# *Line Identification and Modeling*

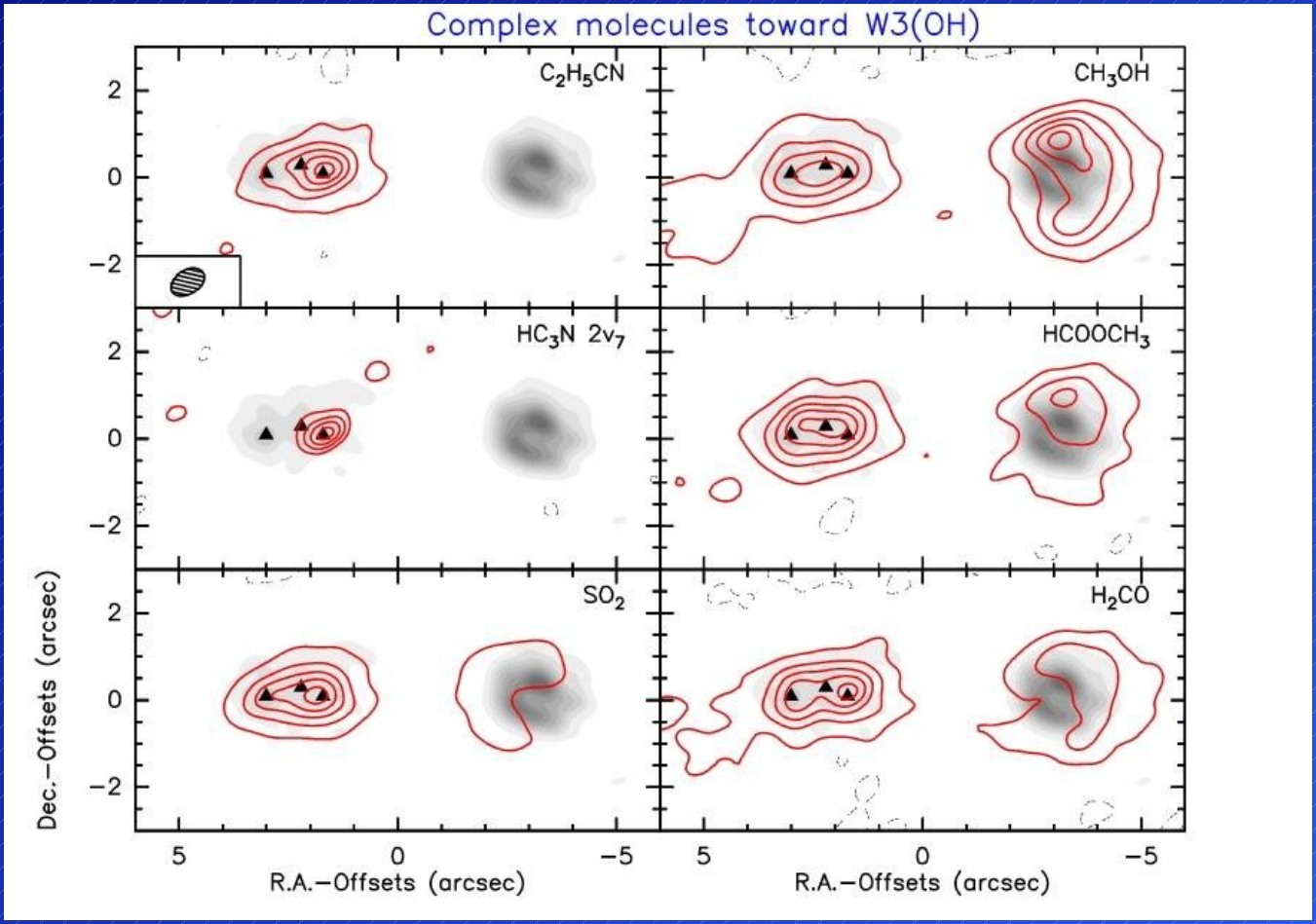
## The XCLASS approach

***Peter Schilke, MPIfR***

# *Why again are we doing this?*

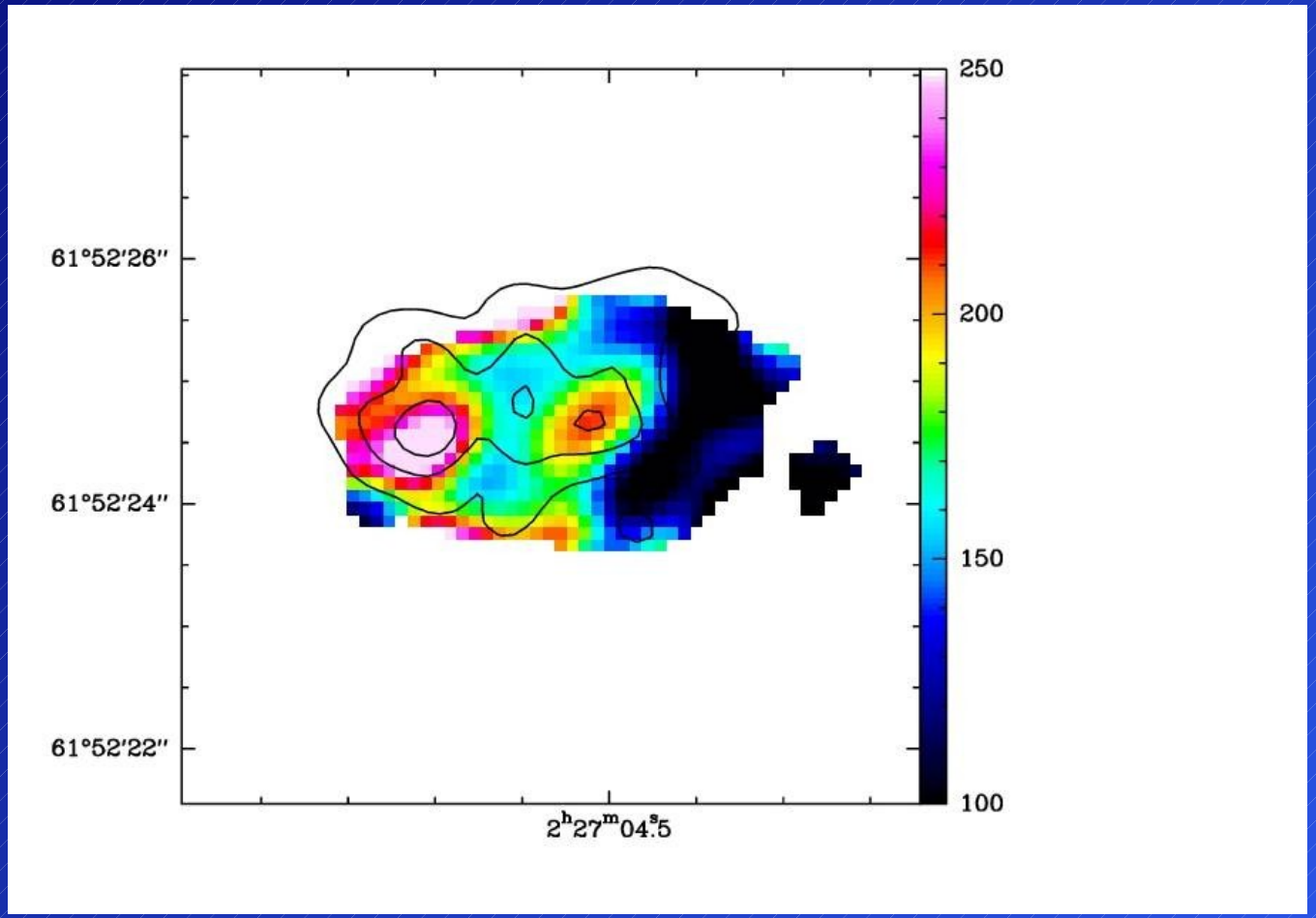
- Understanding physics and chemistry of star forming regions
- Single Dish line surveys have hundreds of lines for some species
  - very strong constraints for modeling source structure
  - has never been fully exploited
- Interferometric line surveys have hundreds of maps
  - nothing even remotely exploiting all the information has ever been done

