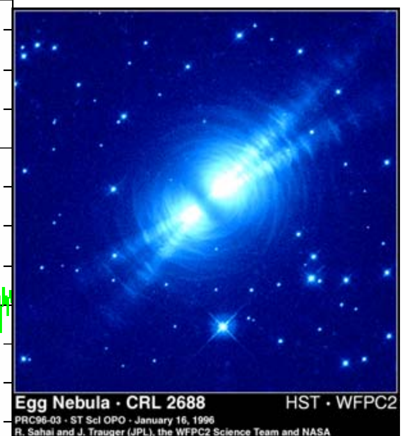


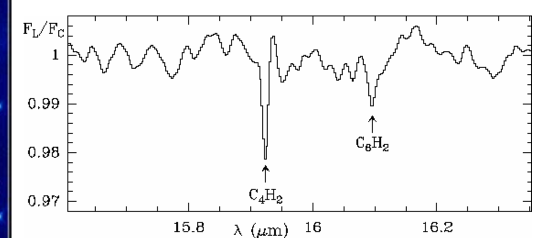
1 mm window : Data & final model

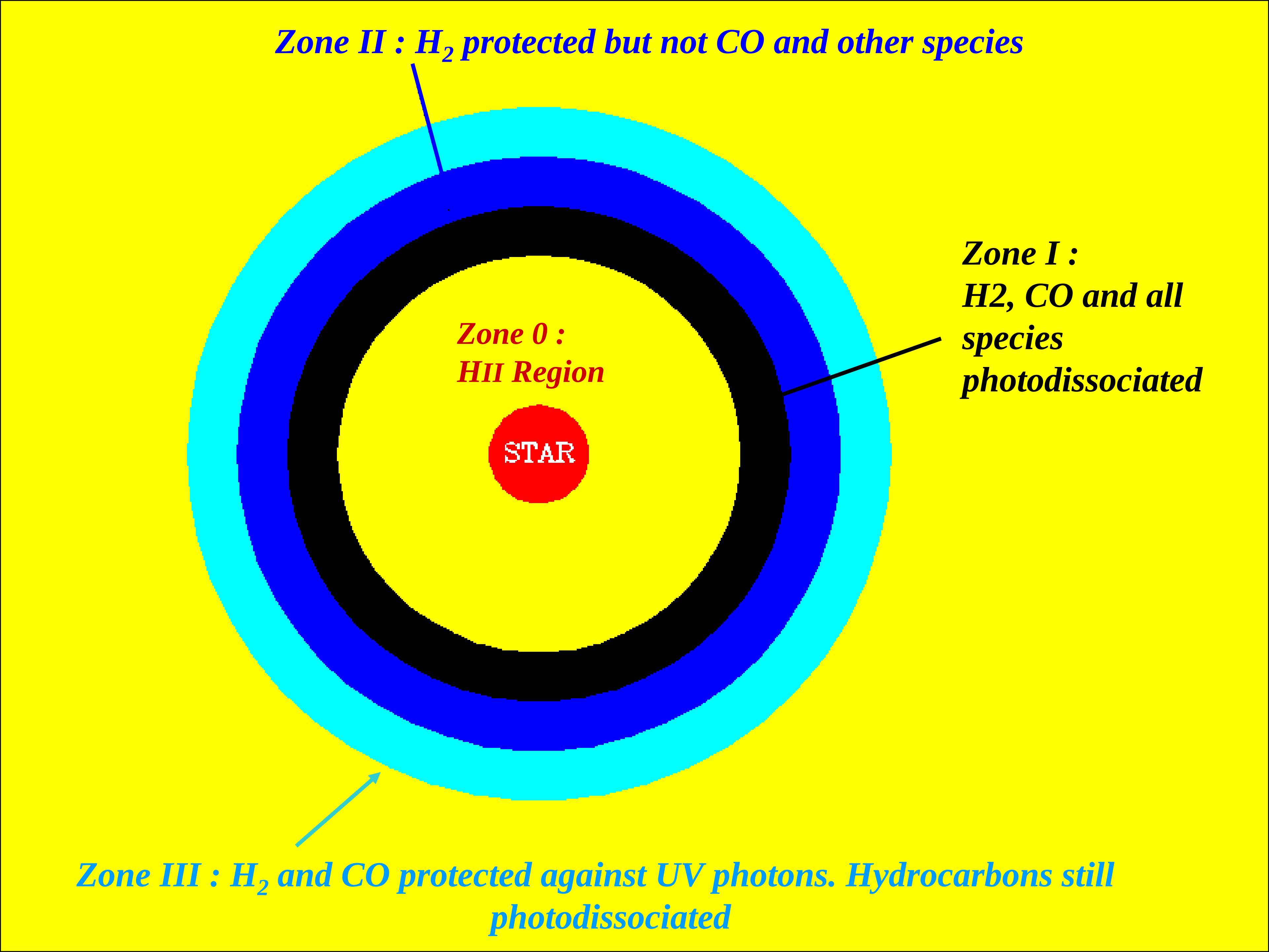


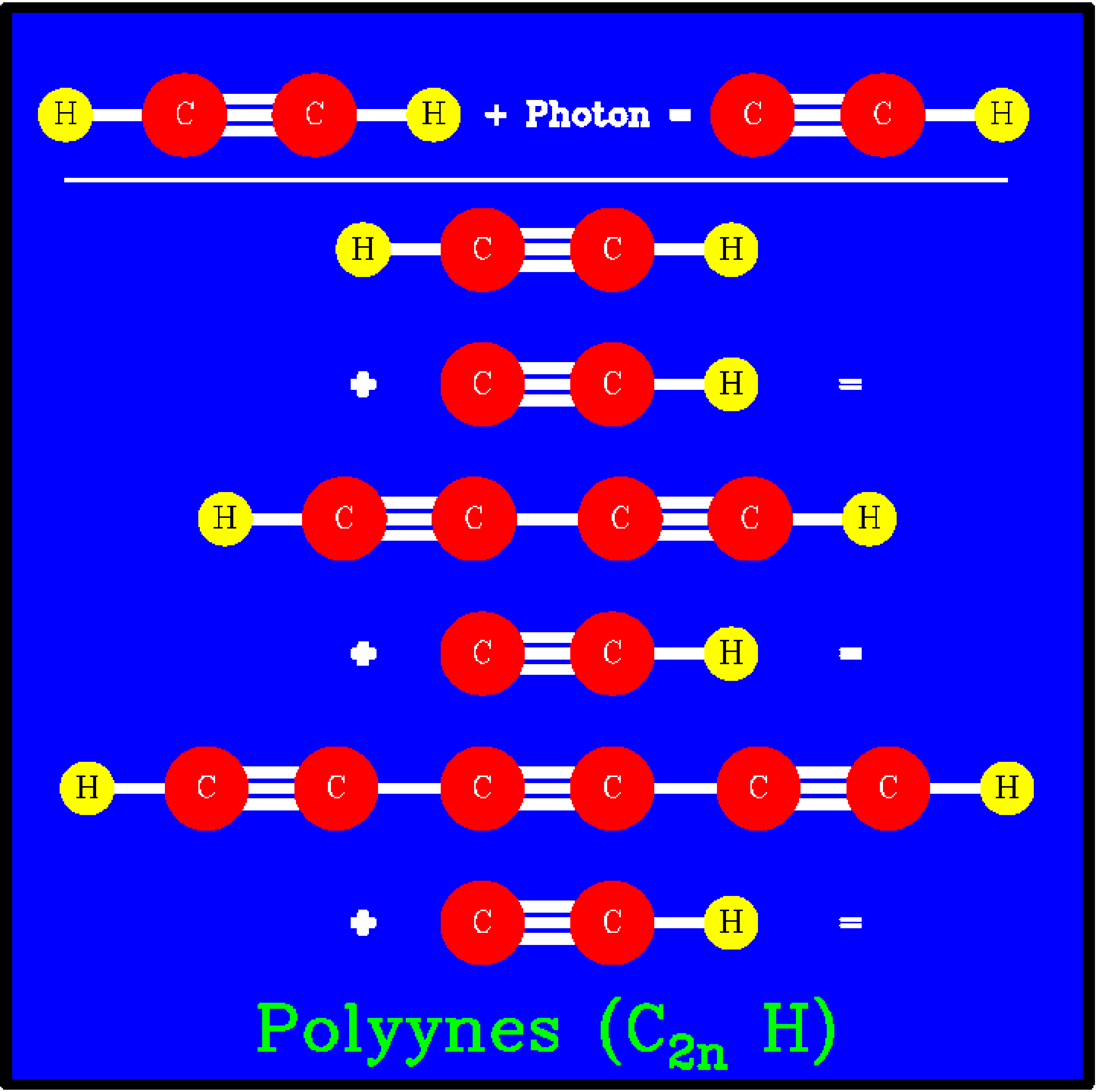

NGC7027
CRL2688
CRL618
F_L/F_c
3
2
1
1.2
1
1
0.9
5.5
6
6.5
7
$\lambda(\mu m)$


Planetary Nebula NGC 7027
HST • WFPC2
PRC96-05 • ST ScI OPO • January 16, 1996 • H. Bond (ST ScI) and NASA


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


F_L/F_C
1
0.99
0.98
0.97
C_4H_2
C_6H_2
15.8
λ (μm)
16
16.2


Zone II : H_2 protected but not CO and other species
Zone I :
H2, CO and all species photodissociated
Zone 0 :
HII Region
STAR
Zone III : H_2 and CO protected against UV photons. Hydrocarbons still photodissociated



