RELOADED

A 3-D MODEL OF THE DISTRIBUTION AND DEUTERATION OF H_2O IN SGR B2(M)

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and the HEXOS team

DEUTERIUM FRACTIONATION

- Abundance of deuterated counterpart of a molecular species is enhanced with respect to the cosmic ratio:
    - **[XD]/[XH] > [D]/[H] ~ 10^{-5}**
- Important tool to infer physical conditions in molecular clouds:
    - kinetic isotope effect: gas-phase fractionation is efficient in cold gas
    - freeze out on dust grains + grain-surface reactions
    - released into gas phase when ices sublimate in warm environments

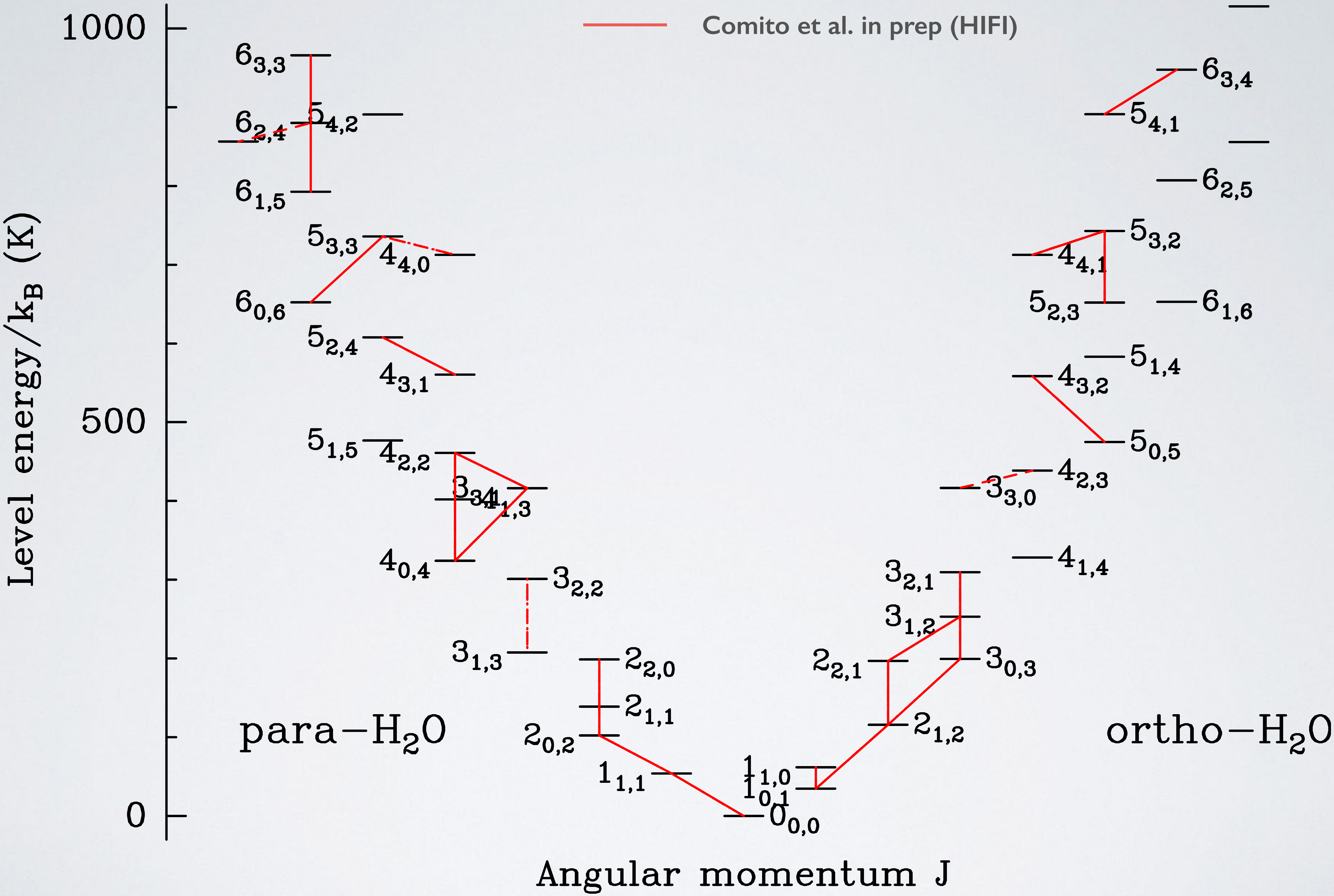
► **window onto “fossile" chemistry**

HERSCHEL/HIFI OBSERVATIONS OF EXTRAORDINARY SOURCES: HEXOS

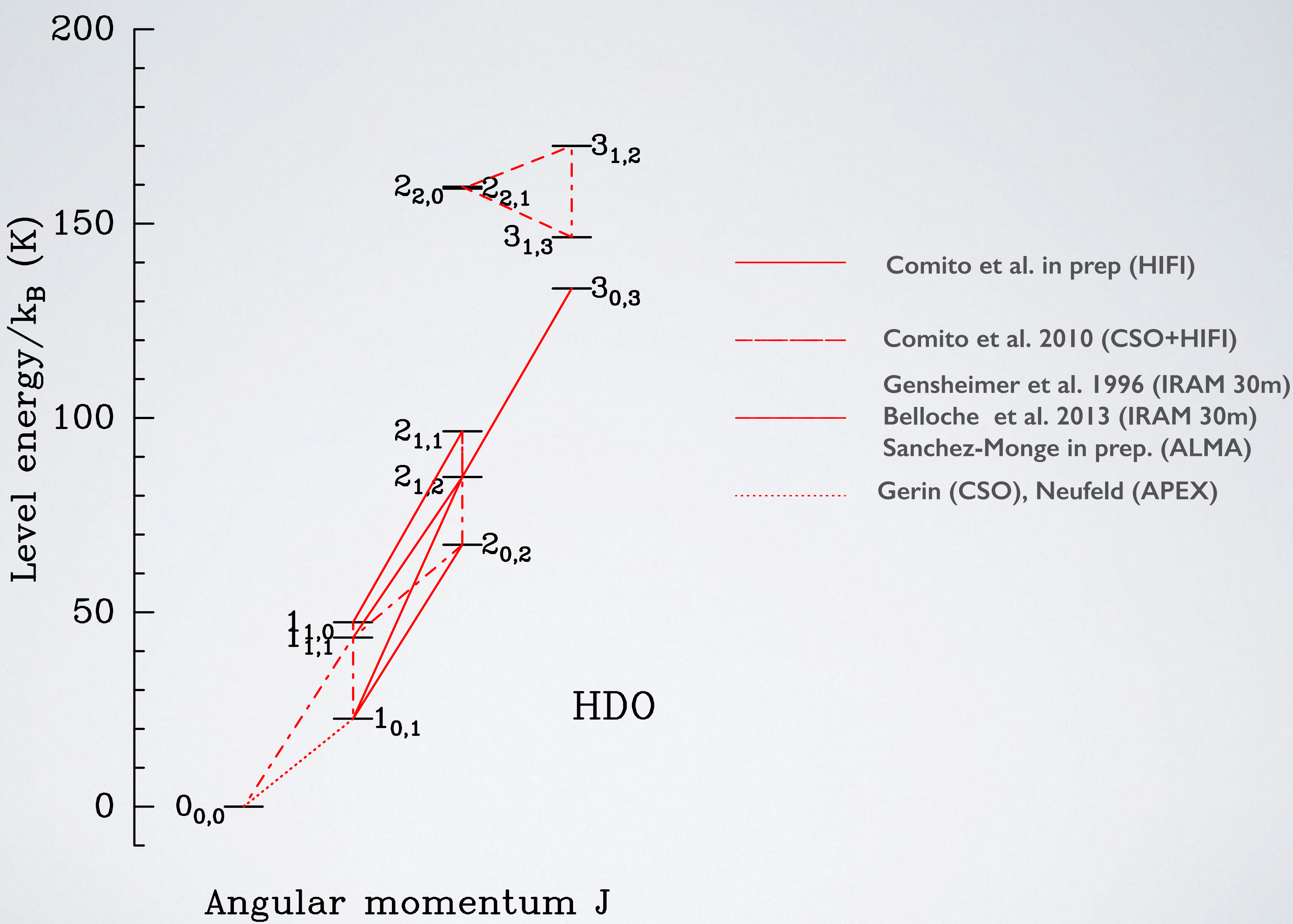
- **Herschel/HIFI SgrB2(M) line survey** acquired in 2010/2011 (GT KP **HEXOS**, Bergin+ 2010). We have detected (or not detected…):
  - 15 HDO transitions
  - 11 (ortho) + 12 (para) $H_2{}^{16}O$ transitions
  - 12 (ortho) + 12 (para) $H_2{}^{18}O$ transitions
  - 9 (ortho) + 12 (para) $H_2{}^{17}O$ transitions

