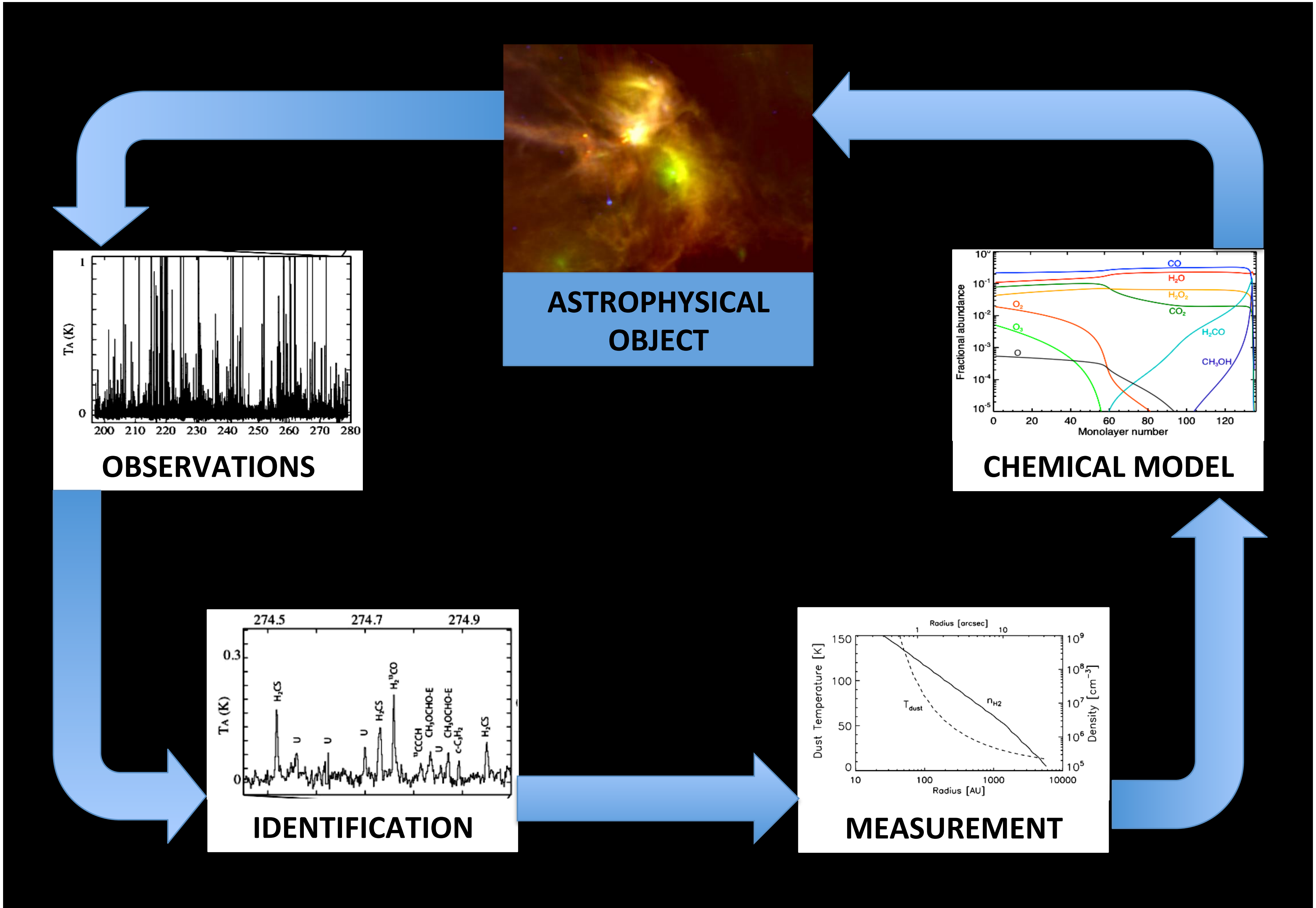
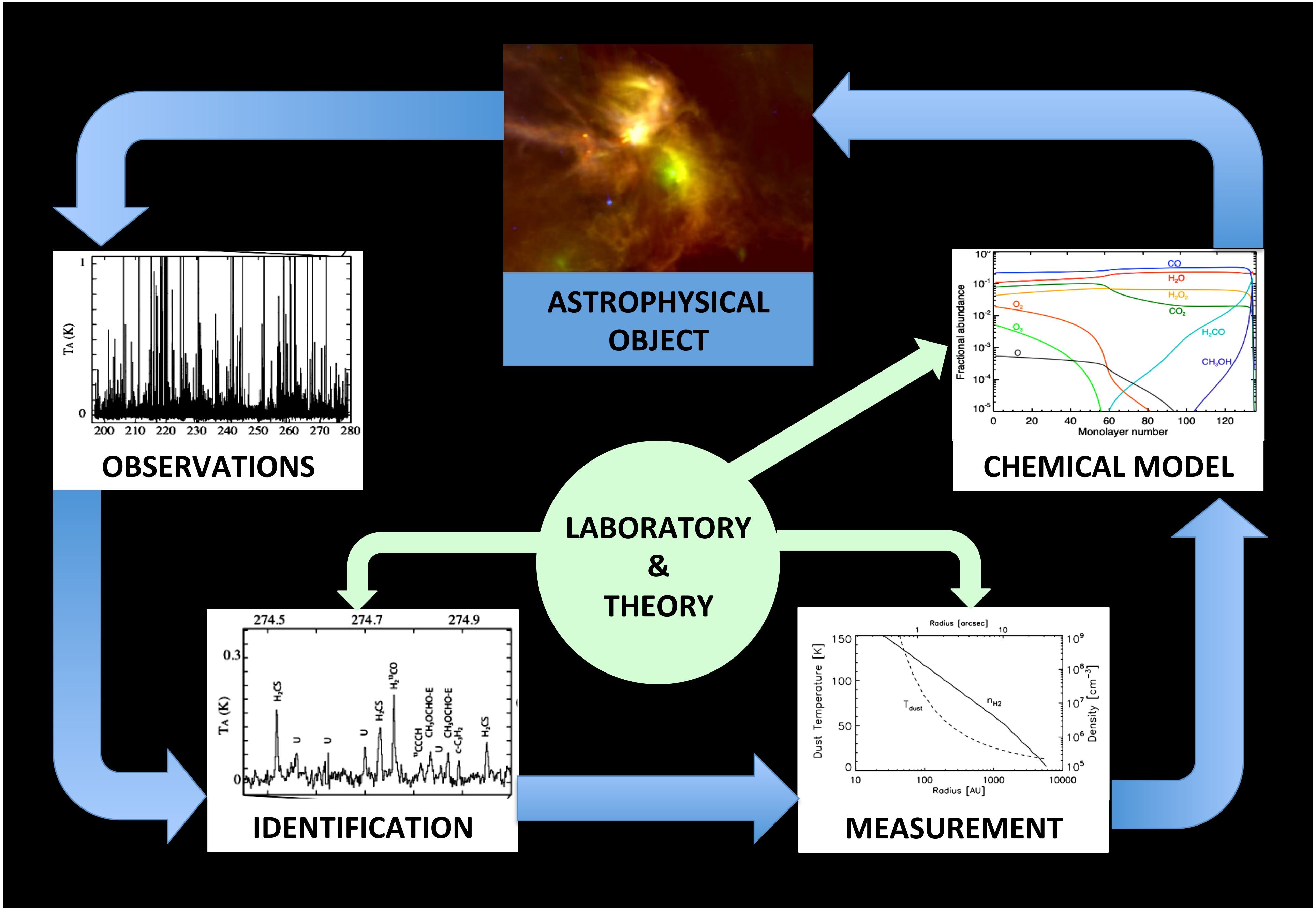
OBSERVATIONAL ASTROCHEMISTRY

Cecilia Ceccarelli
Institut de Planétologie et d'Astrophysique de Grenoble


ASTROPHYSICAL OBJECT
OBSERVATIONS
TA (K)
200 210 220 230 240 250 260 270 280
IDENTIFICATION
274.5 274.7 274.9
H2CS
U
H2 13CO
13CCCH
CH3OCHO-E
c-C3H2
MEASUREMENT
Radius [arcsec]
Dust Temperature [K]
Density [cm-3]
Radius [AU]
Tdust
nH2
CHEMICAL MODEL
Fractional abundance
Monolayer number
CO
H2O
H2O2
CO2
O2
O3
O
H2CO
CH3OH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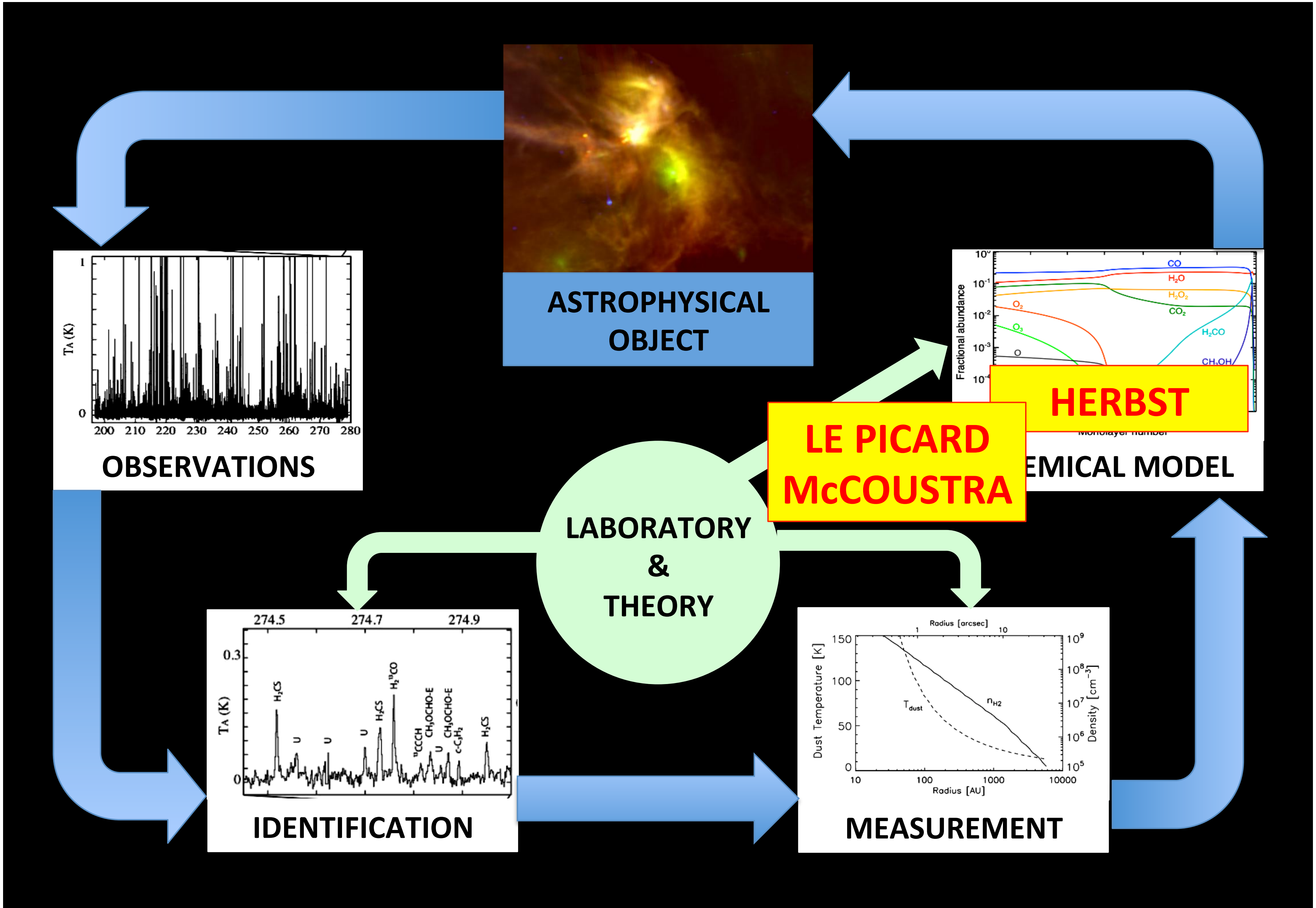
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IDENTIFICATION
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TA (K)
H2CS
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U
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H2CS
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CH3OCHO-E
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CH3OCHO-E
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MEASUREMENT
Radius [arcsec]
1 10
150
100
50
0
Dust Temperature [K]
T dust
n H2
10 100 1000 10000
Radius [AU]
Density [cm-3]
LABORATORY & THEORY
LE PICARD McCOUSTRA
HERBST
EMICAL MODEL
Fractional abundance
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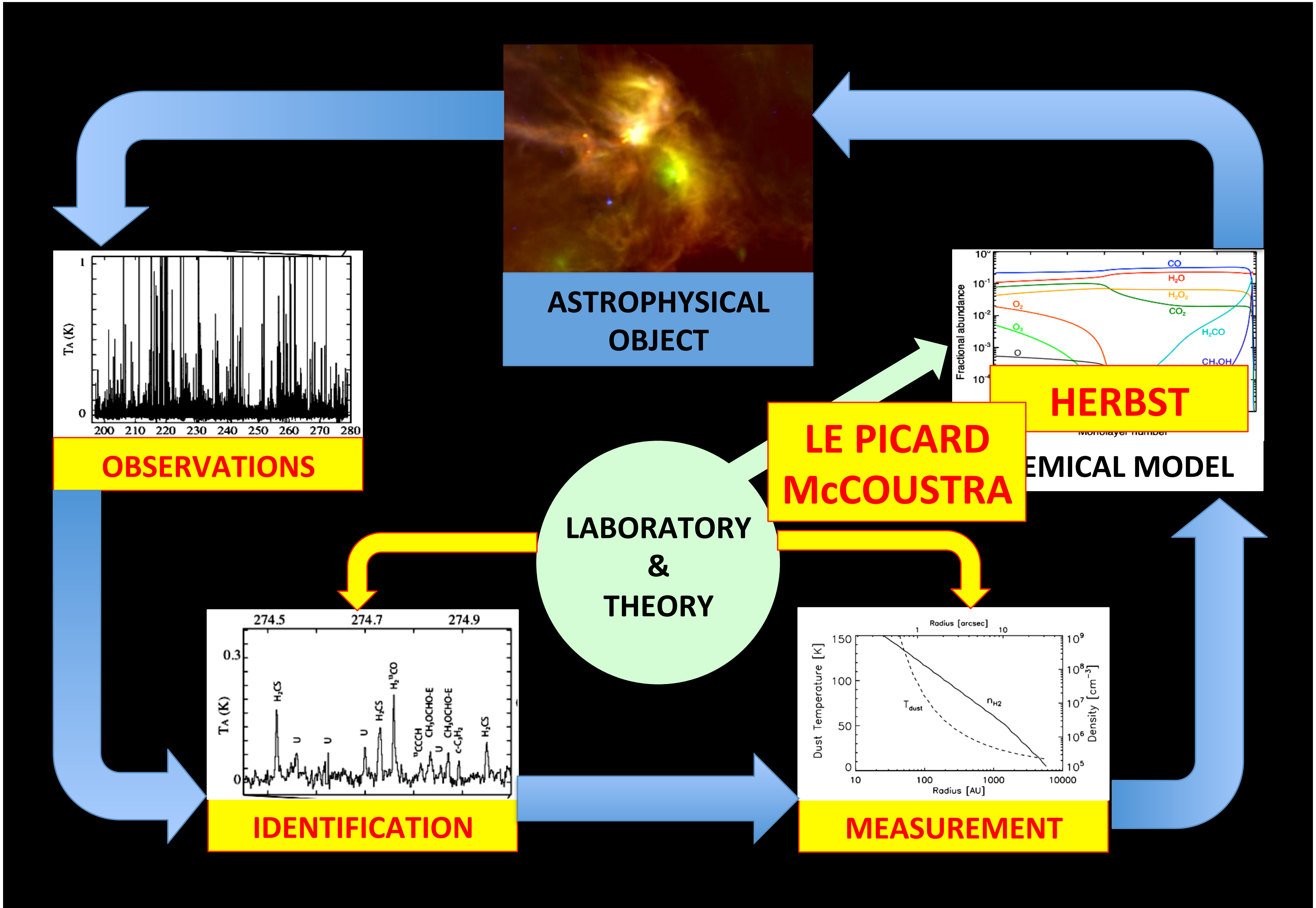
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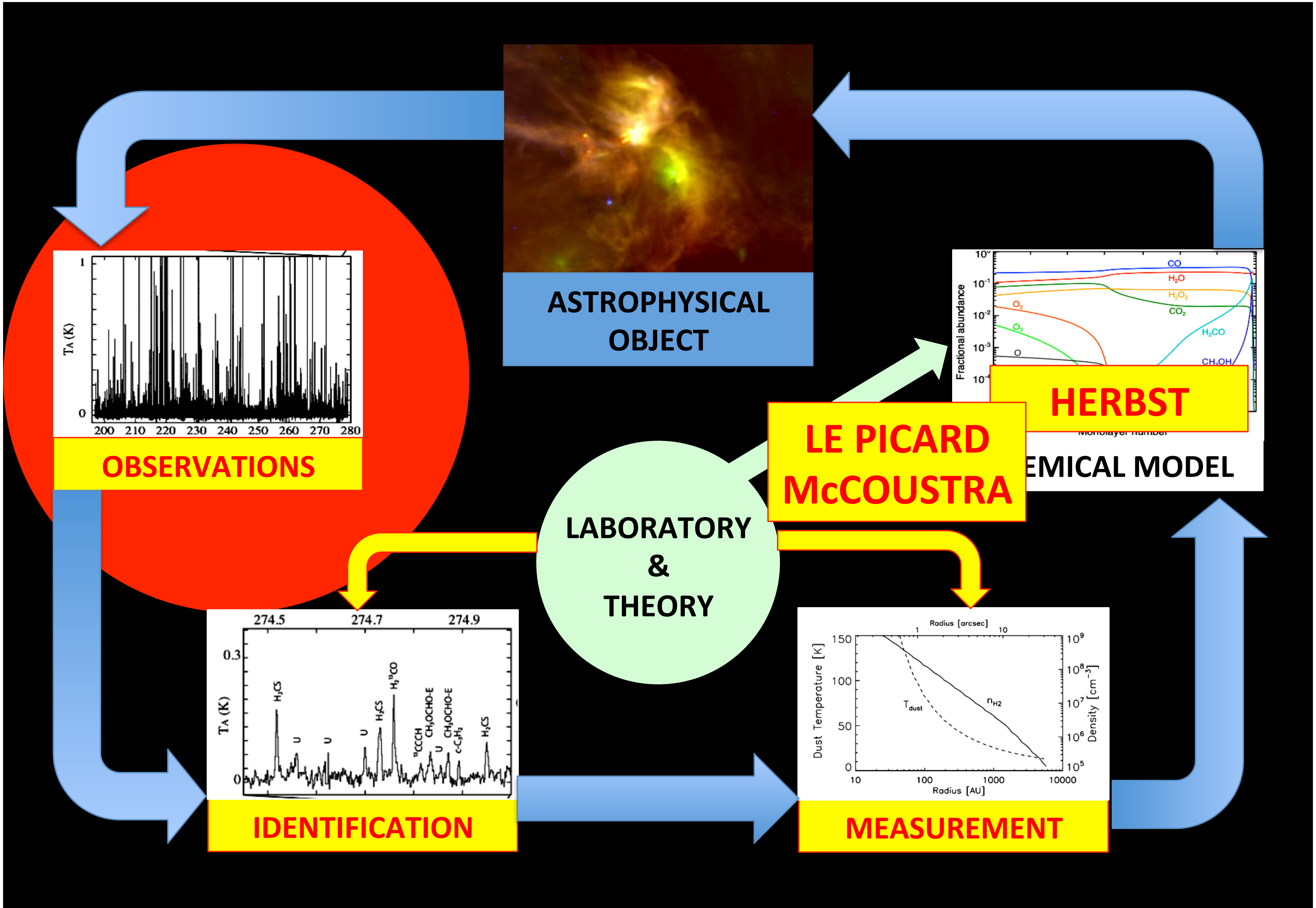
ASTROPHYSICAL
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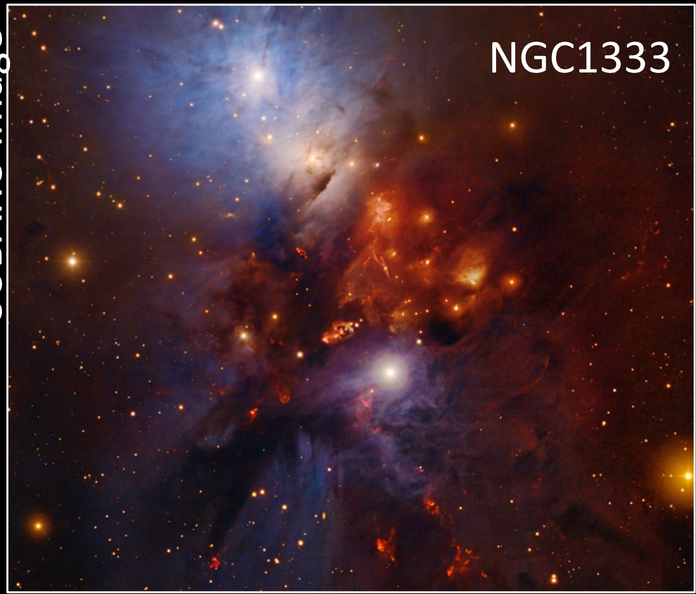
Fractional abundance

