PREPARATORY SCIENCE ACTIVITIES FOR HERSCHEL

(and for same price also for ALMA)

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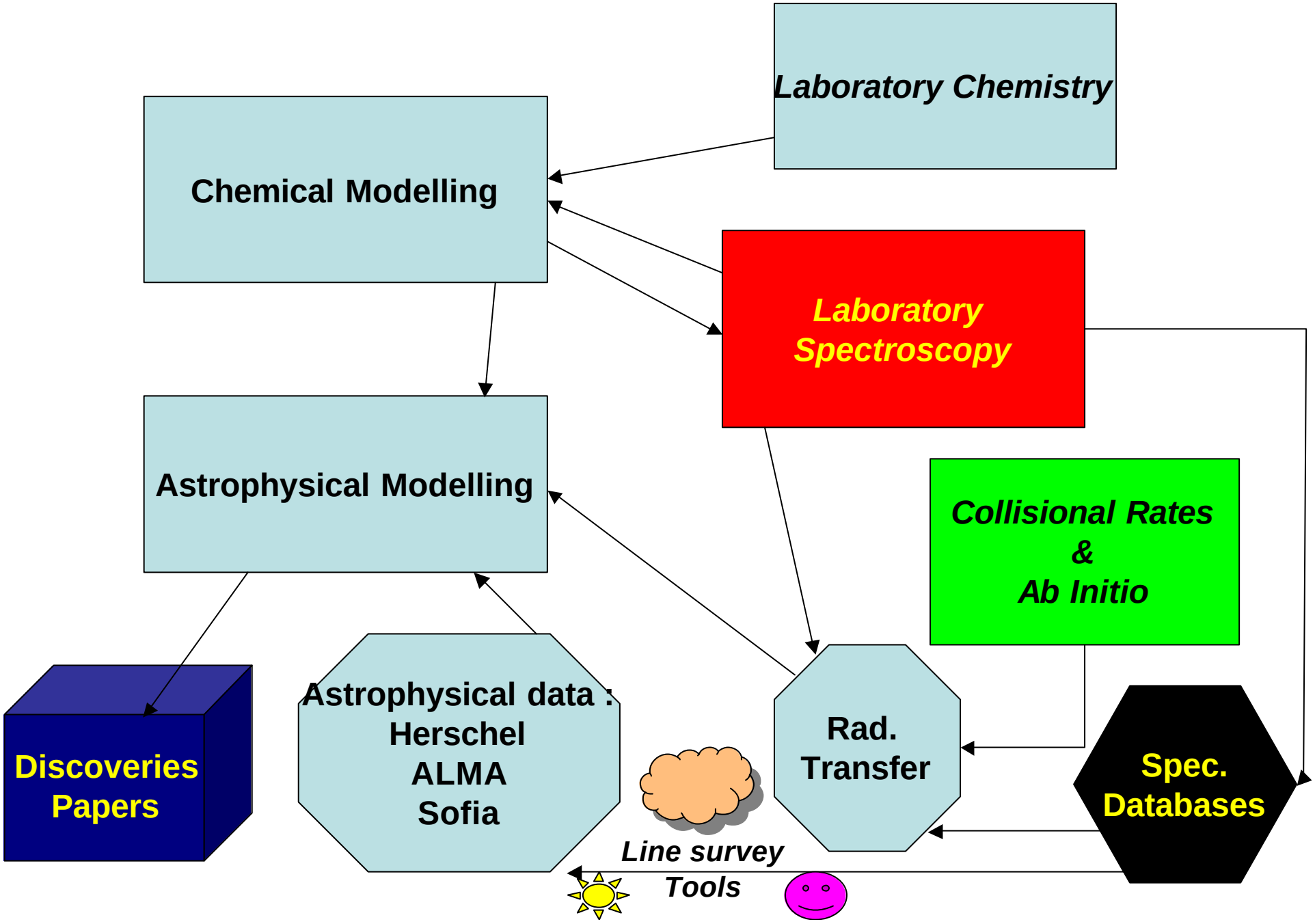
Preparatory Science Activities For Herschel

- **Why it is necessary to prepare the science that Herschel (ALMA) will do ?**
- **What is needed ?**
- **How we can reach the goals of Herschel/ALMA ?**
- **Who can participate ?**
- **What has been done ?**


Laboratory Chemistry
Chemical Modelling
Laboratory Spectroscopy
Astrophysical Modelling
Collisional Rates & Ab Initio
Discoveries Papers
Astrophysical data : Herschel ALMA Sofia
Rad. Transfer
Spec. Databases
Line survey Tools

Why looking for low abundancy species ?

- Some times these species play a crucial role in the chemistry and in the dynamical evolution of the clouds.
- From a spectral point of view because many of these molecules have been never observed in the Earth (complex radicals) : Lab. Chemistry.
- Gas phase and dust grain chemistry need of clear discrimators

The quest for complex molecules

- Understanding the chemistry
- Looking for O-bearing species in C-rich environments (H_2O, H_2CO,…), organic molecules

  in star forming regions,….
- Looking for derivatives of molecules assumed to be formed in the dust grains
- Looking for isotopic species : isotopic abundances : nuclear processes in AGB stars and supernova
- BUT !

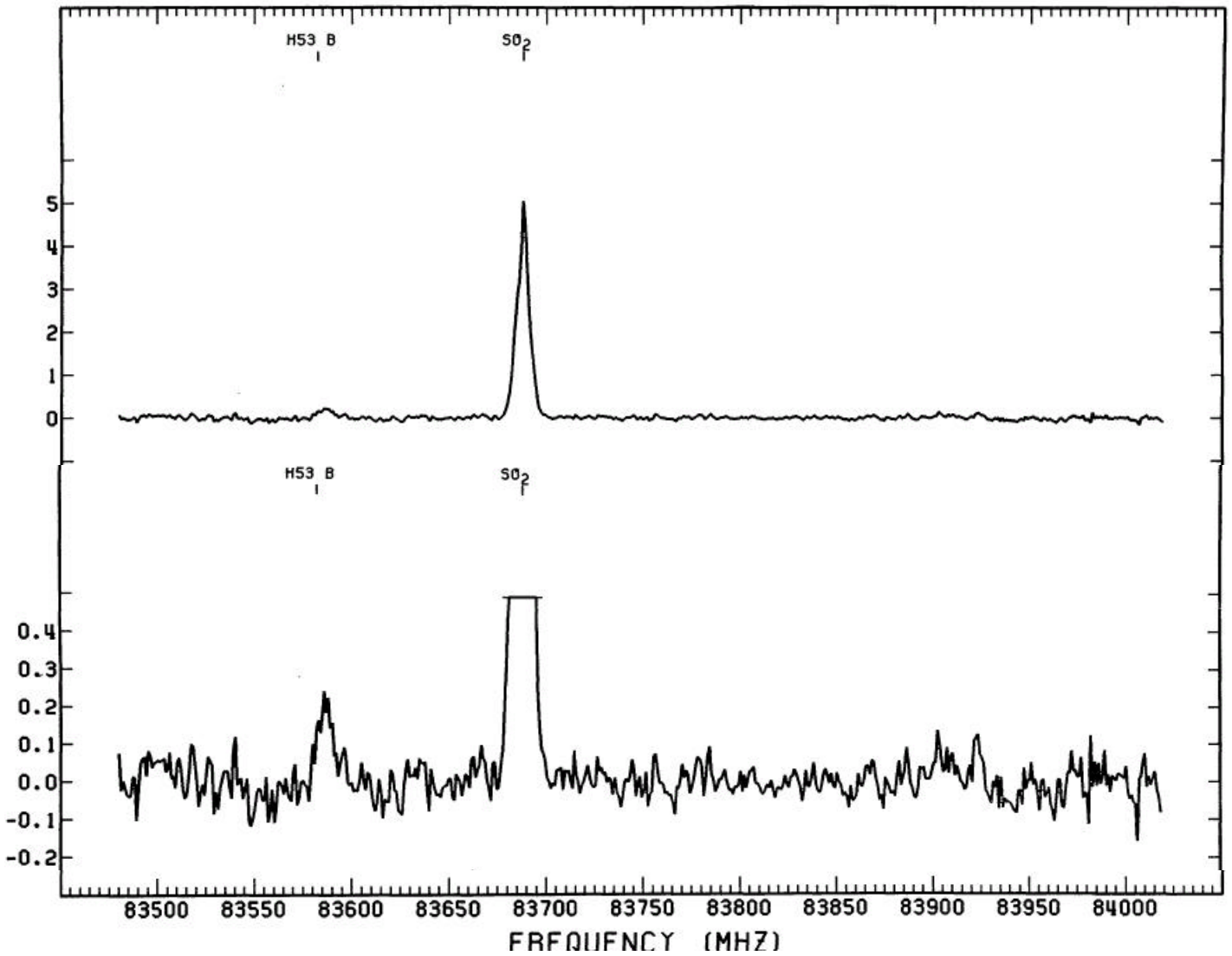
- How to interpret spectra with thousands of lines
- What methods have to be implemented to deal with these expected line forests ?
- Automatic procedures ?
- What we get from line surveys ?

Selecting the sources

- The most prominent sources (Orion, SgrB2, IRC+10216, CRL618) have to be completely understood before confident searches can done in other similar objects !!