We are attempting to fit **>80 rotational transitions between ~0.5 and ~1.8 THz** simultaneously.

Non-detections are detections, too!



Comito et al. in prep (HIFI)
Level energy/k_B (K)
Angular momentum J
1000
500
0
para−H_2O
ortho−H_2O
$6_{3,3}$
$6_{2,4}$
$5_{4,2}$
$6_{1,5}$
$5_{3,3}$
$4_{4,0}$
$6_{0,6}$
$5_{2,4}$
$4_{3,1}$
$5_{1,5}$
$4_{2,2}$
$3_{3,1}$
$4_{1,3}$
$4_{0,4}$
$3_{2,2}$
$3_{1,3}$
$2_{2,0}$
$2_{1,1}$
$2_{0,2}$
$1_{1,1}$
$0_{0,0}$
$1_{1,0}$
$1_{0,1}$
$2_{1,2}$
$2_{2,1}$
$3_{0,3}$
$3_{1,2}$
$3_{2,1}$
$4_{1,4}$
$3_{3,0}$
$4_{2,3}$
$5_{0,5}$
$4_{3,2}$
$5_{1,4}$
$5_{2,3}$
$6_{1,6}$
$4_{4,1}$
$5_{3,2}$
$6_{2,5}$
$5_{4,1}$
$6_{3,4}$



200
150
100
50
0
Level energy/k_B (K)
Angular momentum J
HDO
0_0,0
1_0,1
1_1,0
1_1,1
2_0,2
2_1,2
2_1,1
2_2,0
2_2,1
3_1,3
3_1,2
3_0,3
Comito et al. in prep (HIFI)
Comito et al. 2010 (CSO+HIFI)
Gensheimer et al. 1996 (IRAM 30m)
Belloche et al. 2013 (IRAM 30m)
Sanchez-Monge in prep. (ALMA)
Gerin (CSO), Neufeld (APEX)

THE PROBLEM

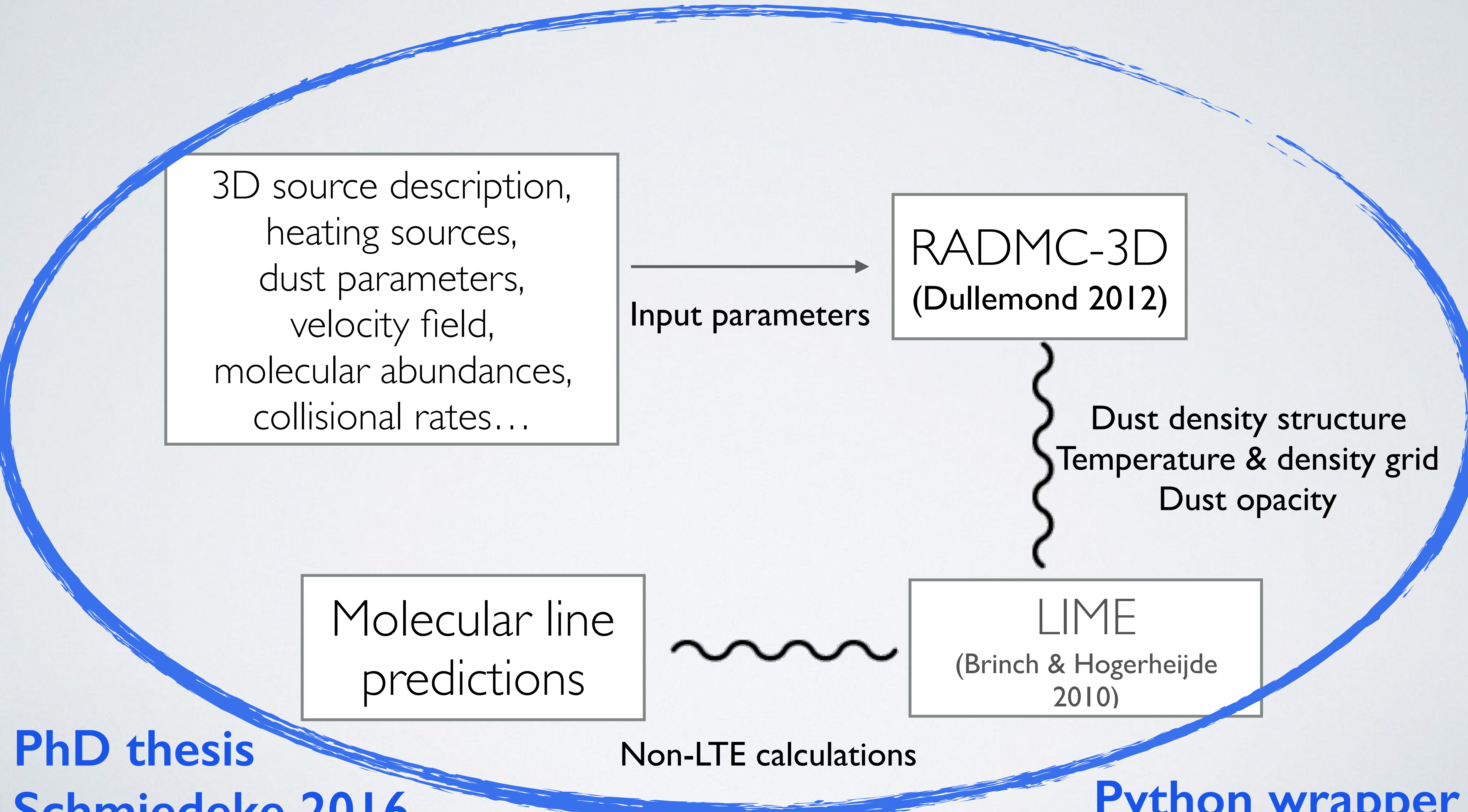
- Simultaneous fit of many transitions from complex source