1. OBSERVATIONS

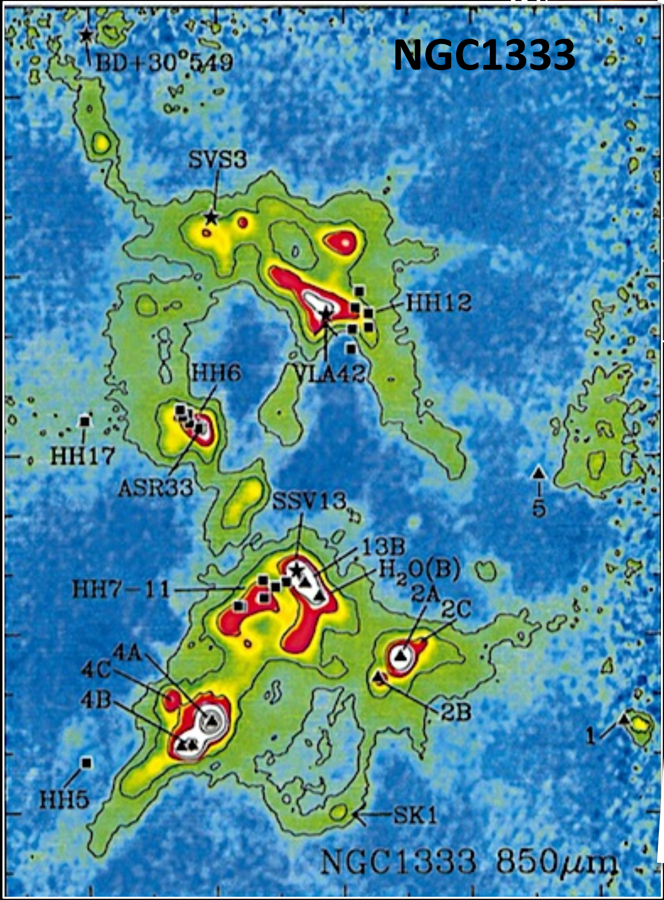
SUBARU image



1. OBSERVATIONS

SINGLE DISH: JCMT

Sandell+2001



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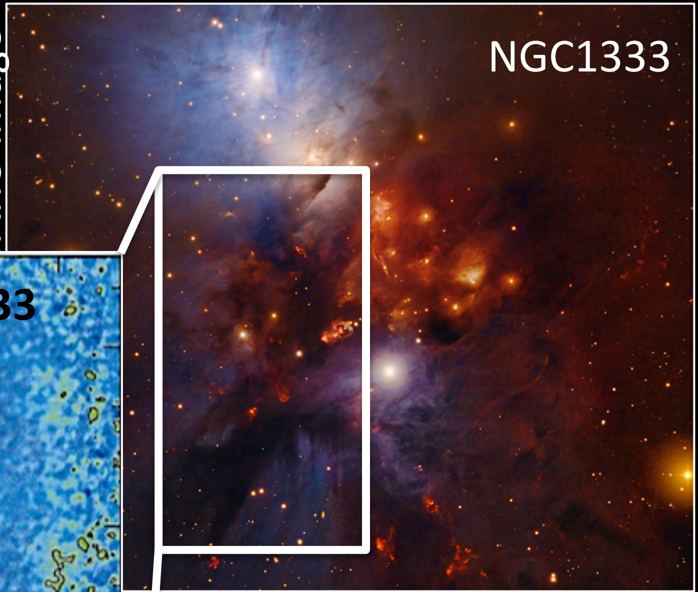
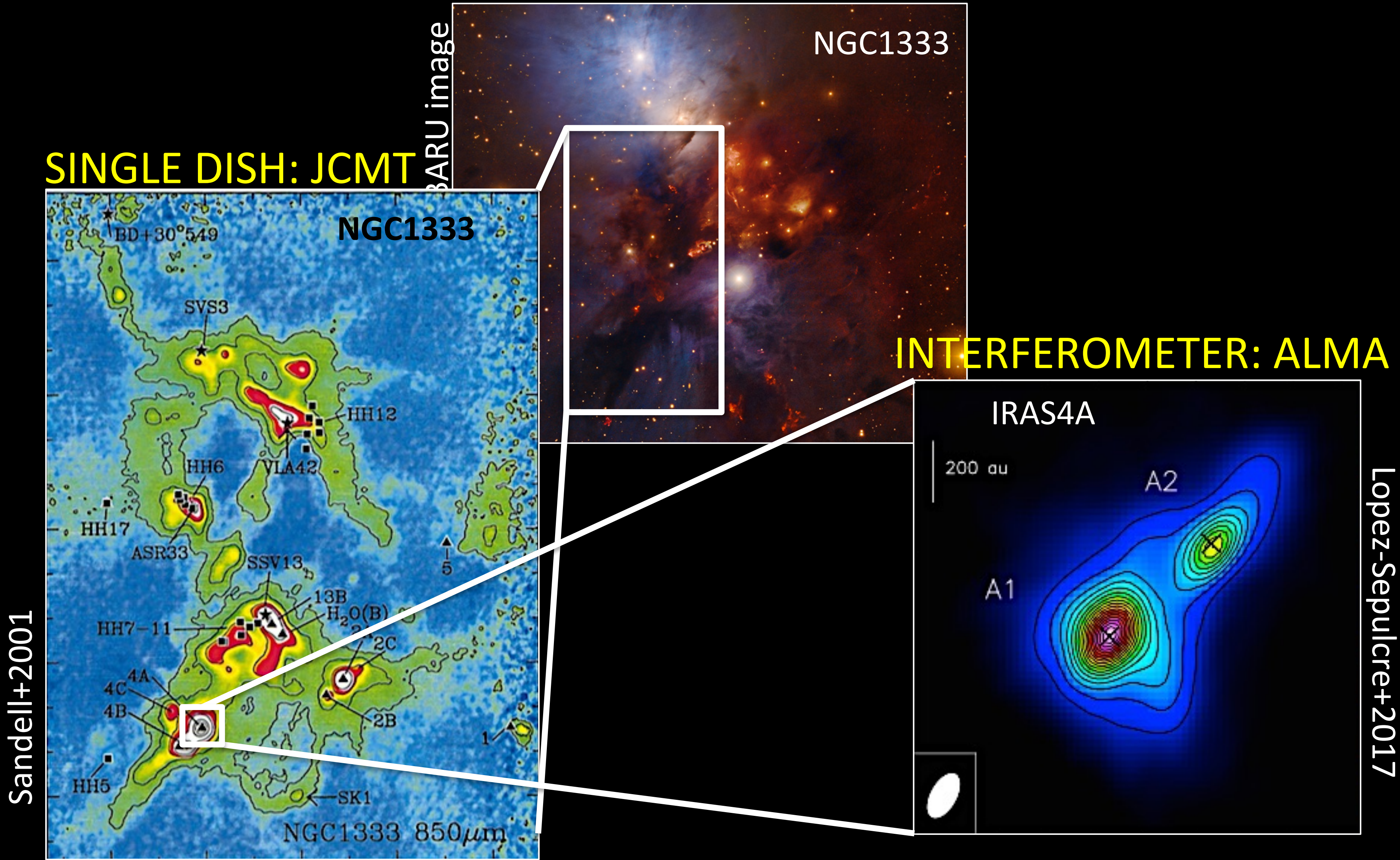


1. OBSERVATIONS

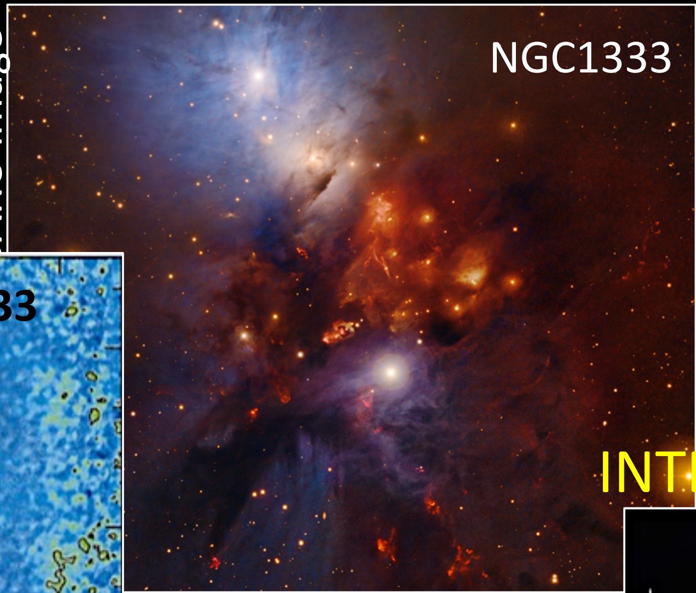
SINGLE DISH: JCMT

INTERFEROMETER: ALMA

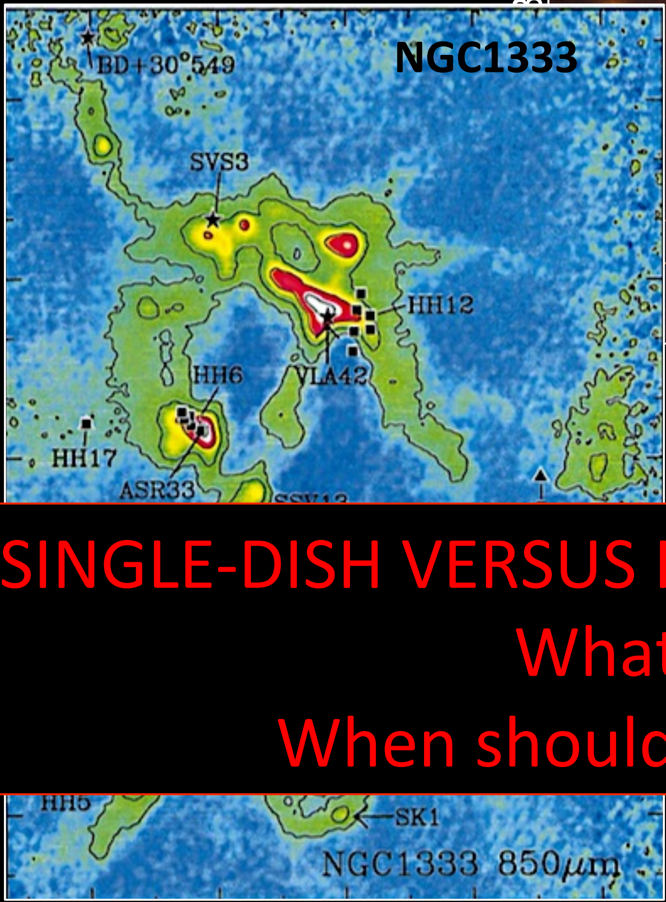


1. OBSERVATIONS

BARU image



SINGLE DISH: JCMT



Sandell+2001

INTERFEROMETER: ALMA

Lopez-Sepulcre+2017

SINGLE-DISH VERSUS INTERFEROMETRIC OBSERVATIONS

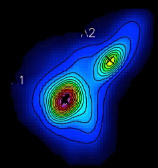
What is the difference ?

When should we use one or the other ?

SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS

ALMA

IRAS4A



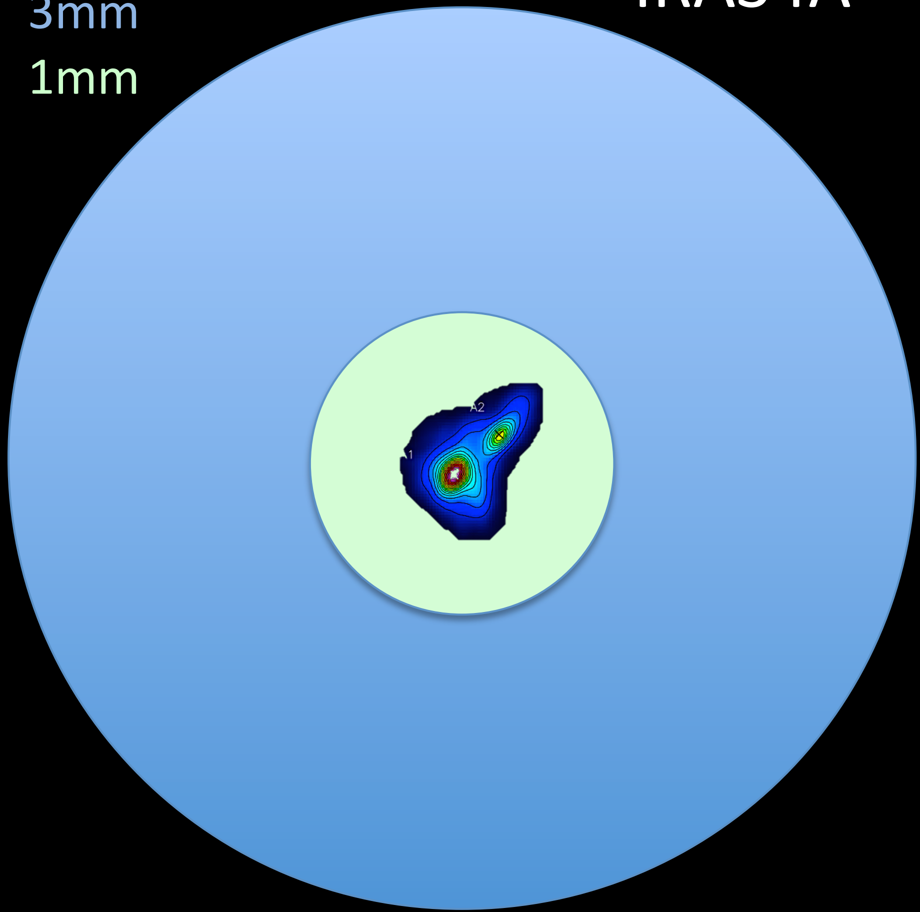
SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS

IRAM 30m

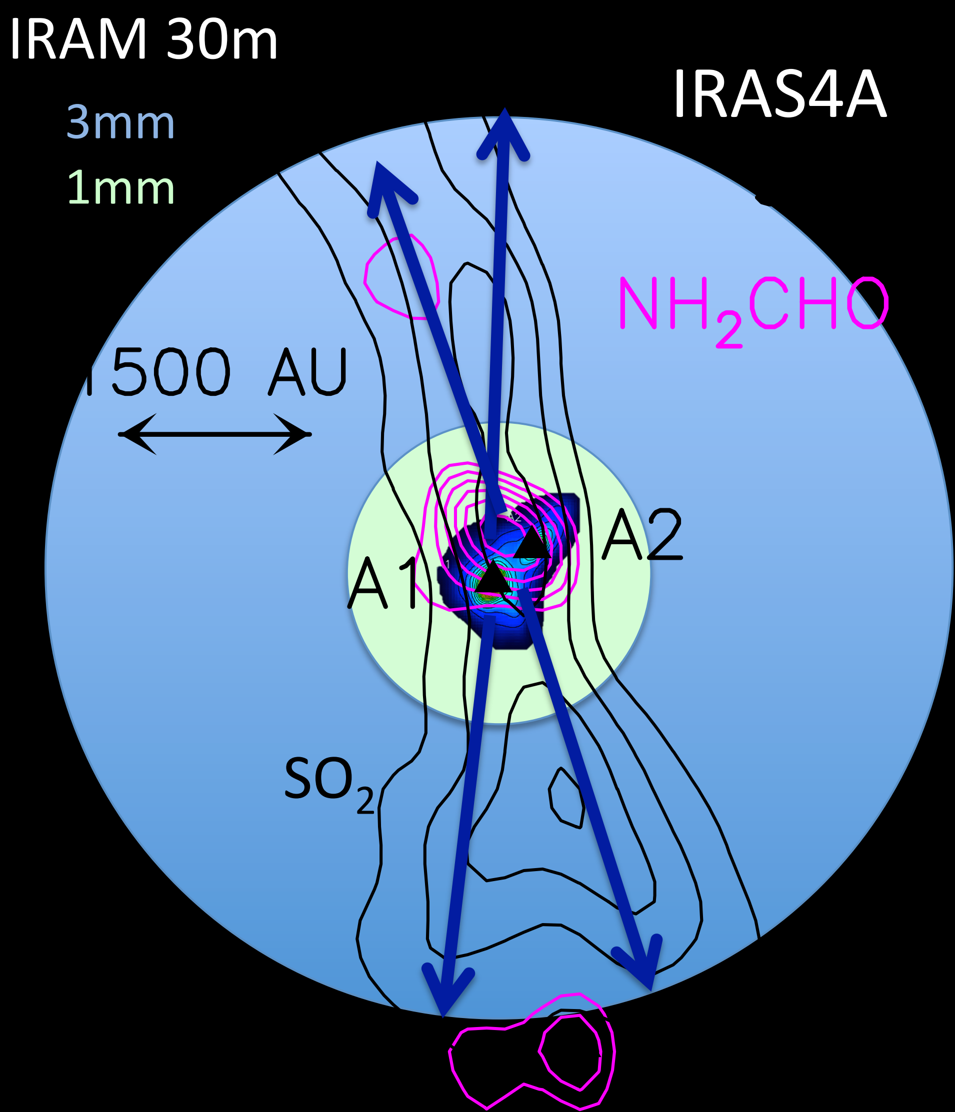
IRAS4A

3mm

1mm



SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS



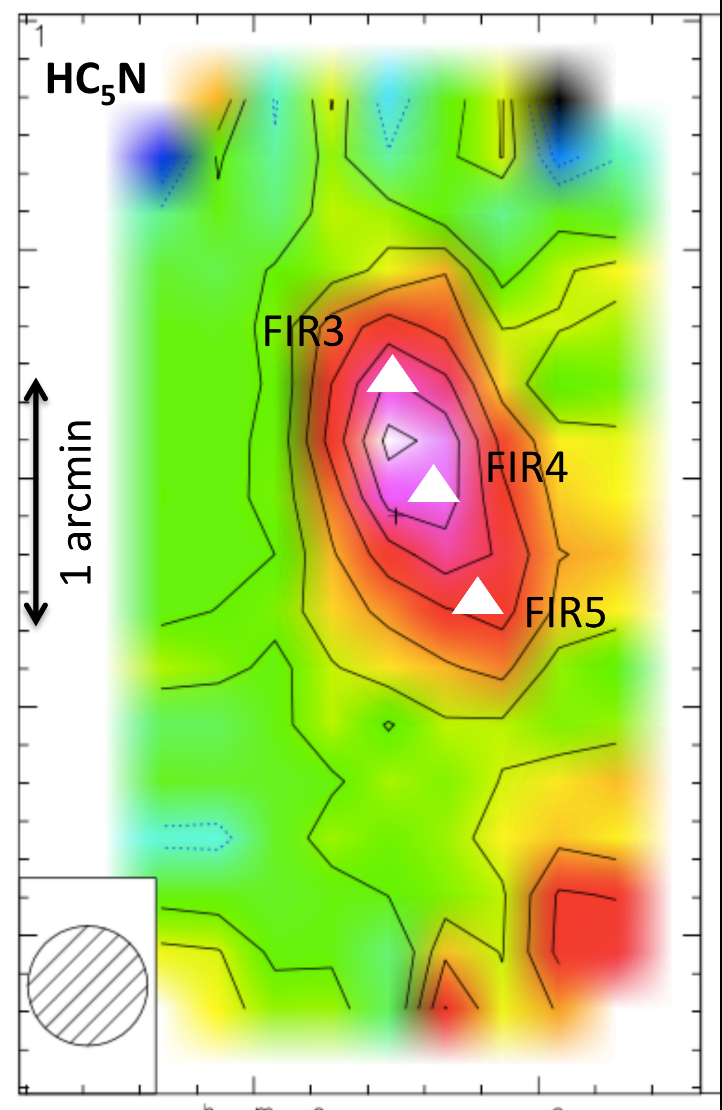
SEVERAL PHYSICAL COMPONENTS MIGHT BE PRESENT WITHIN THE SINGLE-DISH BEAM

➔ INTERFEROMETERS NECESSARY TO STUDY SMALL AND COMPLEX OBJECTS

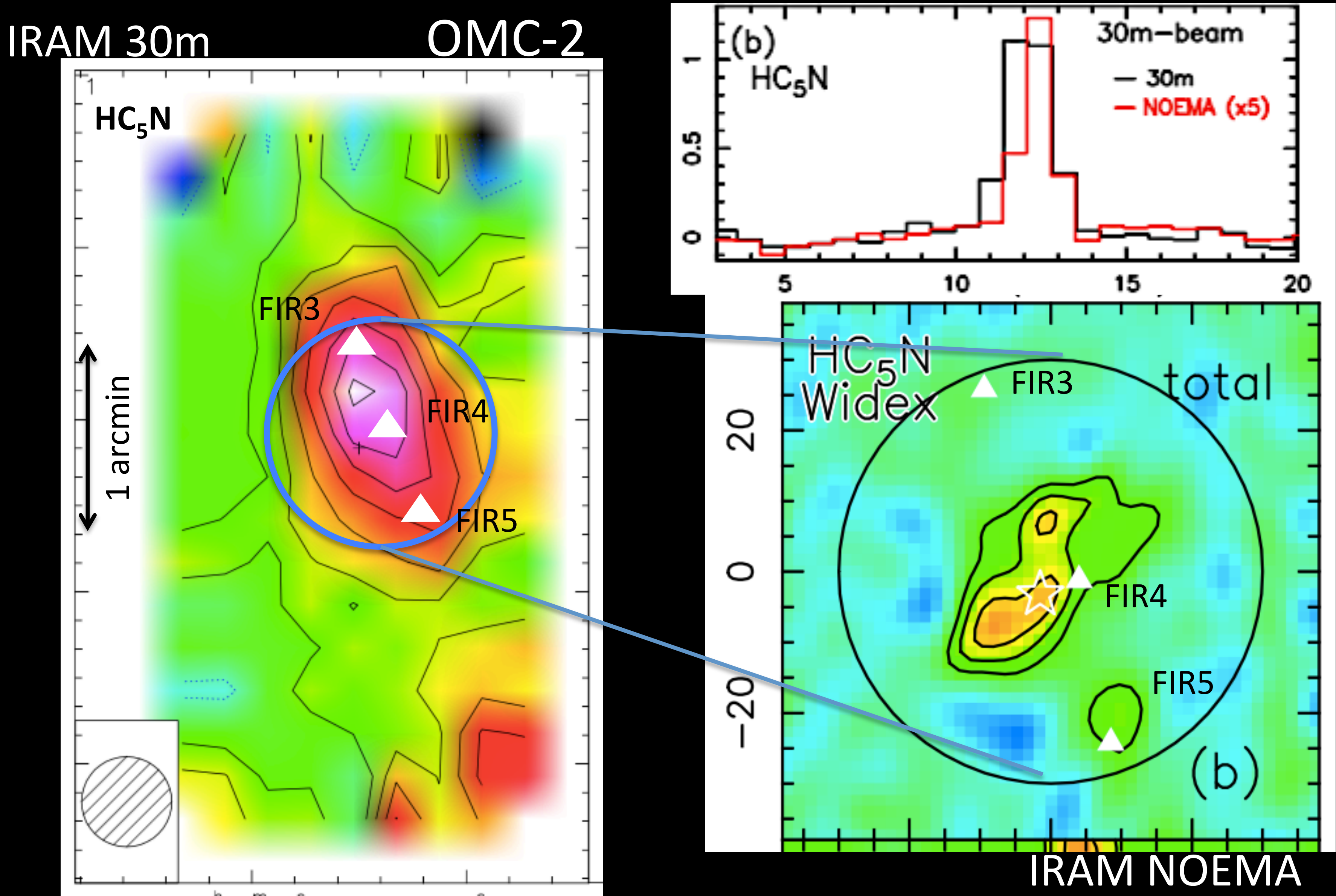
SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS

IRAM 30m

OMC-2

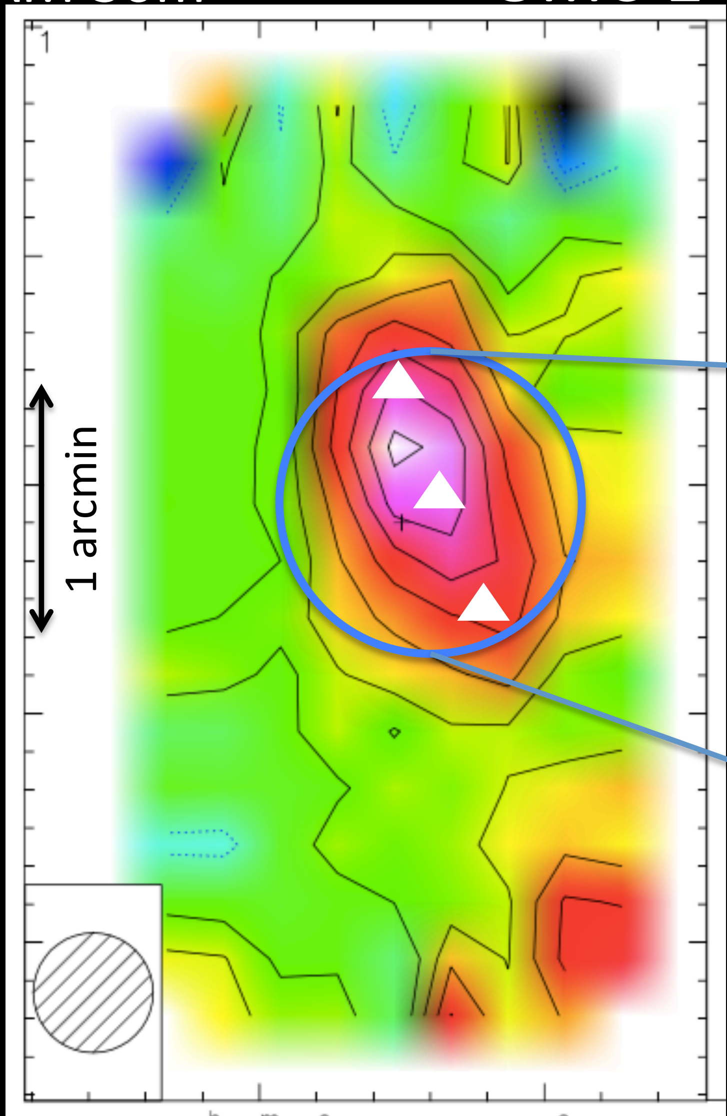


SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS



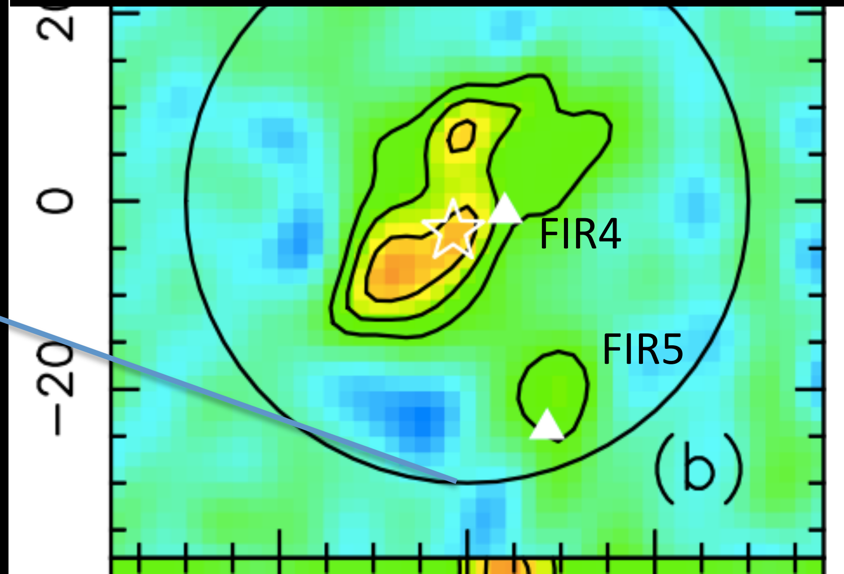
SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS

IRAM 30m OMC-2



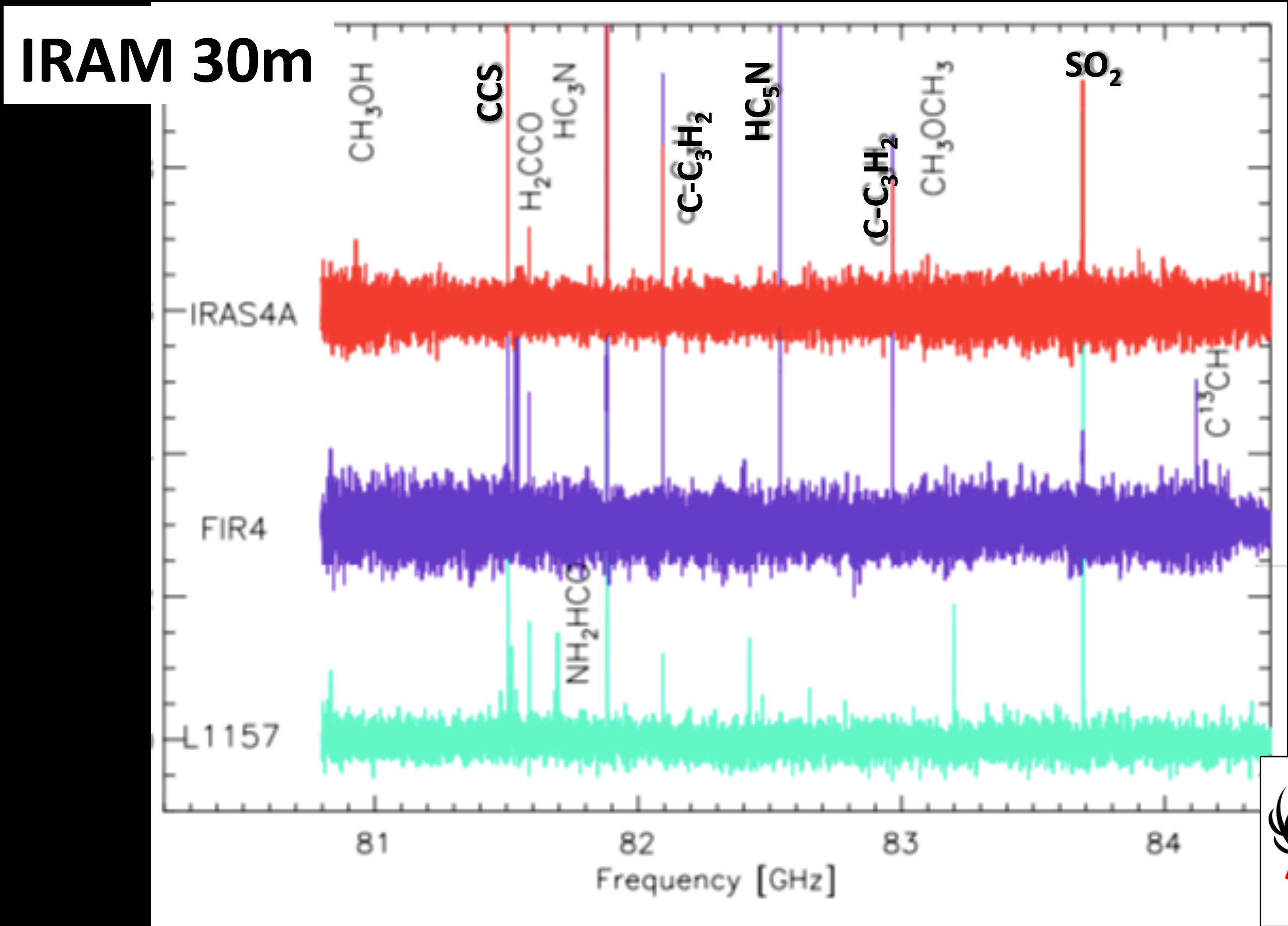
INTERFEROMETERS FILTER-OUT EXTENDED EMISSION

