Les chaines carbonées dans l'atmosphère de Titan

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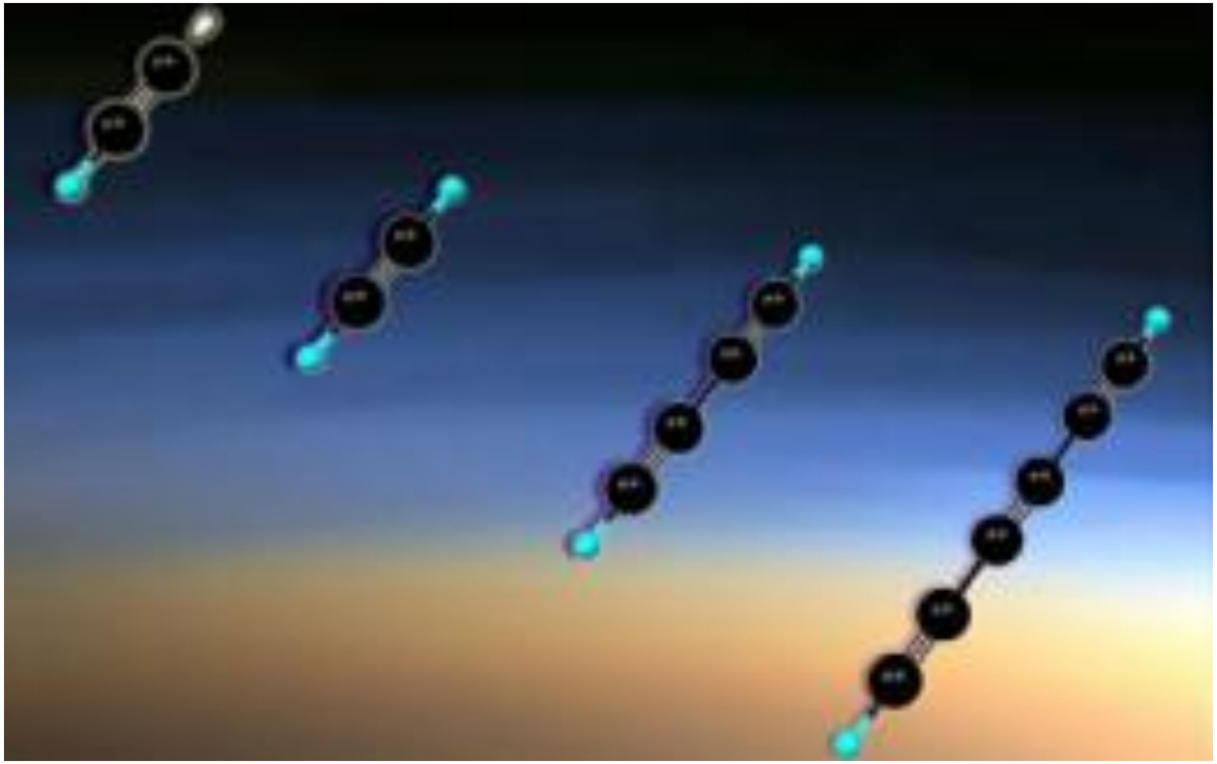
H−C≡C−C≡N

H−C≡C−H

H−C≡C−C≡C−H



N≡C−C≡N

C2H2, C4H2,…C6H2, HC3N, ….HC5N, C2N2, …..C4N2

ESEP, Paris, 07.11.2013

The LISA « Spectroscopy group for Planetology » in CRETEIL (Université Paris-Est)

- Synthesis and purification of organic molecules and isotopes.
- Absolute band intensity measurements on pure samples.
- High resolution spectra and global line analysis (positions, intensities).
- Line lists for the CIRS team, GEISA and HITRAN databases.

Synthesis are done in Créteil or in Rennes (J-C. Guillemin group).
Experiments in the infrared are done in Créteil, Paris and the SOLEIL synchrotron facility in Saclay (Far infrared domain).
Theoretical developments are done in Créteil, Université de Bruxelles (Michel Herman group) and Louvain la Neuve (Pr. André Fayt)

- Band Intensity measurements for: HC_3N, HC_5N, C_4H_2, C_6H_2, C_8H_2, C_2N_2, C_4N_2
  ….and also for isotopes: C_2HD, DC_3N, $HC_3{}^{15}N$, DC_5N, $NCC^{15}N$
- Line lists have been completely renovated: HC_3N, C_4H_2, C_2N_2.
  ………..and others where newly introduced: C_2HD, $H^{13}CCCN$, $HC^{13}CCN$, $HCC^{13}CN$, $HCCC^{15}N$, $H^{13}CCCCH$, $HC^{13}CCCH$, $N^{13}CCN$, $^{15}NCCN$.

All the new line lists have been used by the CIRS Team to improve the analysis of the observation of Titan's atmosphere by the CASSINI-CIRS instrument.

- Refinements for the abundance of already detected species: HC_3N, C_4H_2, C_2N_2
- First detection and abondance determination for isotopic species: C_2HD, $H^{13}CCCN$, $H^{13}CCCCH$.
- Still looking for $^{15}NCCN$, $HCCC^{15}N$ ………………..and also C_6H_2, HC_5N and **C_4N_2**

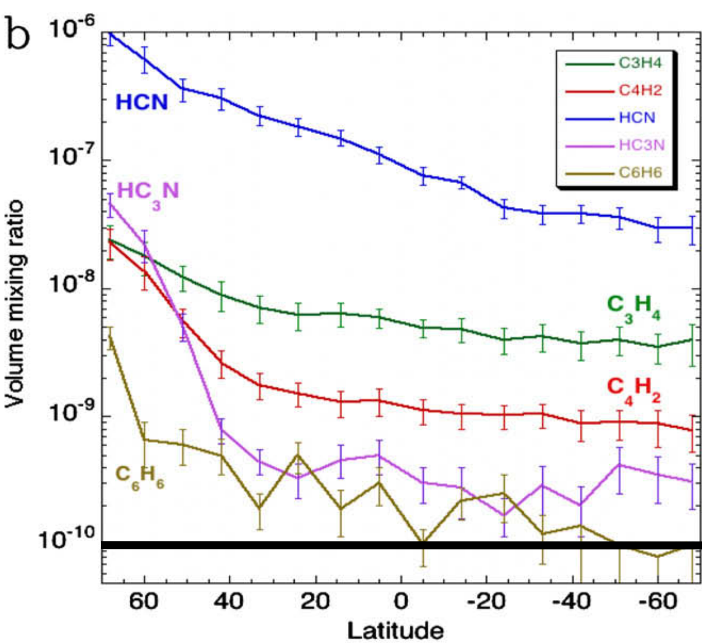
Searching for longer carbon chains:

Interstellar medium: in the microwave $HC_{11}N$ (Bell et al 1982)
Circumstellar medium: HC_5N et C_6H_2 in the infrared (CRL618) (Cernicharo et al. 2001)

C_6H_2 :
622 cm^{-1} (Shindo et al. 2003)
UV (Shindo et al. 2003)
105 cm^{-1} (measured in 2012)
C_8H_2 :
621.5 cm^{-1} (Shindo et al. 2001)

HC_5N :
642 cm^{-1} (Benilan et al. 2007)
VUV (Fray et al. 2010)

C_4N_2:
472 cm^{-1} (Khlifi et al. 1997)
107 cm^{-1} (measured in 2012)
VUV et UV (to be published)

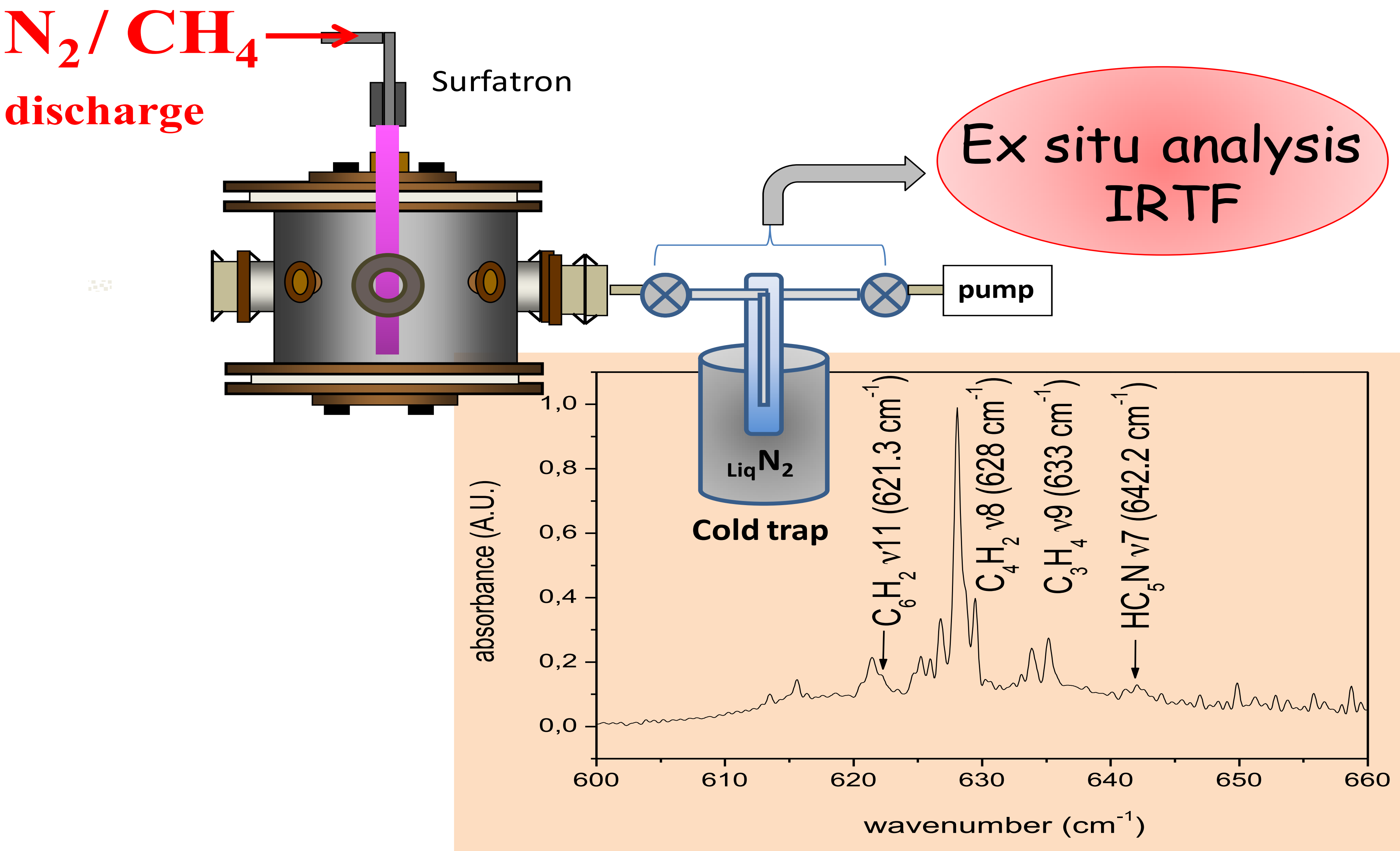


Detection of $^{13}C_4H_2$: 2-3 10^{-10}
C_6H_2 / C_4H_2 < 1 %

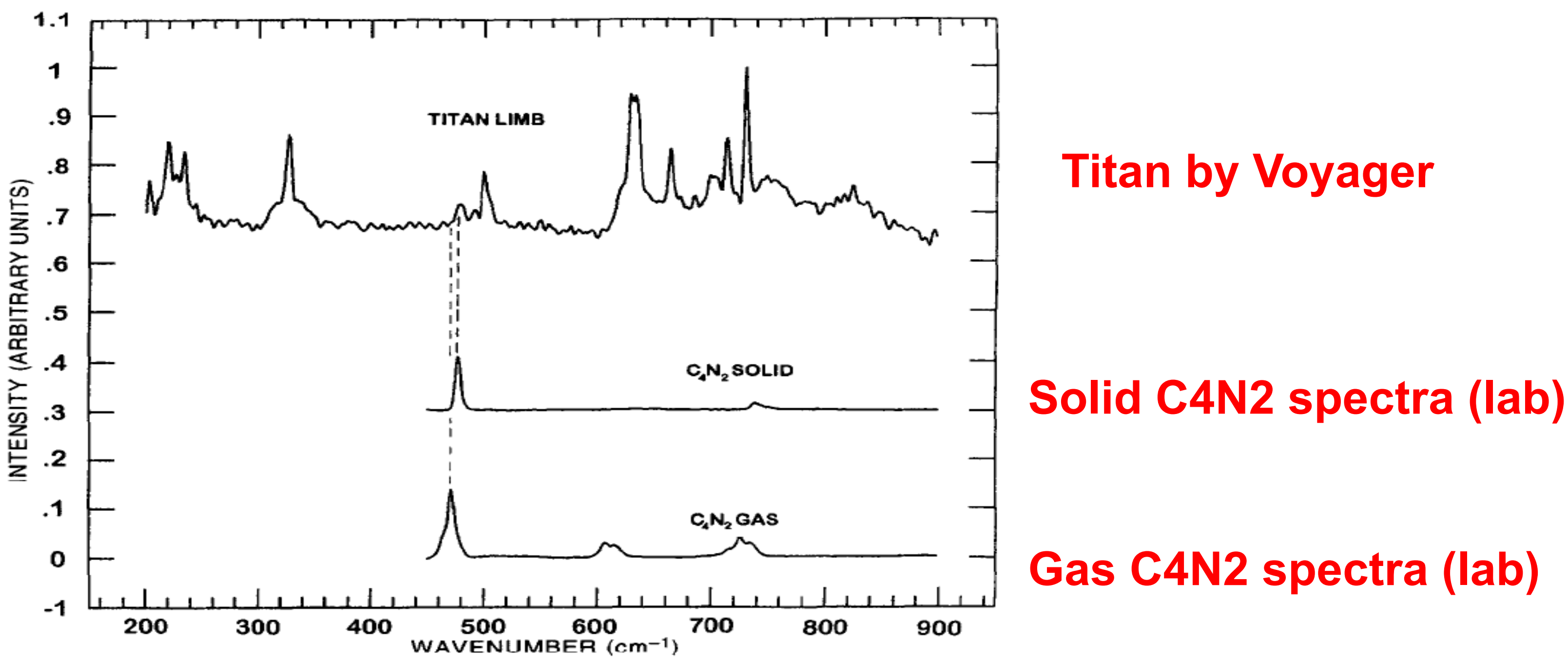
Abundance max HC_3N: 5 10^{-8}
Abundance min HC_3N: 7 10^{-11}

Detection limit: about 10^{-11}-10^{-10}

Long carbon chains can be found ……………………………in the laboratory by simulating Titan's atmosphere.