- Water is all over the place! Line of sight within the HIFI beam affected by high-mass star formation on all scales. Hot cores, clumps, HII regions, envelope (+ filaments, outflows…).

- Common simplifications (LTE) do not apply over such a wide range of densities and temperatures.

► Full radiative transfer.

BRINGING TOGETHER RADMC-3D AND LIME: PANDORA

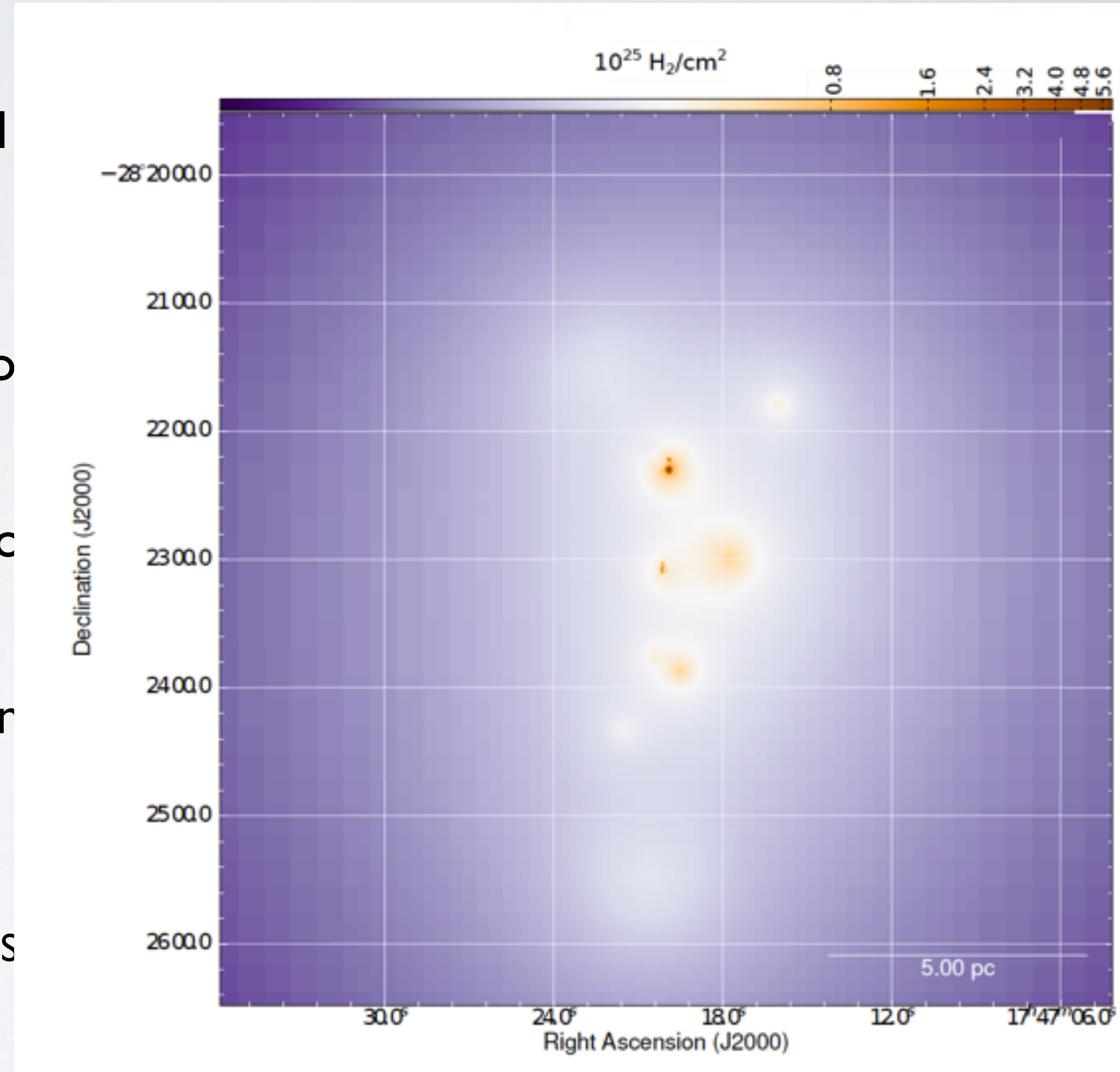


PhD thesis Schmiedeke 2016

Python wrapper

SGR B2: CONTINUUM

- Model C from **Schmiedeke+ 201**
- 3D Monte Carlo calculations
- Fitting small- and large-scale data, fro
  140 AU to 45 pc.
- Multi-wavelength dataset, from cm tc
  IR wavelengths.
- Temperature and density distributior
  of the dust ► starting point for
  prediction of molecular spectra.
- Figure: Blue: JCMT - SCUBA 850 micron, green: CS
  –Sharc II 350 micron, red: Herschel – PACS 70
  micron