# W3(OH/$H_2O$): complex molecules



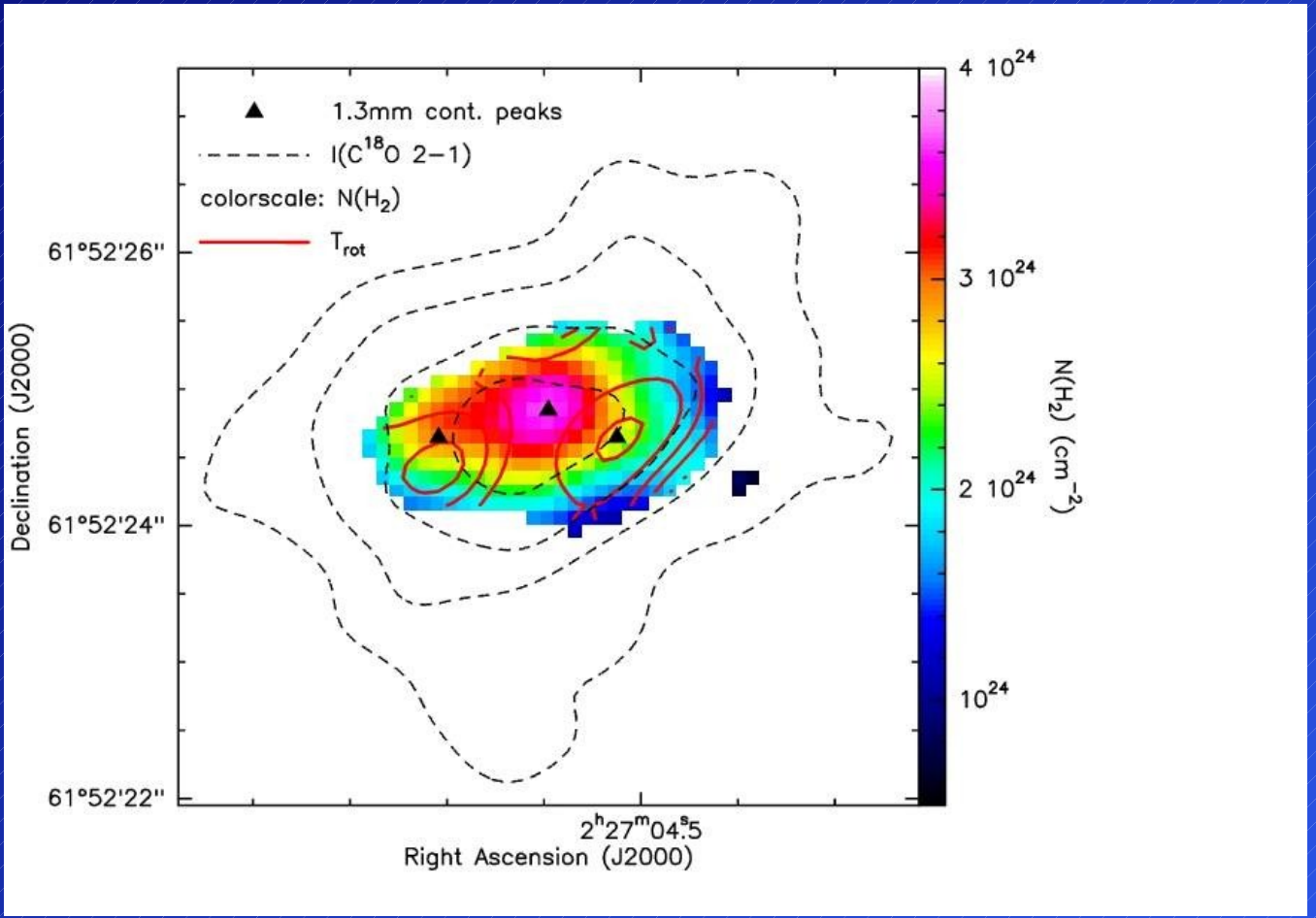

Wyrowski et al. 1999

# W3($H_2O$): temperature



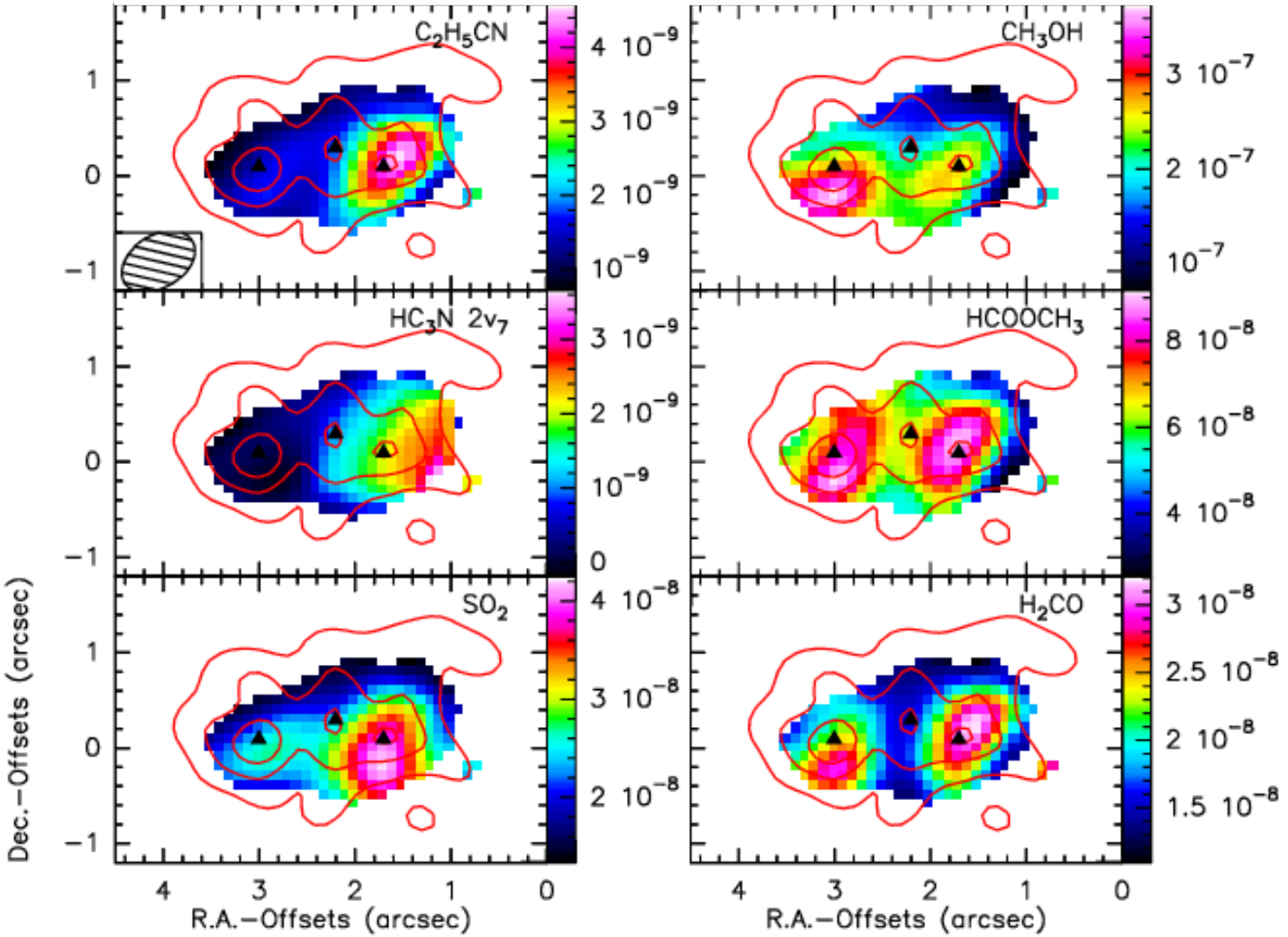

Wyrowski et al. 1999

# W3($H_2O$): $H_2$ column density




Wyrowski et al. 1999

# W3(OH) abundances

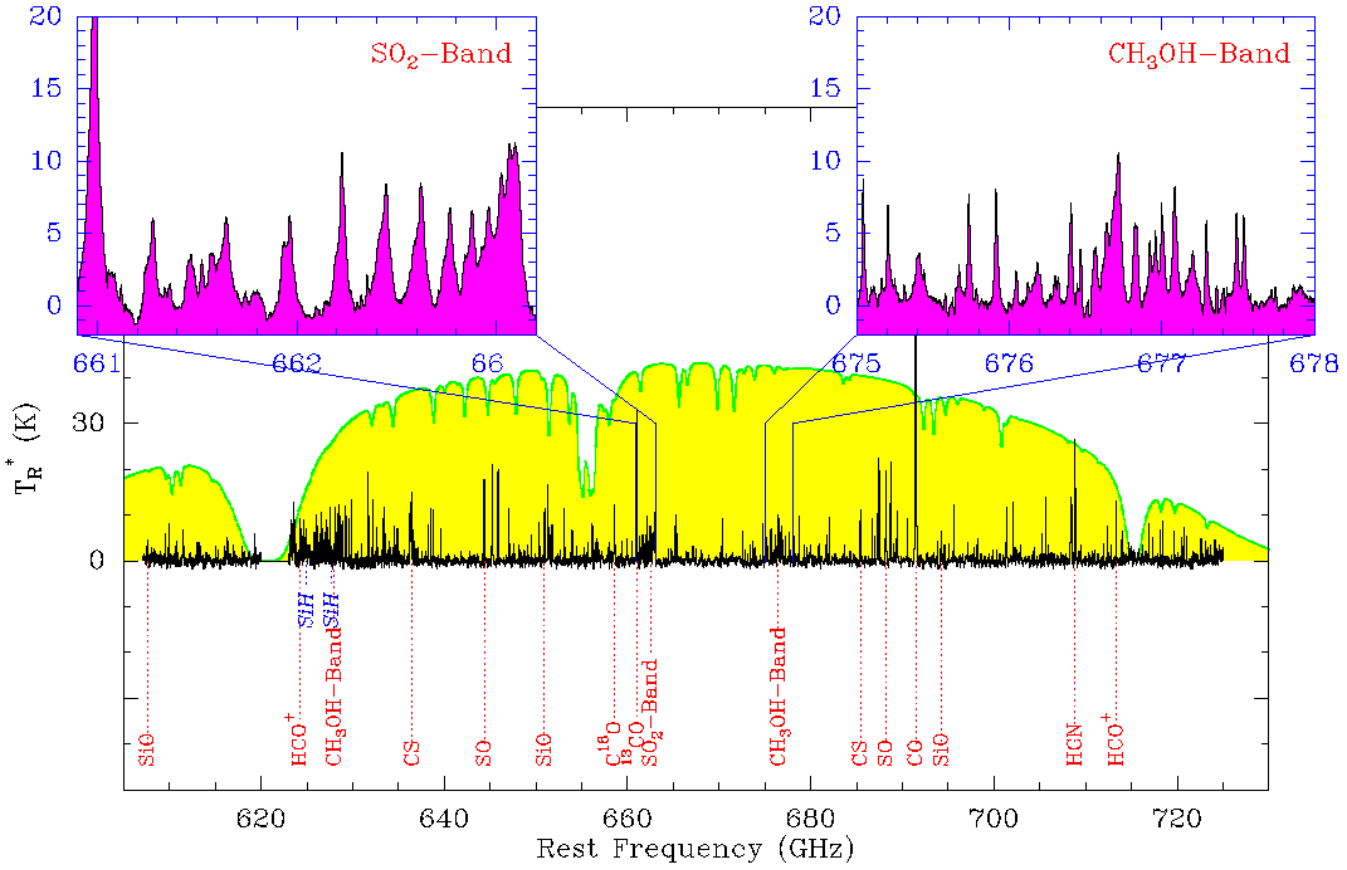



Wyrowski et al. 1999