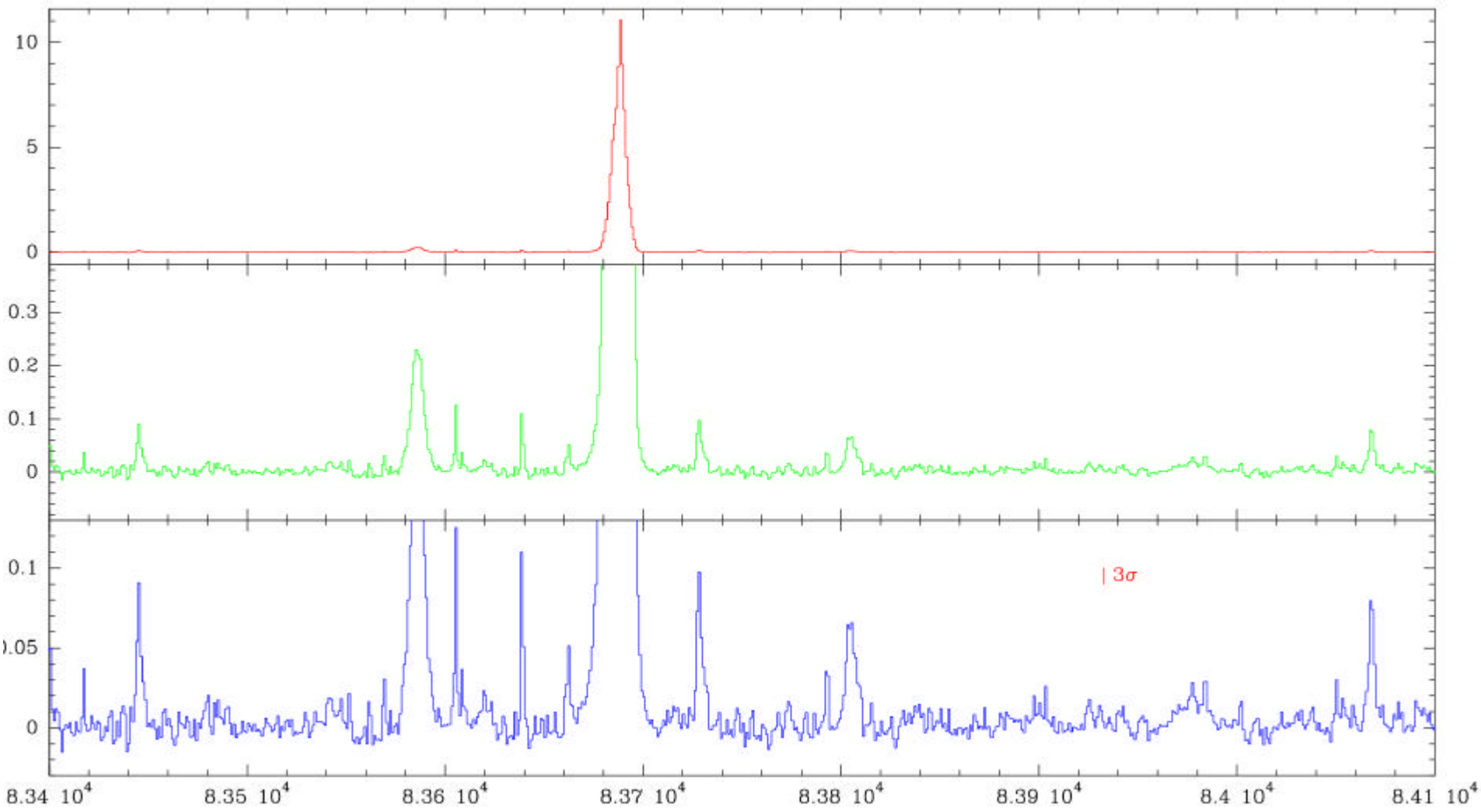
- They are templates for ALMA, Herschel & SOFIA future observations. For ALMA hundreds of sources will look like Orion with present instruments !!!

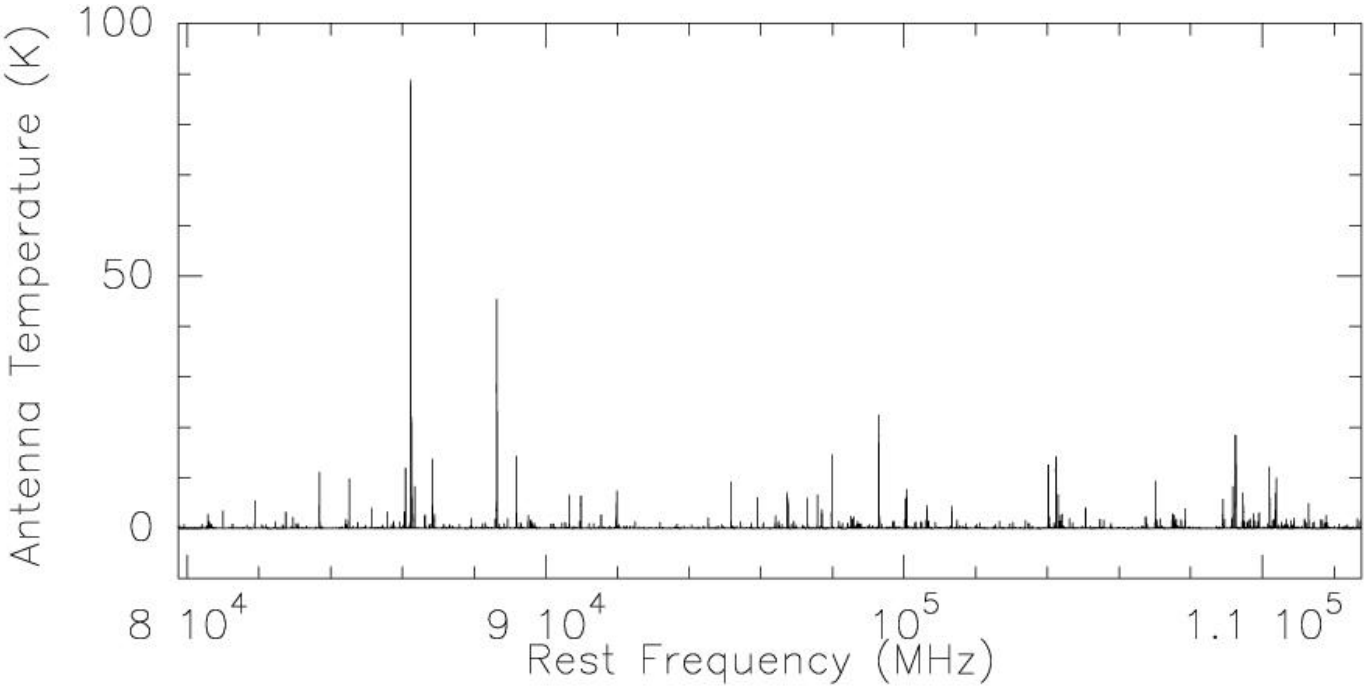
- Each source has its peculiarities : special adapted models, special entries in the spectral catalogs



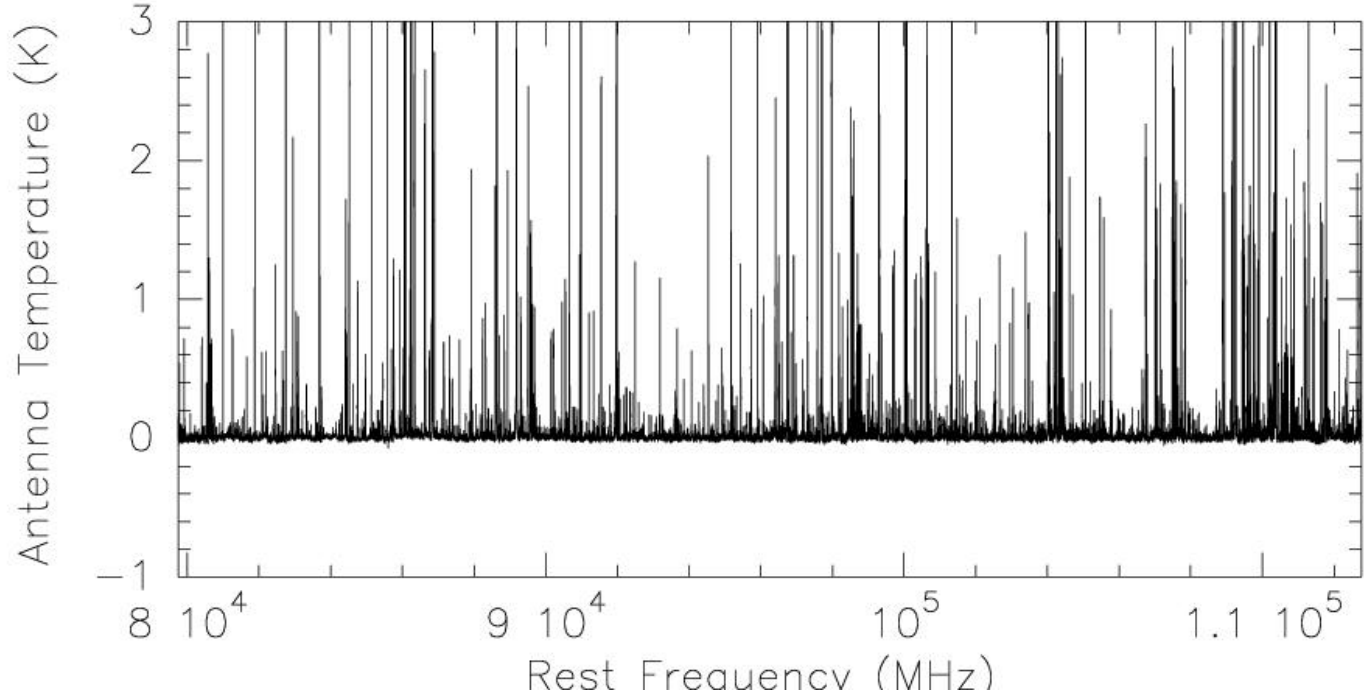
•Onsala line survey of Orion. State of the art in the 80’s