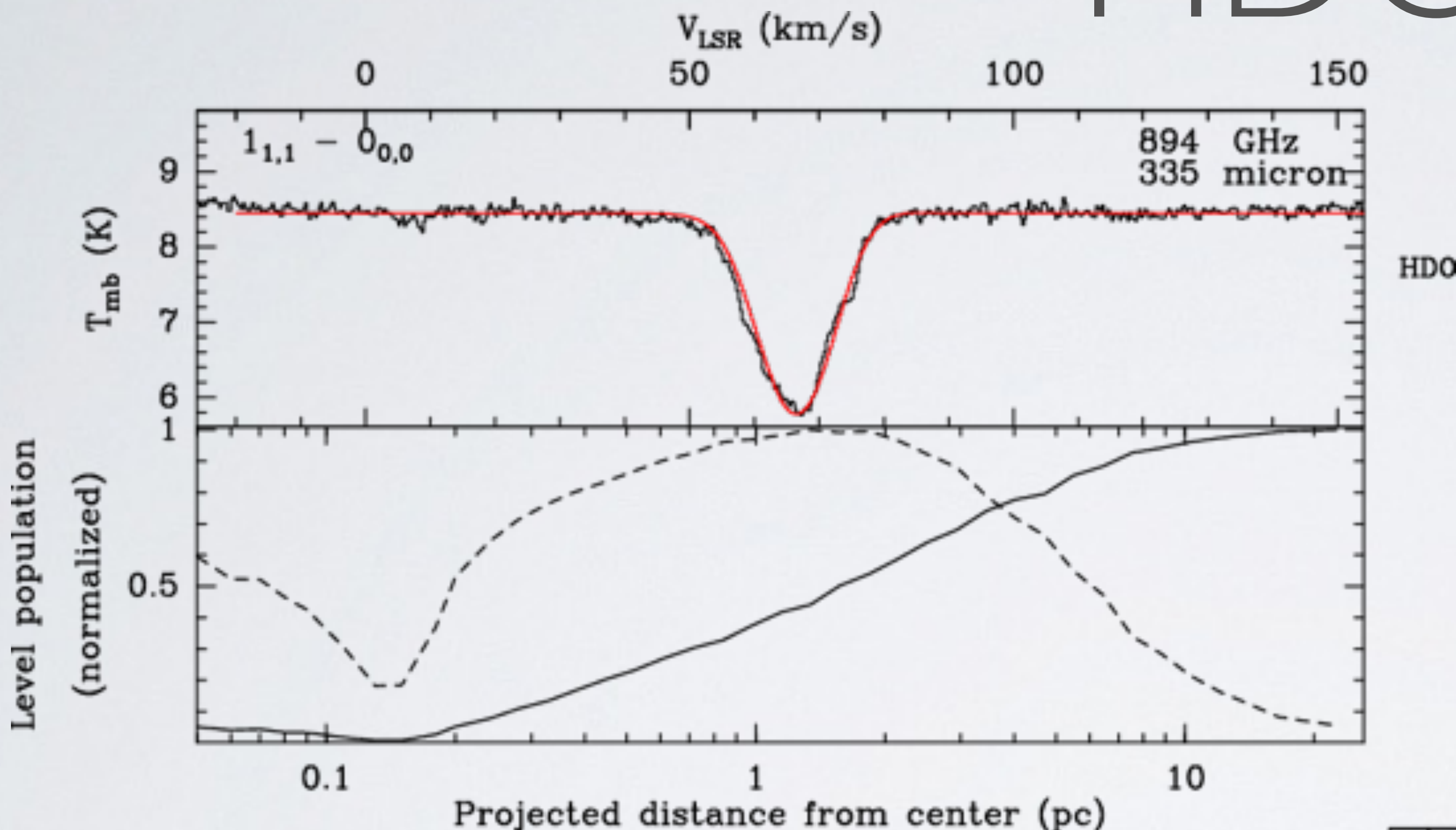


Schmiedeke+ 2016

MODEL PARAMETERS AND ASSUMPTIONS

- Free parameters: **[HDO]/[H_2]** and **[H_2O]/[H_2]**. Two-step abundance increase:
  - T > 100 K: release of H_2O and HDO from grains into gas-phase
  - T > 250 K: gas-phase production of H_2O (Comito+ 2010: 200 K)
- No LTE approximation ▶ we need collisional rates. From the LAMDA database (Schöier+ 2005):
  - HDO (Faure+ 2012), o-H_2O, p-H_2O (Barber+ 2006, Dubernet+ 2006, Dubernet+ 2009)
  - o/p-$H_2{}^{18}0$ and o/p-$H_2{}^{17}0$ collisional rates based on o/p-$H_2{}^{16}0$
- Ortho/para-H_2O = 3, [^{16}O]/[^{18}O] = 250, [^{17}O]/[^{18}O] = 800 (Wilson & Rood 1994).
- All data are single-sideband (after sideband separation, Comito & Schilke 2002).