One long carbon chain has already been identified in Titan's atmosphere: C_4N_2 in the solide phase (Khanna et al. 1987)!



R. E. Samuelson *et al.: C4N2 ice in Titan's north polar stratosphere, Planet. Space Sci., Vol. 45, No. 8, pp. 941-948, 1997*

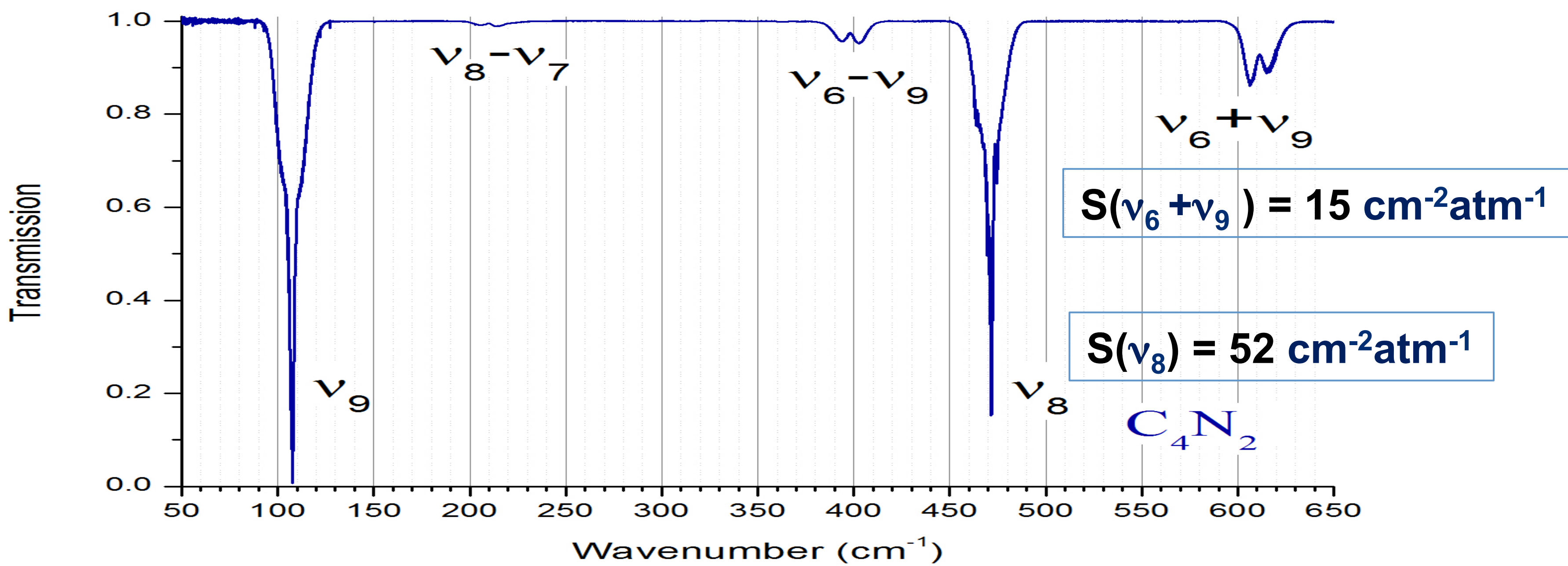
But where is the gas phase?

- Condensate to vapor ratio is two orders of magnitude greater than expected under steady state conditions (Samuelson 97, de Kok 2008)?
- **Is solid C_4N_2 confirmed by CASSINI-CIRS ?**
- **Is gaseous C_4N_2 observed? If not, what is the gaseous abundance upper limit for C_4N_2 ?**

Gaseous abundance Upper limits of C_4N_2 using old experimental spectroscopy work:

- $4\ 10^{-10}$ from ν_8 band (472 cm^{-1},Samuelson 97 (abs coeff = 5.2 $cm^{-2}atm^{-1}$)
- $9\ 10^{-9}$ (winter pole) from $\nu_6 + \nu_9$ band (614 cm^{-1},de Kok 08) (abs coeff = 34.4 $cm^{-2}atm^{-1}$)