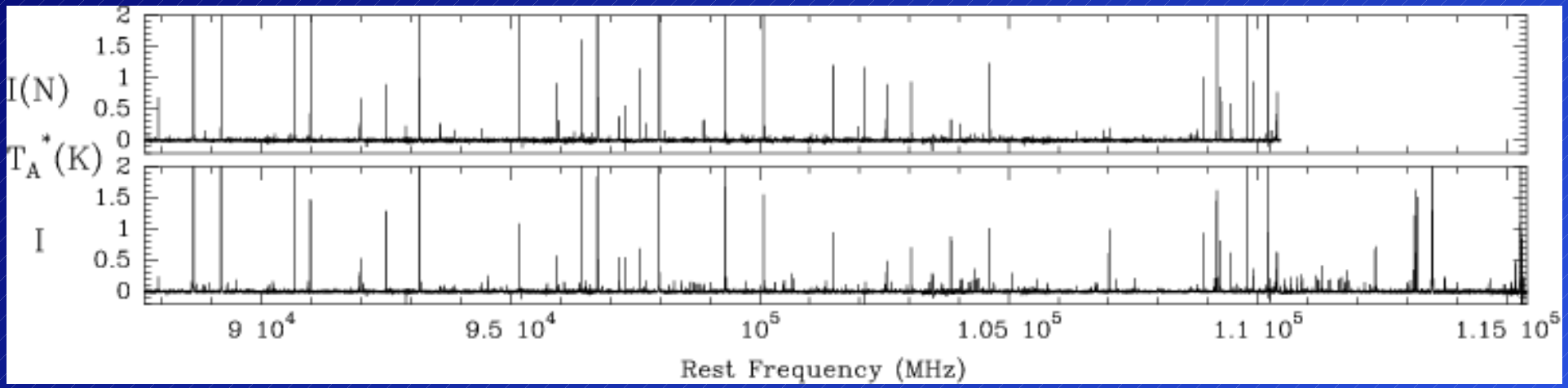
# *Motivation for writing XCLASS*

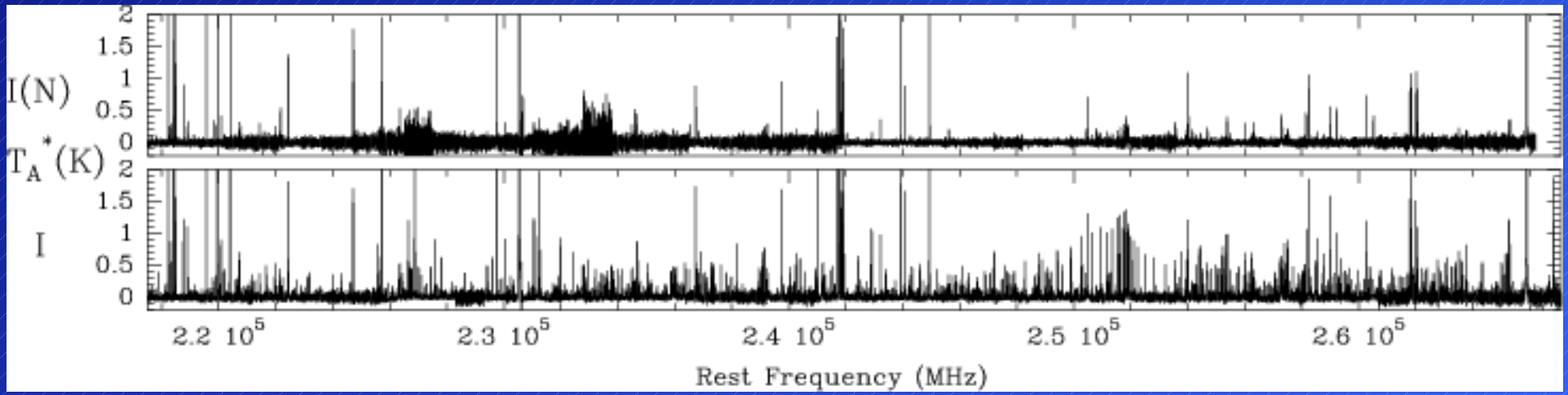
- Grew out of analysis of CSO submm line surveys of Orion
- versatile toolbox:
  - sideband deconvolution
  - line identification
  - spectral modeling
- Properties of line surveys in line-rich sources:
  - heavy blending
  - high opacities in many lines