C-rich circumstellar envelope

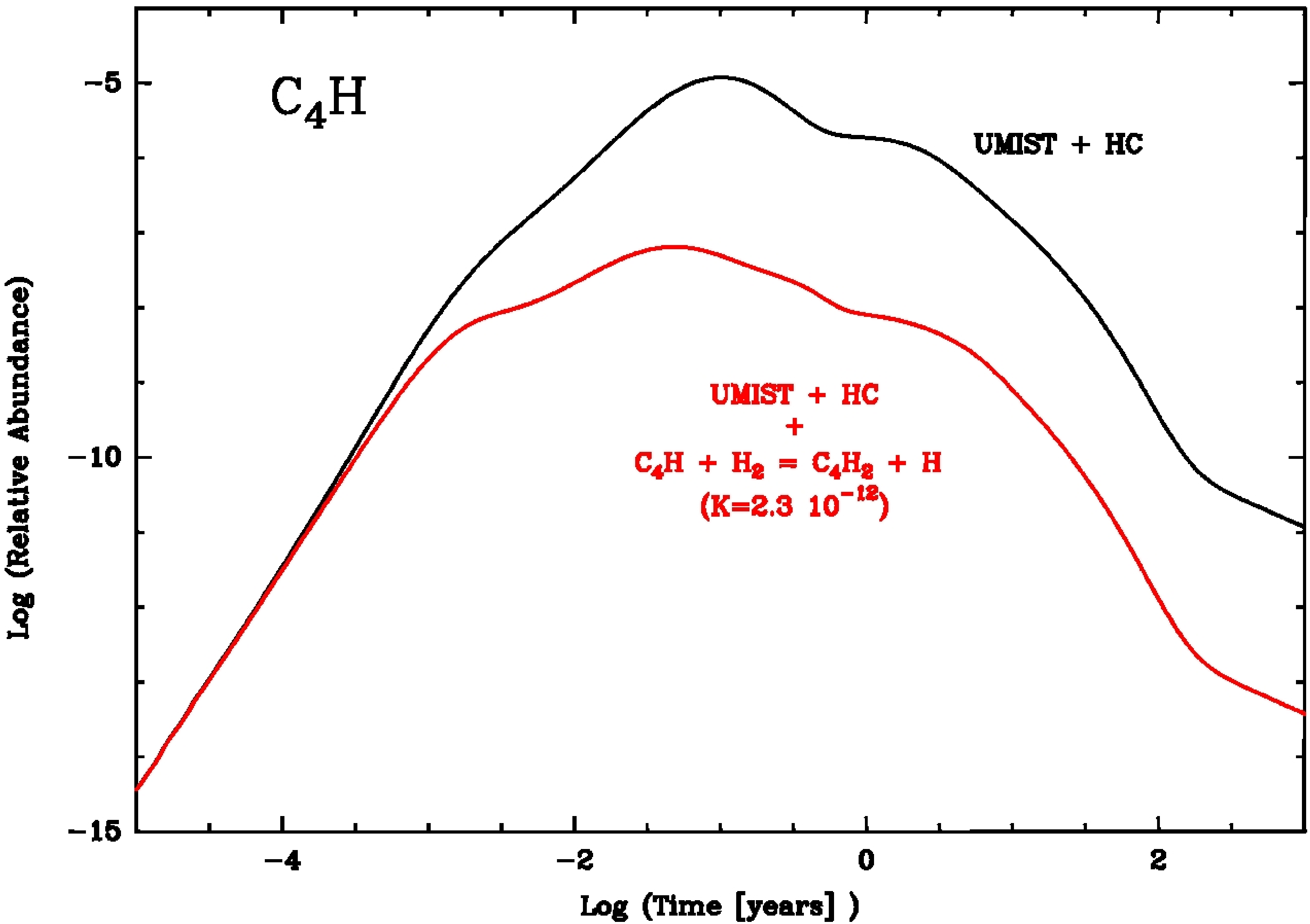
+

Photons from a hot central star

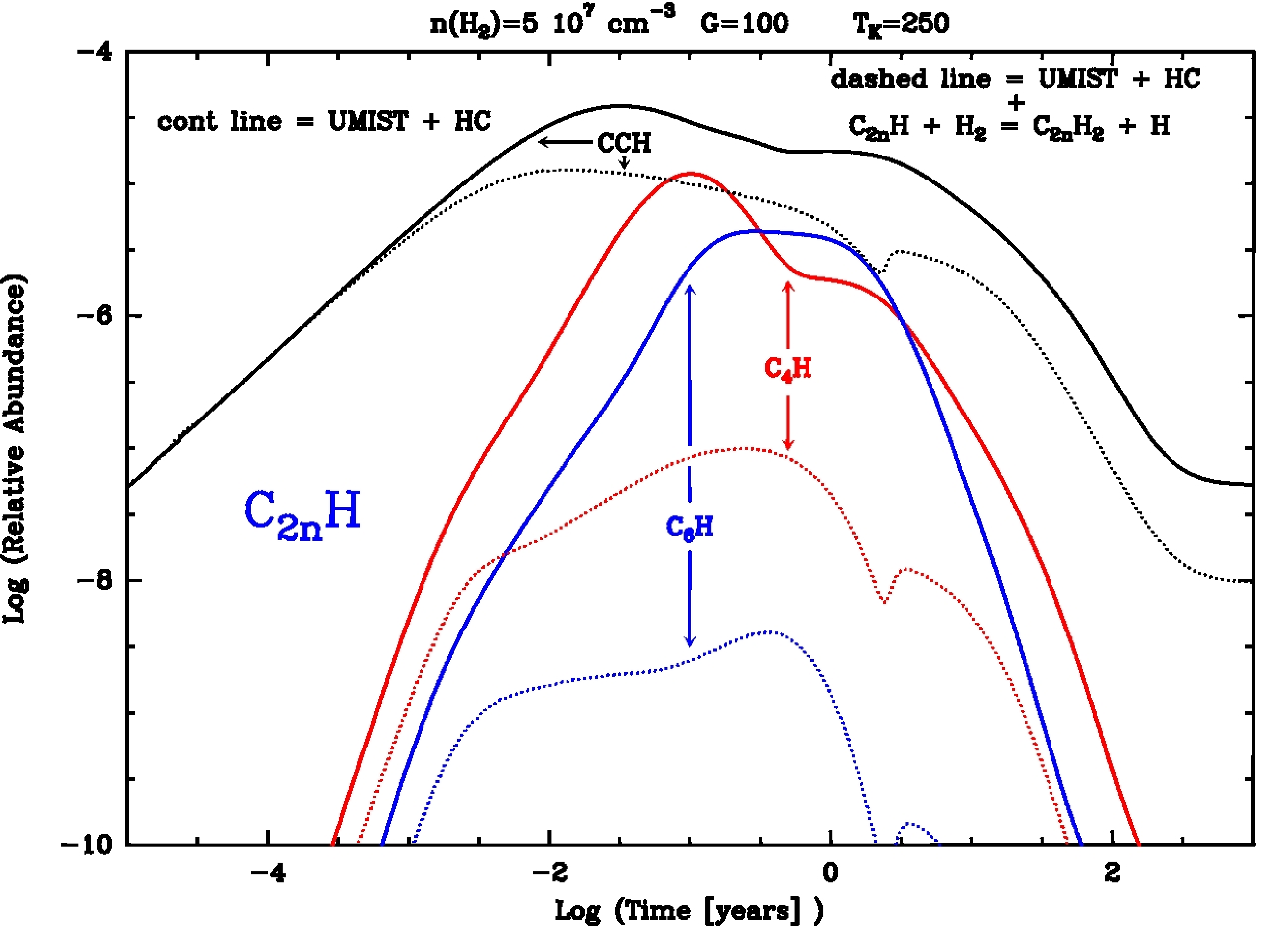