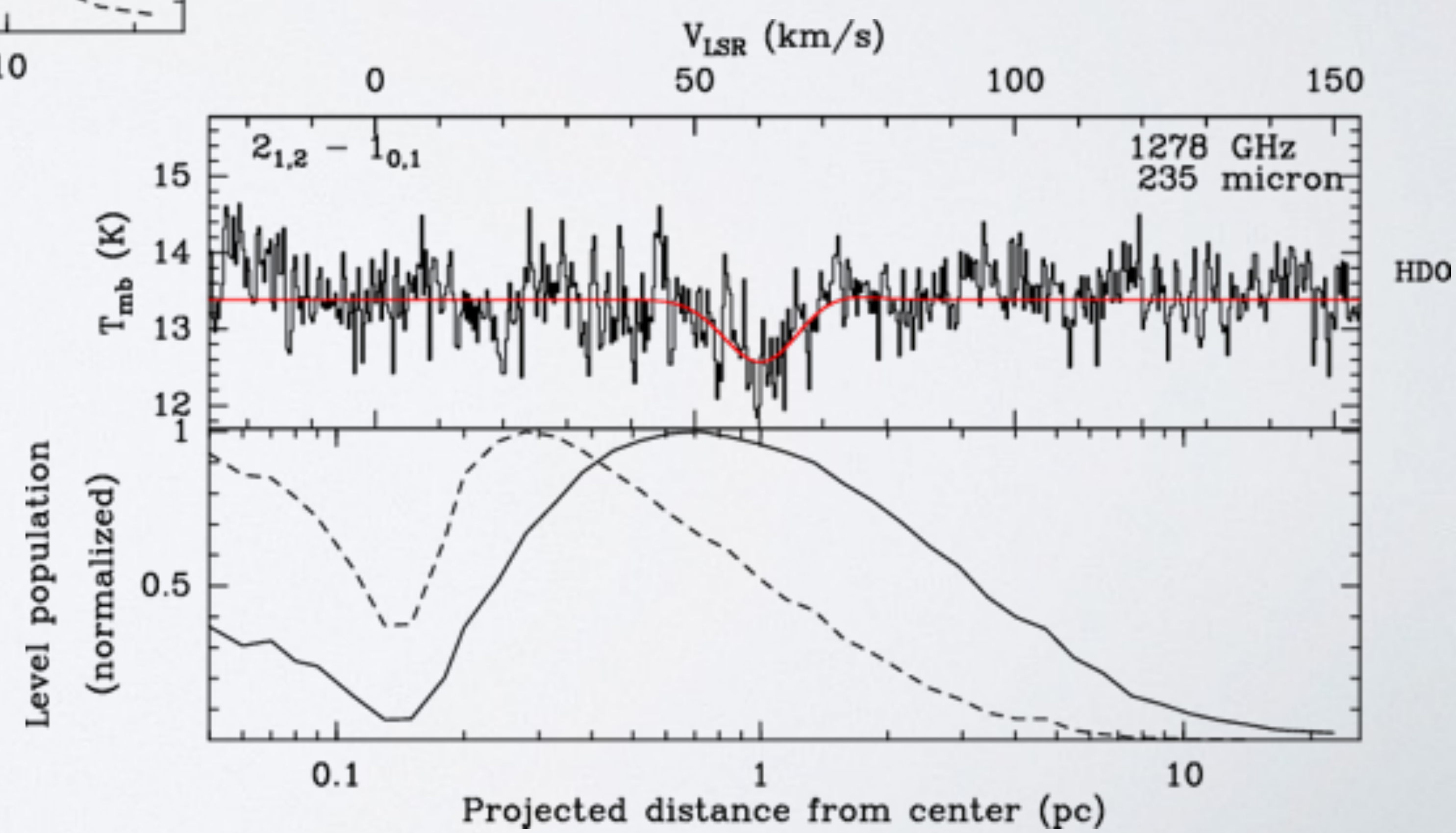
OUTER ENVELOPE (T< 100 K): HDO



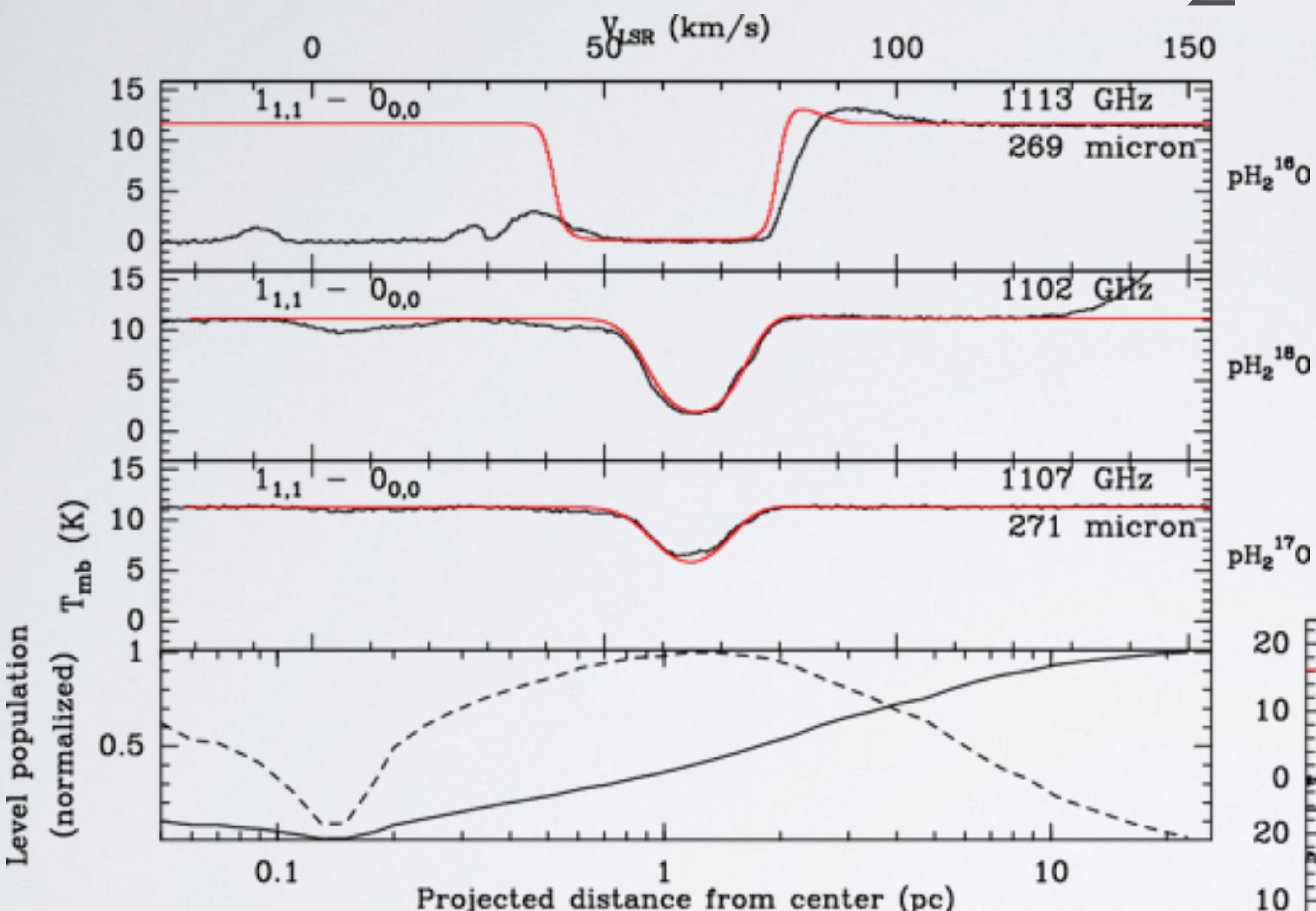