➔ SINGLE-DISH TELESCOPES NECESSARY TO STUDY LARGE OBJECTS



IRAM NOEMA

SINGLE-DISH VS INTERFEROMETERS OBSERVATIONS



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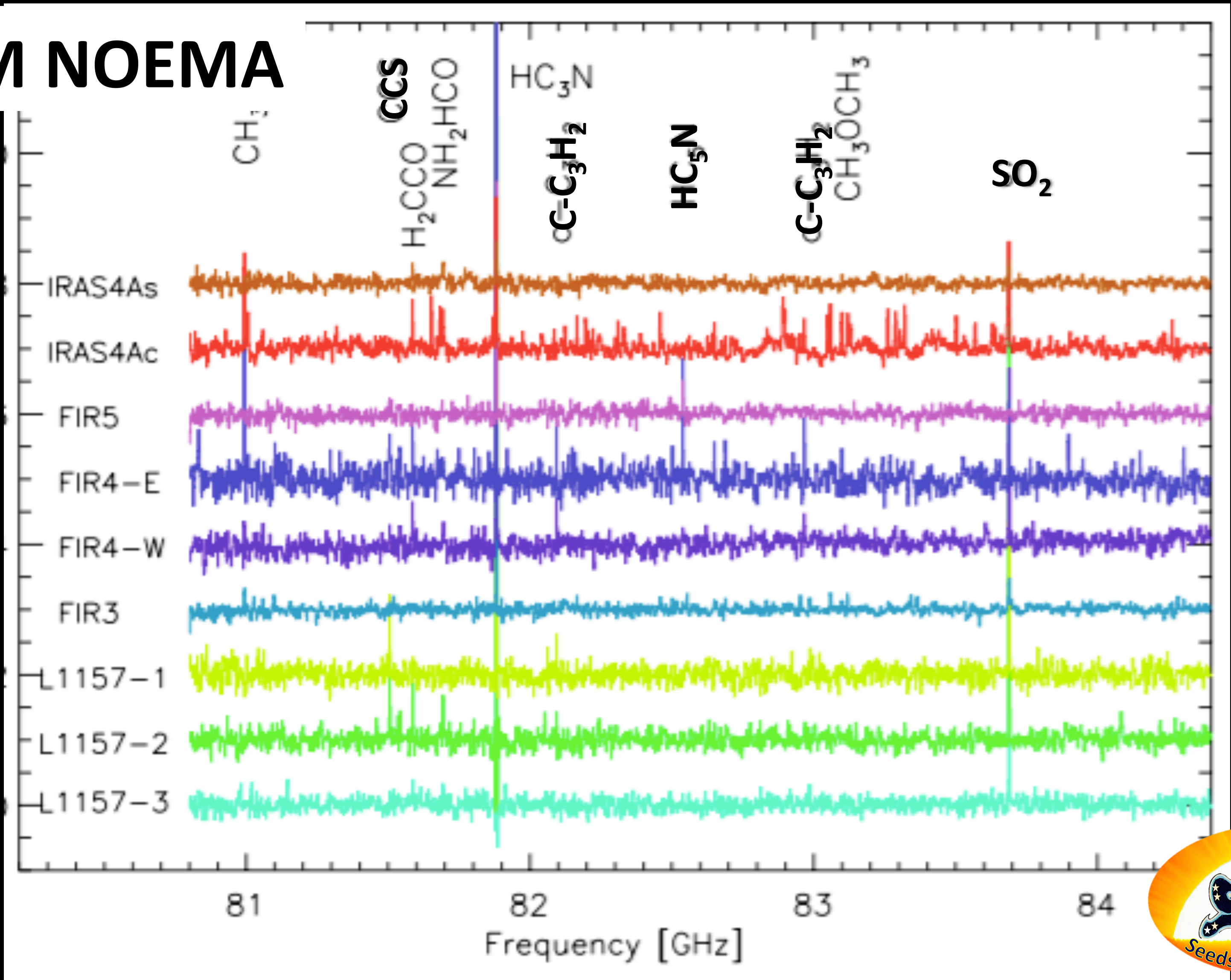
IRAM NOEMA



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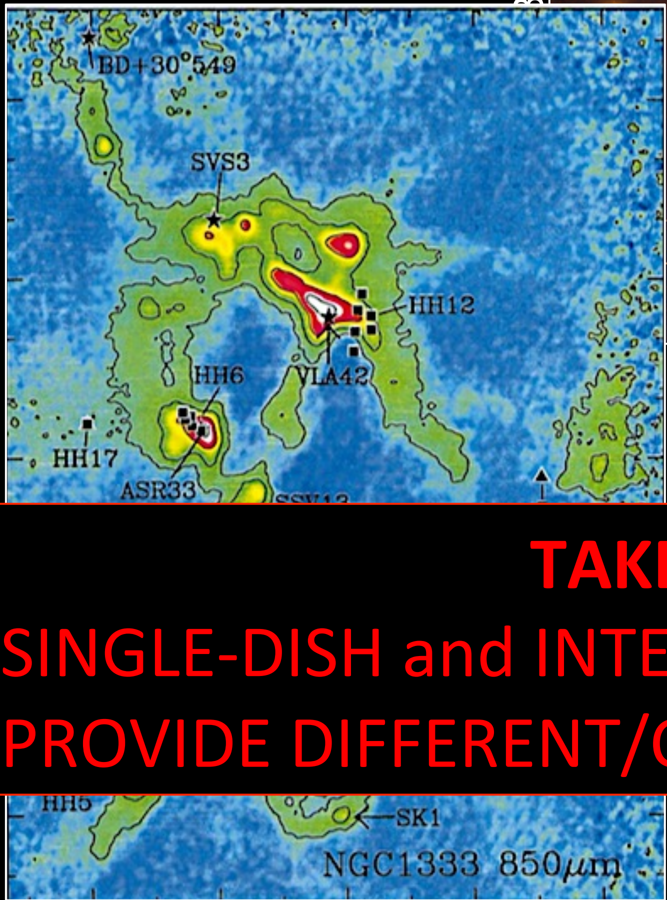
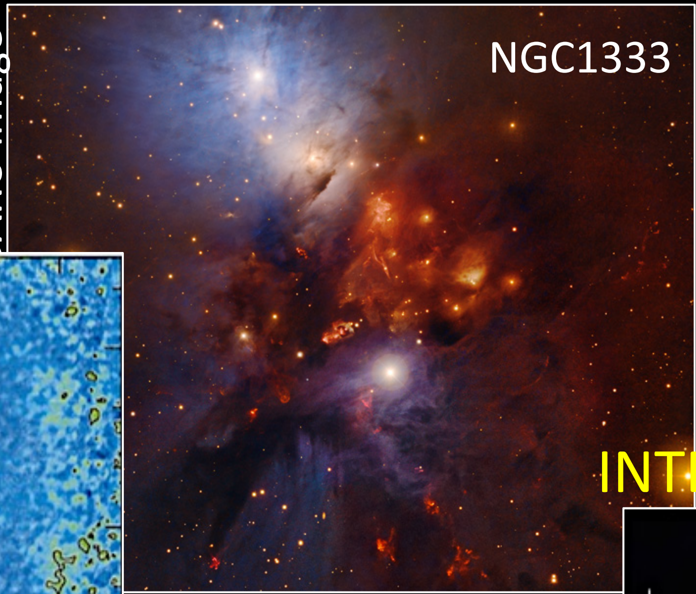
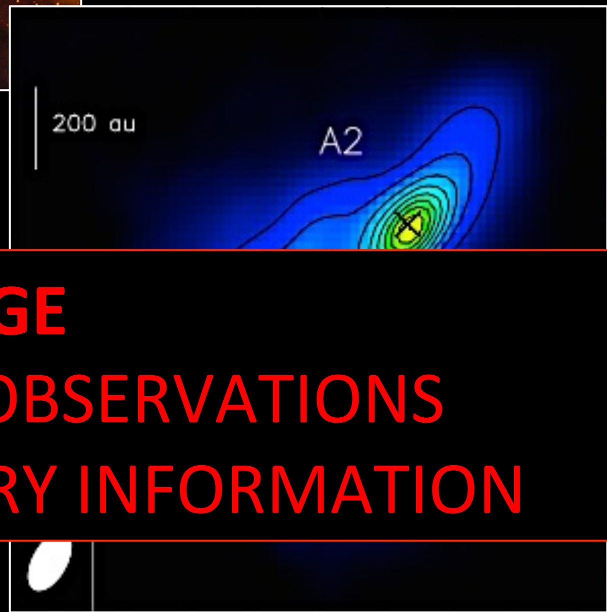


Sandell+2001



BARU image

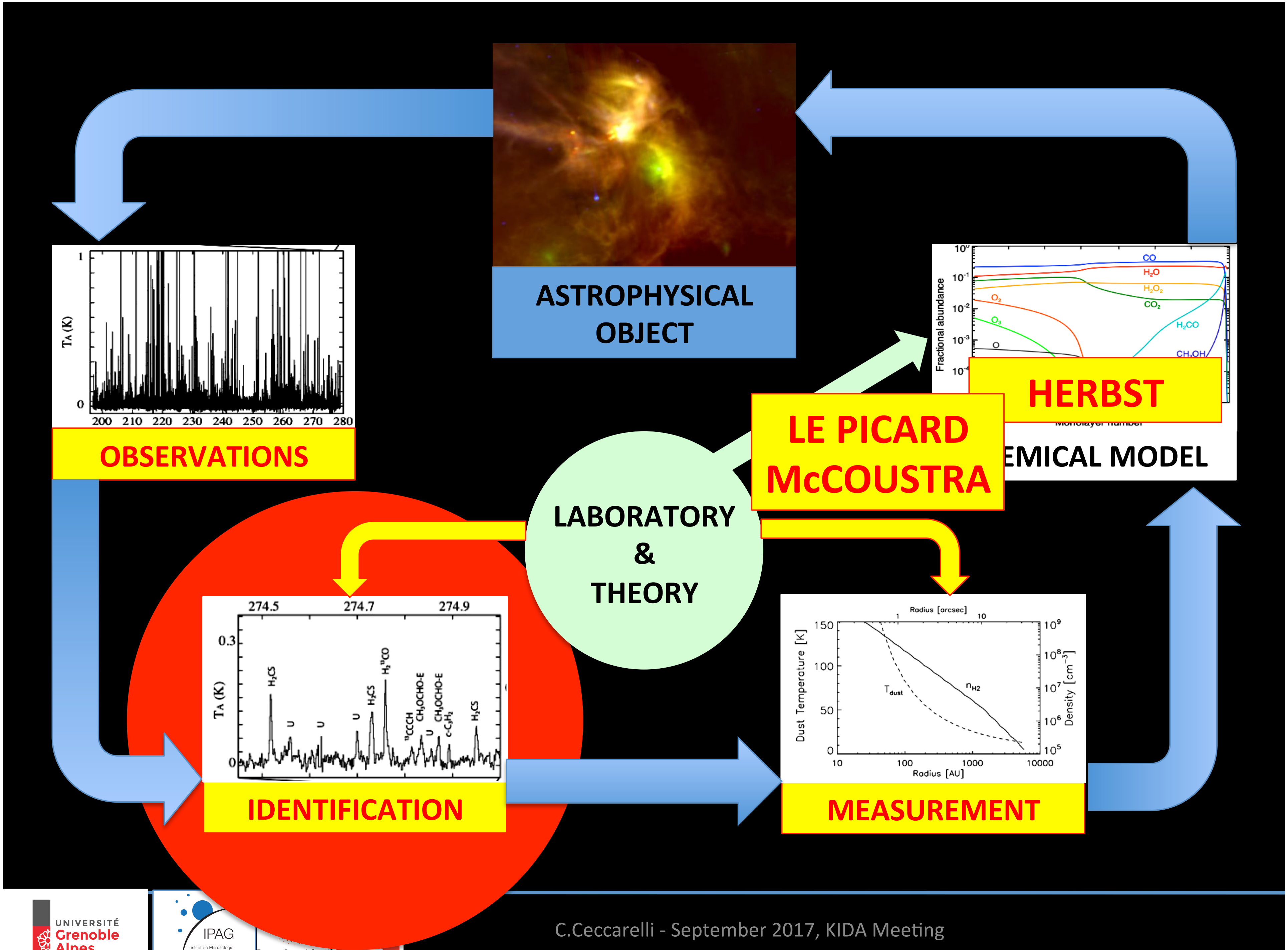
INTERFEROMETER: ALMA



Lopez-Sepulcre+2017

TAKE HOME MESSAGE

SINGLE-DISH and INTERFEROMETRIC OBSERVATIONS PROVIDE DIFFERENT/COMPLEMENTARY INFORMATION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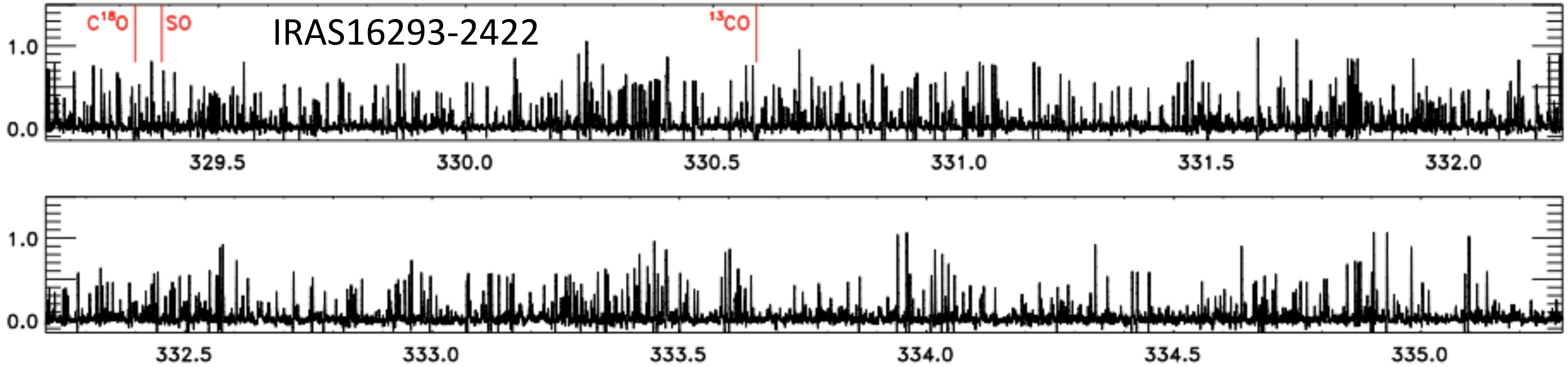
2. IDENTIFICATION



Jorgensen et al. 2016

A MOLECULE IS IDENTIFIED BECAUSE OF THE COINCIDENCE OF OBSERVED AND LABORATORY FREQUENCIES

- TWO DATABASES AVAILABLE: JPL AND CDMS

→ ONE STRONG LINE FROM ABUNDANT (USUALLY SIMPLE) MOLECULES IS USUALLY ENOUGH

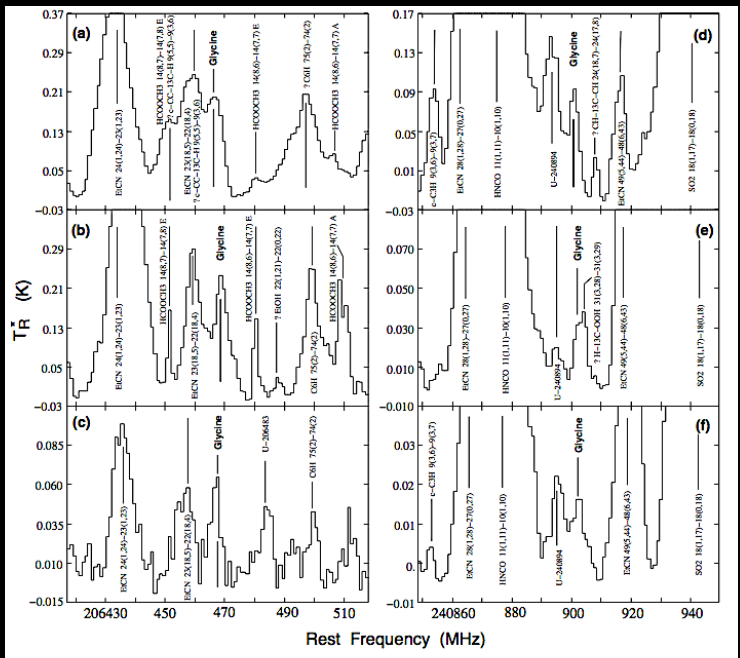
→ SEVERAL MORE WEAK LINES ARE NECESSARY TO IDENTIFY LARGE MOLECULES (USUALLY LESS ABUNDANT and WITH LARGE Q)

IDENTIFICATION FROM WEAK LINES

EXAMPLE: (NON) DETECTION OF GLYCINE

Orion KL (SgrB2 , W51)

Kuan et al. 2003



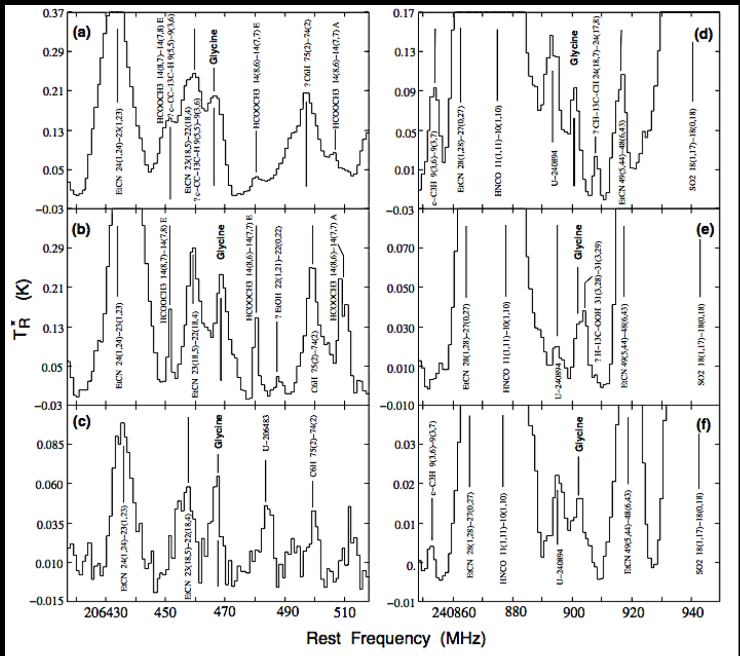
IDENTIFICATION FROM WEAK LINES

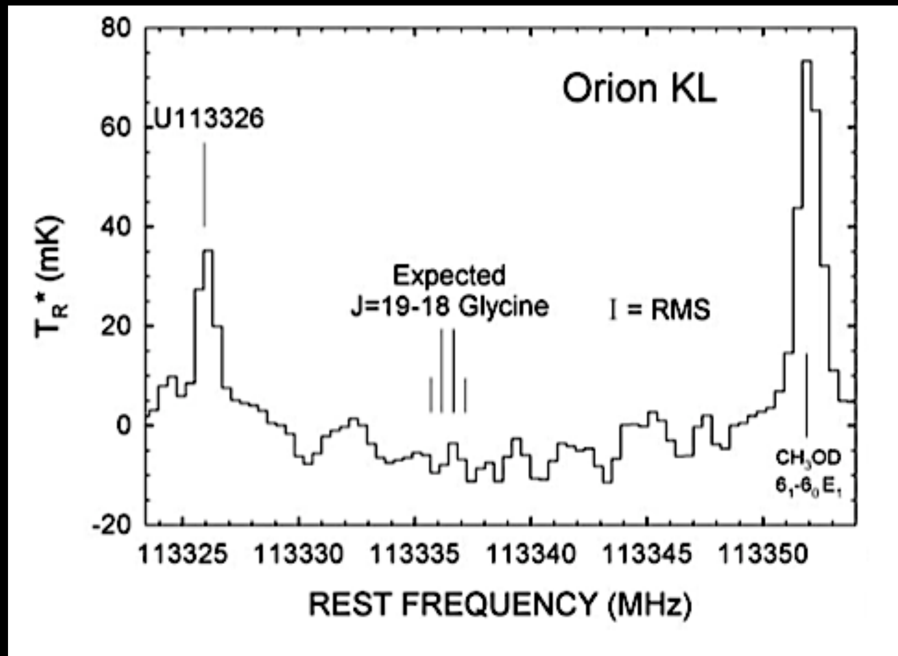
EXAMPLE: (NON) DETECTION OF GLYCINE

Problem 1- *MISIDENTIFICATION*: THE COINCIDENCE OF OBSERVED AND MEASURED LINES IS CASUAL

- → THE LARGER THE NUMBER OF LINES THE SMALLER THE PROBABILITY OF CASUAL COINCIDENCE
- → LINE INTENSITIES TO BE CONSISTENT WITH PREDICTIONS