# Example: Orion-KL @ 650 GHz (HIFI and ALMA Band)



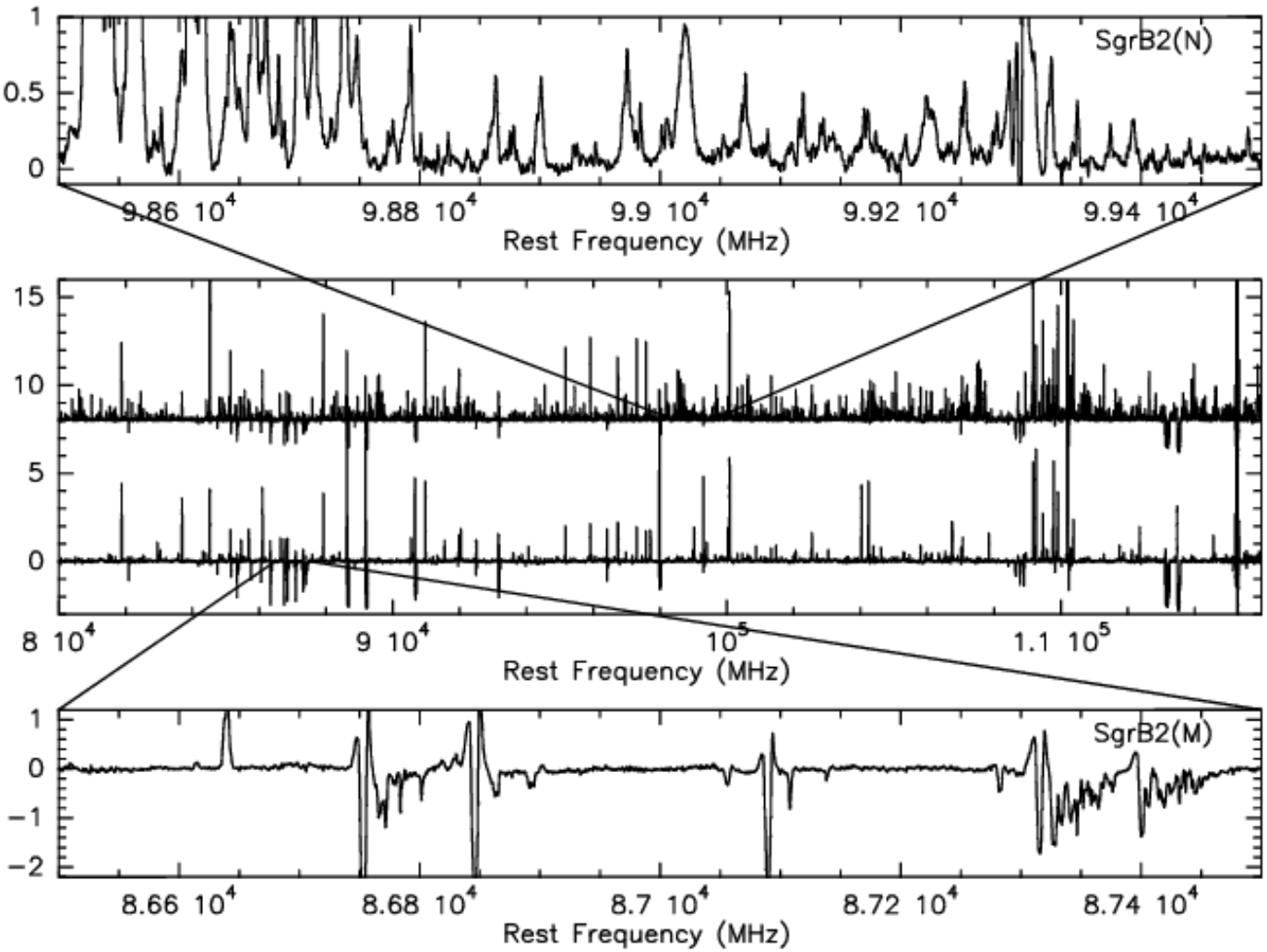
# NGC 6334 I




Thorwirth et al. in prep

# SgrB2(M+N) at 3mm 30 m telescope

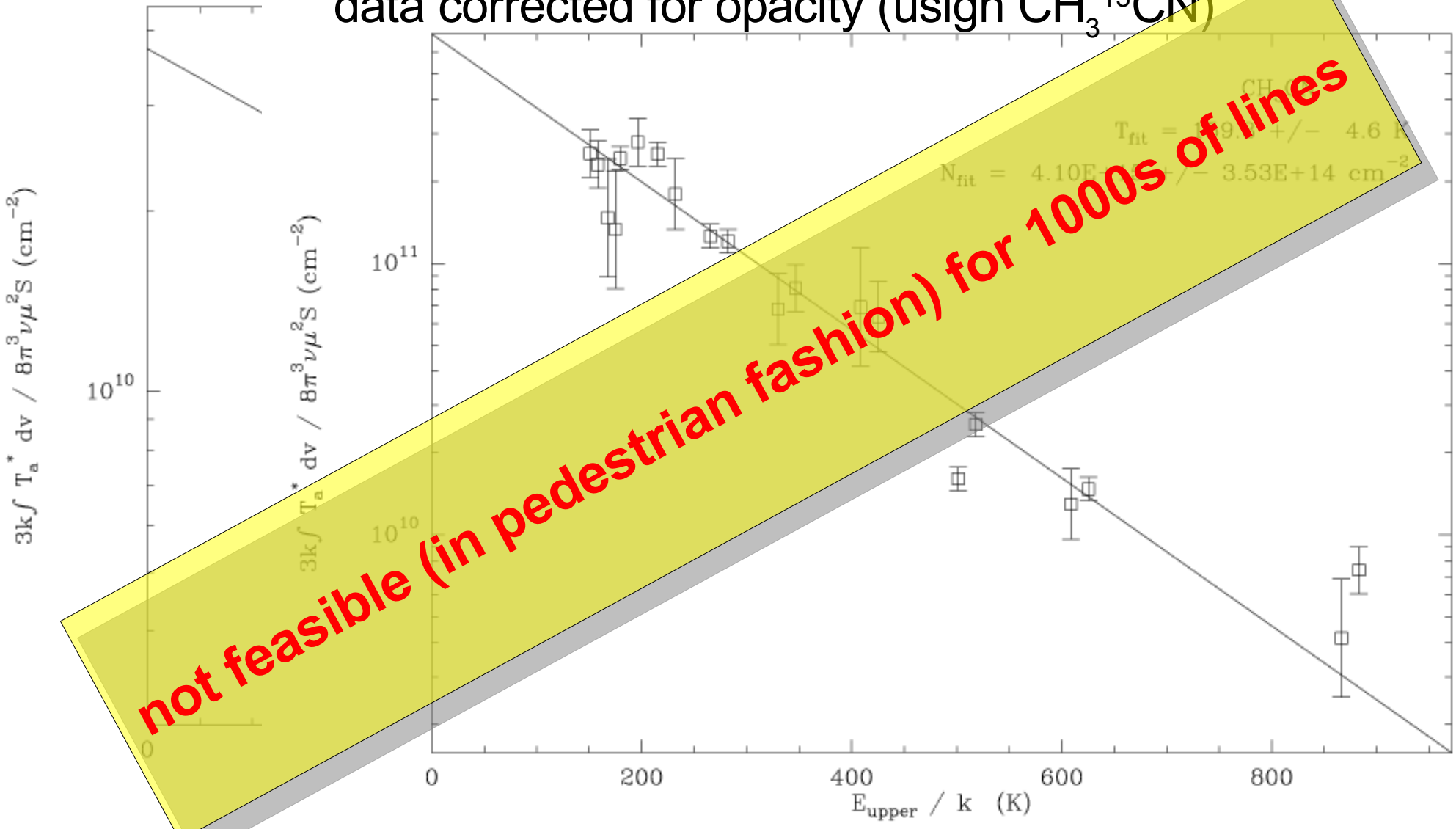



Belloche, Comito, Hieret, Menten, Schilke, in prep.

# Traumatic event

data out of the box

data corrected for opacity (usign $CH_3{}^{13}CN$)




not feasible (in pedestrian fashion) for 1000s of lines

# *Line identification*

- For large line surveys in rich sources, pedestrian approach does not work
- too many plausible candidates
  - automatic labeling is not an option
- line blends
- need some criteria for assign plausibility of line ID

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tralfamadore:~/Projects/articles/NGC6334Survey/dat

Session Edit View Bookmarks Settings Help

```
myXCLASS_4> id

 Lower sideband:    807254.871520996        807264.871520996

connection to xclass succeeded
Freq query succeeded!

User time:     0.07
Real time:     0.00

nRows found: 8

User time:     0.00
Real time:     0.00


Molecule                  Transition                              Frequency
                (MHz)     Error     (K)      (D^2)
C2H3CN                 43 3 40 2      - 42 2 41 2                807256.375