Comito+ 2003, 2010

best fit for T<100 K:
$[HDO]/[H_2] = 3.4x10^{-11}$

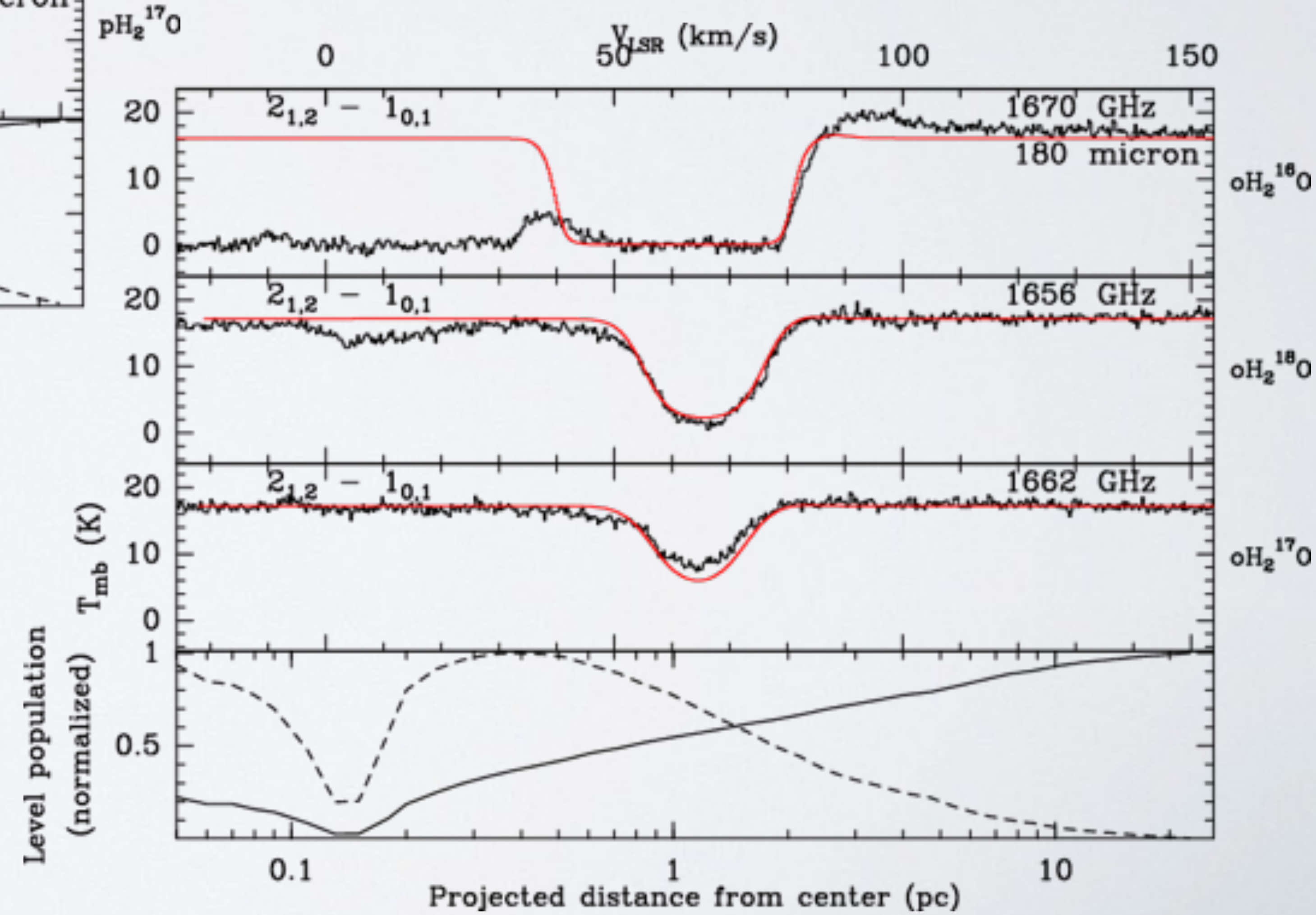
Comito+ in prep.