Kuan et al. 2003





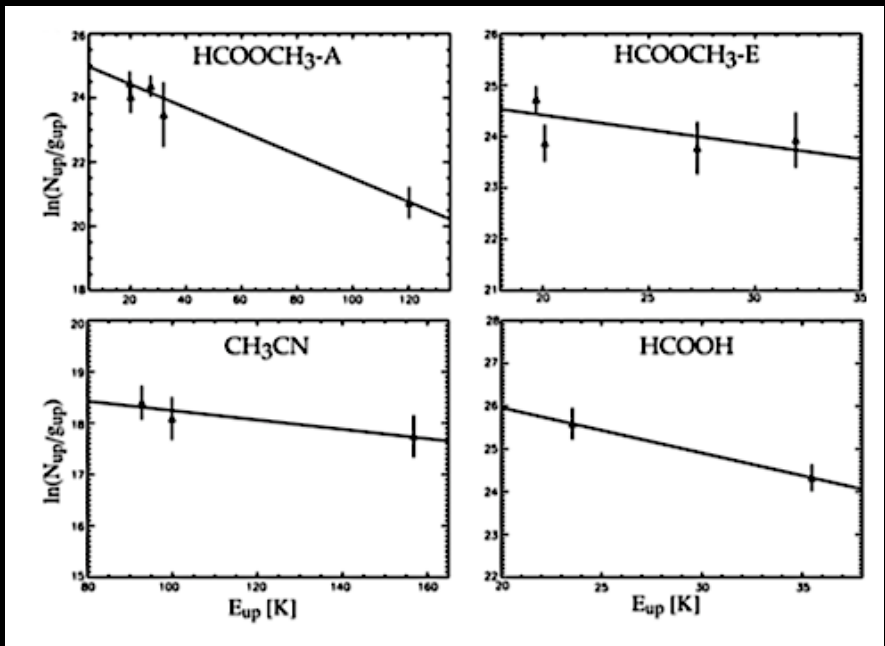
Snyder et al. 2005

IDENTIFICATION FROM WEAK LINES

Problem 2- *MISEVALUATION*: THE NUMBER OF OBSERVED LINES IS NOT LARGE ENOUGH TO MEASURE THE PROPERTIES OF THE MOLECULE (e.g. abundance)

L1157-B1

Arce et al. 2008



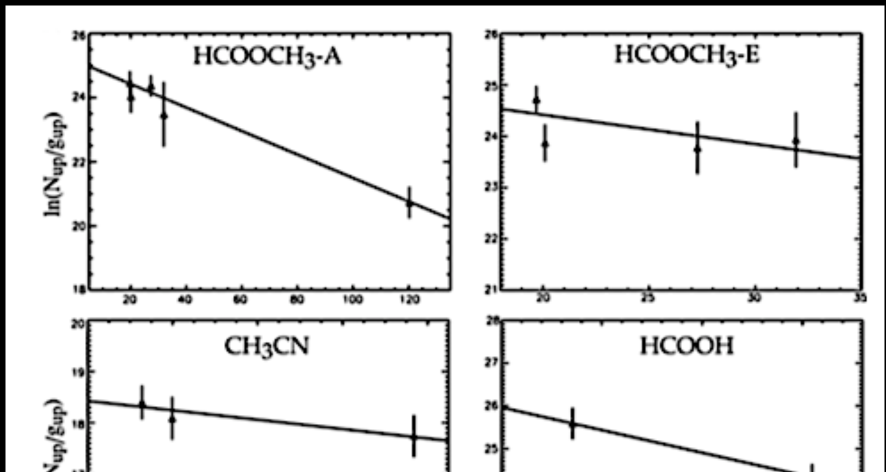
IDENTIFICATION FROM WEAK LINES

Problem 2- *MISEVALUATION*: THE NUMBER OF OBSERVED LINES IS NOT LARGE ENOUGH TO MEASURE THE PROPERTIES OF THE MOLECULE (e.g. abundance)

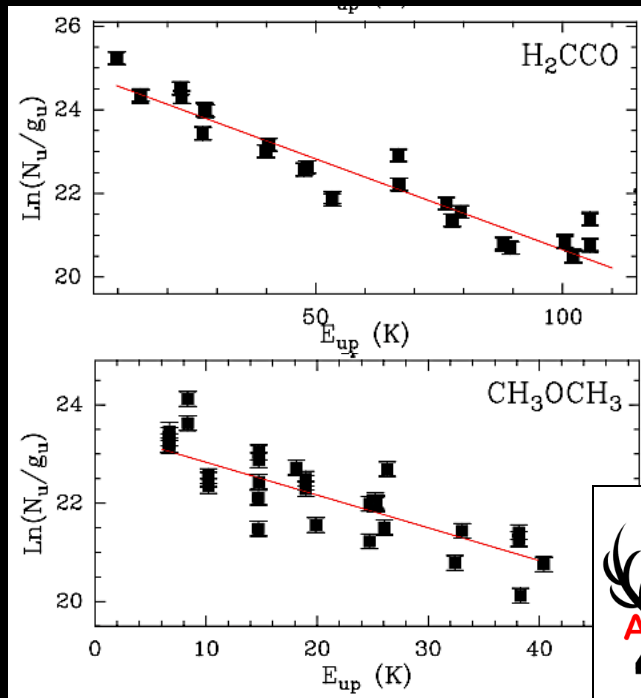
→ THE LARGER THE NUMBER OF LINES THE SMALLER THE PROBABILITY OF MISEVALUATION

→ SIMULATIONS OF LINE INTENSITIES

Arce et al. 2008



NEW ESTIMATES PROVIDE ABUNDANCES DIFFERENT BY UP TO A FACTOR 10

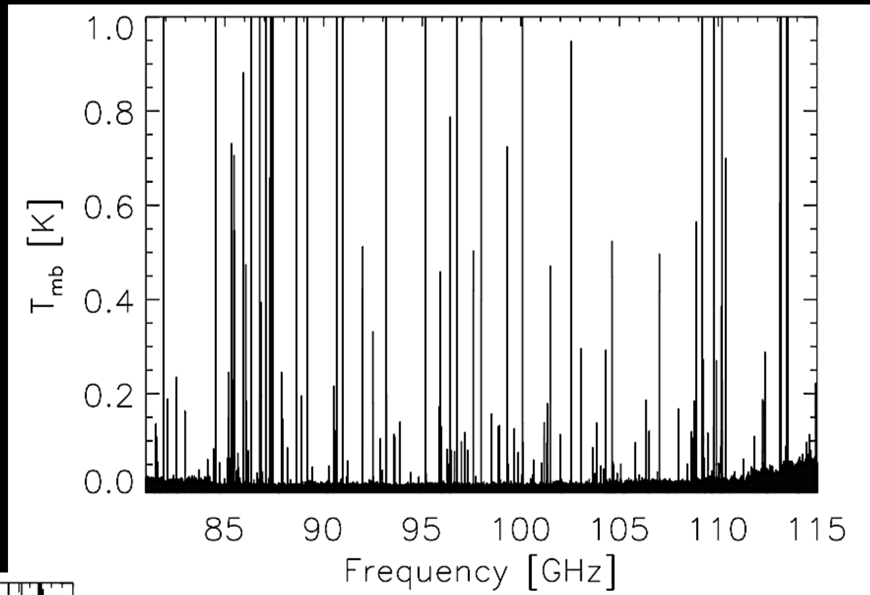


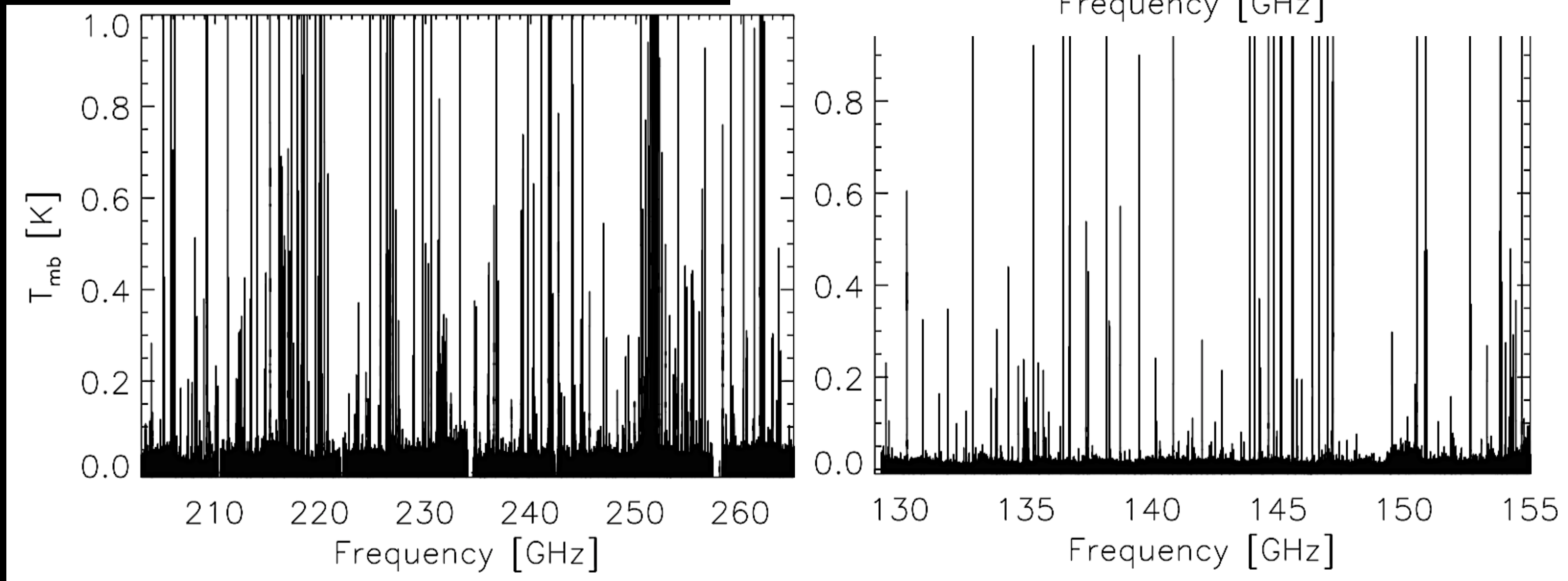
Lefloch et al. 2017

NEW ERA: UNBIASED SPECTRAL SURVEYS

ADVANTAGES

- MANY LINES FROM THE SAME SPECIES
- COMPLETE CENSUS OF THE COMPOSITION
- UNEXPECTED DISCOVERIES (e.g. new species)



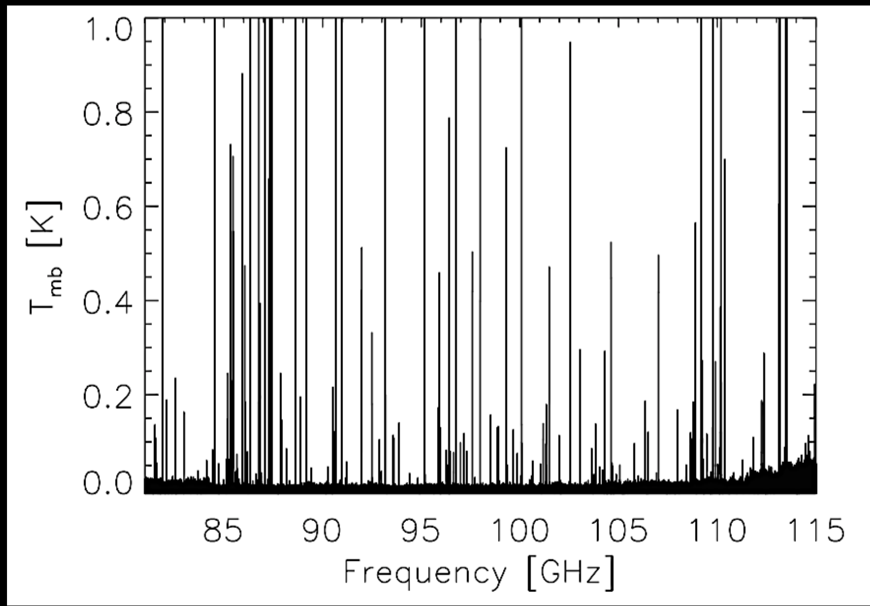


OMC-2 FIR4 by Lopez-Sepulcre et al.

NEW ERA: UNBIASED SPECTRAL SURVEYS

DISADVANTAGES

- MANY LINES FROM THE SAME SPECIES



OMC-2 FIR4 by Lopez-Sepulcre et al.

SEVERAL METHODS ALL BASED ON LTE EMISSION

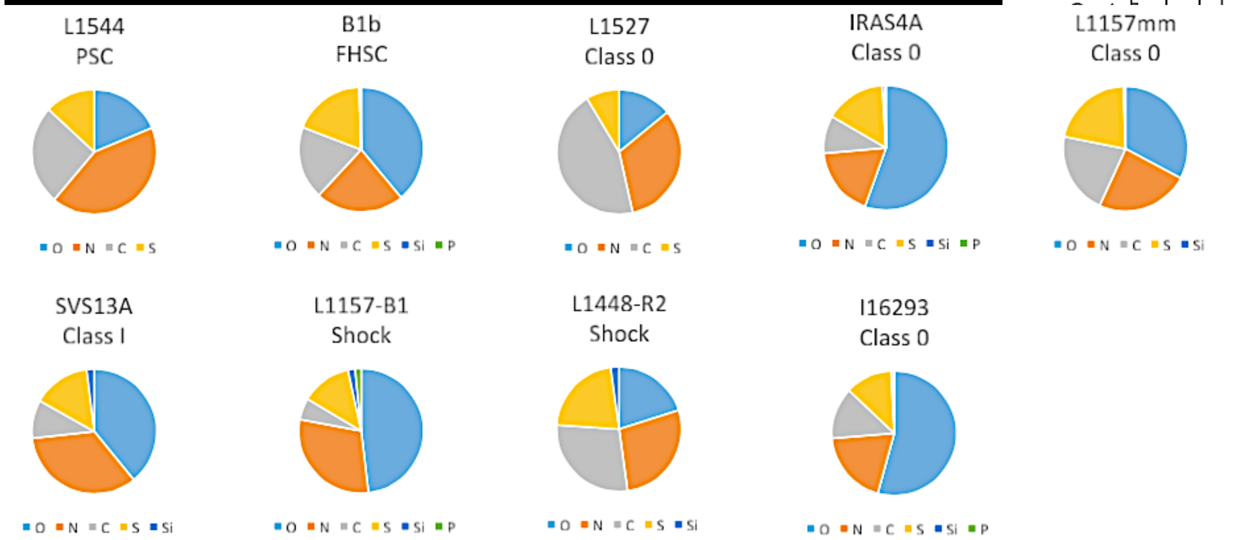
→ SEMI-AUTOMATIC LINE IDENTIFICATION METHODS, Publicly available (e.g. XCLASS, CASSIS, WEEDS…) or private owned (MADEX @ Madrid, ULSA @ IPAG …)