C2H3CHO                38 6 33 0      - 37 5 32 0                807258.438
H2CN                   11 4 8 14 11   - 10 4 7 18 10             807258.500
NH2CH2CH2OH            32 13 20 0     - 32 9 23 0                807262.000
aa-(C2H5)2O            59 18 42       - 58 17 41                 807262.250
aa-(C2H5)2O            59 18 41       - 58 17 42                 807262.250
NH2CH2CH2OH            50 16 35 2     - 50 13 38 2               807263.188
NH2CH2CH2OH            50 16 34 2     - 50 13 38 2               807263.312

 Upper sideband:    818754.878479004        818764.878479004

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Real time:     0.00

nRows found: 3

User time:     0.00
Real time:     0.00

 back from extract_lines

Molecule                  Transition                              Frequency   Freq   E lower  mu^2 S
                (MHz)     Error     (K)      (D^2)
CH3C-13-CH             48 1           - 47 1                     818756.250   1.459   931.35   26.990
CS-34,v=0,1            17 0           - 16 0                     818758.375   0.004   314.51   65.166
CH3OH,vt=0,1           17 -8 10 1     - 16 -8 9 1                818759.938   0.065   989.92   10.678
myXCLASS_4>
```
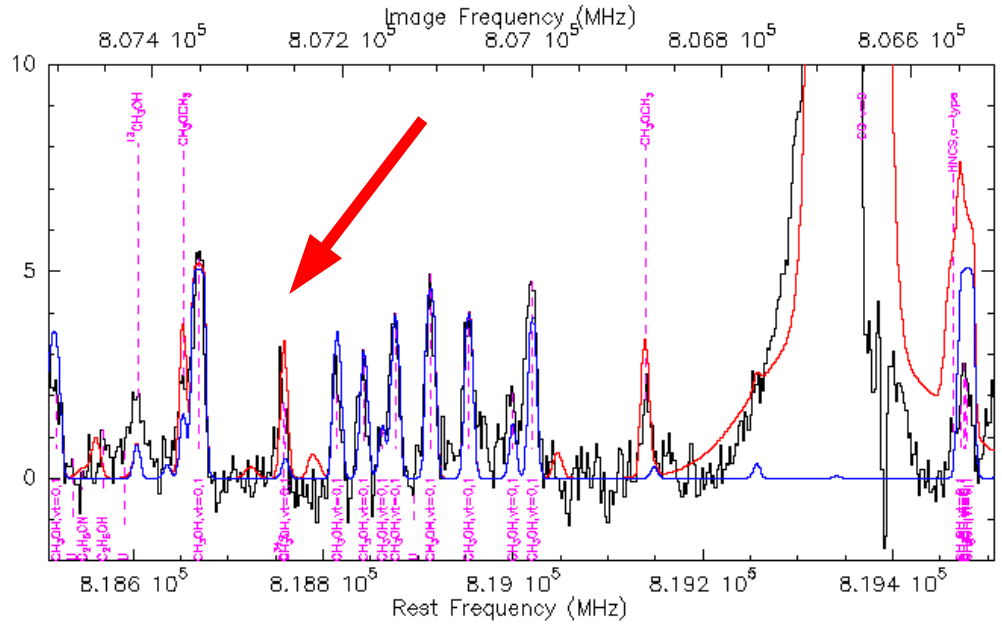