=

C-rich protoplanetary nebula. Enhancement of the abundance of polyynes.

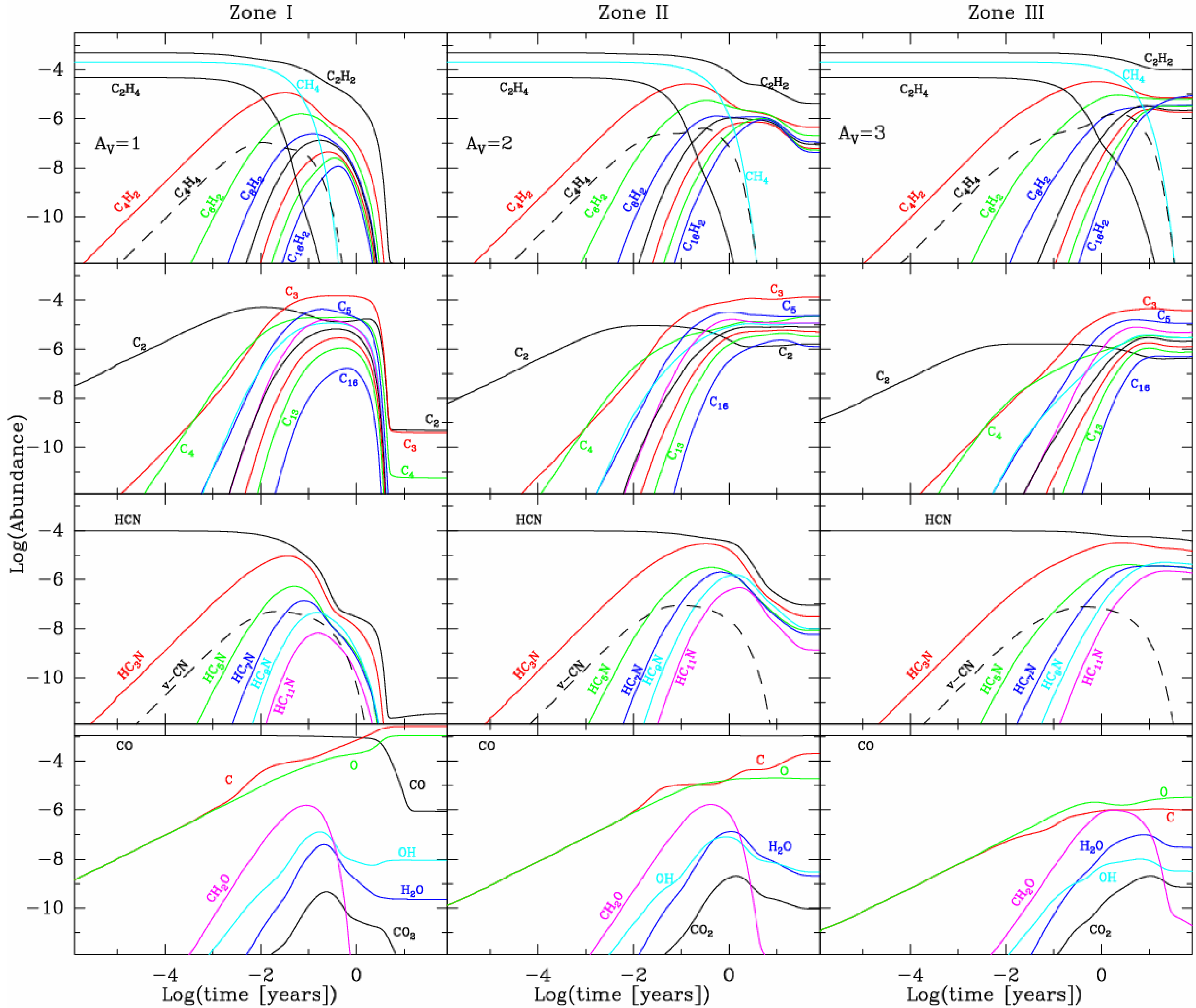
Polymerisation of acetylene.