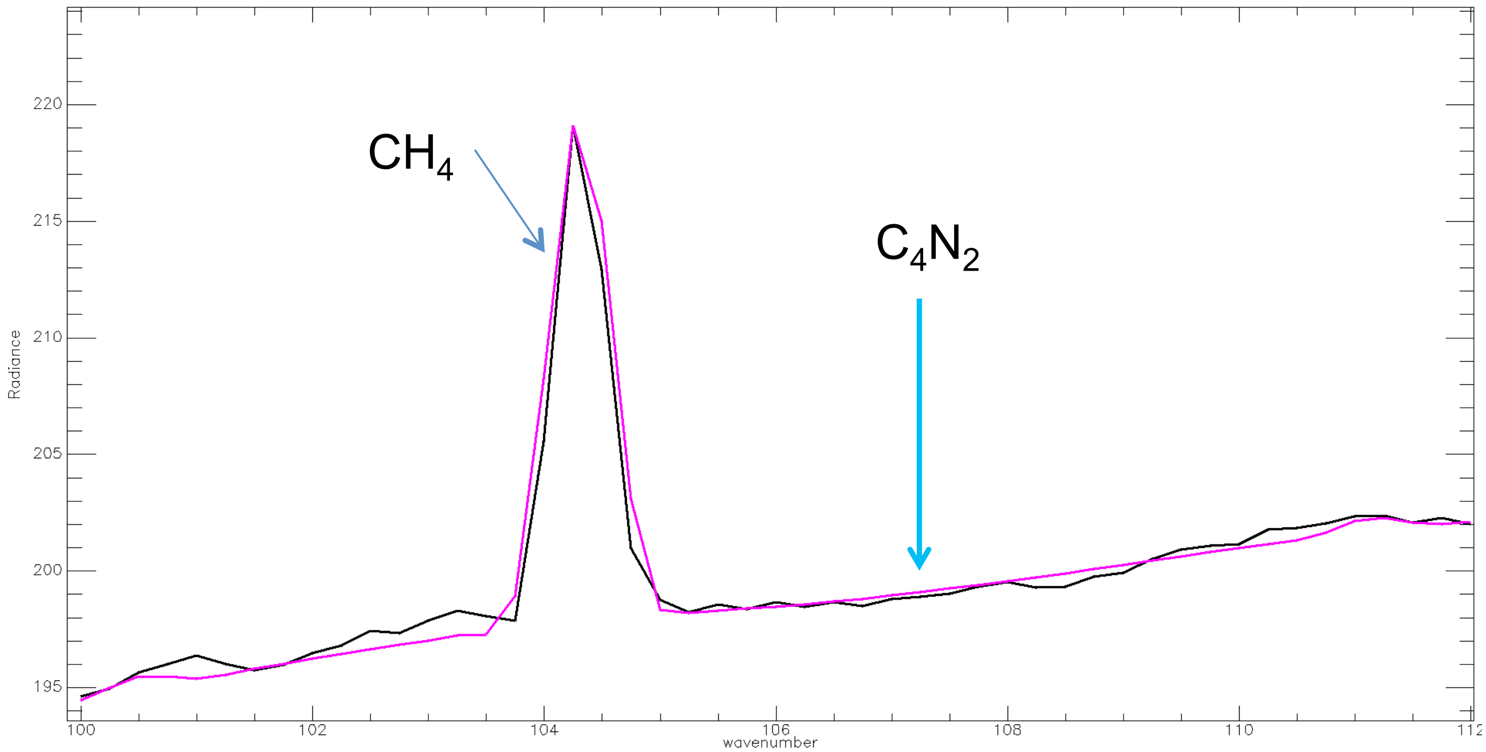
New experimental work on C_4N_2 : Infrared spectra from 50 to 650 (cm^{-1})



Experimental results for C_4N_2 : First intensity measurements for the 107 band:

- Samuelson's abundance upper limit is to be reduced to: $4\ 10^{-11}$
- Intensity for ν_9 (107 cm^{-1}) larger than for ν_8 (472 cm^{-1})! Surprise!
- **C_4N_2 at 107 cm^{-1} ????**

Average of 1888 CIRS nadir spectra of Titan Northern (60° – 90°) winter (2007), where the gas is predicted to increase substantially. No C_4N_2 is observed.

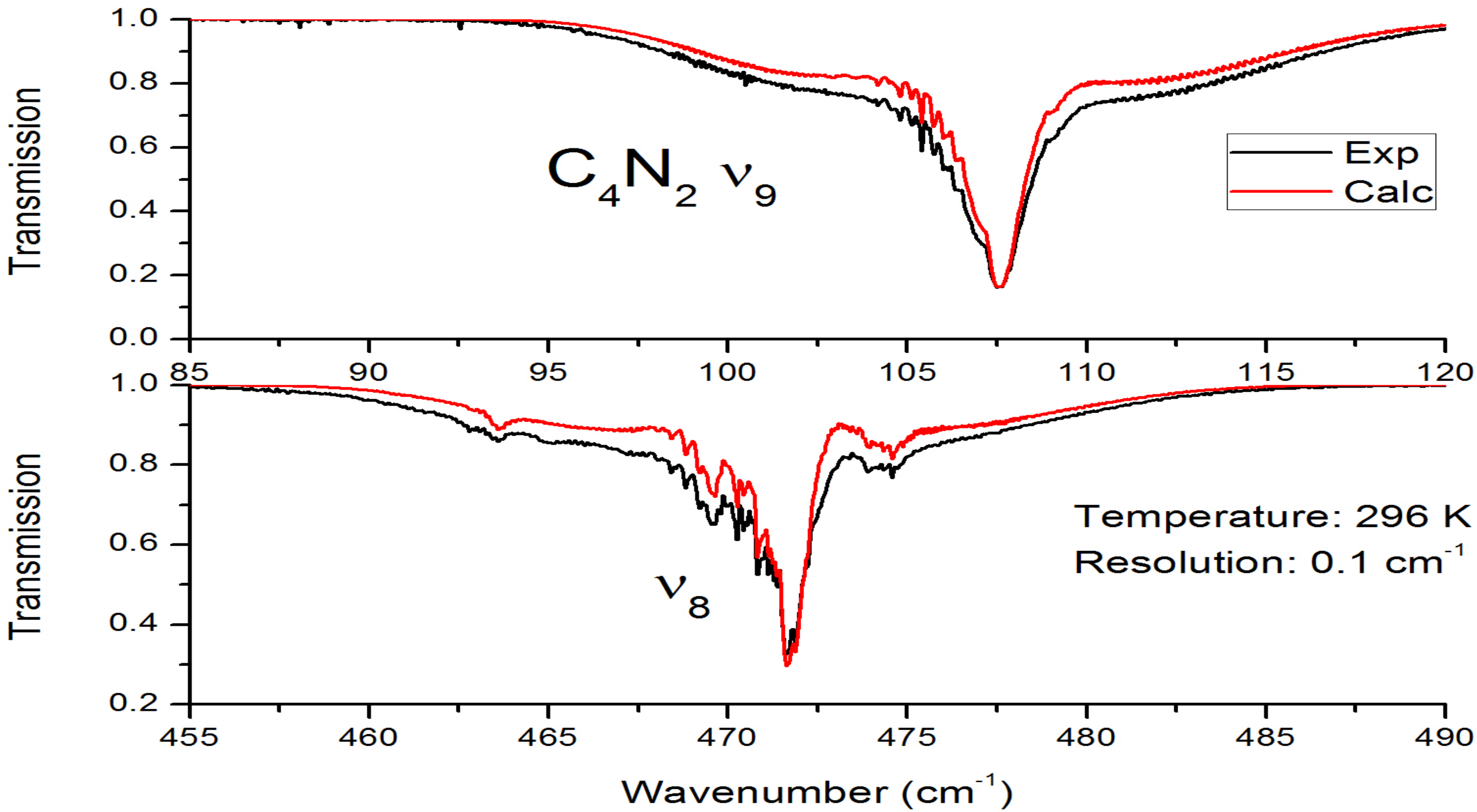


Upper limit determination of gaseous C_4N_2 using 107 cm^{-1} band:

- Using a radiative transfer code and a line list.
- Comparing with another observed molecule.

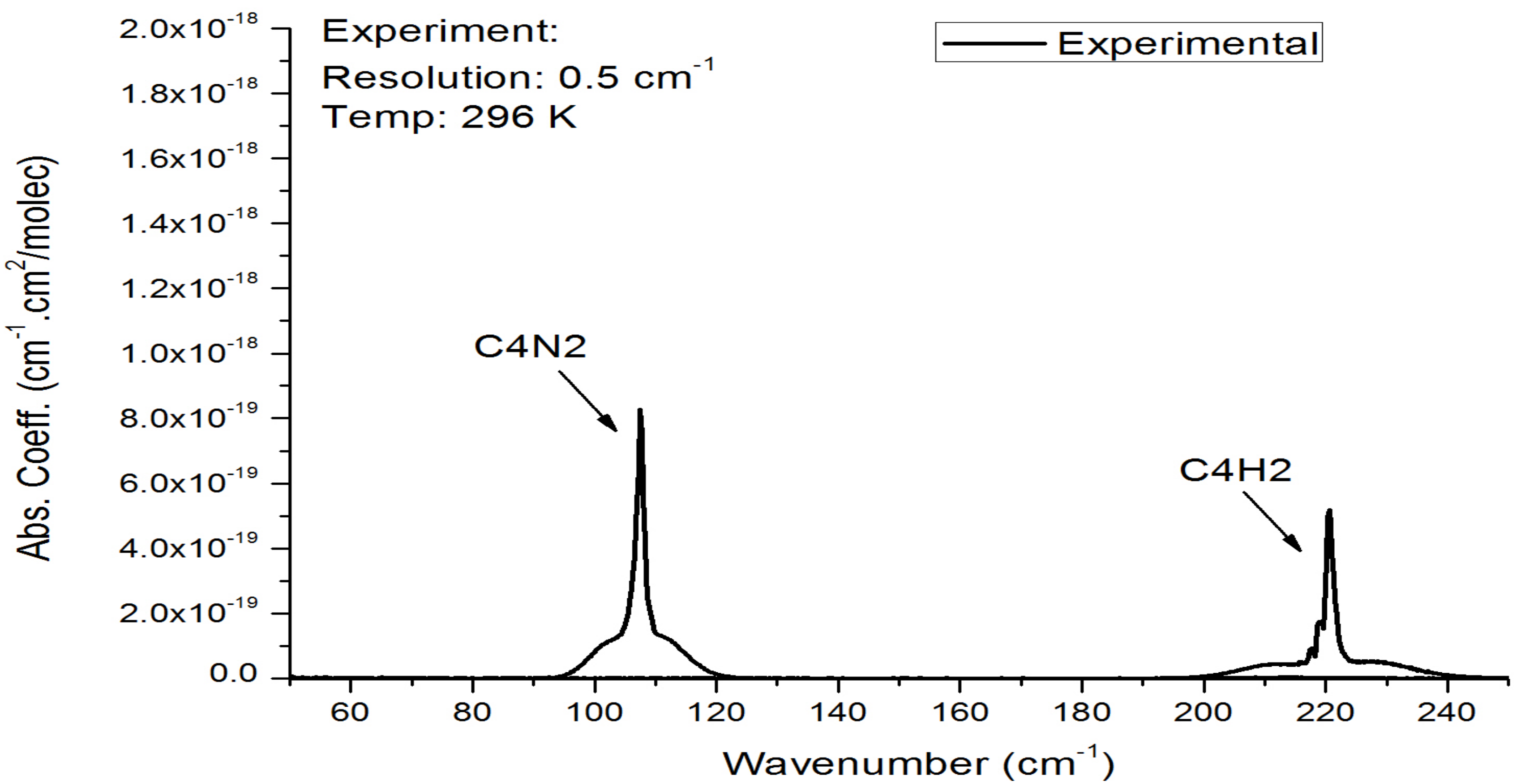
The first line list of C4N2 has been computed thanks to the global analysis method developped by Pr. André Fayt:
Only problem: it contents 468 198 lines (only for ν_9) !!!

Comparison between room temperature lab spectra of C_4N_2 and calculated spectra using the new line list.



- Introducing the C4N2 line list in the radiative transfer code not yet possible.
- Other method: comparing with C4H2 band at 220 cm^{-1}.

Both bands are similar in intensity and in shape. Peak maximum of C_4N_2 is stronger.