Shell | Shell No. 2 | Shell No. 3

<GREG 0

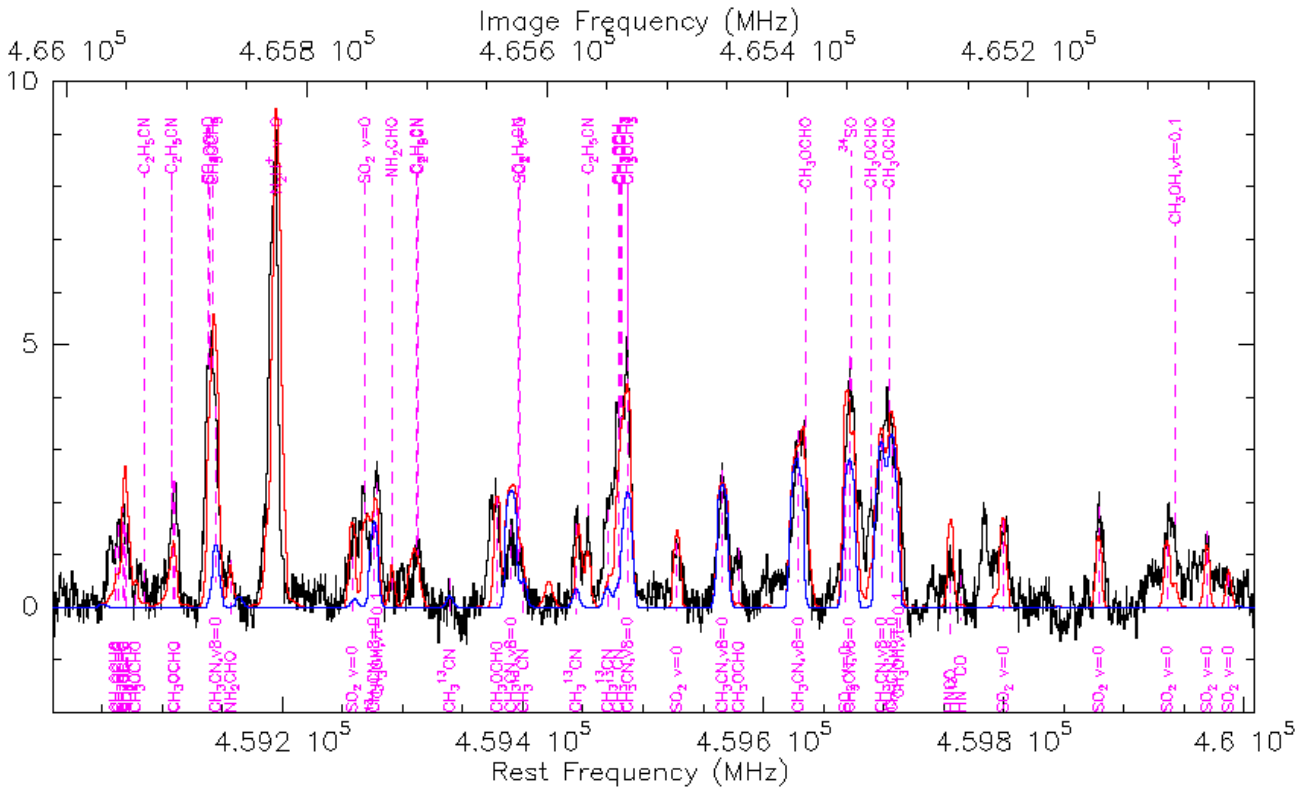


# *Identification of weak lines*

- Holistic approach
  - line identification of any line (except the strong, boring ones) requires a good model of the *whole* spectrum
    - only this gives an idea of how well the spectrum is known
    - including isotopologues (important to constrain optical depths)
  - current approach:
    - LTE, several components
    - Variables:
      - source size
      - kinetic temperature
      - column density
      - velocity, velocity width