C_4H
UMIST + HC
UMIST + HC
+
$C_4H + H_2 = C_4H_2 + H$
($K=2.3\ 10^{-12}$)
−5
−10
−15
−4
−2
0
2
Log (Relative Abundance)
Log (Time [years])



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



Zone I
Zone II
Zone III
Log(Abundance)
Log(time [years])
$A_V=1$
$A_V=2$
$A_V=3$
C_2H_2
C_2H_4
CH_4
C_4H_2
C_4H_4
C_6H_2
C_8H_2
$C_{16}H_2$
C_2
C_3
C_4
C_5
C_{13}
C_{16}
HCN
HC_3N
v–CN
HC_5N
HC_7N
HC_9N
$HC_{11}N$
CO
C
O
CH_2O
OH
H_2O
CO_2

COMPLEX ORGANIC MOLECULES IN COMETS & METEORITES:

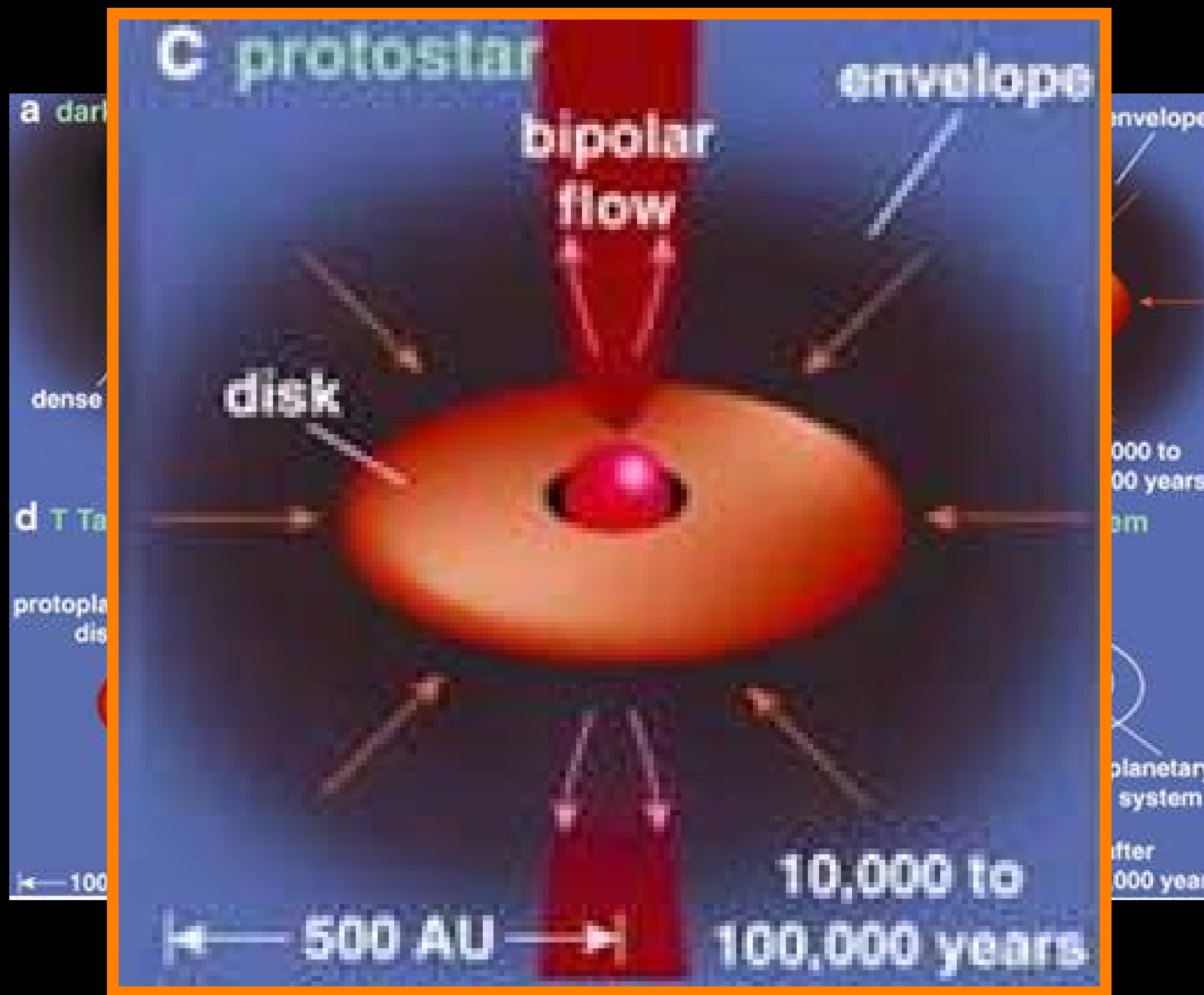
C-, O- AND N- bearing COMPLEX ORGANIC MOLECULES (COMs) ARE FOUND IN COMETS : methanol, formaldehyde, formic acid, methyl

formate, cyanoacetylene, formamide, ethyl amine, methyl amine.... (e.g. Bockelee-Morvan et al. 2000; Sandford et al. 2006)

...UP TO THE AMINO ACIDS FOUND IN THE MURCHISON METEORITE

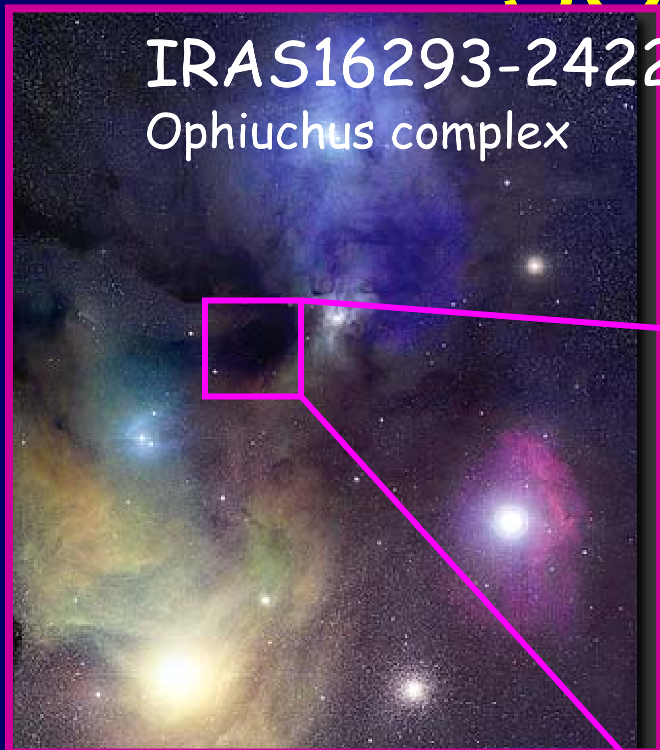
(e.g. Pizzarello et al. 2001)

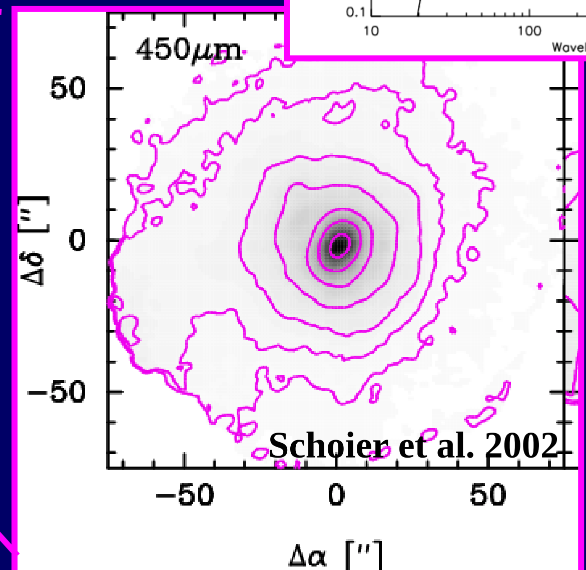
WHERE DO THEY COME FROM ?

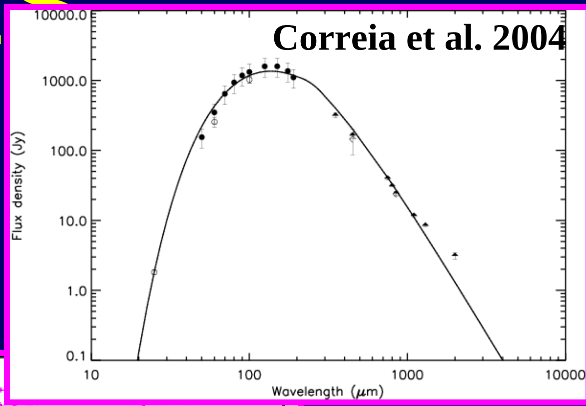


ARE COMs SYNTHESIZED ? WHEN?
WHAT? HOW MUCH? WHY?