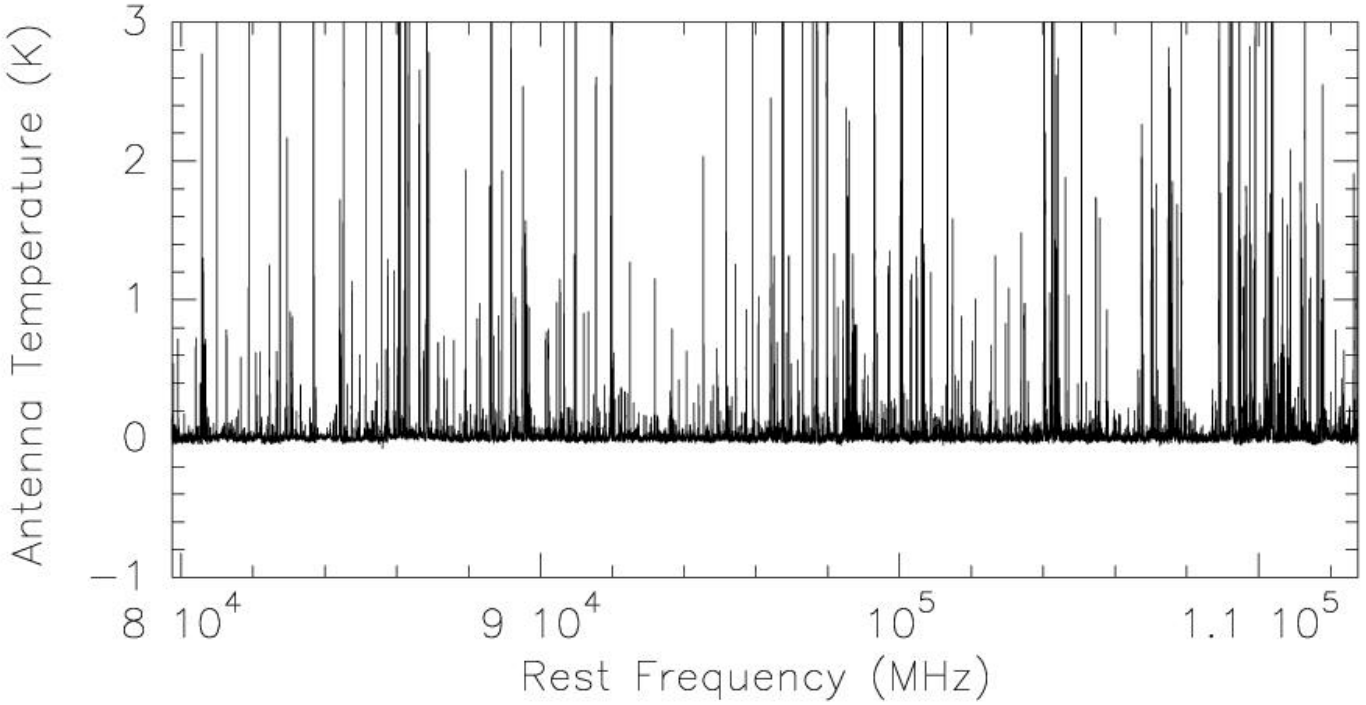
IRAM 30m spectrum; 40 min integration; Tsys=100 K

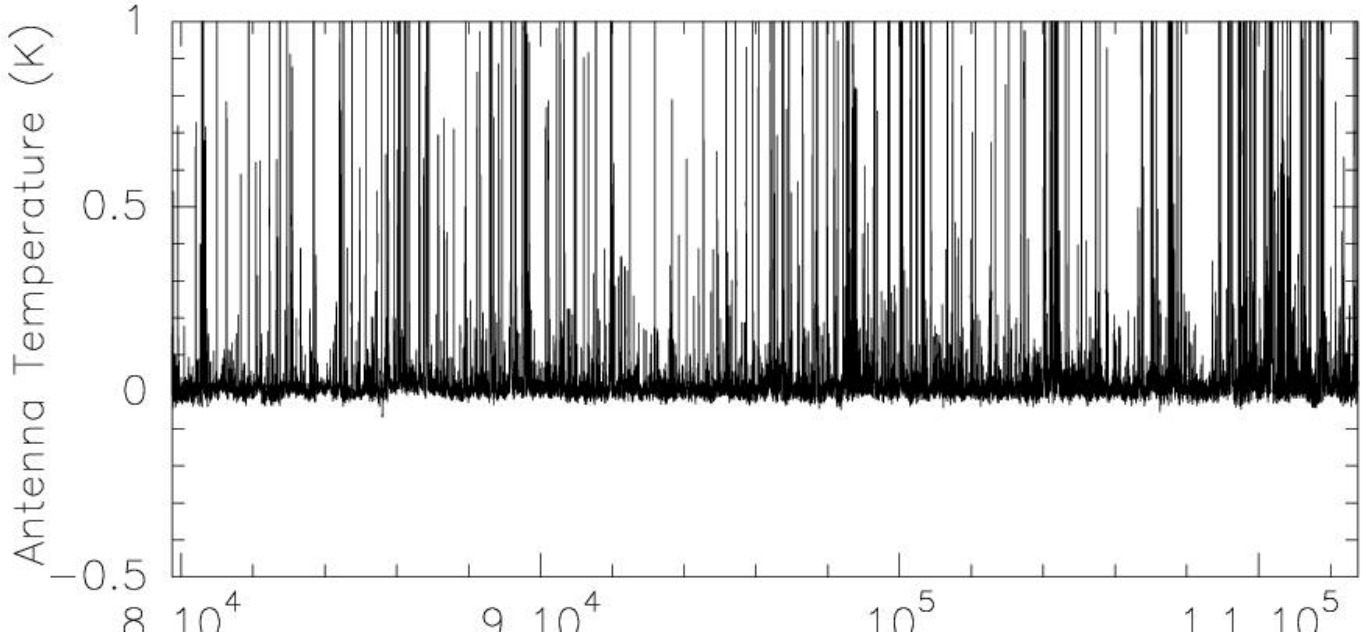


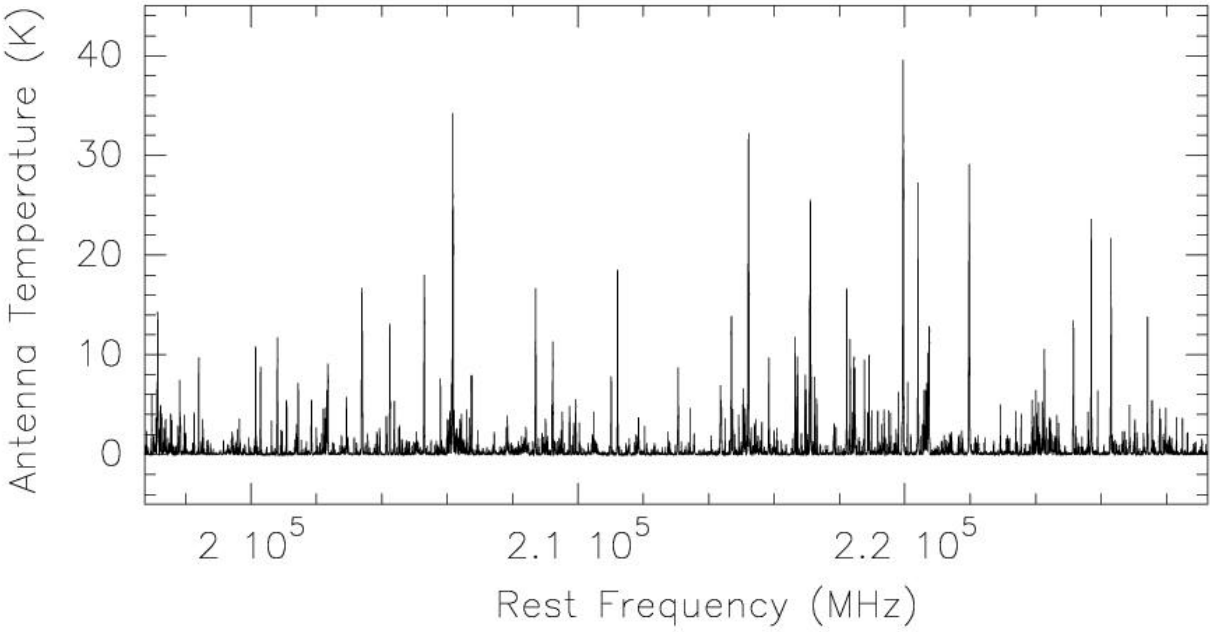


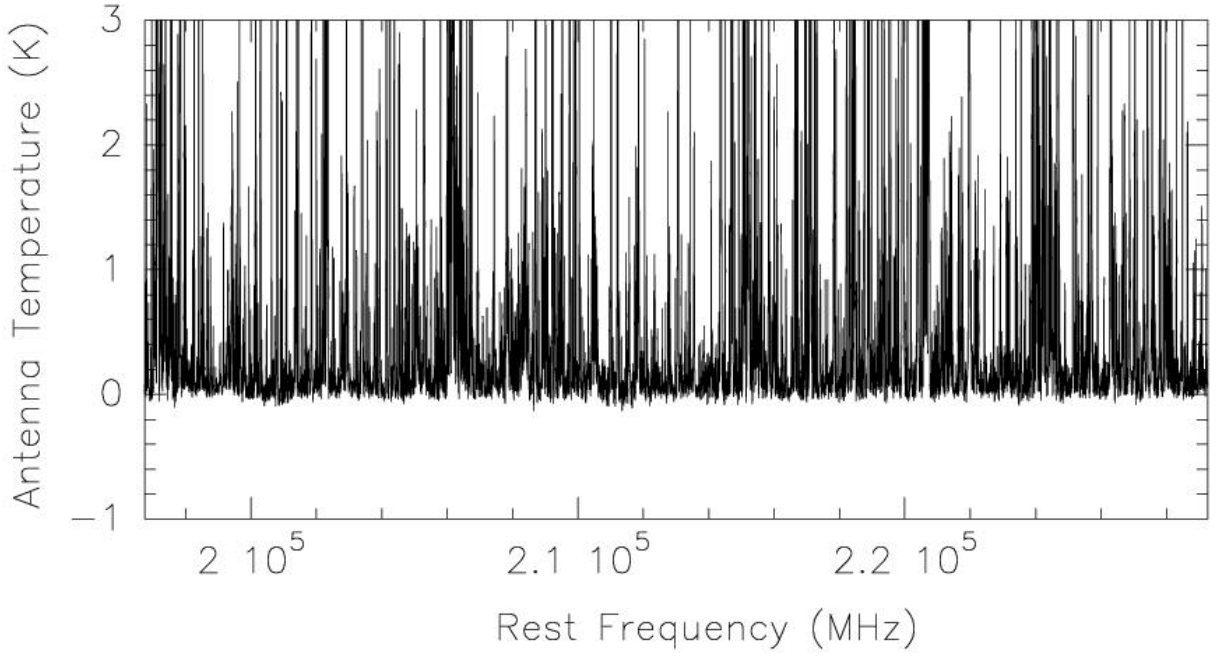
Belen Tercero, PhD, DAMIR




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





Orion as seen with 30-m IRAM Telescope.