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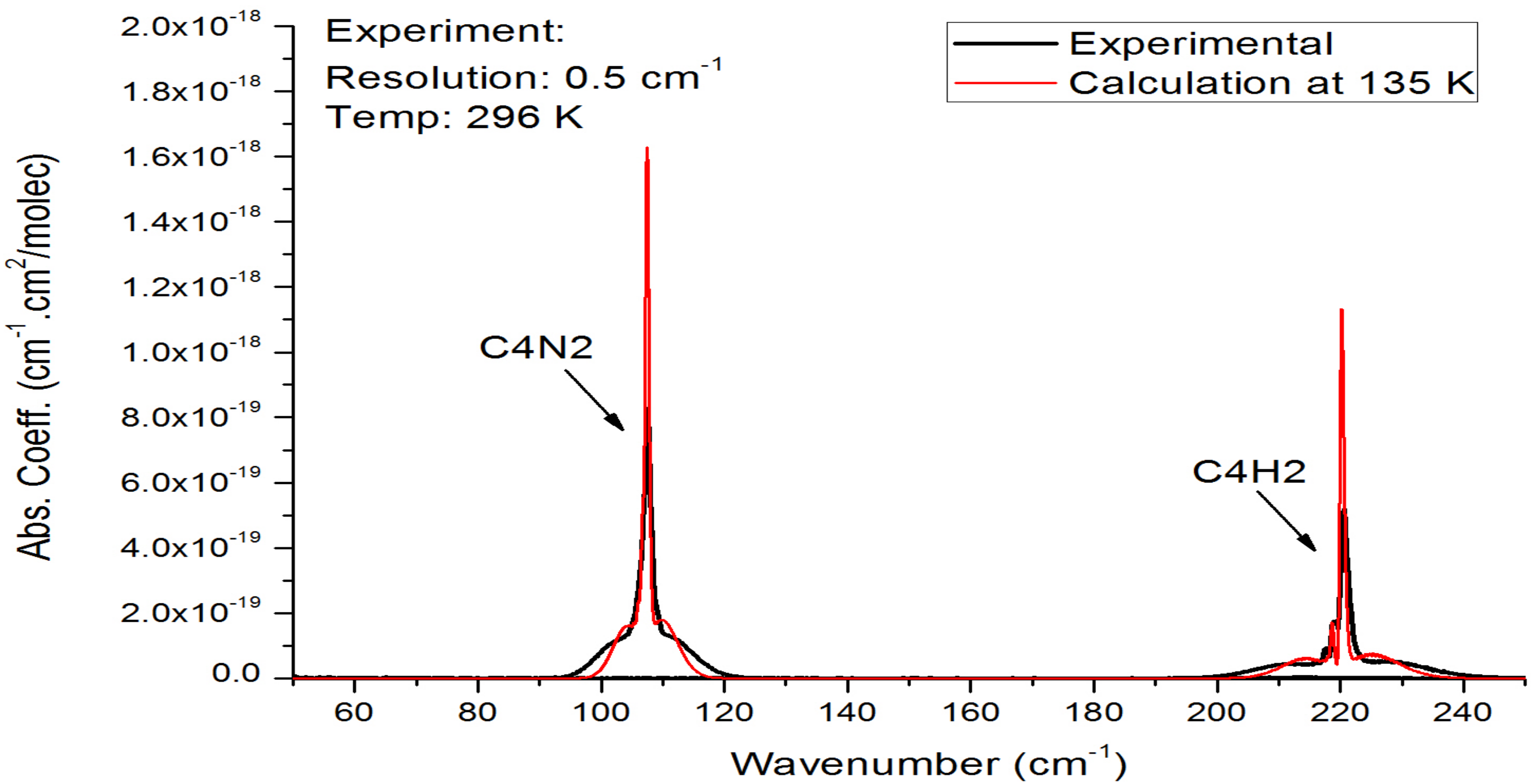
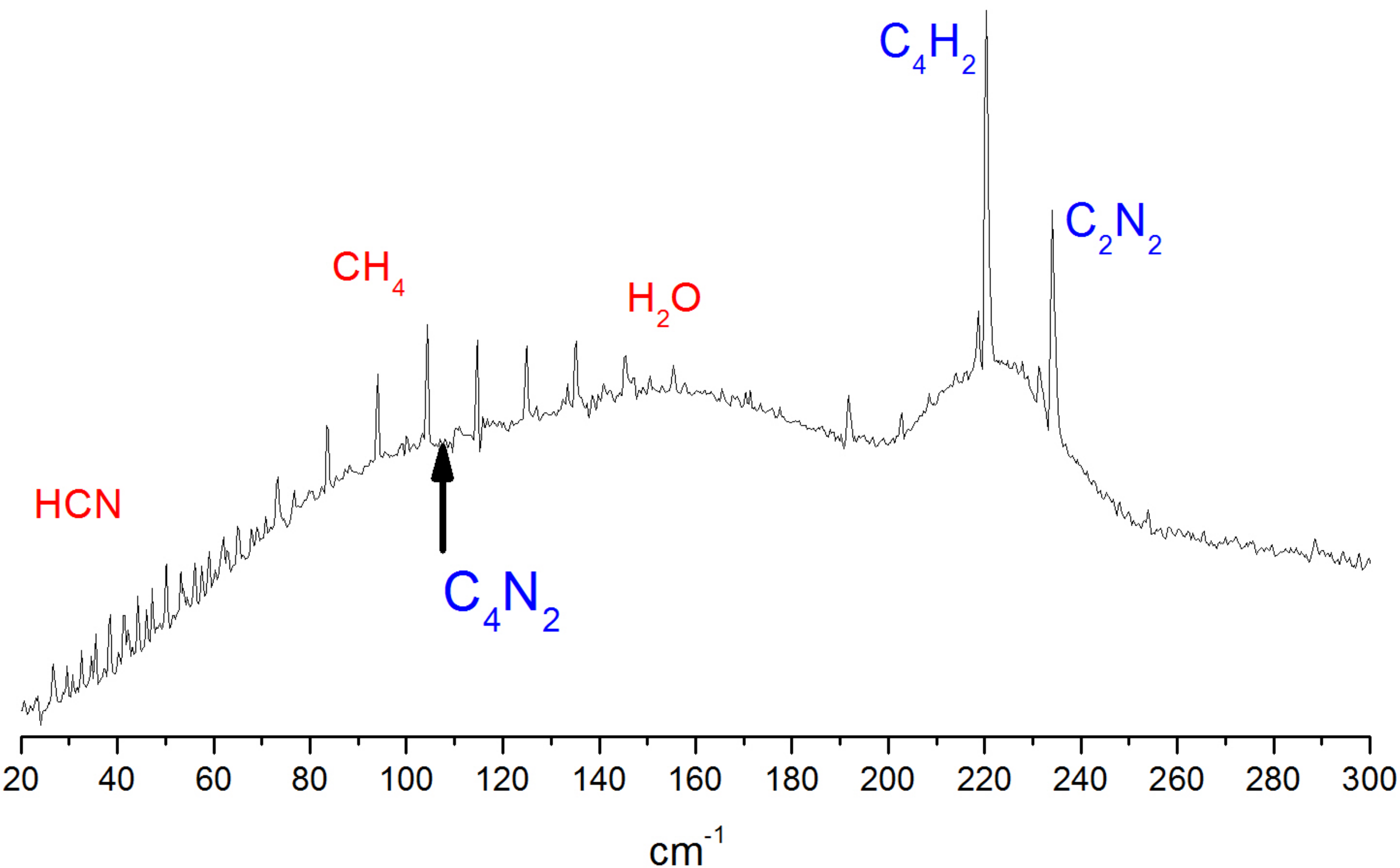
Both bands are similar in intensity and in shape. Peak maximum of C_4N_2 is stronger. The line list is used to predict the ratio of the peak maxima of both bands at 135 K = 1.45