THE YOUNGEST SUN-LIKE PROTOSTARS: CLASS 0 SOURCES

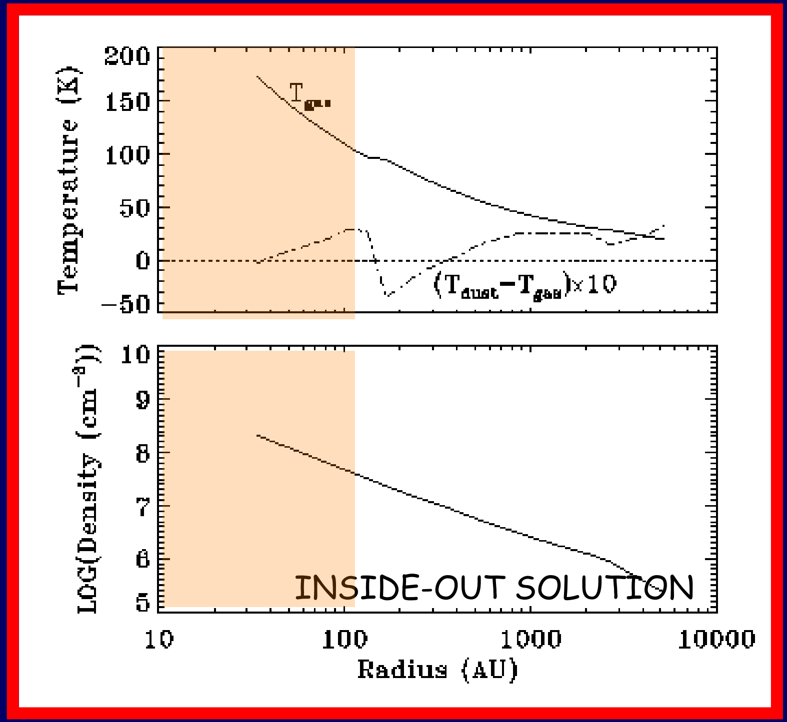


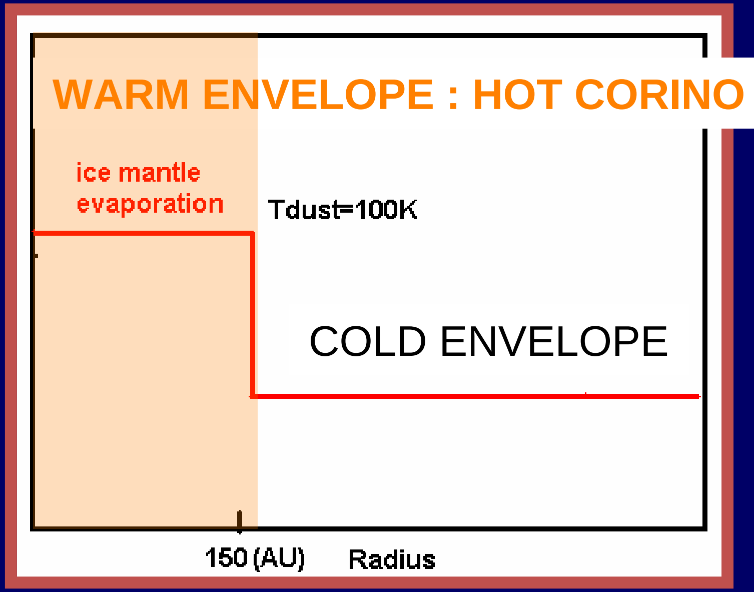




CLASS 0 ARE COLD (<30K) SOURCES OF FEW $M_{\odot}$, EMITTING MOSTLY IN THE mm/submm λs

SUN-LIKE PROTOSTAR STRUCTURE





COLD OUTER ENVELOPE: CHEMISTRY SIMILAR TO PRE-STELLAR-CORES (COLD MOLECULAR CLOUDS)

HOT CORINO ENVELOPE : CHEMISTRY DOMINATED BY THE EVAPORATION OF THE GRAIN MANTLES

HOT CORINOS : COMPACT (<150AU), WARM (~100K), DENSE (>$10^7 cm^{-3}$) REGIONS ENRICHED OF COMs

Source	Molecules	Ref.
IRAS16293-2422	HCOOH, CH_3CHO, CH_3OCHO, CH_3OCH_3, $HCOOCH_3$, CH_3CN, C_2H_5CN, CH_3CCH	Cazaux et al. 2003 ; Kuan et al. 2004; Bottinelli et al. 2004b; Chandler et al. 2005; Remijan & Hollis 2006
NGC1333-IRAS4A	HCOOH, $HCOOCH_3$, CH_3CN	Bottinelli et al. 2004a, 2007b
NGC1333-IRAS4B	$HCOOCH_3$, CH_3CN	Sakai et al. 2006, Bottinelli et al. 2007a
NGC1333-IRAS2A	CH_3CN , CH_3OCH_3	Jorgensen et al. 2005; Bottinelli et al. 2007a

HOW ARE COMs FORMED ?

GAS PHASE versus GRAIN SURFACES

GAS PHASE FORMATION

THREE STEPS:

1. MANTLE FORMATION DURING PRE-COLLAPSE → H_2CO, CH_3OH & NH_3….
2. MANTLE SUBLIMATION e.g. BECAUSE OF THE HEATING OF THE FORMING STAR
3. GAS PHASE REACTIONS BURN H_2CO & CH_3OH and FORM MORE COMPLEX COMs

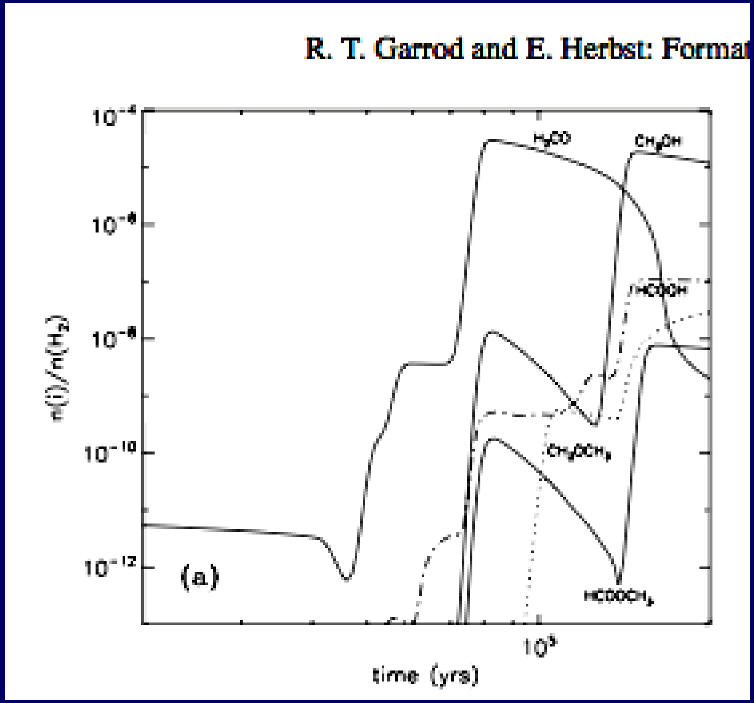
« OLD » MODELS SEEMED TO REPRODUCE OBSERVATIONS BUT… NEW LAB EXPERIMENTS CHALLENGE THE USED REACTION ROUTES AND RATES

NO CURRENT MODELS REALLY ACCOUNT FOR THE OBSERVED ABUNDANCES

GRAIN SURFACES FORMATION

TWO STEPS:

1. MANTLE FORMATION DURING PRE-COLLAPSE → H_2CO, CH_3OH & NH_3….
2. MANTLE SUBLIMATION e.g. BECAUSE OF THE HEATING OF THE FORMING STAR



NO CURRENT MODELS REALLY ACCOUNT FOR THE OBSERVED ABUNDANCES

HOW ARE COMs FORMED ?