10 min observing time/GHz

30 GHz at 1mm &

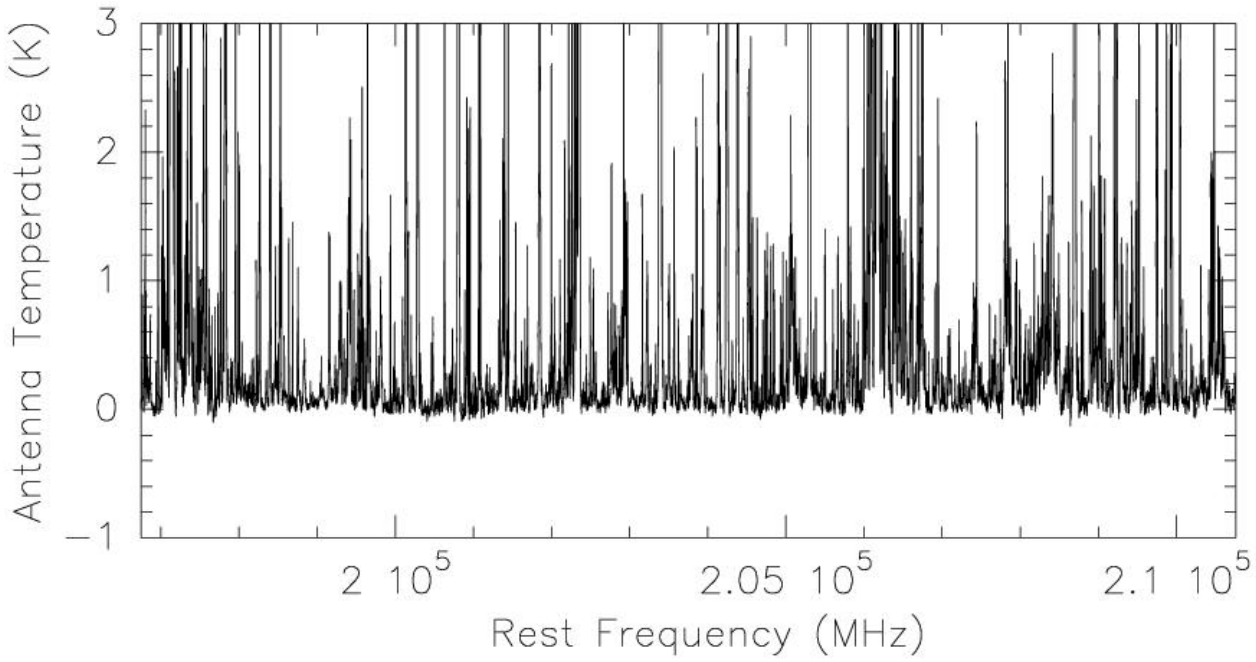
30 GHz at 3mm

Simultaneously

+ many 2'x4' maps

= 35 hours observing time

B. Tercero & Cernicharo

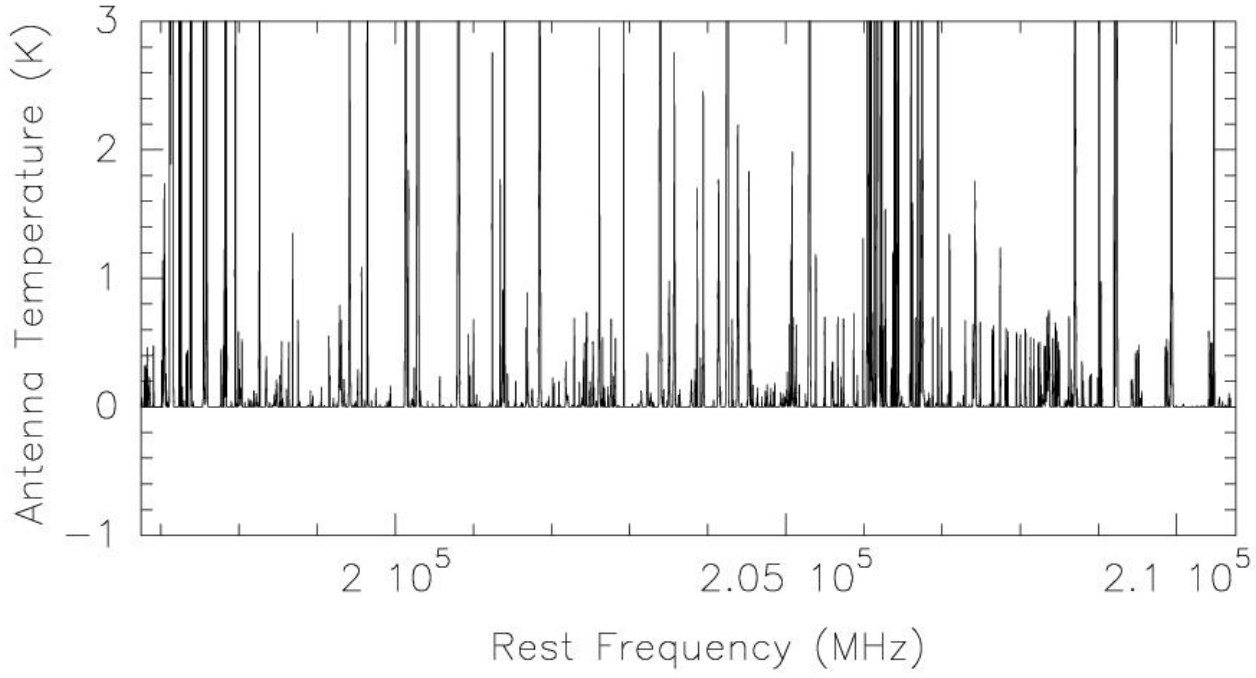


- Vibrational states
- Isotopes

CH_3OCH_3

CH_3CH_2CN

$HCOOCH_3$,….



New species :

Alcohols, X-CN,

Ethers, (X-O-Y)

Cetones (X-CO-Y)

Isomers, …

ALMA will provide hundreds of Orions !!

- 30m telescope = 16000 lines in Orion

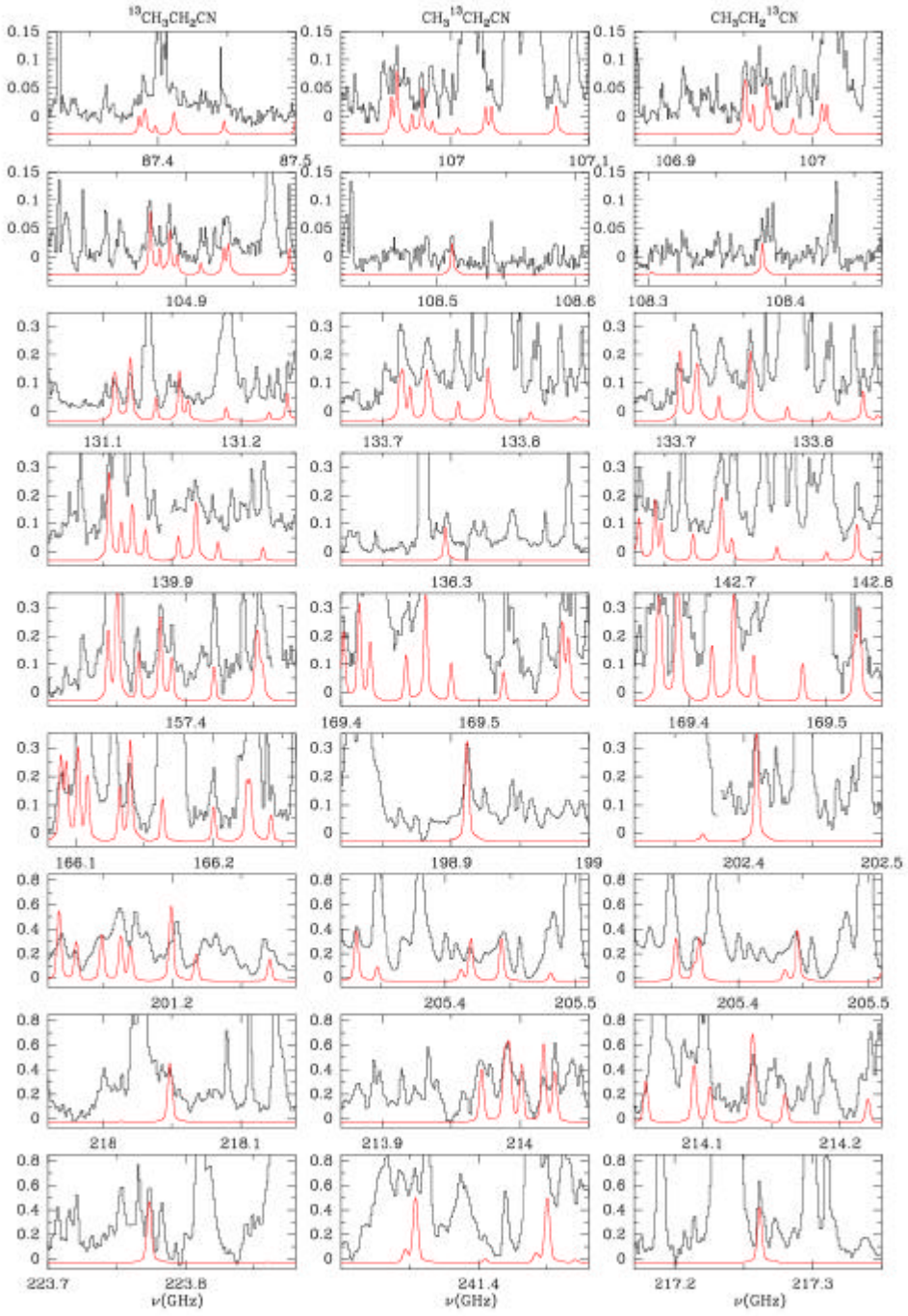
  8000 unassigned !!

How to proceed ?

What to do ?

How to proceed in the real world?

- Modelling the main isotope of a given species
- Finding the best isotopic ratios from full modelling of the spectrum of each isotopologue
- Finding vibrational temperatures for vib excited of molecules. In Orion all vib states with energies below 600 K easily detected.
- More energetic states within the line confusion limit



A search from JPL frequencies for ^{13}C isotopes provided some identications but also many missing lines (wrong frequencies; old constants)

Collaboration with Karine Demyk (Lille). New Frequencies + Astronomical modelling ➔

More than 700 lines detected from the three ^{13}C isotopologues !