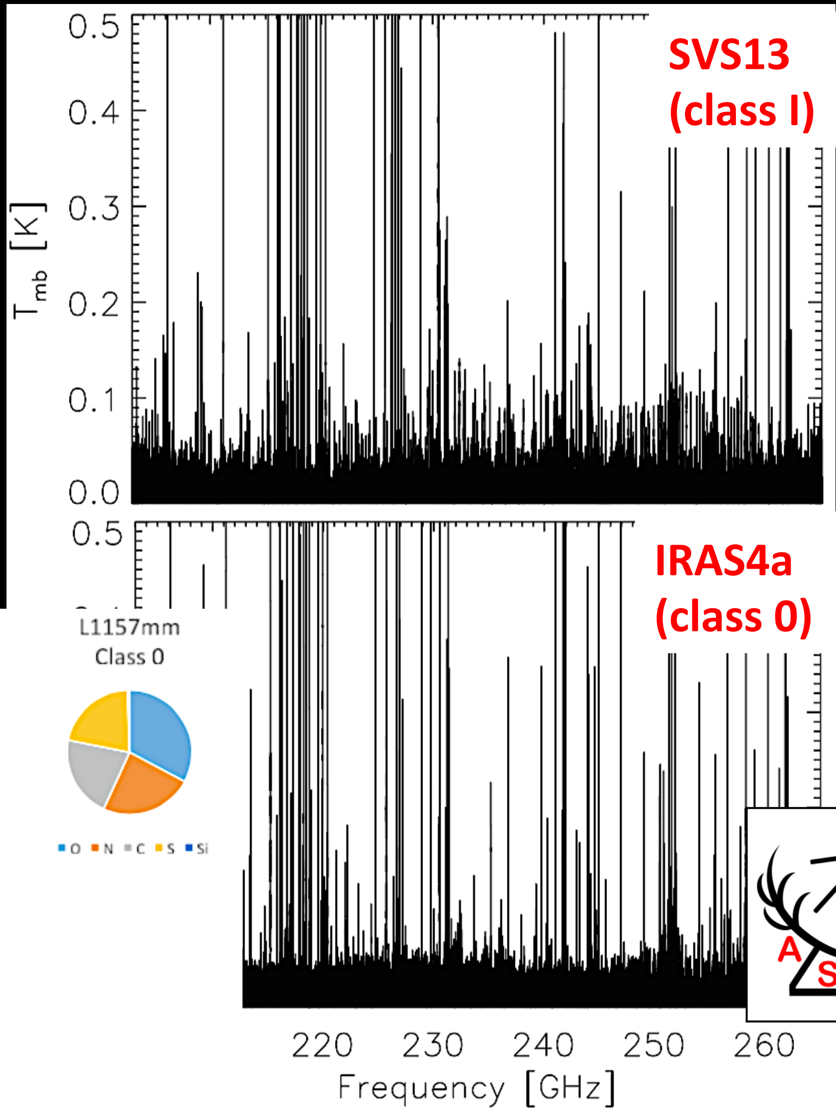
→ BAYESIAN-BASED METHODS (Gratier et al. 2016)

NEW ERA: UNBIASED SPECTRAL SURVEYS

ADVANTAGES

- COMPARISON OF THE CHEMICAL COMPOSITION OF DIFFERENT SOURCES



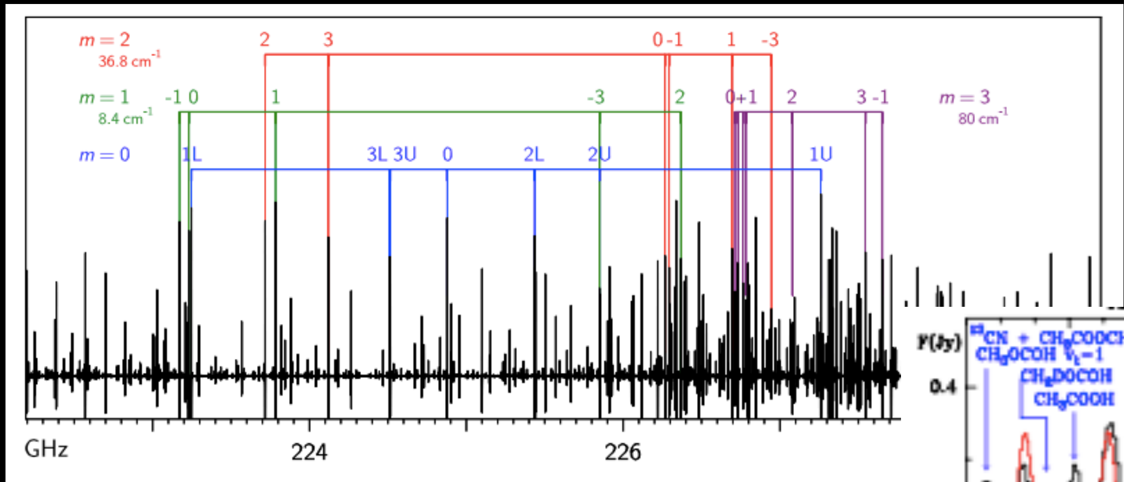


ASAI by Lefloch & Bachiller et al.

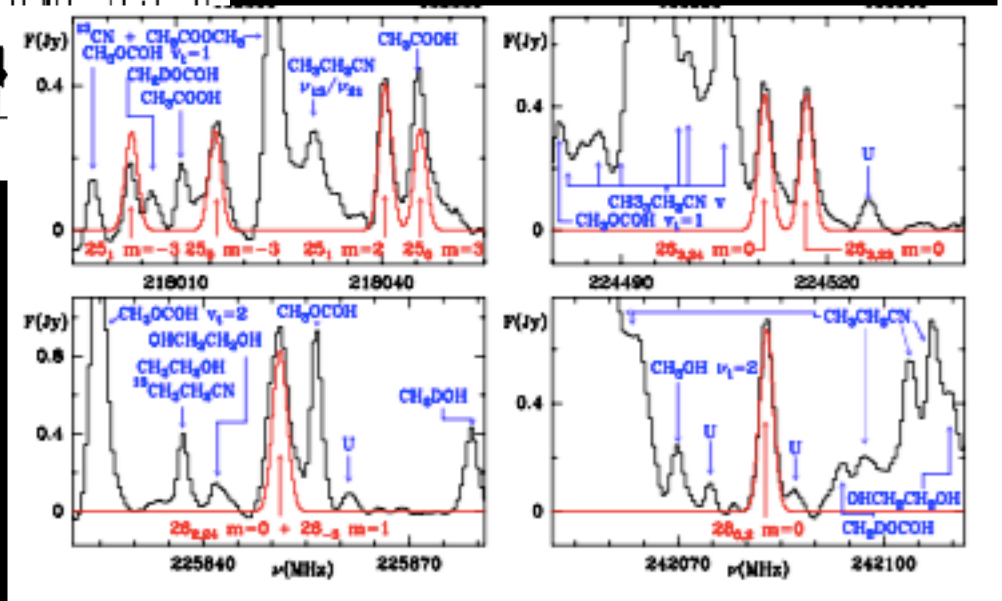
WRONG OR UNKNOWN FREQUENCIES

EXAMPLE OF CH_3NCO (methyl isocyanate) (Cernicharo et al 2016)

EXTENSIVE LABORATORY WORK TO CHARATERIZE THE MM SPECTRUM

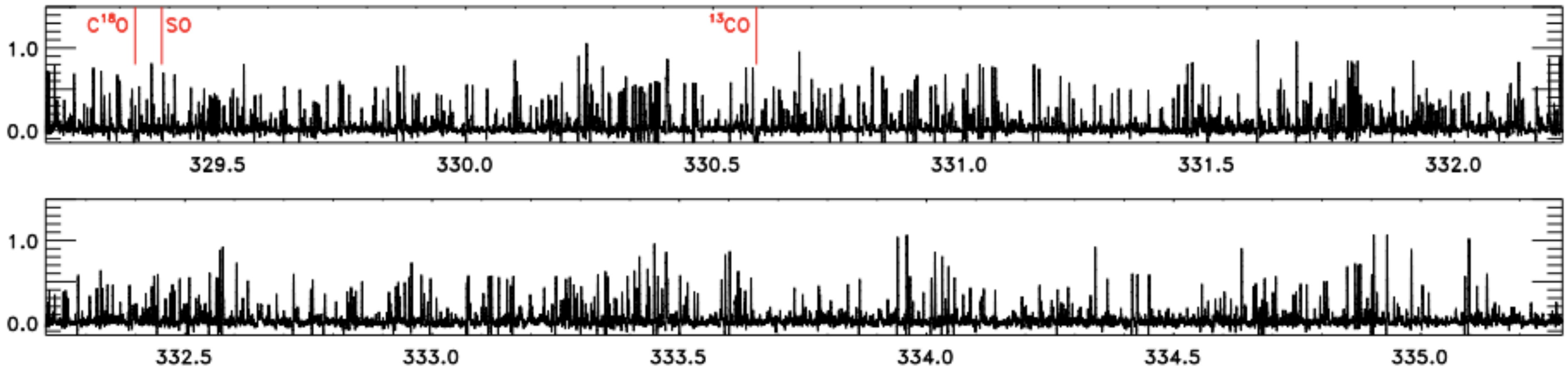


PLUS OBSERVATIONS OF 339 LINES



NEEDED FOR A RELIABLE ESTIMATE OF THE CH_3NCO ABUNDANCE

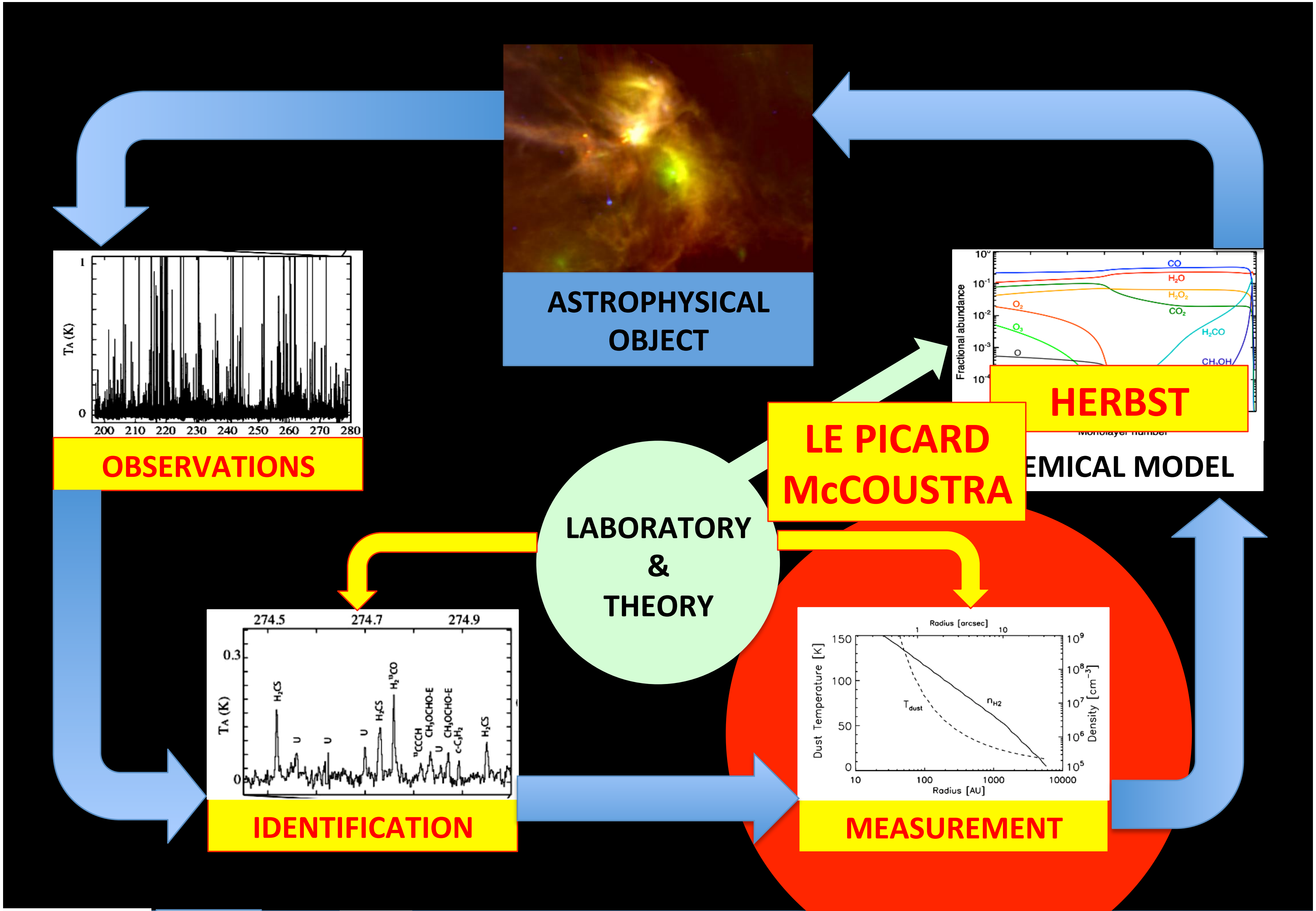
2. IDENTIFICATION



TAKE HOME MESSAGES

IDENTIFICATION OF TRACE AND LARGE MOLECULES IS A DELICATE BUSINESS THAT REQUIRES MUCH ATTENTION

STILL MUCH WORK NEEDED TO PROVIDE LINES FROM POTENTIAL ISM MOLECULES (AND FEED THE DATABASES)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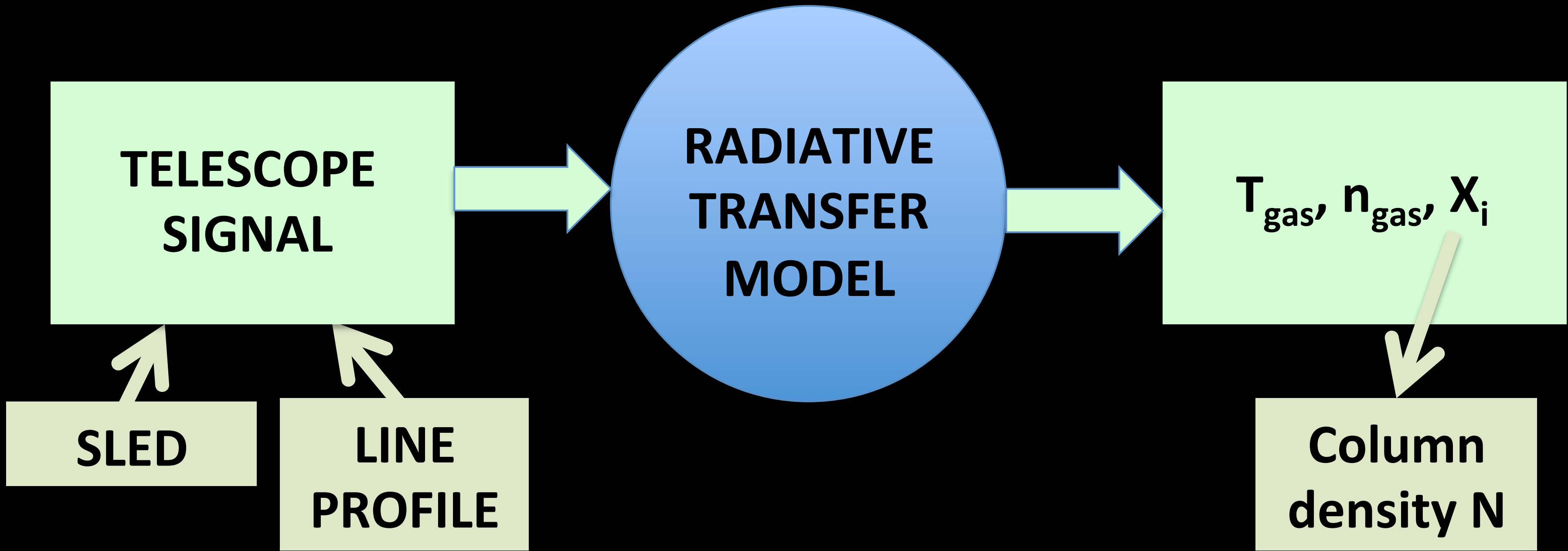
3. MEASUREMENT

HOW TO EXTRACT ASTROCHEMICAL-USEFUL DATA: TEMPERATURE, DENSITY AND ABUNDANCE COLUMN DENSITY

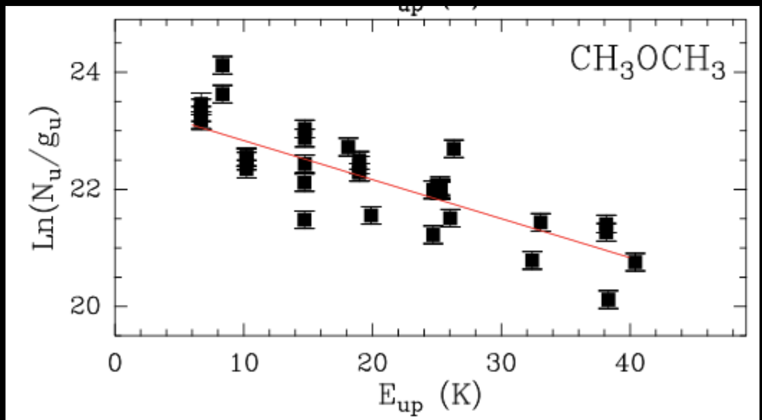


RADIATIVE TRANSFER MODELS: a ZOO

LTE
(RD, PD, τ ….)

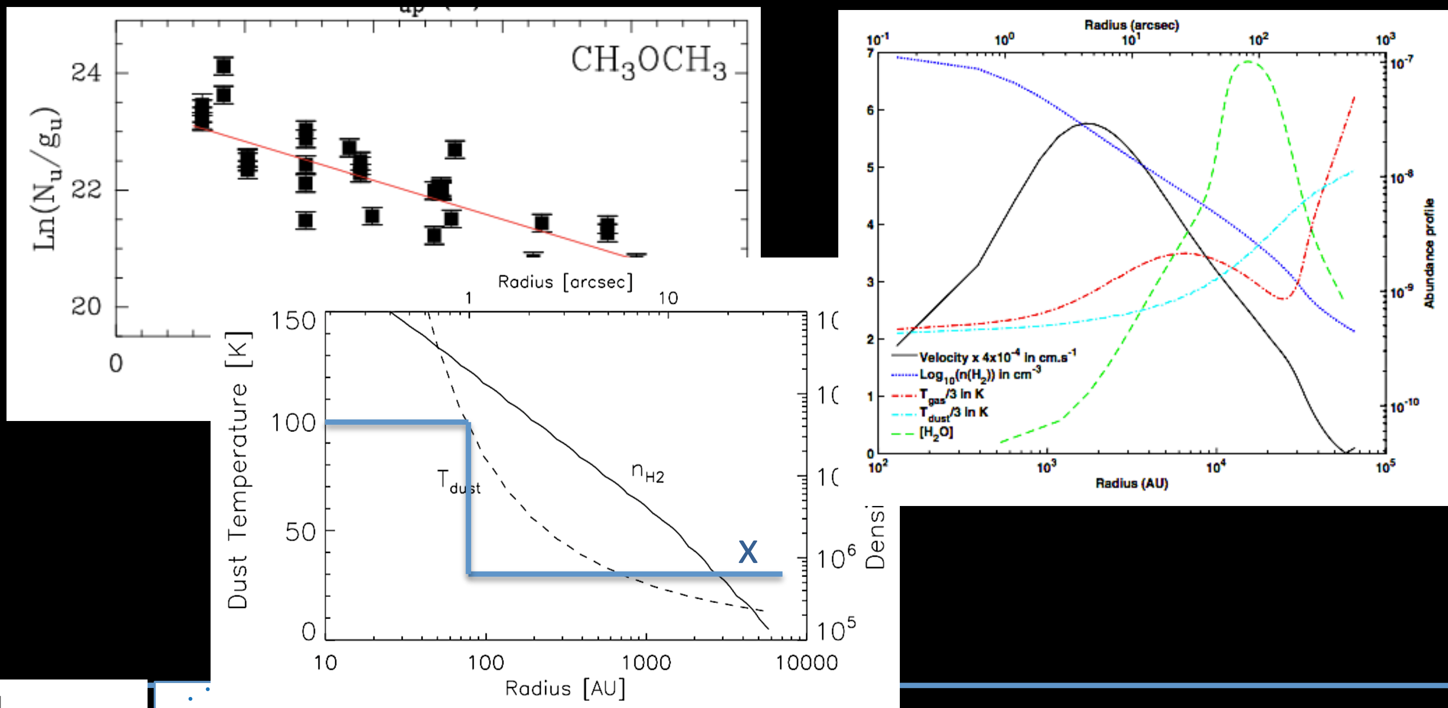
vs

non-LTE
(LVG, β, MC, Λ-acc ….)