GAS PHASE versus GRAIN SURFACES

TOO LITTLE IS KNOWN → LABORATORY EXEPERIMENTS + THEORY ARE NEEDED !

Chemistry in Planetary disks : The role of strong UV field

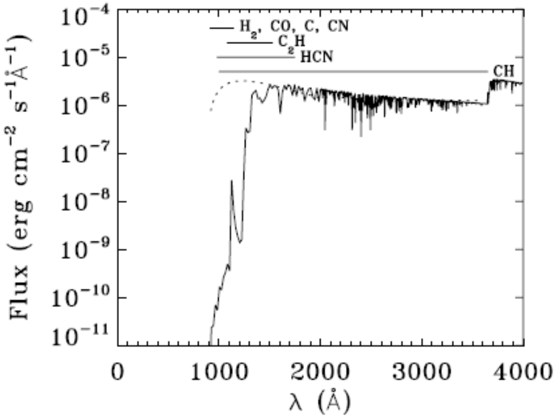
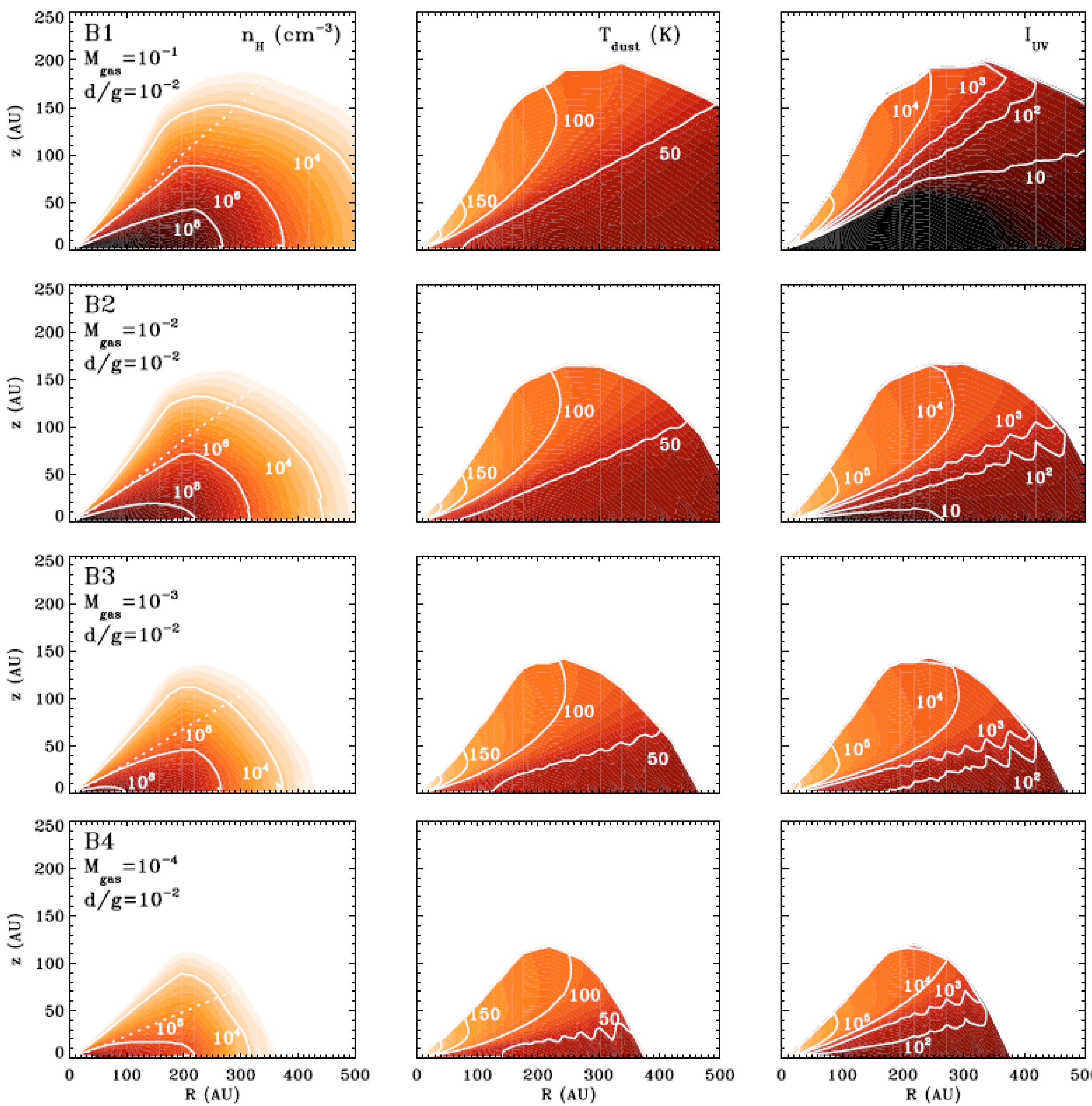
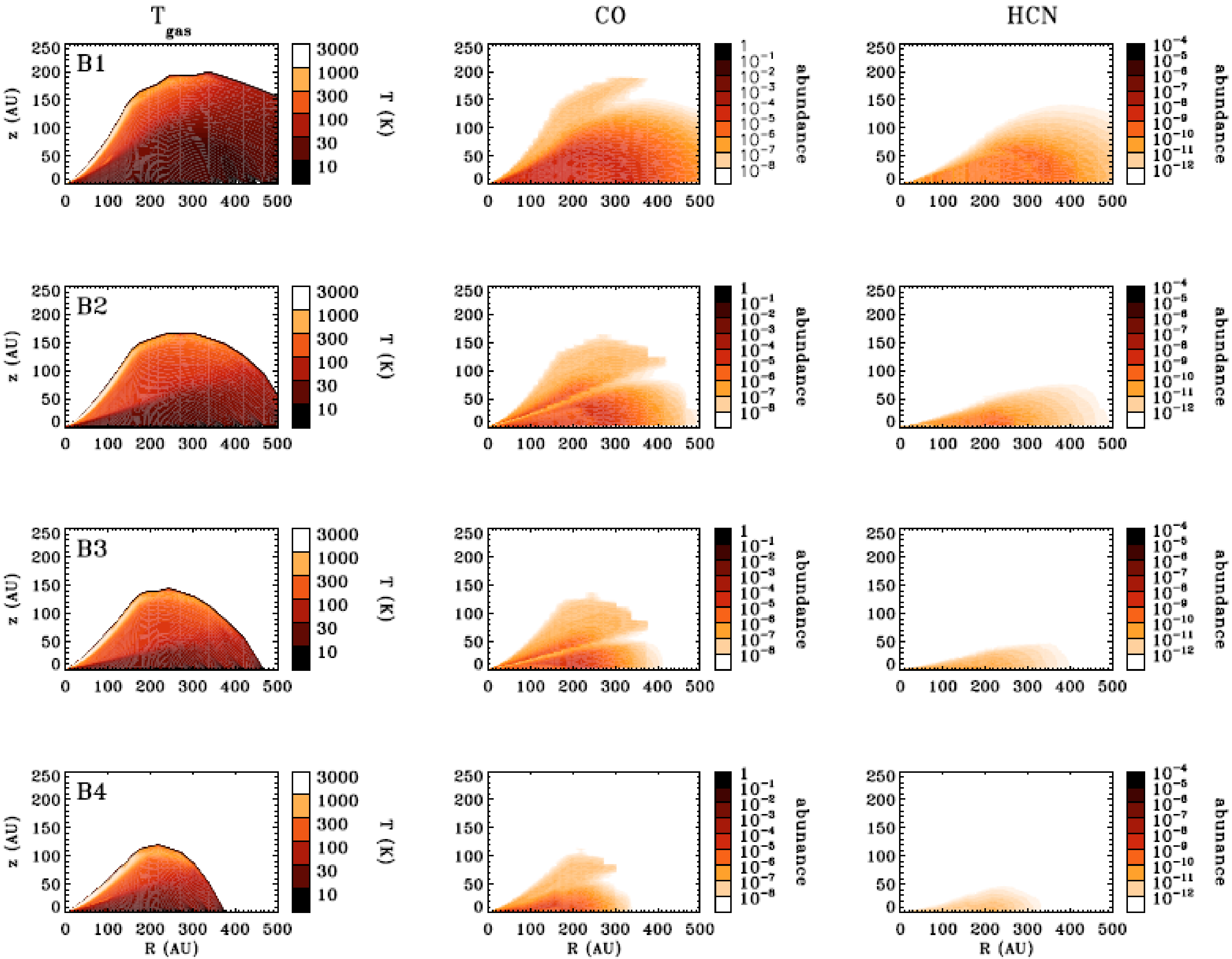