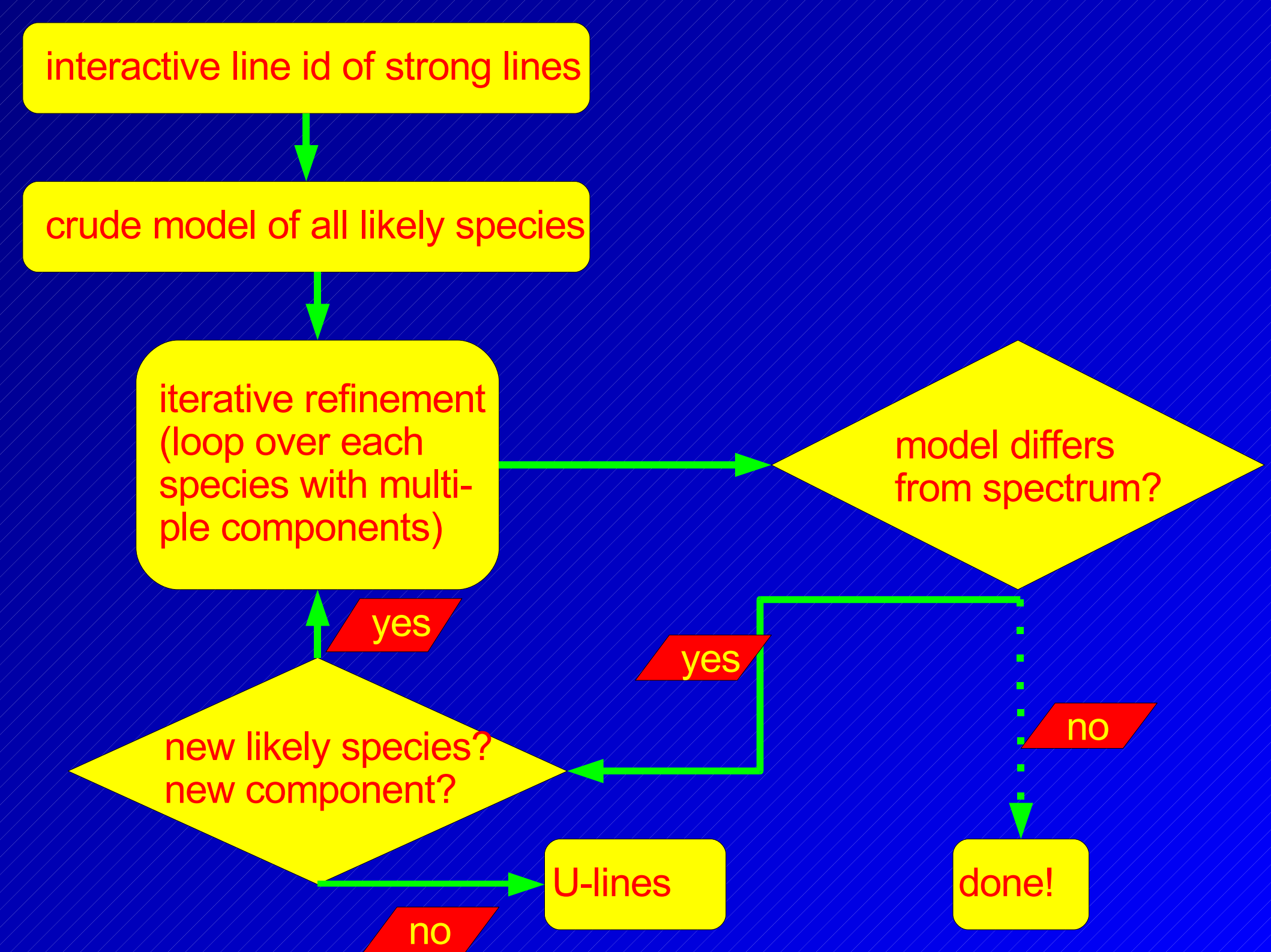
blue: $CH_3CN$

red: all species



# *Practical approach*

- interactive line ID
- crude model of all likely species
- iterative refinement
  - species by species
  - fit *all* lines in *all* frequency ranges
  - take blending into account
  - allow for multiple components
- then look for deviations
  - previously overlooked species
  - different excitation ranges (very highly excited lines)
  - U-lines


interactive line id of strong lines
crude model of all likely species
iterative refinement (loop over each species with multi-ple components)
model differs from spectrum?
yes
yes
no
new likely species? new component?
U-lines
done!
no

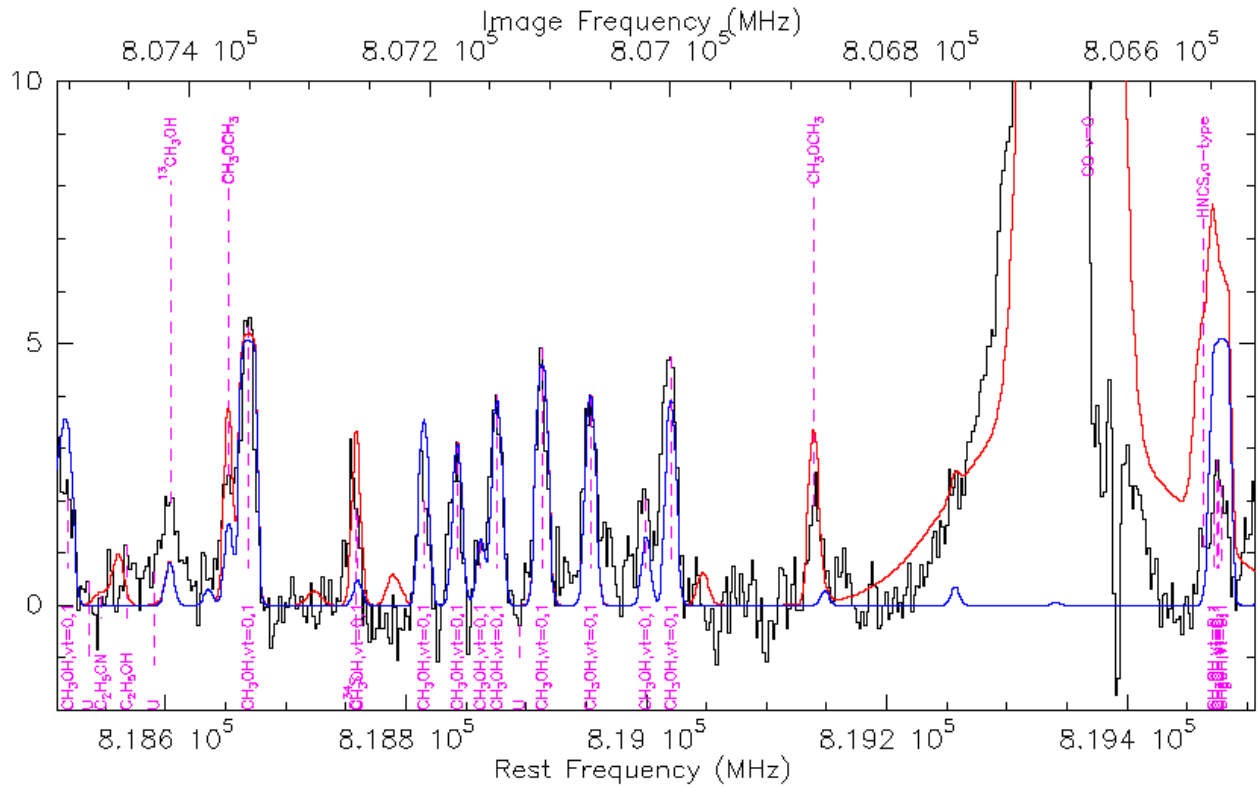
# script for modeling and visual inspection

emacs@tralfamadore.m

File Edit Options Buffers To

```
!
!  Time-stamp: <2006-03-24 17
!
def char yn*1 mol*20
let mol &1
let yn &2
file in ngc6334_corr.apex
$ ./make_class.pl
s\lim /en 0 2000
freq 450000 475000
if (yn.eq."y") then
        readm molfit_ngc6334.
        freq 450000 475000
        mods 12 /iso
        mem model400
        maketau
        mem tau400
        freq 800000 830000
        mods 12 /iso
        mem model800
        maketau
        mem tau800
        $ ls molfit_ngc6334*
        readm all_ngc6334.mol
        freq 450000 475000
        mods 12 /iso
```