Missing spectroscopy for CH_3CH_2CN

- $CH_3CH_2{}^{15}N$
- CH_2DCH_2CN, CH_3CHDCN, CH_3CDHCN

CHD_2CH_2CN + other D-combinations

(In the plane + torsion + out of the plane (CCN) v> 1)

Double ^{13}C isotopes (ALMA)

A goog example : CH_2CHCN

- CH_2CHCN, $^{13}CH_2CHCN$, $CH_2{}^{13}CHCN$,
- $CH_2CH^{13}CN$, $CH_2CHC^{15}N$, HCDCHCN
- DCHCHCN, HCDCDCN, DCHCDCN, CD_2CHCN (Colmot et al., 1997; data for most isotopes of CH_2CHCN)
- V_{11}=1,2,3 V_{15}=1
- All lines with intensities > 0.05 K in the 80-280 GHz domaine detected (>1500 lines)
- Missing spectroscopic data for v_{15}=2, $v_{11}+v_{15}$ and high transitions of some isotopes

Real World too complex for simple identication procedures as soon as the lines are in the confusion limit (and even above that limit)

- Systematic modelling needed for each source and for each molecule (look the case of CRL618 by Pardo & Cernicharo)

- Example (Orion)

  Tvib (CH_2CHCN) < Tvib(CH_3CH_2CN)

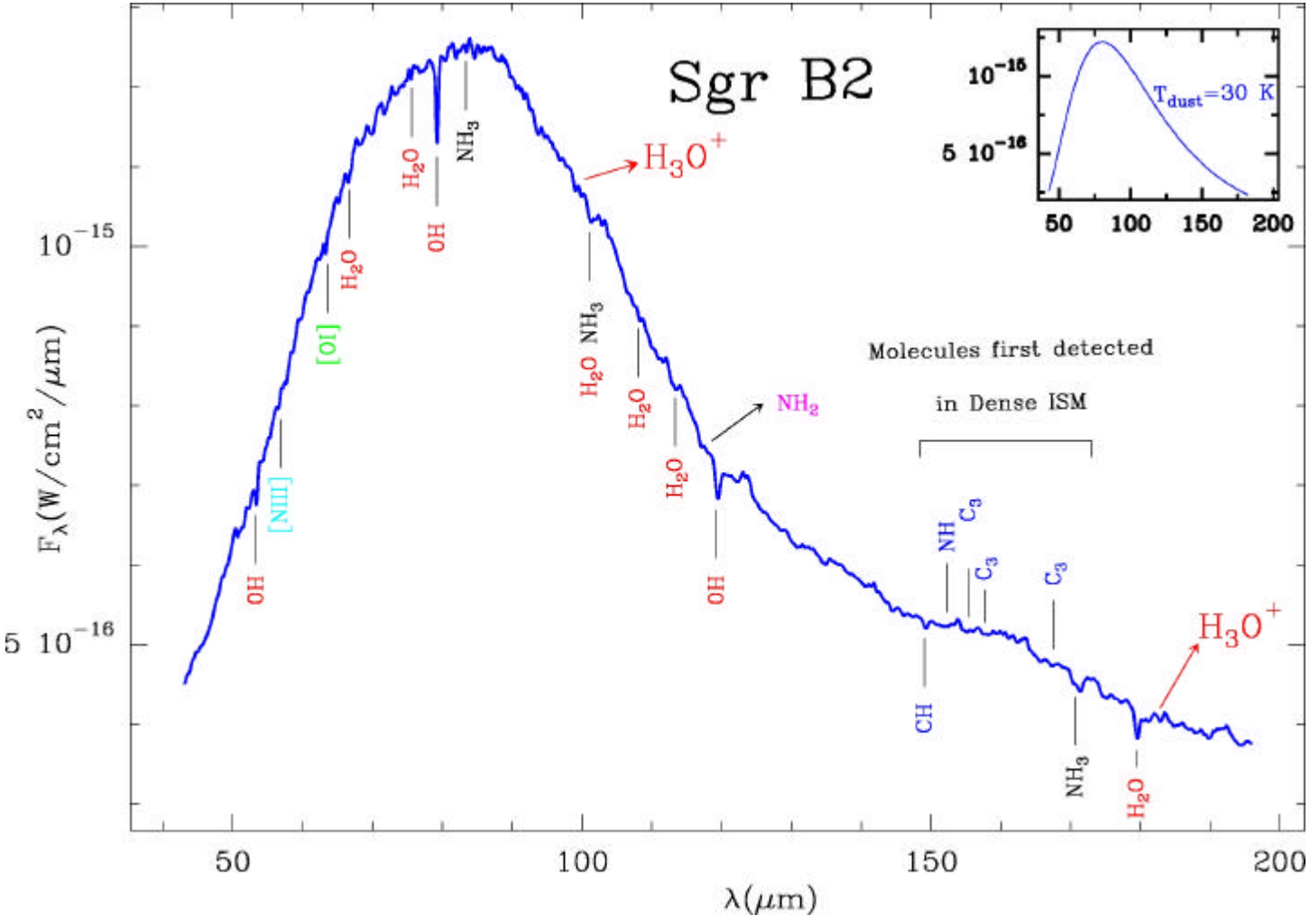
Astron. Astrophys. 323, L25–L28 (1997)