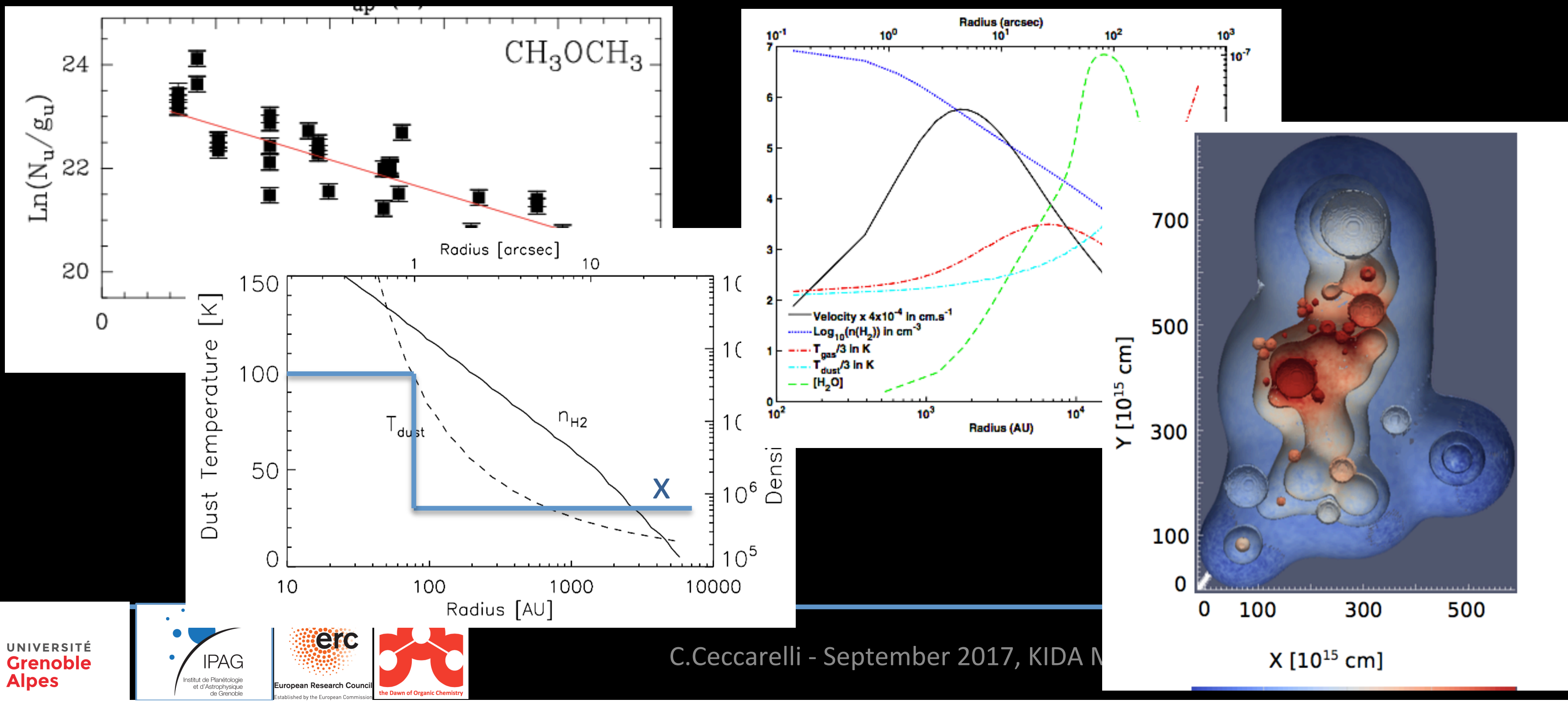
RADIATIVE TRANSFER MODELS: a ZOO

LTE (RD, PD, τ ….)	vs	non-LTE (LVG, β, MC, Λ-acc ….)
constant T_{gas}, n_{gas}, X_i	vs	PhysChemical profile



RADIATIVE TRANSFER MODELS: a ZOO

LTE (RD, PD, τ ….)	**vs**	**non-LTE** (LVG, β, MC, Λ-acc ….)
constant T_{gas}, n_{gas}, X_i	**vs**	**PhysChemical profile**
1D	**vs**	**2D and 3D**



RADIATIVE TRANSFER MODELS: a ZOO

LTE (RD, PD, τ ….)	**vs**	**non-LTE** (LVG, β, MC, Λ-acc ….)
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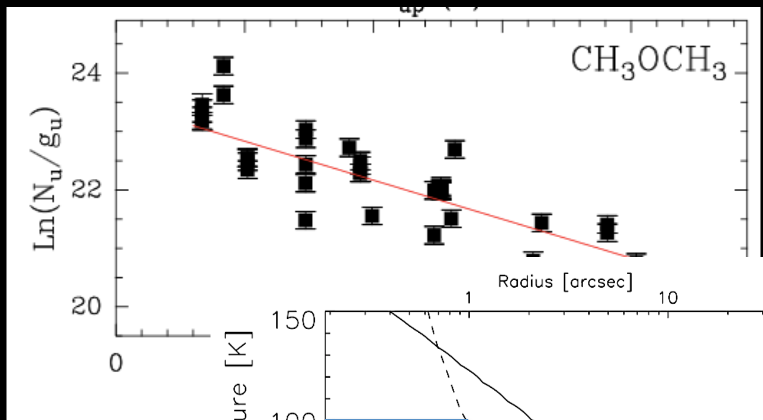
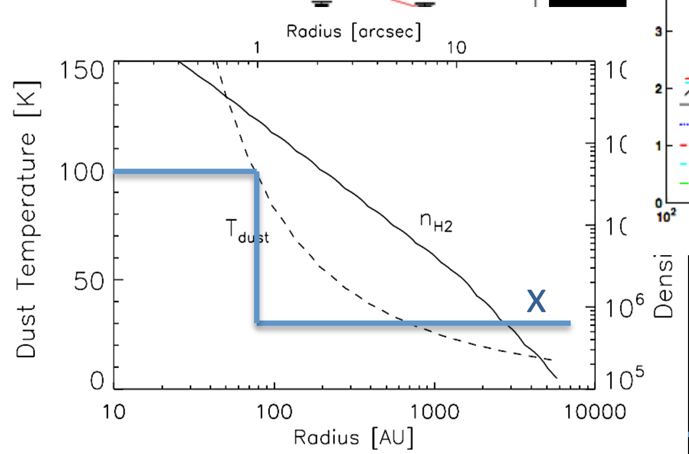
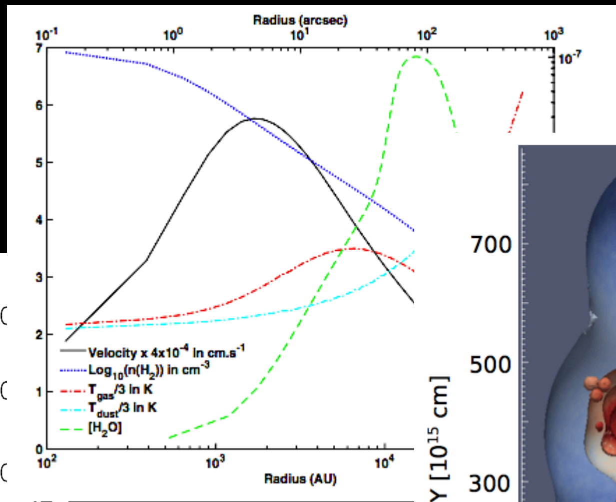
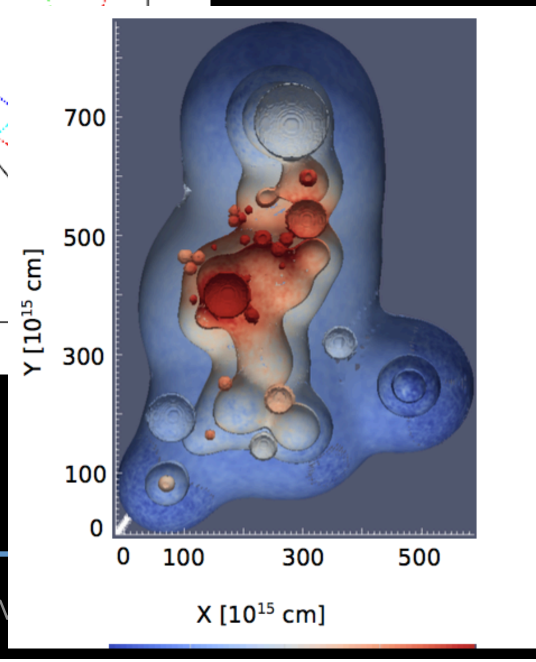






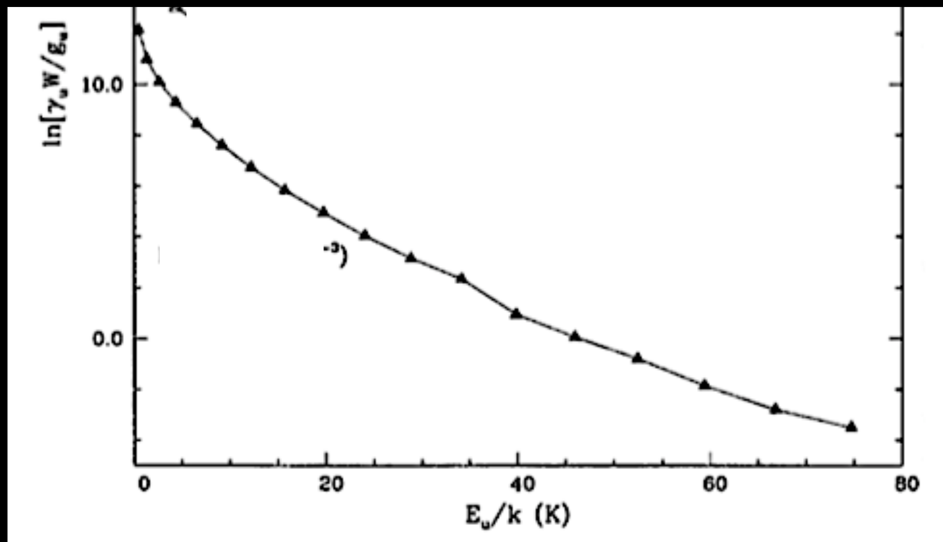


LTE: ROTATIONAL & POPULATION DIAGRAMS

IN GENERAL:

constant T_{gas}, n_{gas}, X_i

$T_{gas} \neq T_{rot}$ & $N_i \approx N_{rot}$ (factor 2: beam-averaged)



LTE: ROTATIONAL & POPULATION DIAGRAMS

constant T_{gas}, n_{gas}, X_i

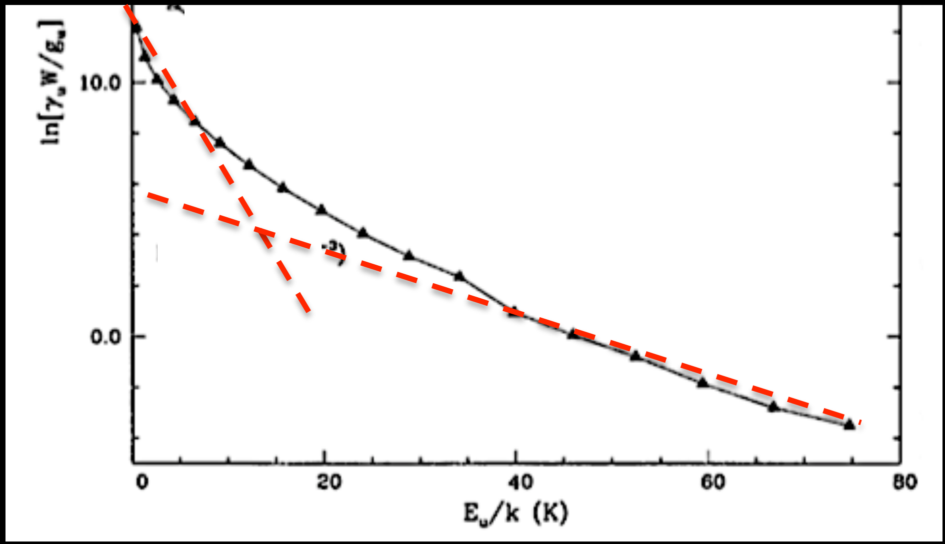
IN GENERAL:

$T_{gas} \neq T_{rot}$ & $N_i \approx N_{rot}$ (factor 2: beam-averaged)

WHEN ARE THEY NOT ENOUGH ?

1- WHEN THE EMISSION IS CLEARLY NOT FROM ONE COMPONENT ONLY:

e.g. due to a cold extended low-abundance region plus a hot core/corino



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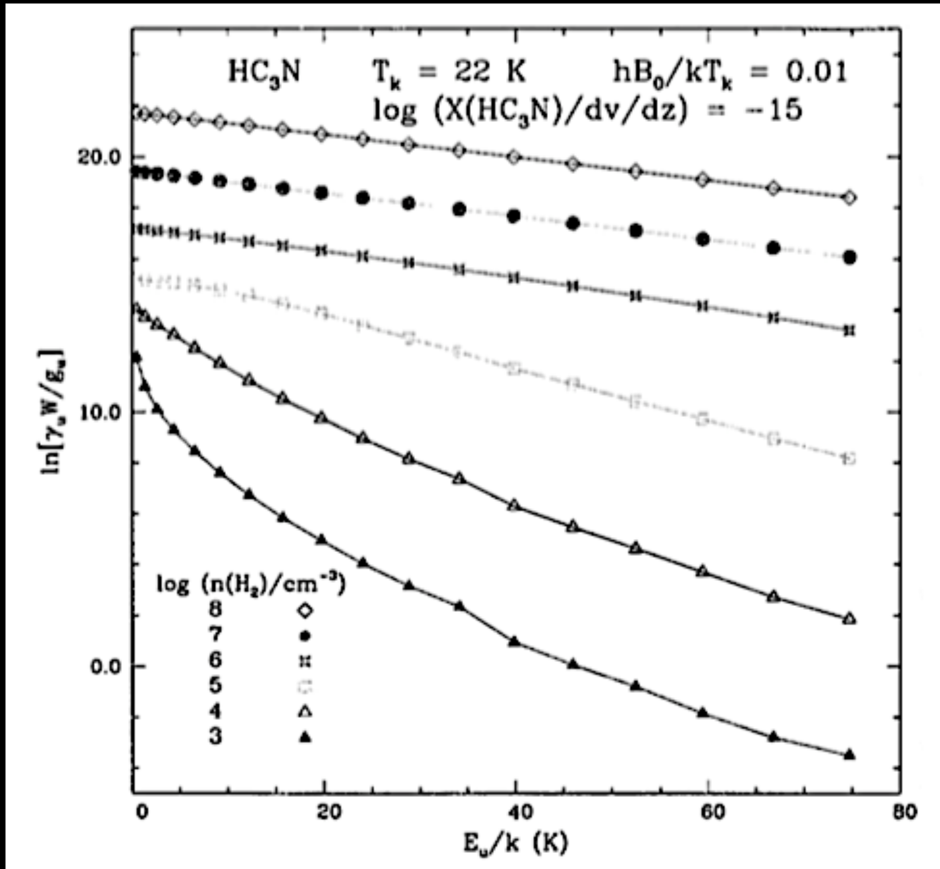
➔ BUT CAREFUL: IT COULD BE A NON-LTE EFFECT INSTEAD