Fig. 3. The radiation fields used in the model. The solid line gives the stellar radiation field, scaled to the interstellar UV field by Draine (1978) (dotted line). The horizontal lines indicate the wavelength ranges where several important molecules are dissociated.

B. Jonkheid et al.: Chemistry and line emission from evolving Herbig Ae disks





HCN abundances below 10^{-8}; but 10^{-5} needed !!!!

Formation of organic molecules in oxygen-rich UV illuminated environments

Marcelino Agúndez and José Cernicharo

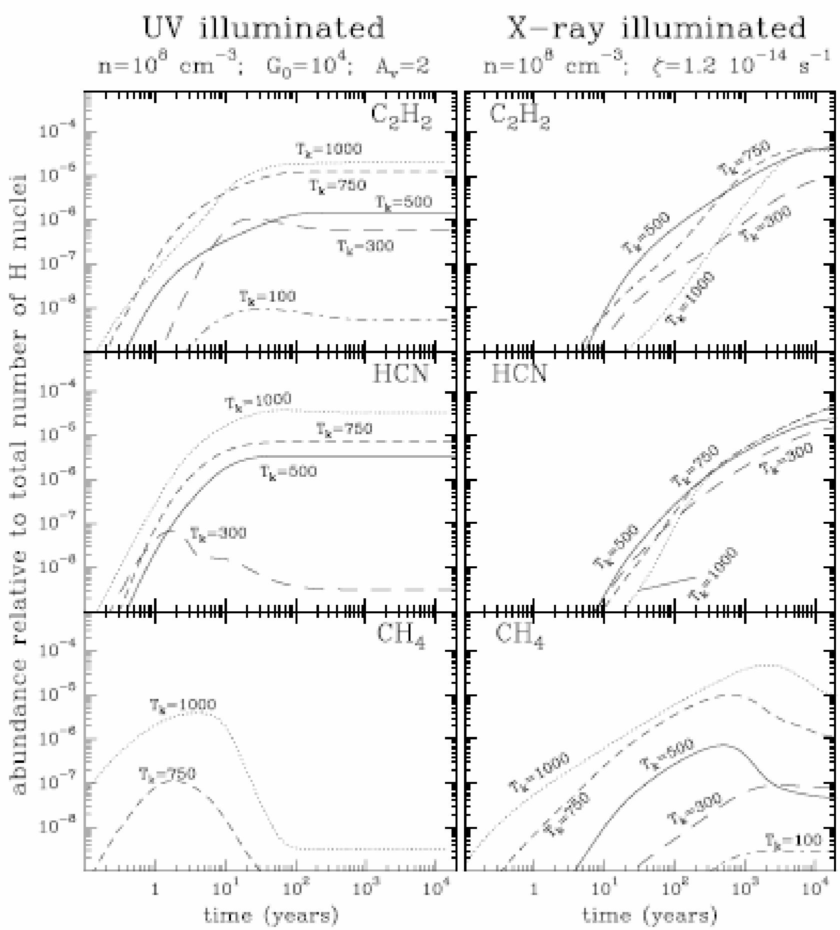


Fig. 2. Evolution of C_2H_2, HCN and CH_4 abundances for a chemistry driven by far-UV photons (left) and by X-rays (right). Different curves correspond to different gas temperatures.

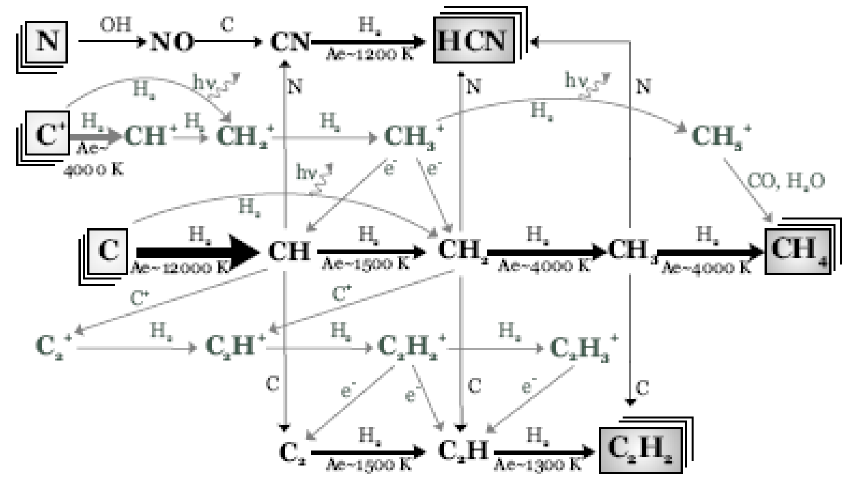


Fig. 3. Scheme with the main synthetic routes for the formation of C_2H_2, HCN and CH_4 from C, C^+ and N. Reactions with a high activation energy (Ae) are indicated by a thick arrow.

Radicals + H_2 very efficient at high T_K and high densities !!