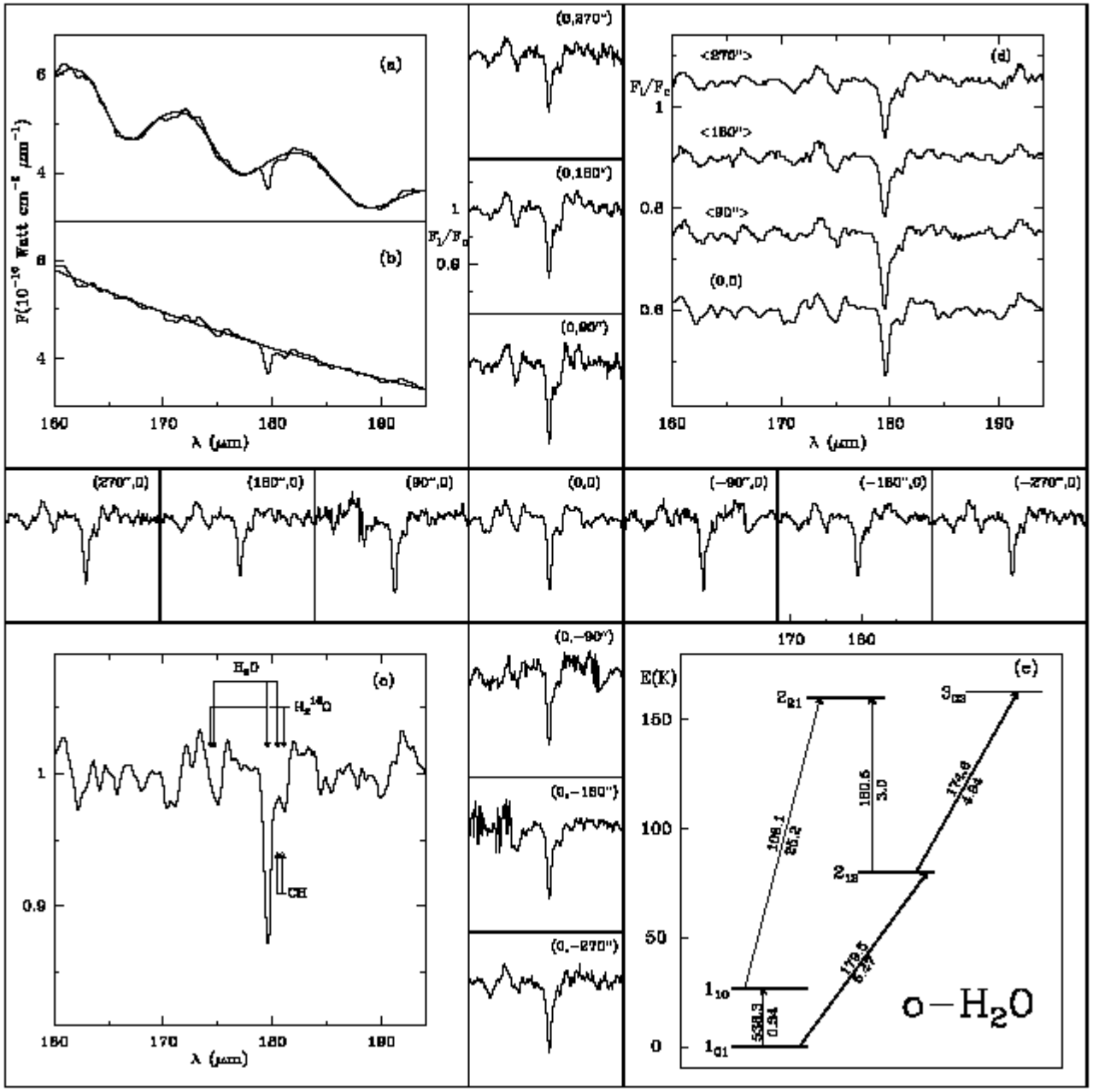
ASTRONOMY
AND
ASTROPHYSICS

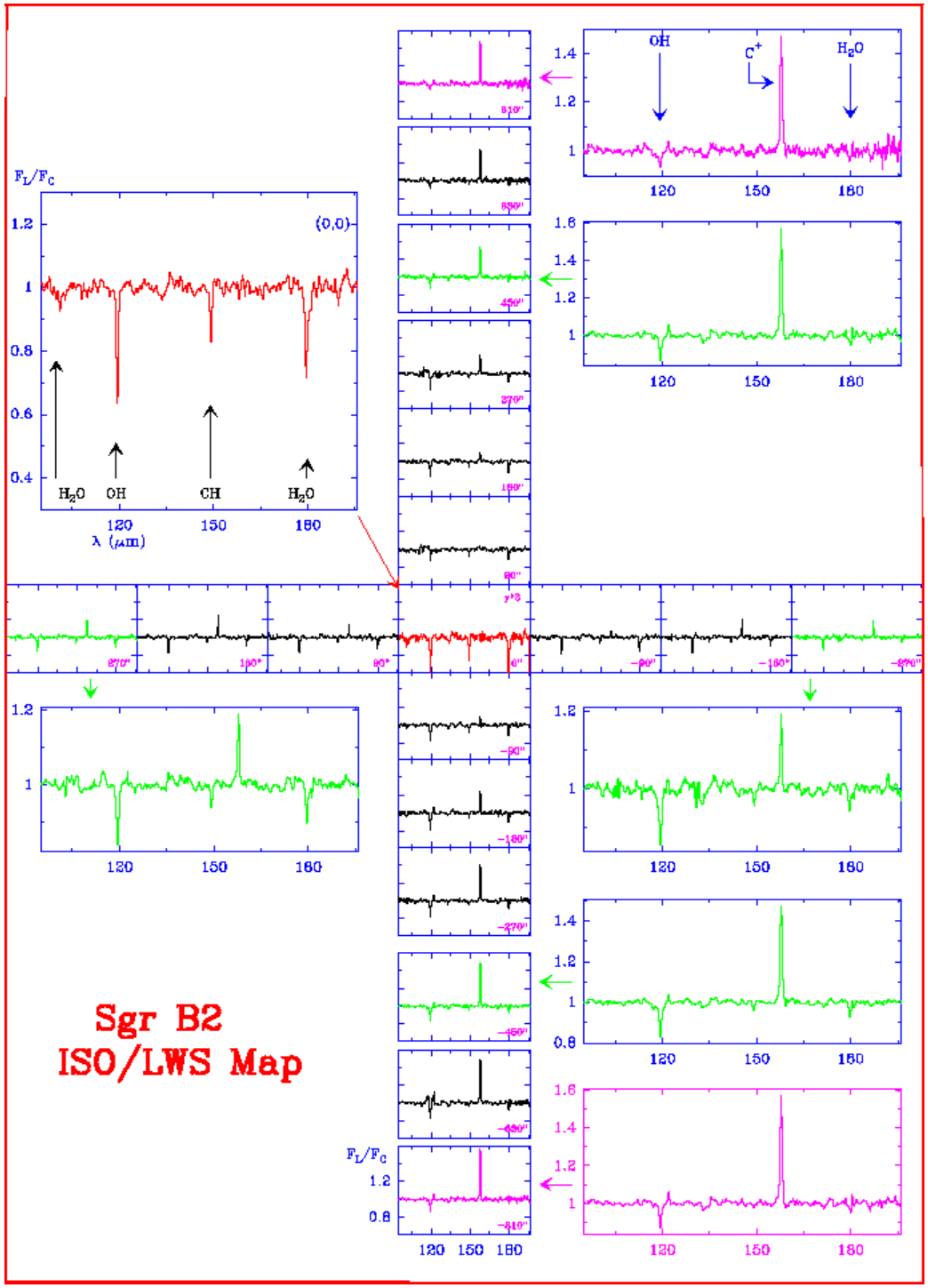
Letter to the Editor

Widespread water vapour absorption in SgrB2[1]

J. Cernicharo[1], T. Lim[2], P. Cox[3], E. González-Alfonso[4,5], E. Caux[6], B.M. Swinyard[7], J. Martín-Pintado[5], J.P. Baluteau[8], and P. Clegg[9]




(a)
(b)
F(10^-19 Watt cm^-2 μm^-1)
λ (μm)
(0,270")
(0,180")
(0,90")
F_l/F_c
(d)
<270">
<180">
<90">
(0,0)
(270",0)
(180",0)
(90",0)
(0,0)
(−90",0)
(−180",0)
(−270",0)
(0,−90")
(0,−180")
(0,−270")
(c)
H2O
H2 18O
CH
E(K)
o−H2O
2_21
3_03
2_12
1_10
1_01
538.3
0.34
179.5
6.47
180.5
3.0
175.9
4.84
108.1
25.2


Sgr B2
ISO/LWS Map
F_L/F_C
(0,0)
H2O
OH
CH
H2O
λ (μm)
OH
C+
H2O

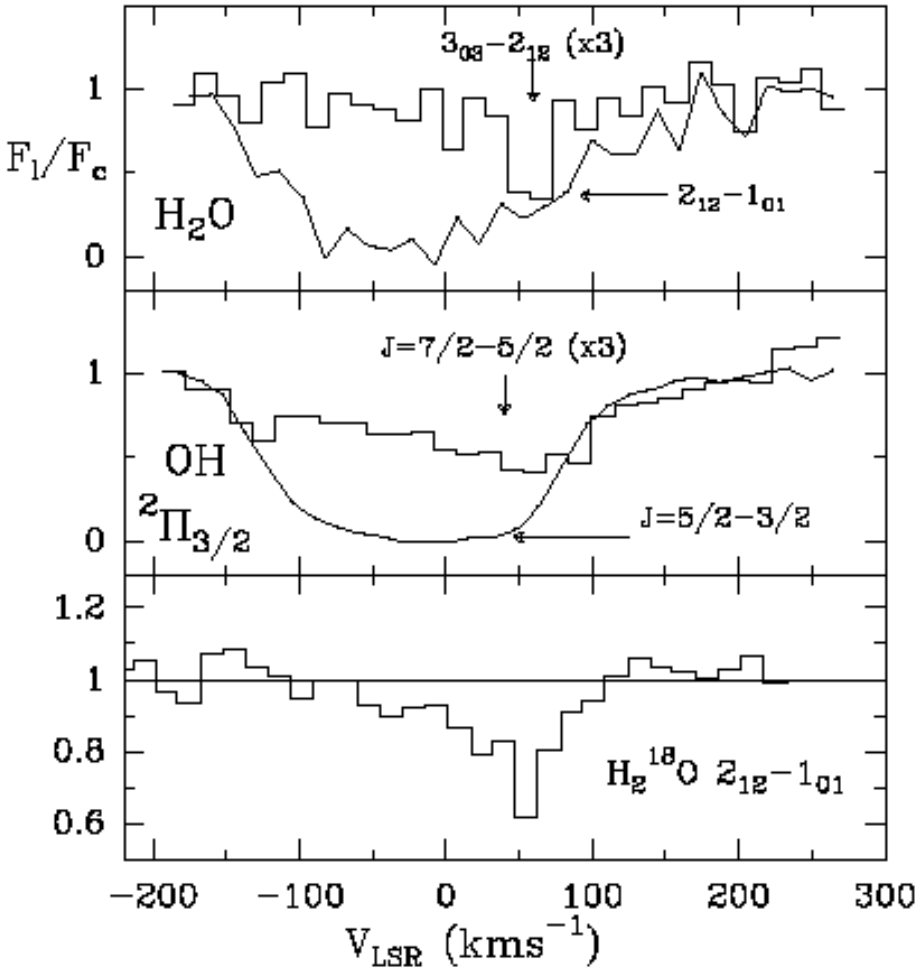


Fig. 2. LWS Fabry-Perot observations of the central position of SgrB2. (a) The 2_{12}-1_{01} and 3_{03}-2_{12} lines of water at 179.52 and 174.6 μm, respectively; (b) the 5/2-3/2 and 7/2-3/2 lines of the $^2\Pi_{3/2}$ state of OH at 119 and 84 μm; (c) the 2_{12}-1_{01} $H_2{}^{18}O$ line at 181.05 μm