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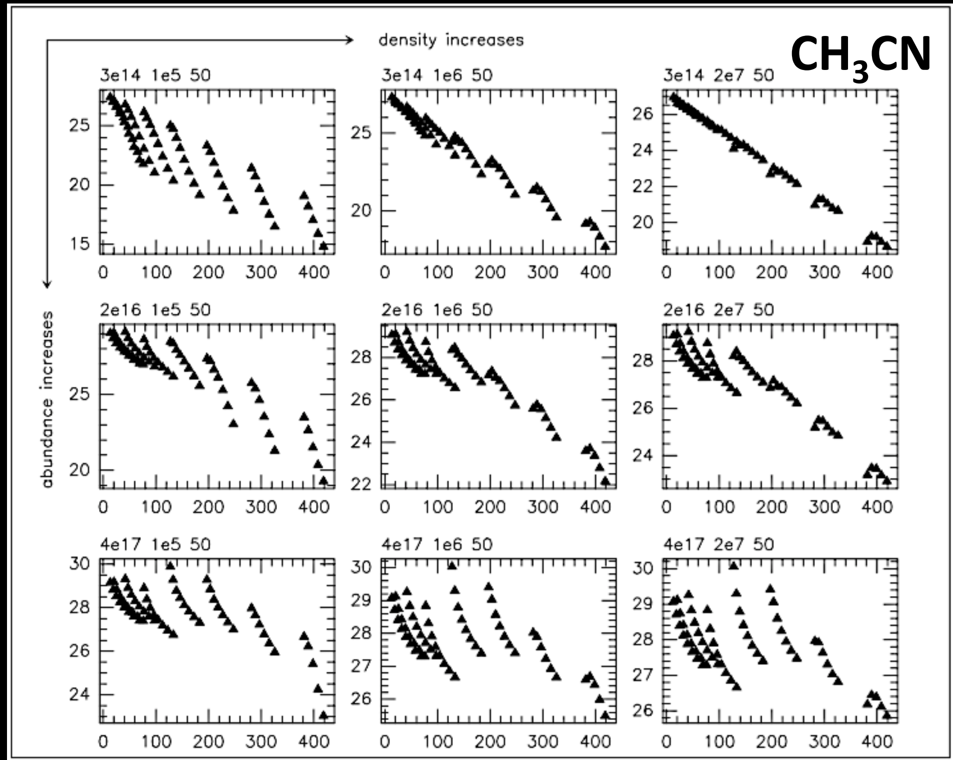
2- WHEN THE EMISSION IS CLEARLY NOT LTE



Non-LTE RADIATIVE TRANSFER MODELS

ONLY FEASIBLE WHEN THE COLLISIONAL COEFFICIENTS ARE KNOWN

TWO PUBLIC DATABASES:
BASECOL (52 molecules) *http://basecol.obspm.fr*
LAMDA (46 molecules) *http://home.strw.leidenuniv.nl/~moldata/*

➔ When considering that about 200 ISM molecules (+ isotopologues) are detected there is still some work to do…

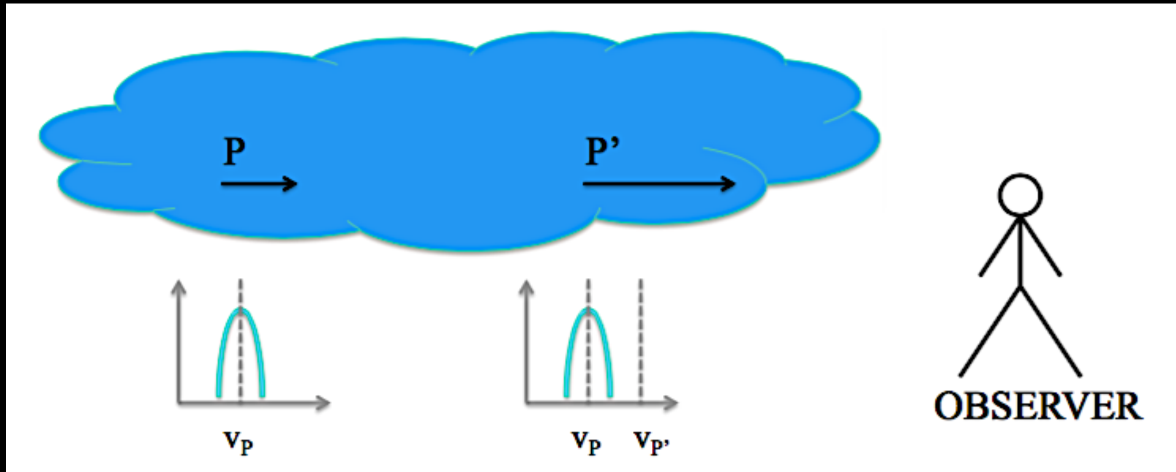
Non-LTE LARGE VELOCITY GRADIENT MODELS

PROVIDE ESTIMATES OF

T_{gas} & n_{gas} + N_i

constant T_{gas}, n_{gas}, X_i

ASSUME THAT PHOTONS EITHER ARE ABSORBED CLOSE TO WHERE THEY ARE EMITTED OR THEY ESCAPE (escape probability formalism)



SEVERAL CODES AVAILABLE

Publicly available (e.g. RADEX)

or private owned (MADEX @ Madrid, lvg_gre @ IPAG …)

Non-LTE LARGE VELOCITY GRADIENT MODELS

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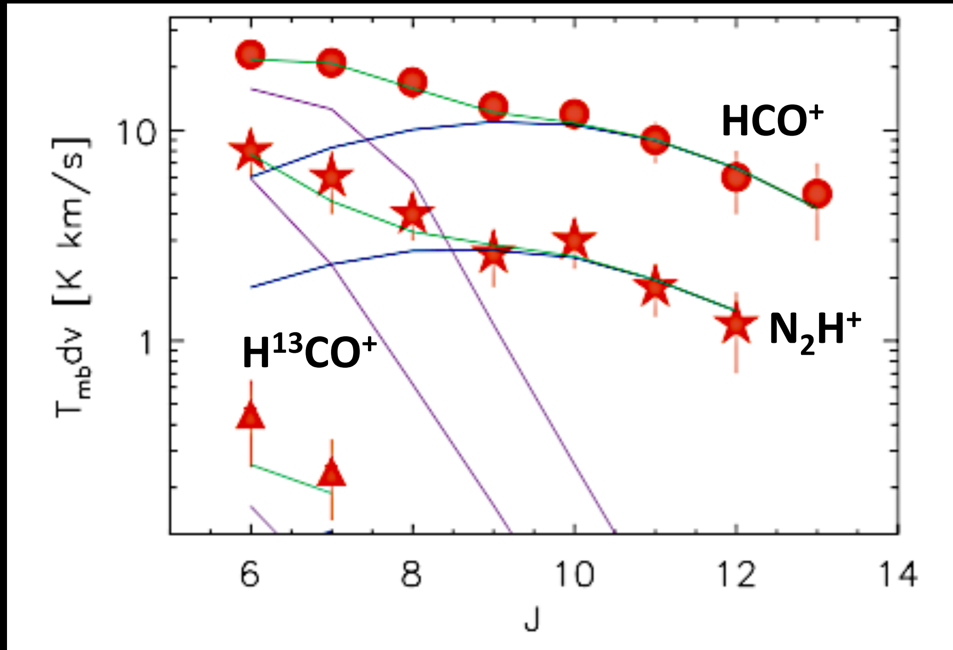

Non-LTE LARGE VELOCITY GRADIENT MODELS

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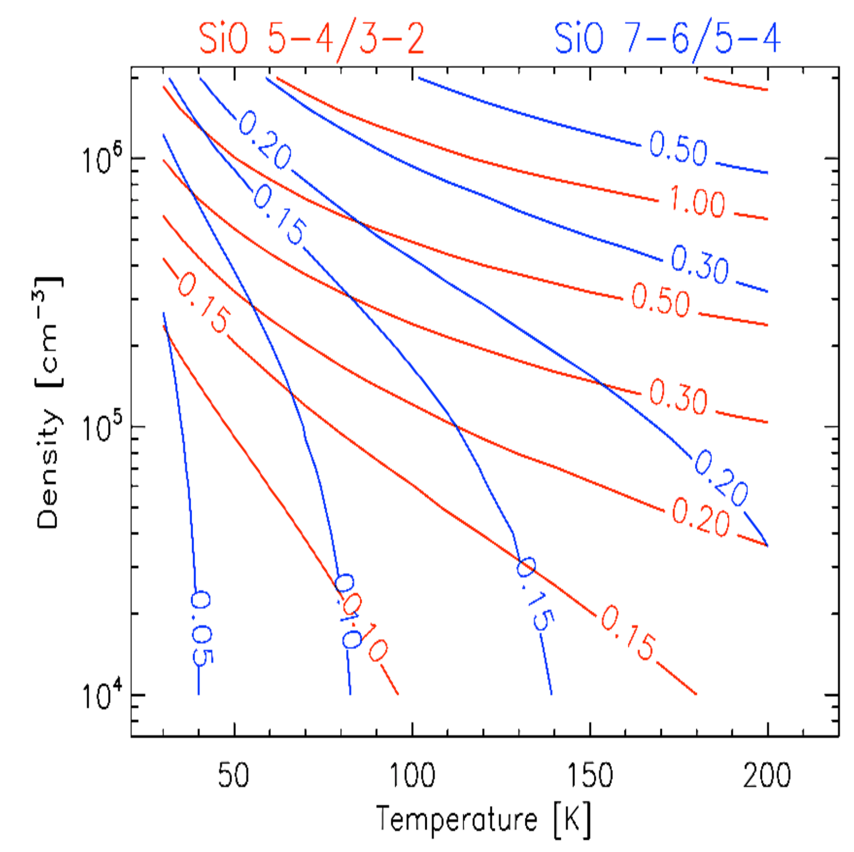
2- WHEN TOO FEW LINES ARE MEASURED:

n_{gas} vs T_{gas} degeneracy



WHAT ABOUT ABUNDANCES?

$$X_I = N_I / N_{H2}$$

MEASUREMENTS OF $N(H_2)$ ARE DIFFICULT AND VERY OFTEN INDIRECT → USING CO LINES OR DUST CONTINUUM

1- CO LINES

ASSUME CO/H_2 ← NOT ALWAYS SO OBVIOUS

2- DUST CONTINUUM

LARGE UNCERTAINTY ON THE DUST EMISSION EFFICIENCY (EASILY BY A FACTOR 2)

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LARGE UNCERTAINTY ON THE DUST EMISSION EFFICIENCY (EASILY BY A FACTOR 2)

ABSOLUTE ABUNDANCES HAVE LARGE UNCERTAINTIES

→ ABUNDANCE RATIOS ARE MUCH MORE RELIABLE ←

RADIATIVE TRANSFER MODELS

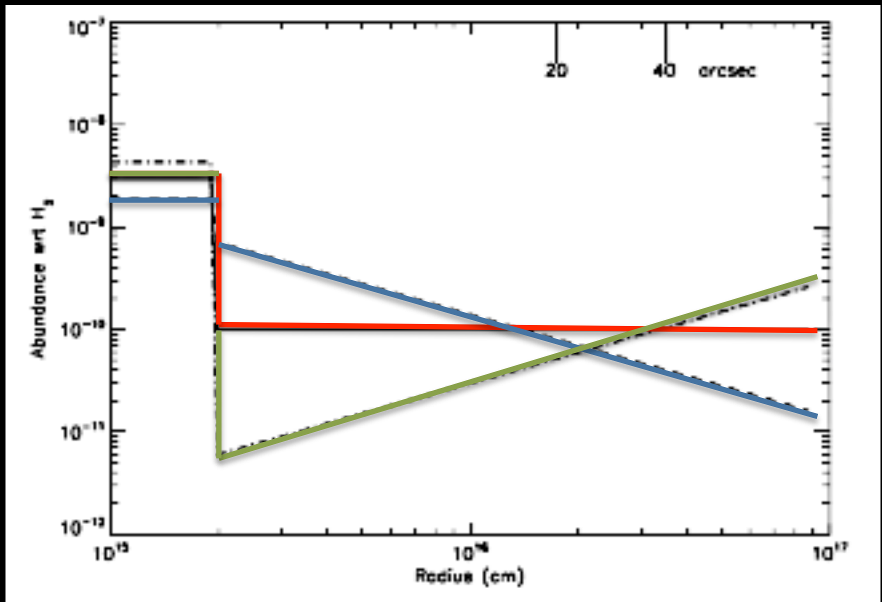
MODEL	T_{gas}	n_{gas}	N_i	X_i	X_a/X_b
ROT.DIAG.	🔴	🔴	🟡	🟡	🟡🟢
POP.DIAG.	🔴	🔴	🟢	🟡	🟢
LVG	🟡🟢	🟡🟢	🟢	🟡	🟢

ARE MORE COMPLICATED MODELS ALWAYS BETTER ?

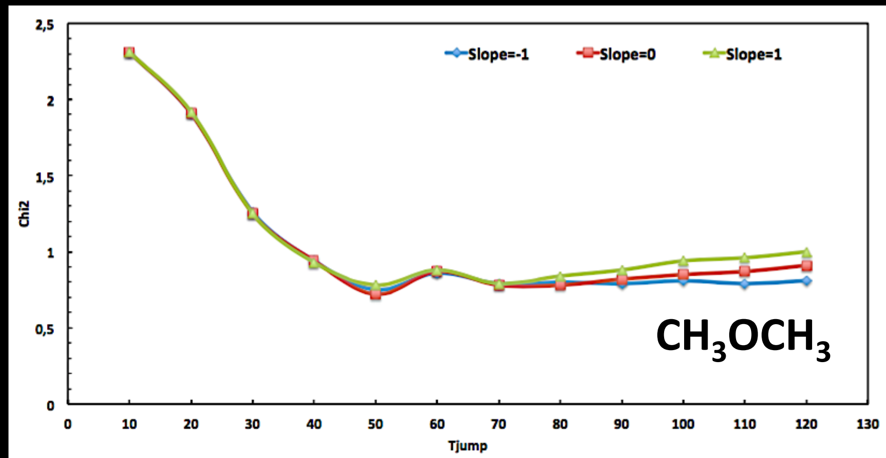
NOT NECESSARELY

IT DEPENDS ON THE DATA YOU HAVE IN HANDS
AND THE OBJECT YOU WANT TO MODEL

EXAMPLE iCOMs IN IRAS16293-2422: COMPLICATION USELESS



MODELING OF THE TIMASSS DATA



Jaber et al. 2014

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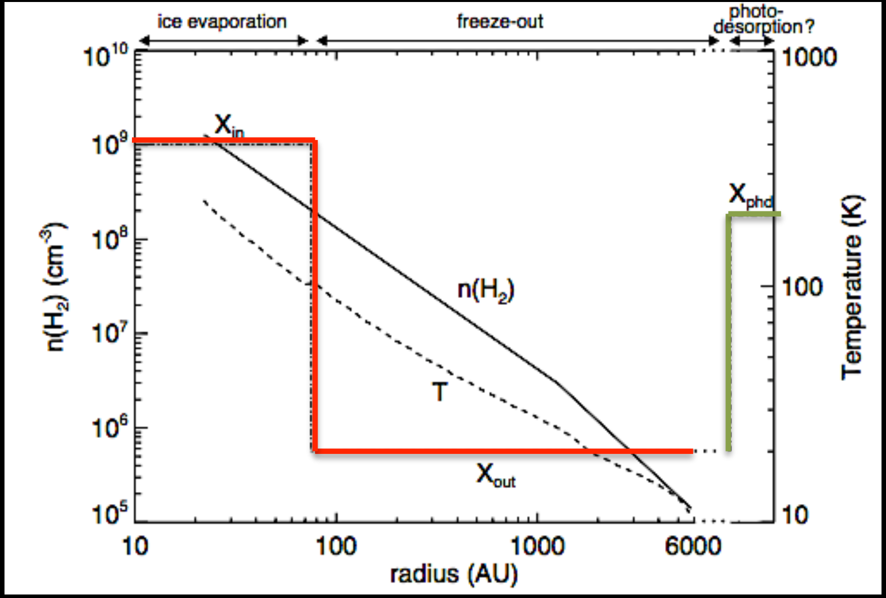
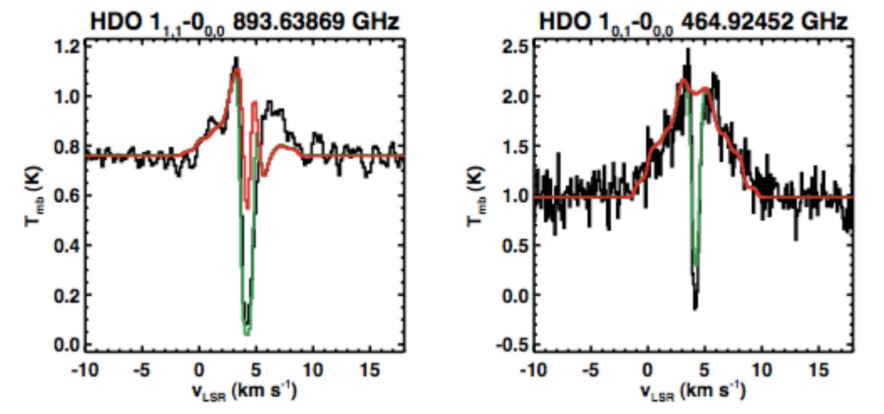
EXAMPLE H_2O IN IRAS16293-2422: COMPLICATION USEFUL



MODELING OF THE CHESS DATA



Coutens et al. 2012

ABUNDANCE OF GASEOUS ELEMENTS

ASTROCHEMICAL MODELS NEED THE ABUNDANCE OF THE SPECIES AND THE ABUNDANCE OF ELEMENTS IN THE GAS

→ DIFFICULT PROBLEM

- RELY ON THE SOLAR PHOTOSPHERE ABUNDANCES AND STUDIES IN THE OPTICAL (e.g. Jenkins 2009)
- OBTAIN THE CENSUS OF THE MAJOR ELEMENT BEARING SPECIES

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ONE EXAMPLE : OXYGEN

CO H_2O O_2 O

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ONE EXAMPLE : OXYGEN

CO H_2O O_2 O

3. MEASUREMENT

HOW TO EXTRACT ASTROCHEMICAL-USEFUL DATA: TEMPERATURE, DENSITY AND ABUNDANCE

TAKE HOME MESSAGES

NOT AN EASY JOB : FROM pizza TO haute cuisine !

FOR NON-LTE MODELS MORE COLLISIONAL COEFFICIENTS ARE NEEDED

ABUNDANCE RATIOS MORE RELIABLE THAN ABSOLUTE ABUNDANCES

ABUNDANCE OF ELEMENTS IN THE GAS ALSO IMPORTANT

WRAP-UP

DESPITE ALL THE CAVEATS AND DIFFICULTIES

LA VIE EST ROSE

THANKS TO THE ADVENT OF SENSITIVE
SINGLE-DISH TELESCOPES AND INTERFEROMETERS
THAT ALLOW UNBIASED SPECTRAL SURVEYS
AND/OR
HIGH SPATIAL RESOLUTION OBSERVATIONS

ASTROCHEMISTRY IS THE NEW BLACK

©KROME crew

Thanks for your attention

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