Titan in the far infrared by CASSINI-CIRS



C_4N_2 upper limit determination

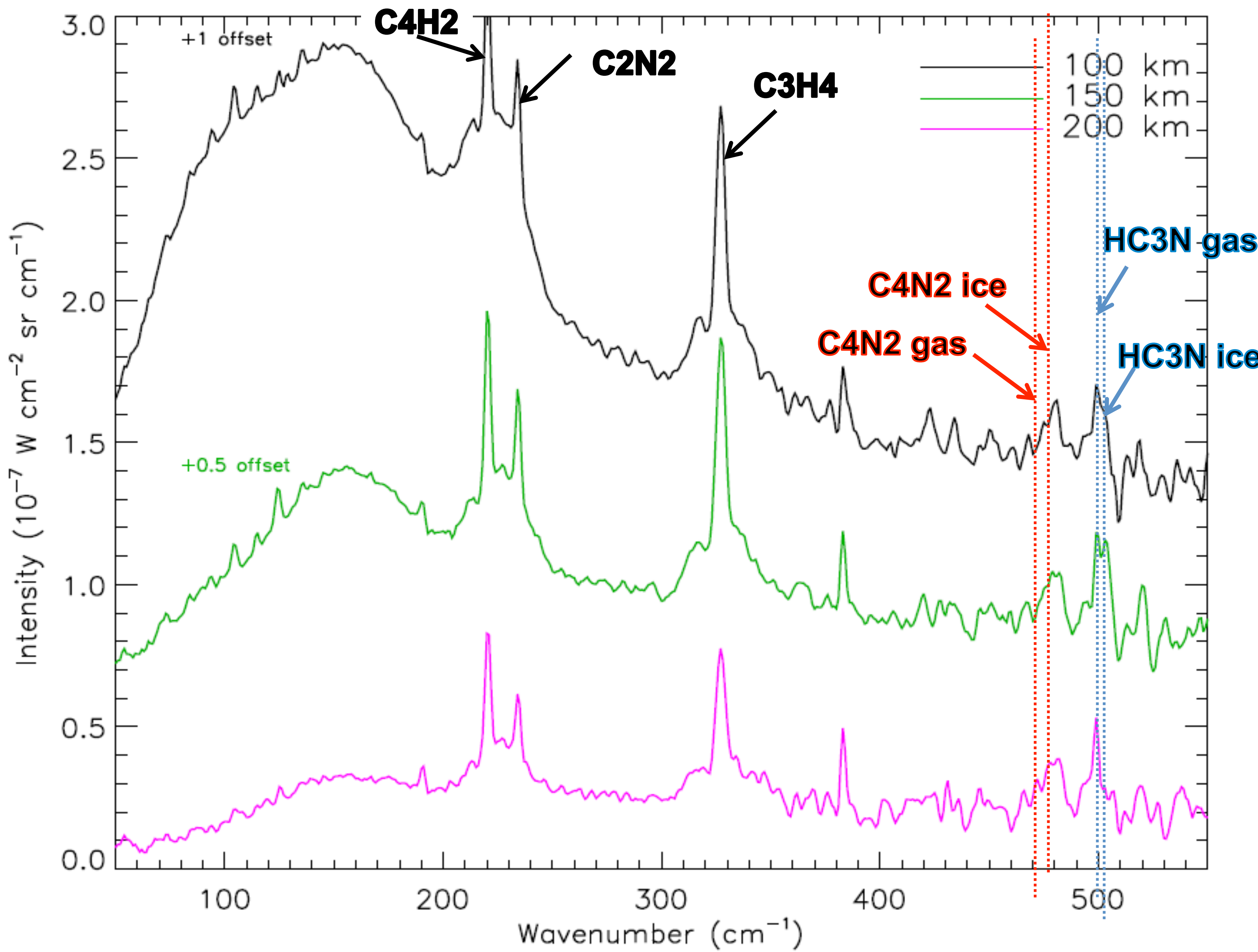
- C_4H_2 retrieved abundance: $q_1 = 2.4*10^{-9}$

- C_4H_2 radiance level : $I_1 = 2.1\ 10^{-8}$
- Standard deviation from residual at 107 cm^{-1} : I_2 $2*10^{-10}$

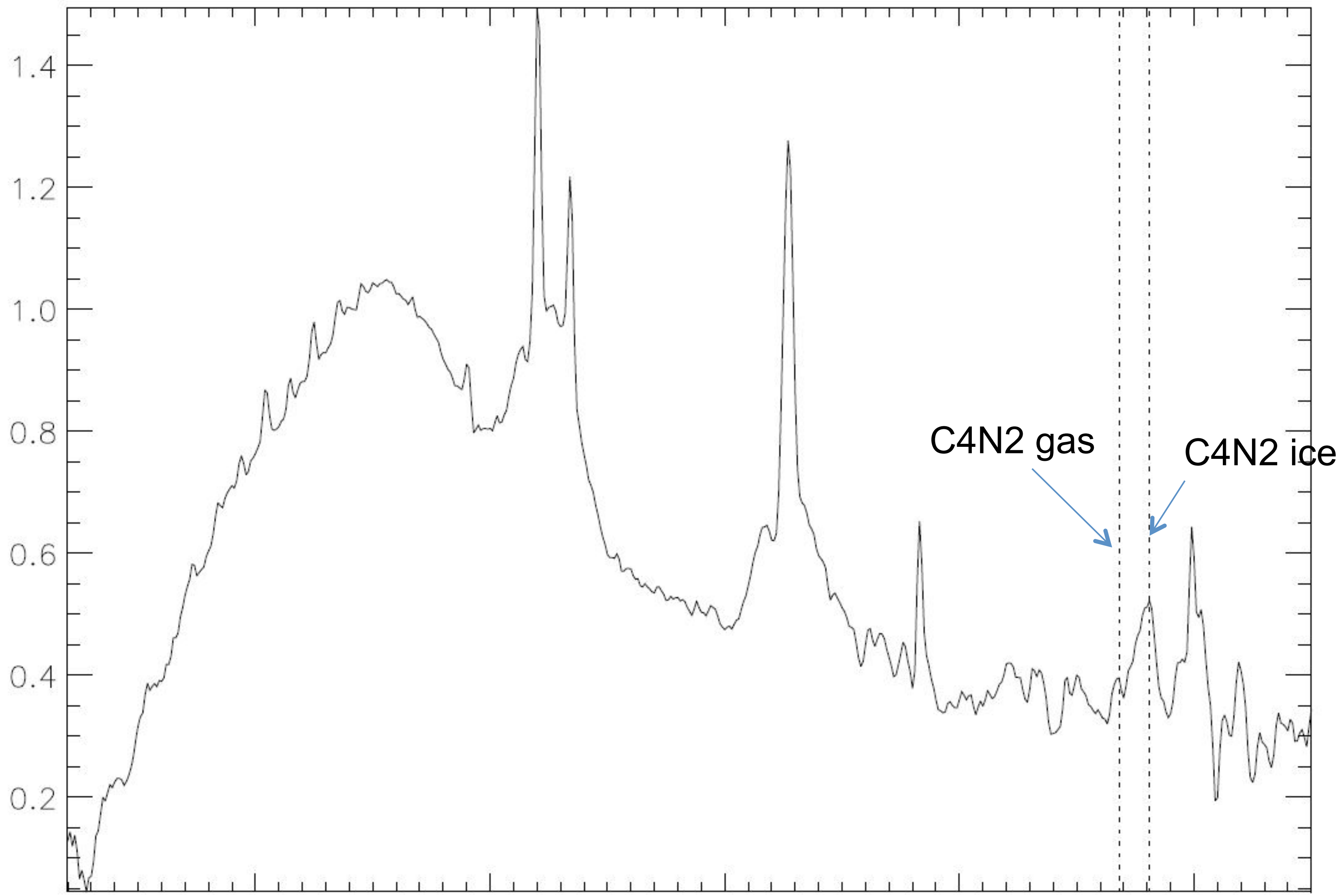
- Peak Max ratio: $S_1/S_2 = 1/1.45$ at 0.5 cm^{-1} spectral resolution and 135 K
- Black body ratio: B_1 (134K (122km) , 220 cm^{-1}) / B_2 (134K (122km, 107cm^{-1}) ~ 2