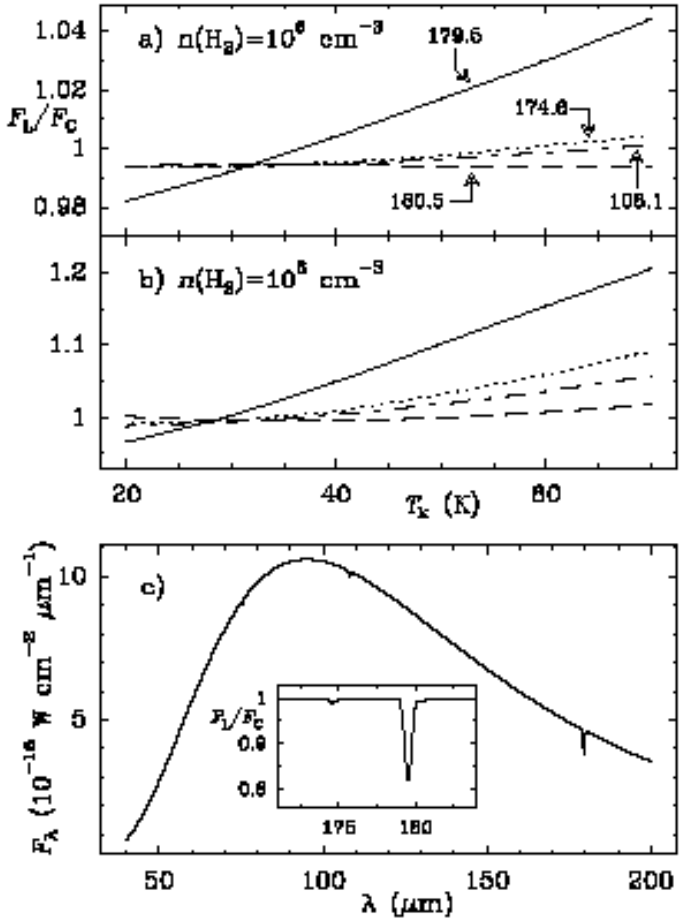
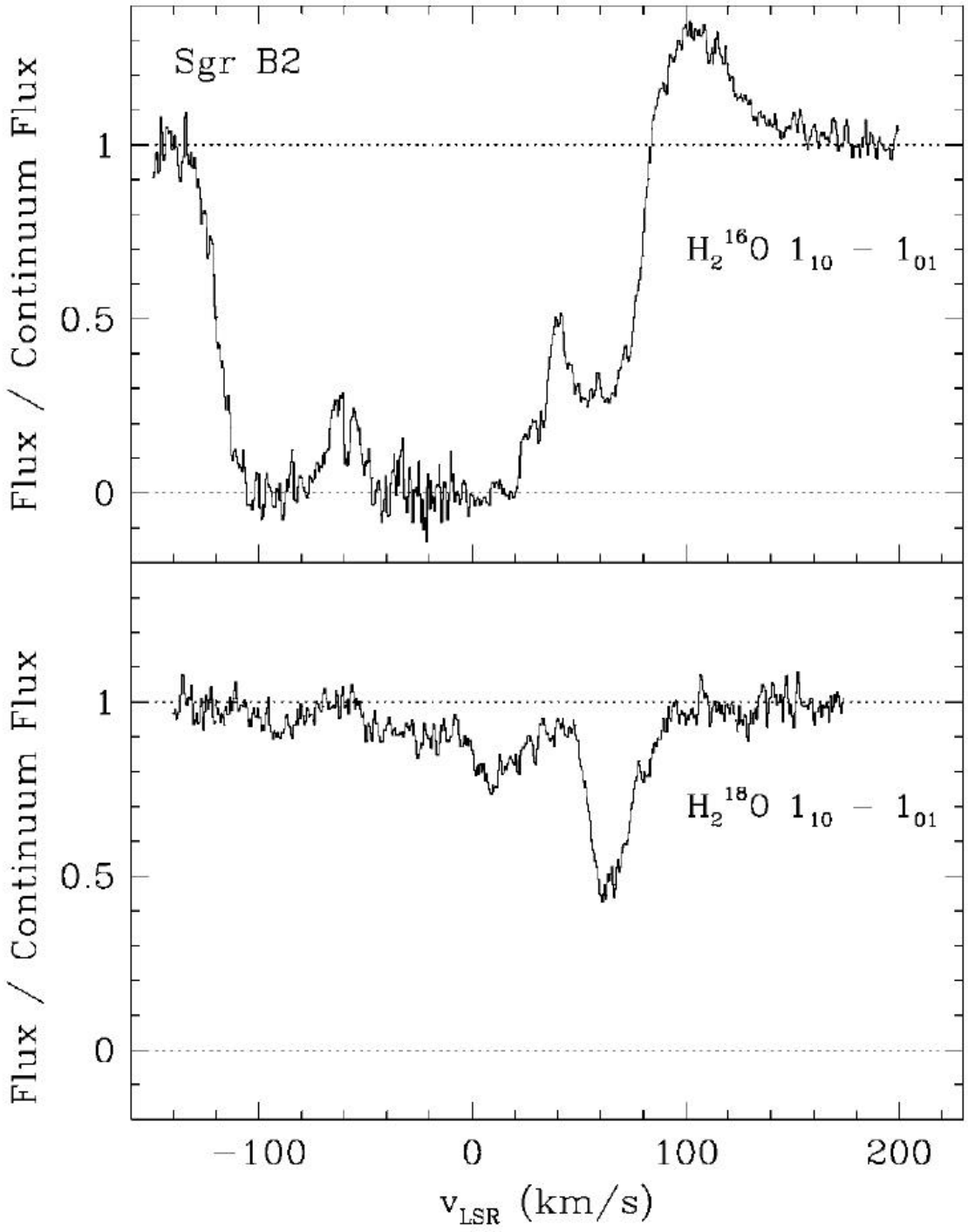
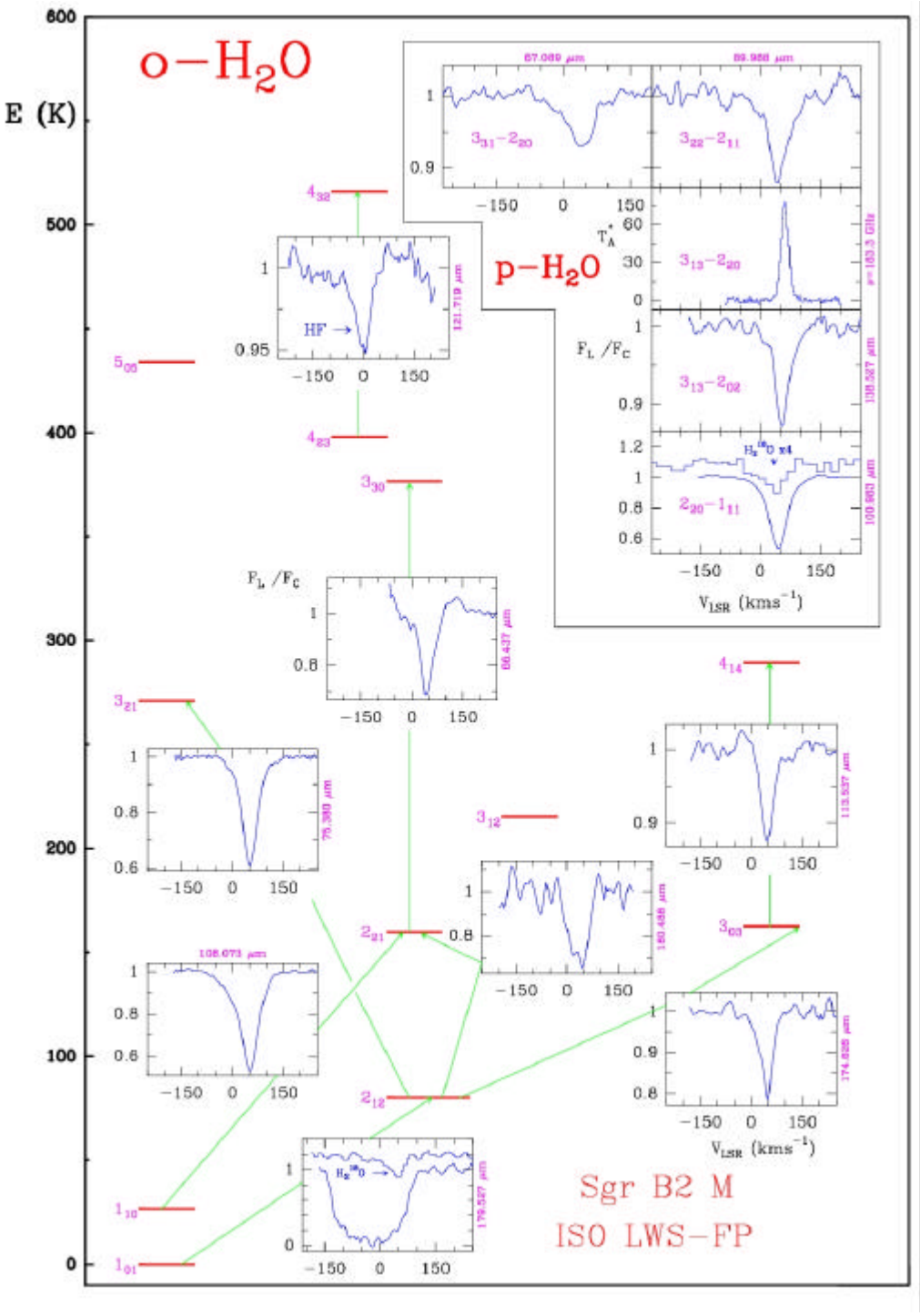


Fig. 3. a) and b) Results of model calculations showing the line over continuum flux ratio of four o-H_2O transitions (labelled with their wavelengths) as a function of kinetic temperature. c) Model spectrum for a cloud with an external absorbing shell (see text for details)



SWAS data in the direction of SgrB2



Modelling water in SgrB2:

Absolute need for 183.3 GHz data

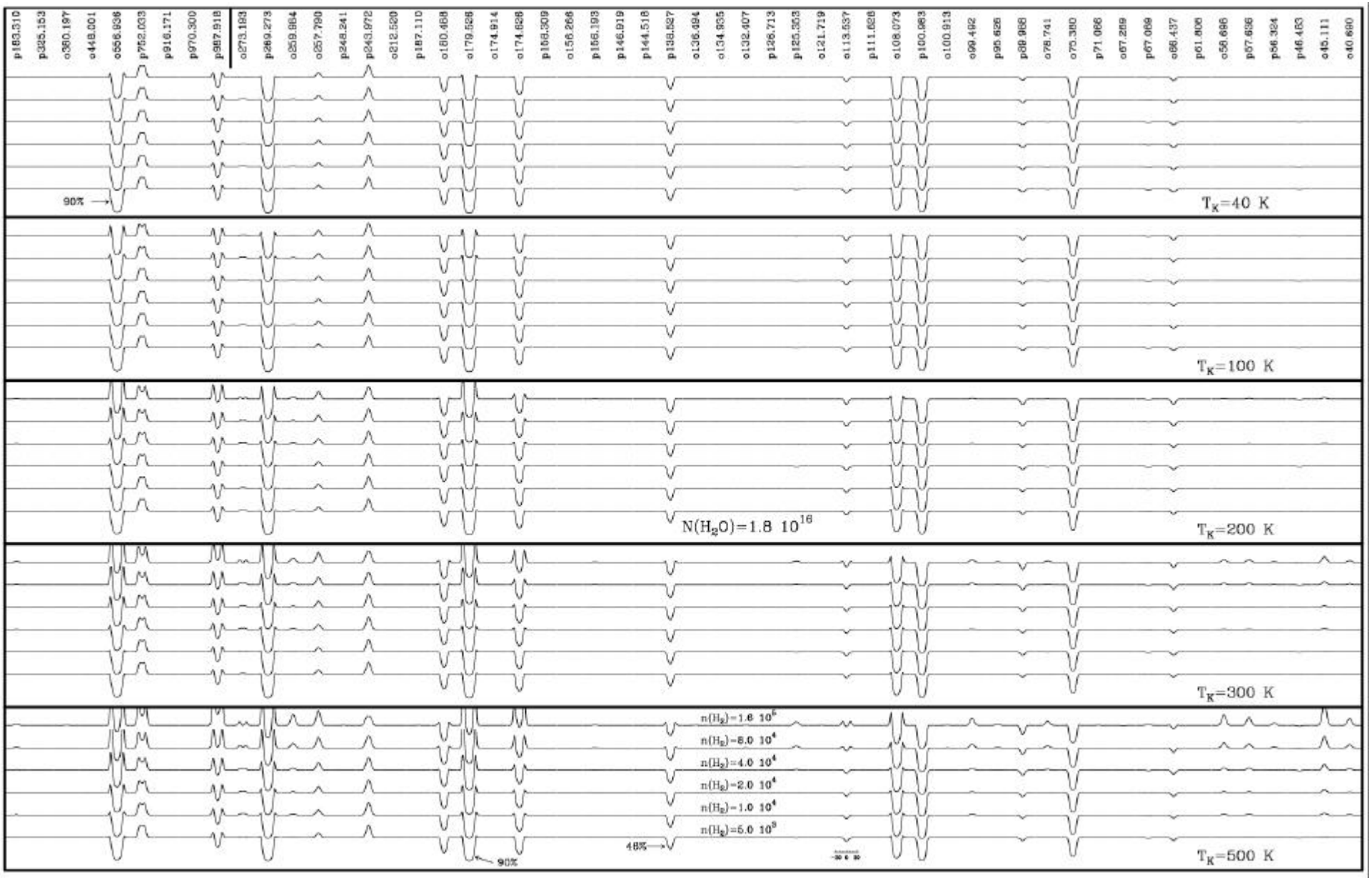
Three different codes :