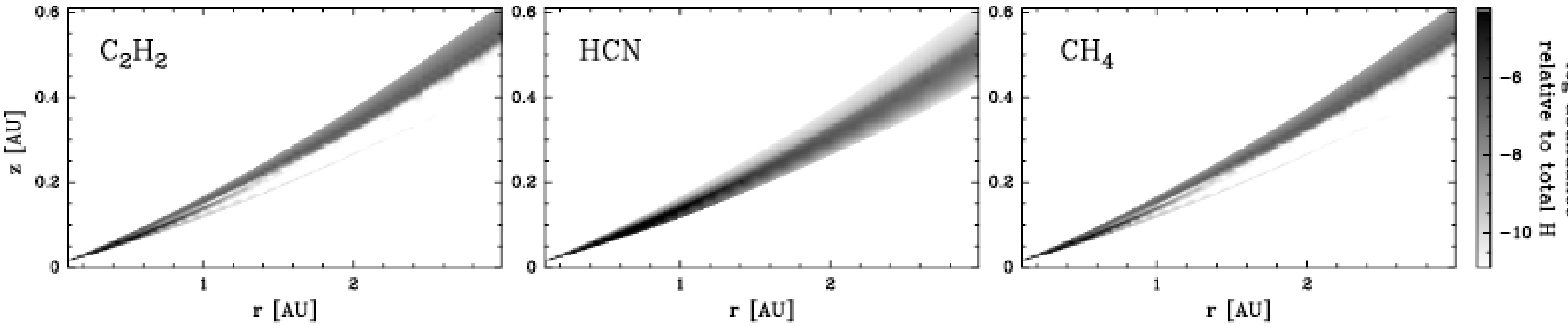


Fig. 4. Distribution of C_2H_2, HCN and CH_4 abundances in the photodissociation region of the inner 3 AU of a protoplanetary disk.

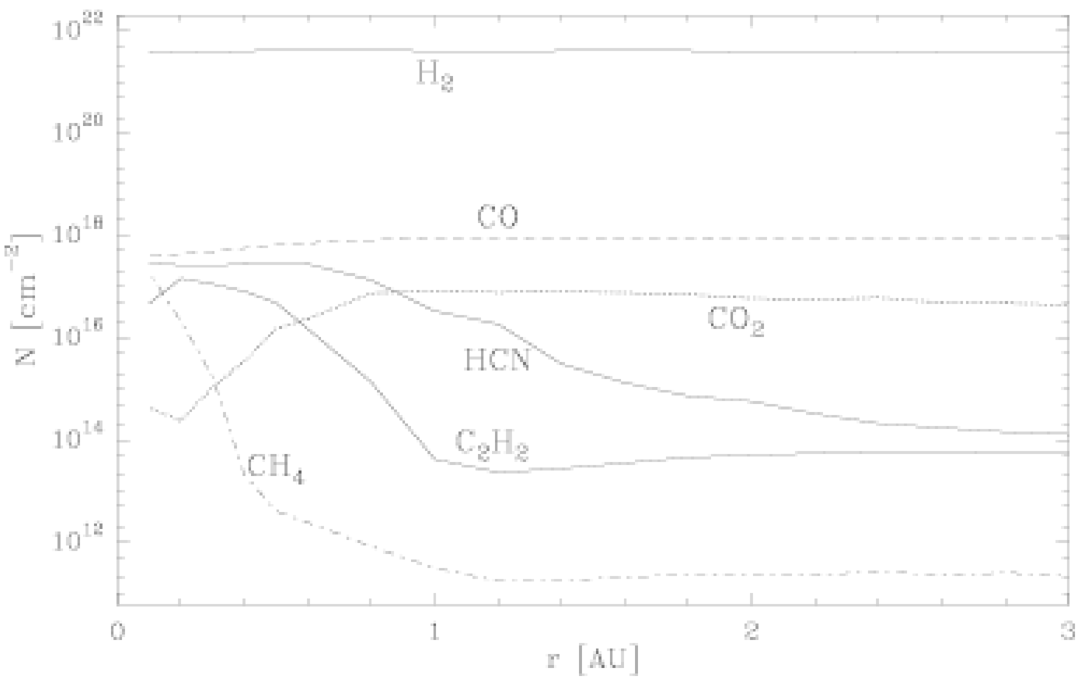


Fig. 5. Vertical column densities within the photodissociation region of the inner 3 AU of a protoplanetary disk.

Geers et al., 2006

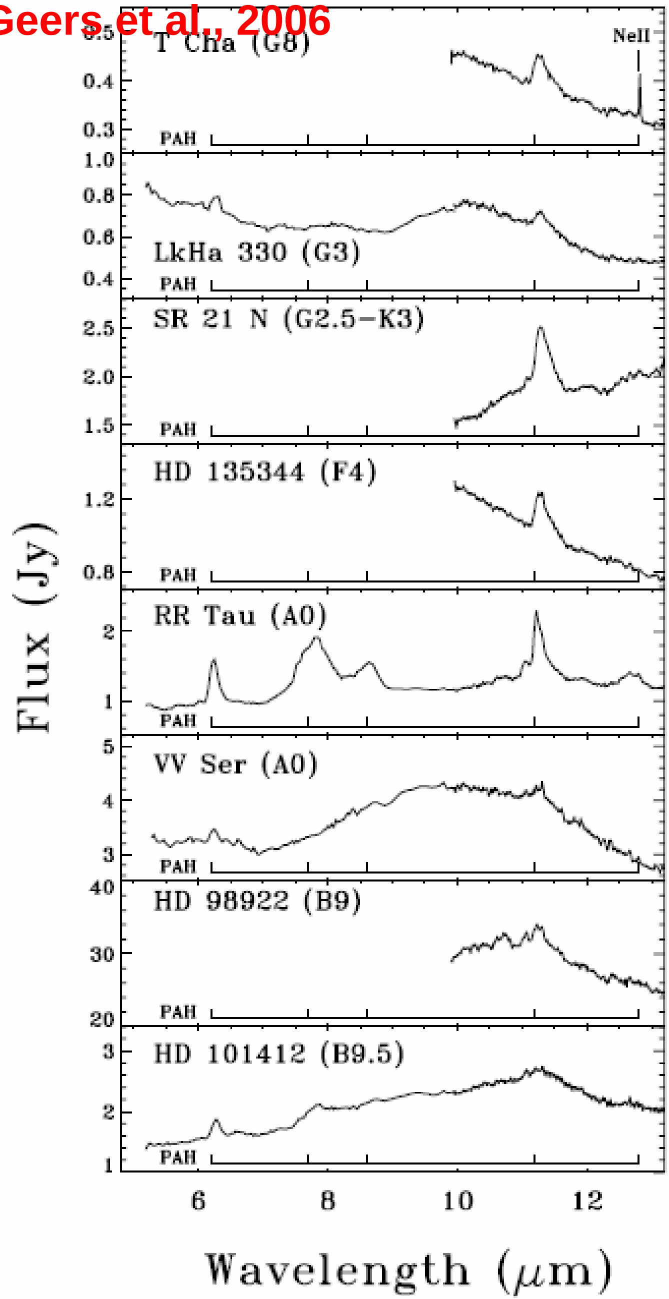


Fig. 1. Spitzer IRS spectra of sources with PAH features, comprised o the SL (5–10 μm) and SH (10–20 μm) modules. The location of PAH features is indicated with markers at 6.2, 7.7, 8.6, 11.2 and 12.8 μm.

Missing chemistry ?
Missing physical processes ?
Role of turbulence in planetary disks
How molecules are formed and can survive near the central star (C_2H_2, HCN,…)
What is the role of dust grain chemistry ?

New observations, new generation of Instruments :
Herschel (IR), ALMA (mm/submm)
IR high spectral resolution ? (ground based)
UV (electronic transitions of most abundant molecules; high spectral resolution needed) –WSO-