<GREG 0




tralfamadore:~/Project

Session Edit View Bookmar

```
I-MODIFY, Beam efficiency set to
-9.0001142578125E+03
I-SIMULATE, IF = -6000, Fsignal =
I-SIMULATE, Using model taken fro
I-SIMULATE, IF = -6000, Fsignal =
I-SIMULATE, Using model taken fro
myXCLASS_3> SIC\PAUSE
myXCLASS_4> c
I-GET, Entry 8 Observation 402; 9
I-MODIFY, Beam efficiency set to
-9.0001162109375E+03
I-SIMULATE, IF = -6000, Fsignal = 819010, Fimage = 807009.
I-SIMULATE, Using model taken from CLASS R-memory.
I-SIMULATE, IF = -6000, Fsignal = 819010, Fimage = 807009.
I-SIMULATE, Using model taken from CLASS R-memory.
myXCLASS_3> SIC\PAUSE
myXCLASS_4>
```

Shell | Shell No. 2 | Shell No. 3

# *Modeling*

- Minimum requirement
  - LTE
  - opacities are dealt with, taking isotopologues into consideration
  - line blends
- Dream Requirement
  - Radiative transfer modeling of all species
  - taking radiation coupling into account
  - taking source structure into account
- Ultimate goal:
  - getting the physics and chemistry of the source

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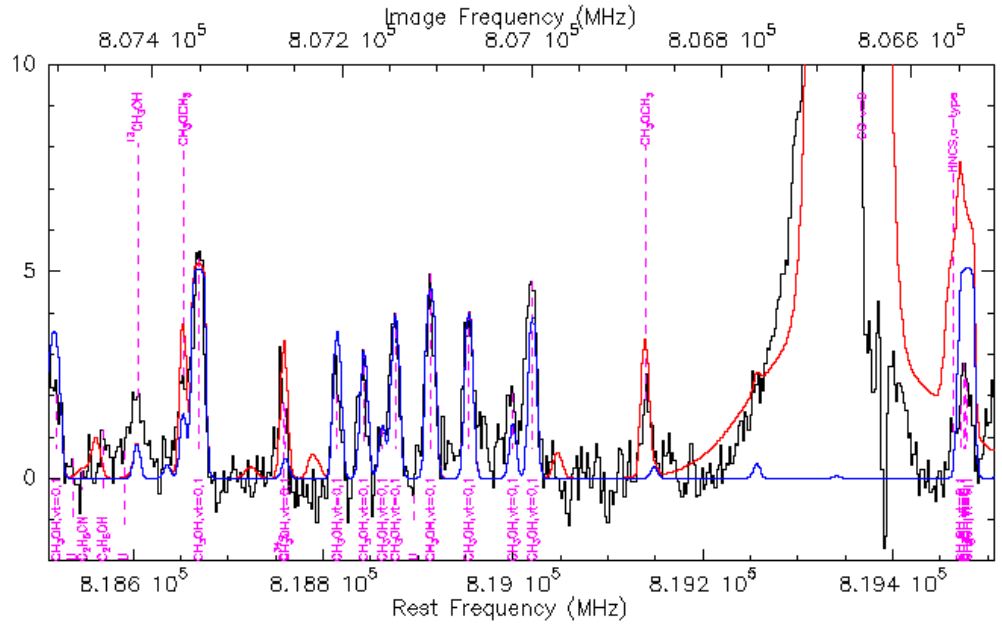


Shell | Shell No. 2 | Shell No. 3

# *Problems*

- Incompleteness and quality of catalogs
  - particulary at submm wavelength
- inadequacy of model
  - LVG approach for methanol
  - OK up to a point (finite number of components)
  - collision rates missing
  - even when collision rates are available, they often are not for the very high levels observed in submm

# *XCLASS now*

- **+**
  - builds on CLASS, has all the commands and
  - scripting language (very important)
  - fast
  - (for us): extensible
- **-**
  - homegrown software – no design to speak of
  - limited documentation
  - very limited manpower available for improvements (CC, PS, AB + students and postdocs)
  - only 1-d

# *What we have*

- XCLASS, CASSIS and some private programs with similar capabilities for single dish surveys
- Utilize private compilations based on CDMS/JPL and maybe some private data sets

# *What we want*

- Must be able to model spectra (data cubes!) using different input models
  - must be able to get input parameters (frequencies, line strengths, collision rates) from database
  - must be able to read data
- Must provide figure of merit ($\chi^2$ or so) for model
- Must provide error estimates for input parameters
- Must run semi-automatically
  - scripting language!
- Must have visualization capability

# *What we really want*

- Should find best fit autonomously
- Should be exportable (run on a laptop in an airplane)
- Should be easily extensible by user
  - models should be plug-ins
  - should be able to re-use existing models (radiative transfer)

# *XCLASS then*

- in development
  - Error analysis of parameters ($\chi^2$)
  - automatic fitting (numerically non-trivial)
  - input from LVG
- desirable
  - full radiative transfer
    - one physical model
    - abundance profiles for each species
  - model maps
    - interferometers: PdB, ALMA

# *Future: MAGIX*

- Collborative effort of MPIfR Bonn (PS, D. Muders) with Obs. Meudon (F. Boone, M.-L. Dubernet), Cologne (CDMS) and Leiden (van Dishoeck, Hogerheijde: radiative transfer models)
- Generic model fitting package: versatile
- Models provided as plugins by users: re-use of existing knowledge
- fitting and feedback by common module

# *Databases*

- CDMS/JPL are great resources
- but they are NOT usable out of the box
  - collection of ASCII files in compressed format
  - special cases: $CH_3OH$
  - lots of content, sparse infrastructure for our applications
- Out-of-the-box databases have to be
  - queried directly from the web in a standard format (VO compatible)
  - provide quality tag for frequencies
  - provide unique answers
  - give more information: energy tables, collision coefficients, ...

# Basecol Database
# http://www.obspm.fr/basecol

Science Team: **M.L. Dubernet[*], N. Moreau, F. Daniel[*], D. Flower[***], A. Grosjean[**]**

Supported by LERMA, VO-Paris Data Center, National Program « Physico-Chimie du milieu interstellaire », NSF "Masse de Données en Astrophysique" project

[*] *LERMA, Paris Observatory*
[**] *Besançon Observatory*
[***] *Durham University, UK*

# Objectives/Content

- Published (de)-excitation rate coefficients
  - Rotational (fine, hyperfine structure)
  - Ro-vibrational, Vibrational (not exhaustive)
  - Currently: 21 Target molecules
  - Perturbers : He, H, $H_2$ (not exhaustive)
  - 76 collisional systems
  - Fully documented and referenced (630 ref.)
  - Fitting coefficients, visualisation tools
- Linked to CDMS and JPL
  - Theoretical and experimental energy levels
  - Einstein coefficients

# Basic package we need

- Data
  - frequencies
  - collision rates
- Infrastructure
  - complete databases
- Models
  - spectra, data cubes
  - versatile, easy to use

# *Role of XCLASS*

- testbed for algorithms and methods
- with current manpower not possible to provide reliable package to wide user community