J. Cernicharo (non local)
A. Asensio (non local)
C. Ceccarelli (LVG)

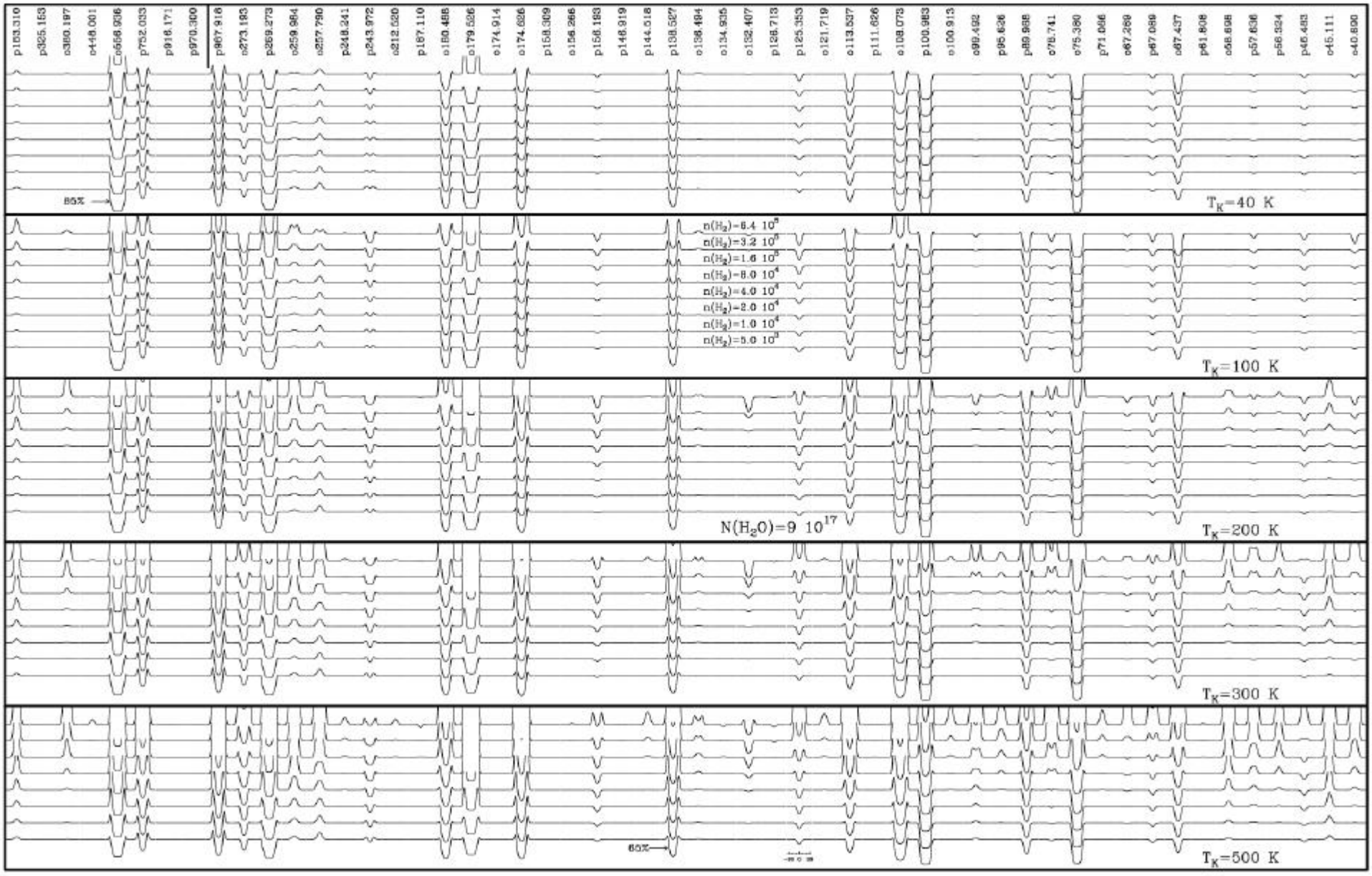
Velocity resolution limits the Interpretation : HERSCHEL

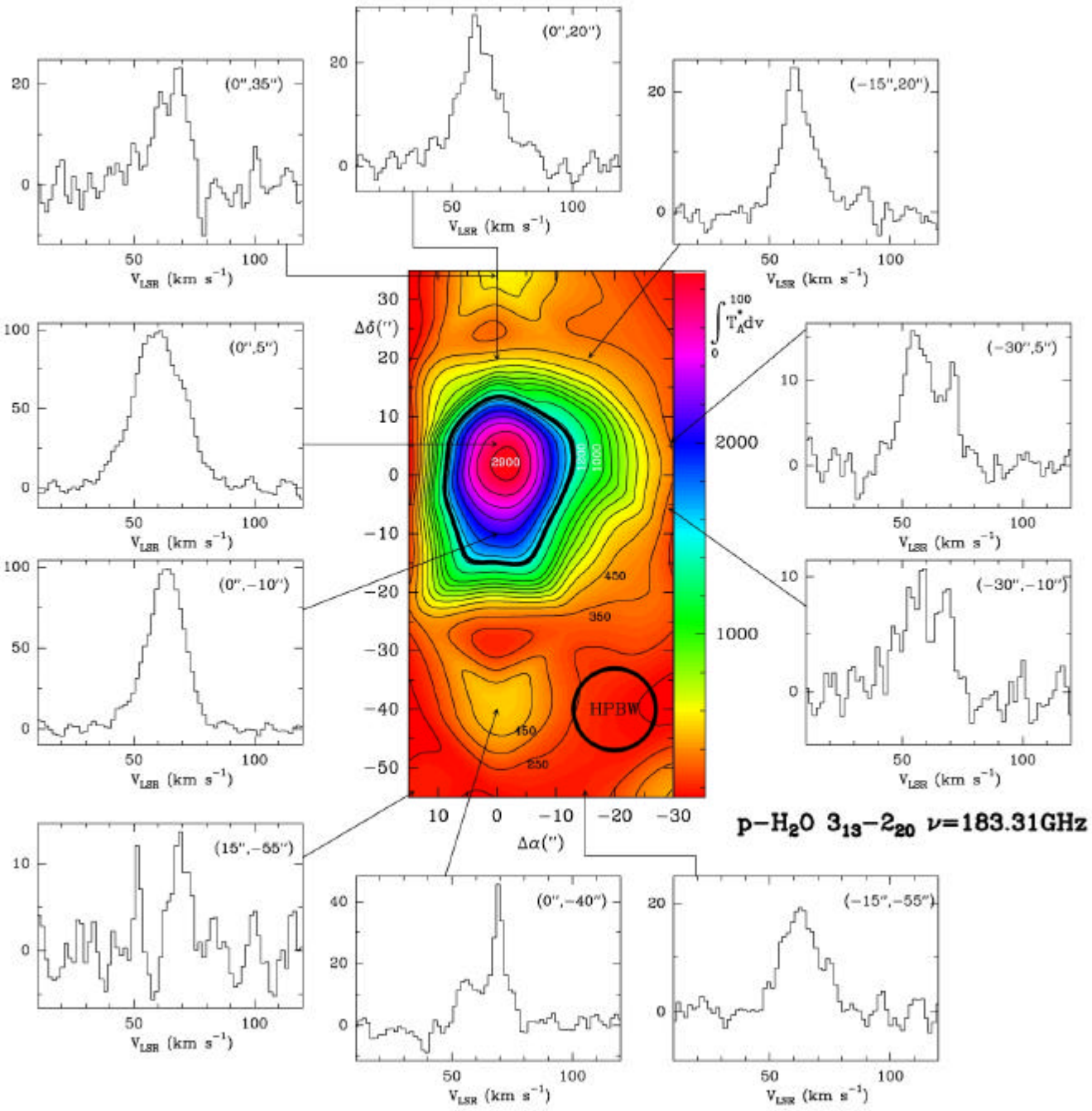
Cernicharo et al. in preparation

$N(H_2O)=1.8\ 10^{16}\ cm^{-2}$



$N(H_2O)=1.8\ 10^{17}\ cm^{-2}$





IRAM
30-m radio
telescope
observations

Herschel will
have a similar
beam

MOLECULAR DATABASES FOR HERSCHEL, ALMA & SOFIA

- Two meetings in the last two years in the Lorentz Center (Leiden).

- **Sessions on :**

  * Laboratory Spectroscopy
  * Laboratory Chemistry
  * PES and Collisional rates
  * Ab Initio Calculations of Molecules of Astrophysical Interest
  * Chemical Modelling
  * Astrophysical Modelling

Herschel / ALMA Desiderata

- **Absolute need for laboratory spectroscopy information**
- **Absolute need for new codes allowing to treat Radiative Transfert in 2,3-D with fast algorithms**
- **Absolute need for chemical modelling predictions about what new molecules could be observed**
- **A good understanding of the observational capacities that these instruments will bring in the millimeter, submillimeter and far-IR domains**
- **Open time KP have to show that the proposers will be able to analyze and interpret the data. A lot of preparatory work has to be done. Tools are needed !**

What we can do in Spain

- J. Cernicharo is taken over, as mission scientist of Herschel, the coordination of the preparatory science activities at the European level.

- DAMIR is doing a lot of effort within the FP6 program “The Molecular Universe”. Computing PES and collisional rates, ab initio calculations, astrophysical modelling

- To find Astrophysical/laboratory/chemistry groups willing to use Herschel /ALMA and motivated to do preparatory science activities

1er CONGRESO NACIONAL DE ASTROFÍSICA MOLECULAR

Ciudad Real, 1-4 Diciembre de 2003

UNA VISIÓN GENERAL DEL POTENCIAL DE LOS GRUPOS DE QUÍMICA ESPAÑOLES ANTE LOS NUEVOS DESAFÍOS DE LA ASTROFÍSICA"

2º CONGRESO NACIONAL DE ASTROFISICA MOLECULAR

- Date : 2007
- Where ?
- Who ?

OBJETIVOS :

Preparar un proyecto CONSOLIDER con los grupos de química-física a nivel nacional (5 MEuros) : Focused on Herschel & ALMA (Title : Molecular Astrophysics)

Definir entre los Astrofísicos las necesidades a nivel nacional para Herschel y ALMA. Colaborar con los químicos-físicos (equipar los laboratorios para obtener información necesaria para interpretar nuestros datos, tesis codirigidas, postdocs comunes,…)

Support Letters from our European and American colleagues are welcome for the proposal (Dec 2007)