$$q_2 = q_1 \frac{I_2}{I_1}\frac{S_1}{S_2}\frac{B_1}{B_2} \approx 2.4*10^{-9} * (2*10^{-10} / 2.1*10^{-8}) /1.45*2$$

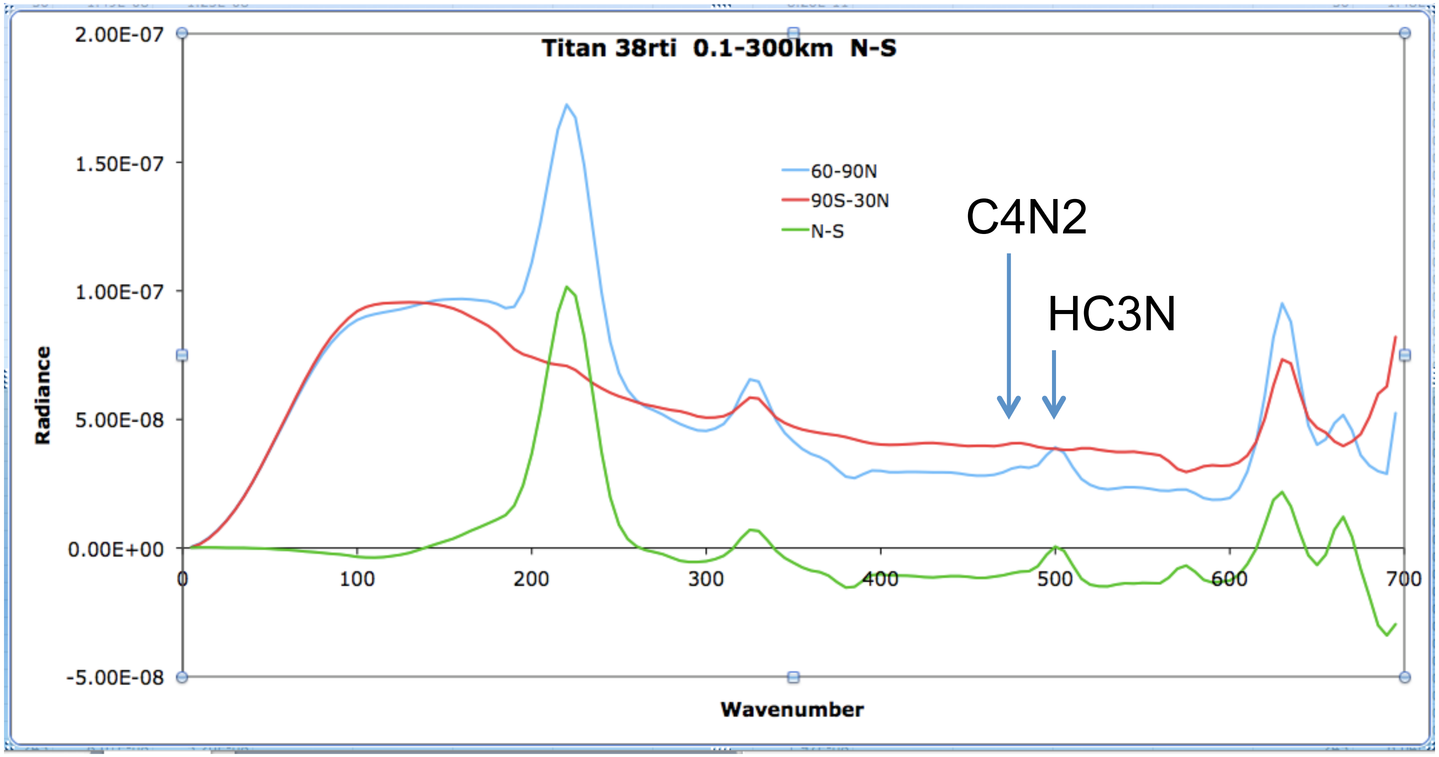
- => The derived C_4N_2 upper limit = $3*10^{-11}$



C4H2
C2N2
C3H4
+1 offset
100 km
150 km
200 km
HC3N gas
C4N2 ice
C4N2 gas
HC3N ice
+0.5 offset
Intensity (10^{-7} W cm^{-2} sr cm^{-1})
Wavenumber (cm^{-1})
3.0
2.5
2.0
1.5
1.0
0.5
0.0
100
200
300
400
500



1.4
1.2
1.0
0.8
0.6
0.4
0.2
C4N2 gas
C4N2 ice



Titan 38rti 0.1-300km N-S
60-90N
90S-30N
N-S
C4N2
HC3N
Radiance
Wavenumber
2.00E-07
1.50E-07
1.00E-07
5.00E-08
0.00E+00
-5.00E-08
0
100
200
300
400
500
600
700