OUTER ENVELOPE (T< 100 K): H_2O

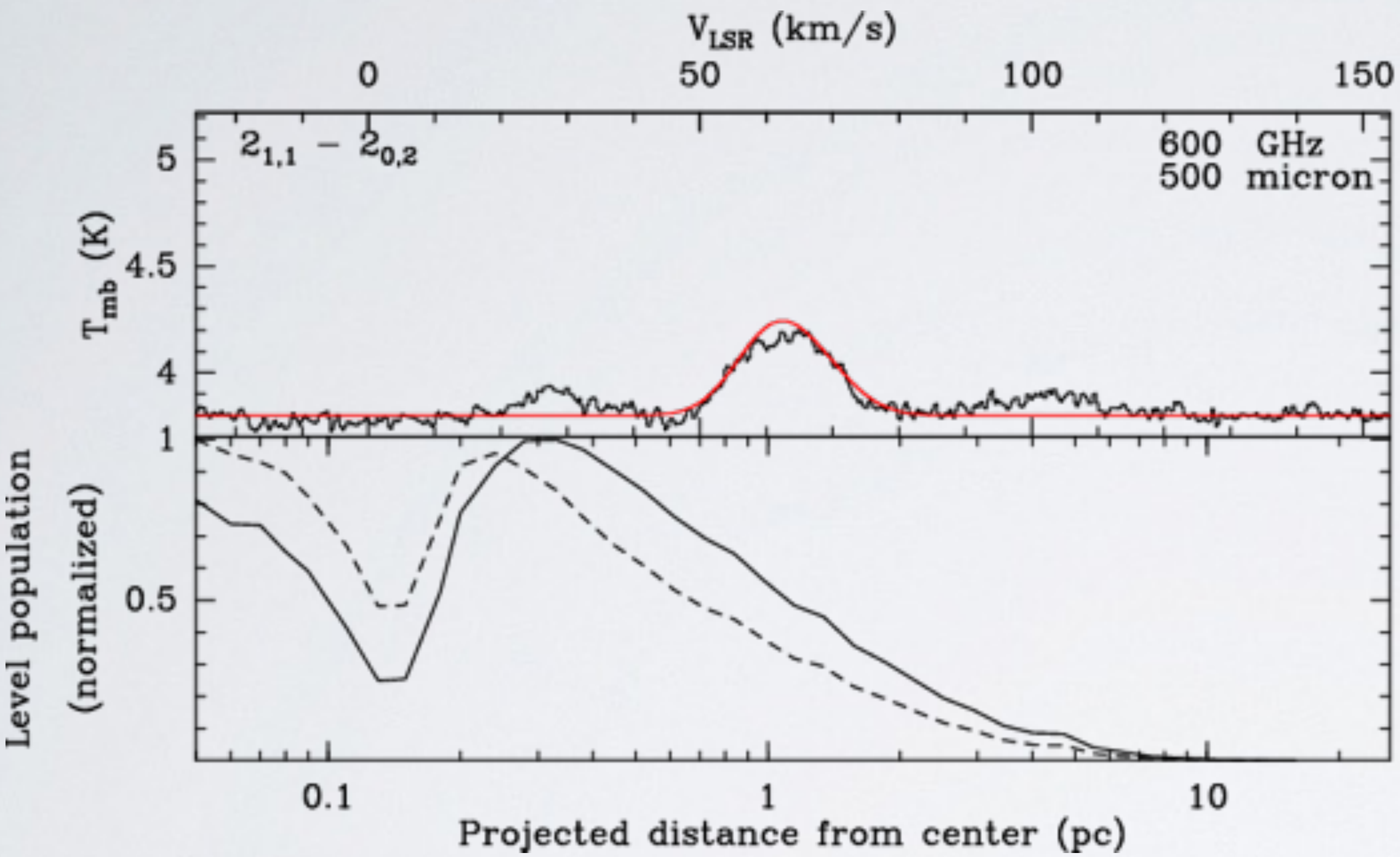


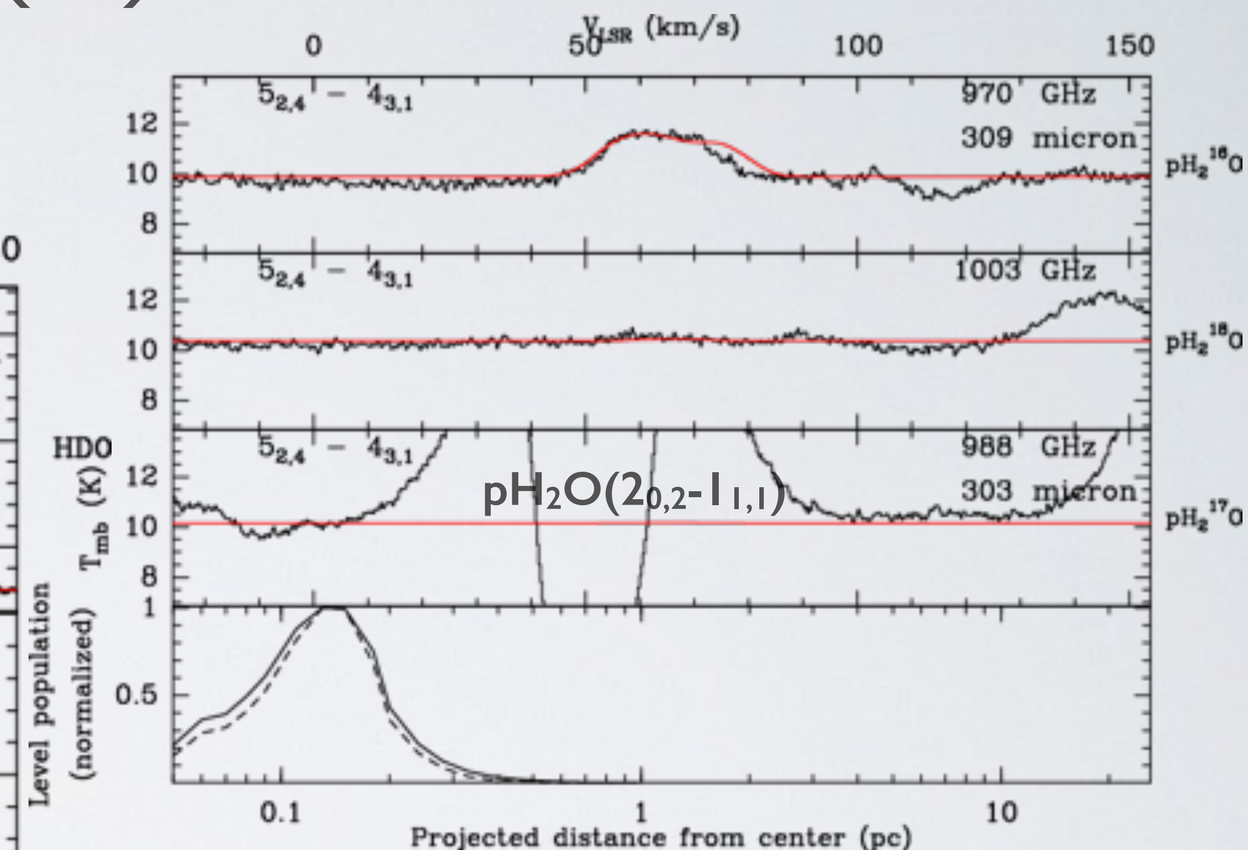
best fit for T<100 K:
$[H_2O]/[H_2] = 1.3x10^{-7}$

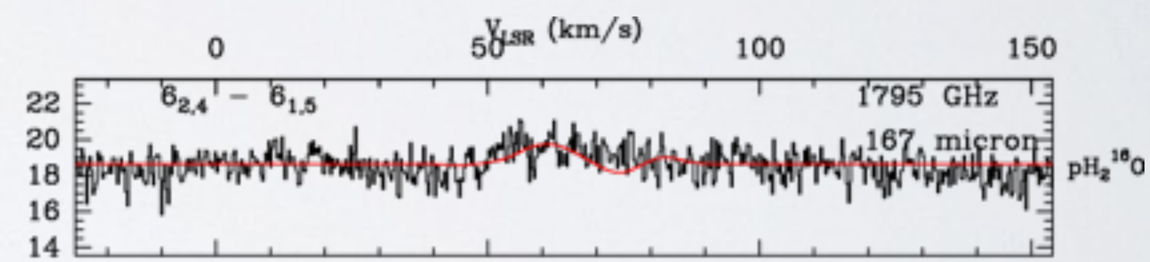


Comito+ in prep.

INNER CORE(S), T > 250 K



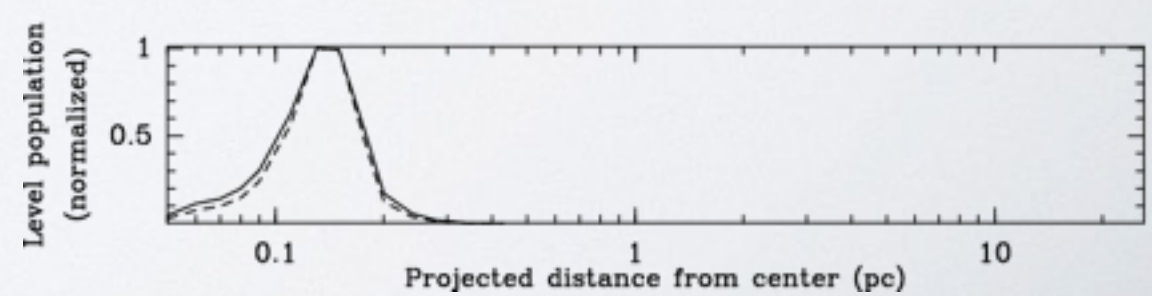




best fit for T>250 K:

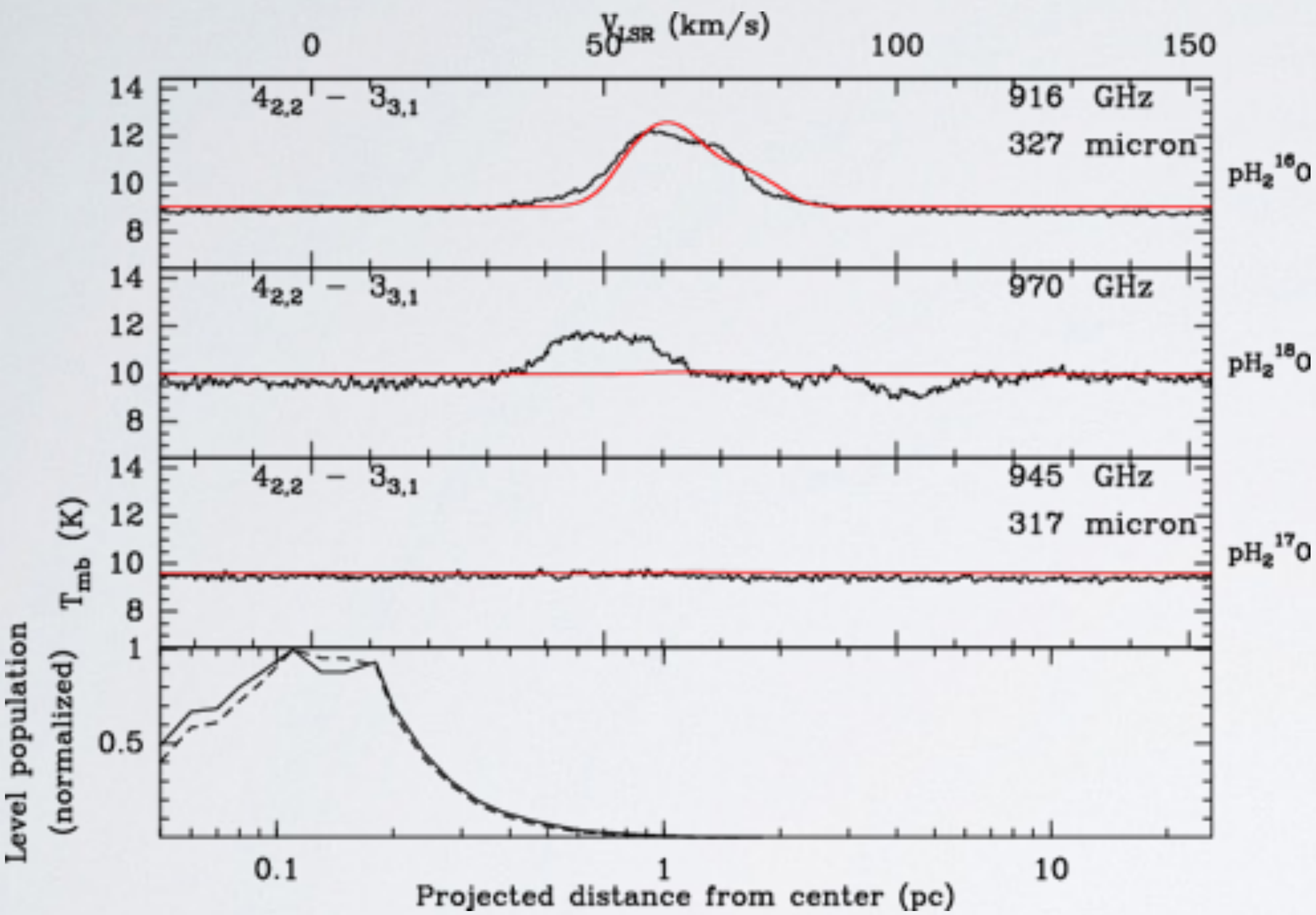
$[H_2O]/[H_2] = 4.2x10^{-6}$

$[HDO]/[H_2] = 8.2x10^{-10}$



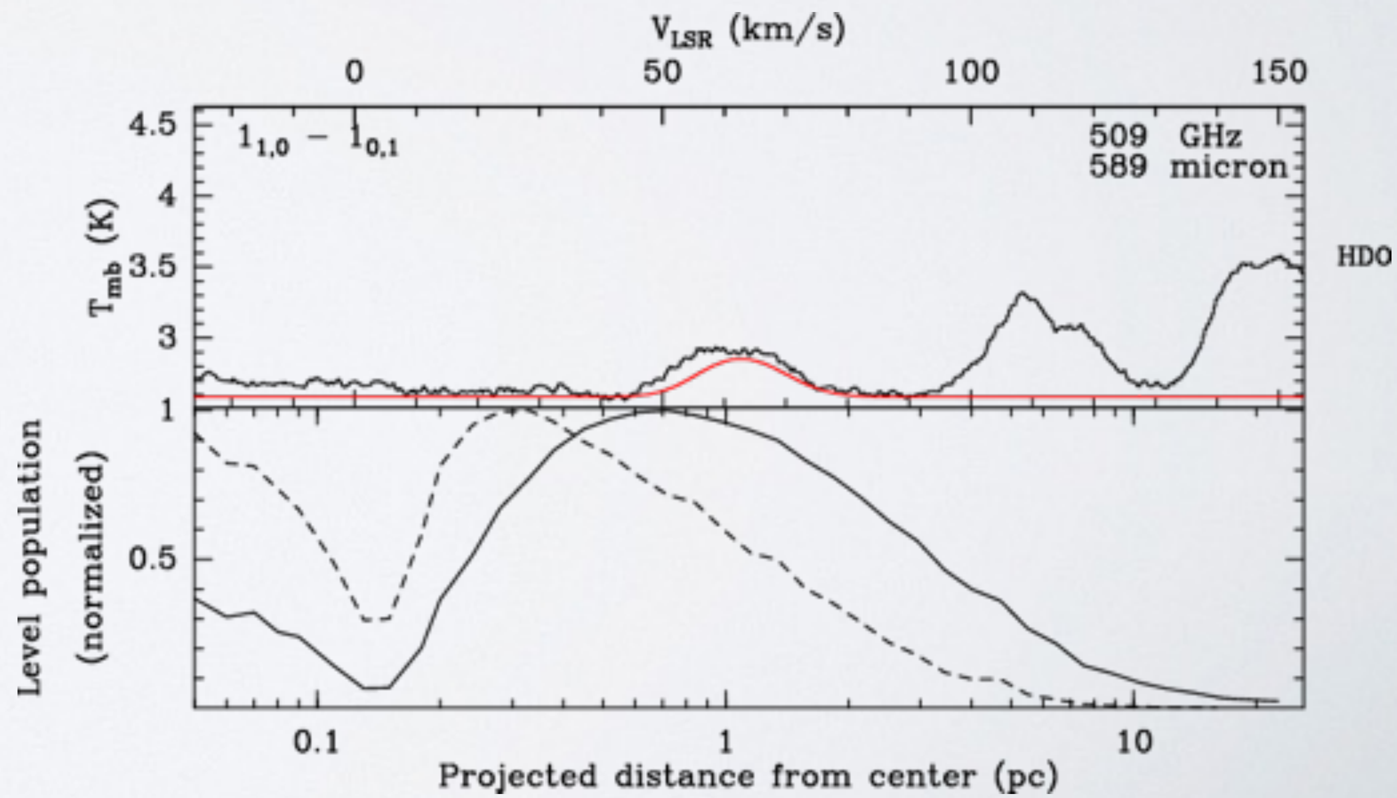
Comito+ in prep.

INTERMEDIATE REGION (100 K < T < 250 K)



best fit for 100 K<T<250 K:
$[H_2O]/[H_2] = 3.5x10^{-6}$
$[HDO]/[H_2] = 8.2x10^{-10}$

Comito+ in prep.



RESULTS PART I

- We have achieved a **simultaneous fit of ~ 80 H_2O and HDO transitions** between 500 and 1800 GHz, and of the continuum emission, towards Sgr B2(M).

- Total H_2O abundance, $[H_2O]/[H_2]$:

  - **1.3 x 10^{-7} when T< 100 K**

  - **3.5 x 10^{-6} when 100 < T< 250 K**

  - **4.2 x 10^{-6} when T > 250 K**

- Consistent with Comito+ 2003, cf. Choi+ (AFGL 2591, $[H_2O]/[H_2]$ up to 2 x 10^{-8}). cf. E. van Dishoeck's review talk

RESULTS PART II

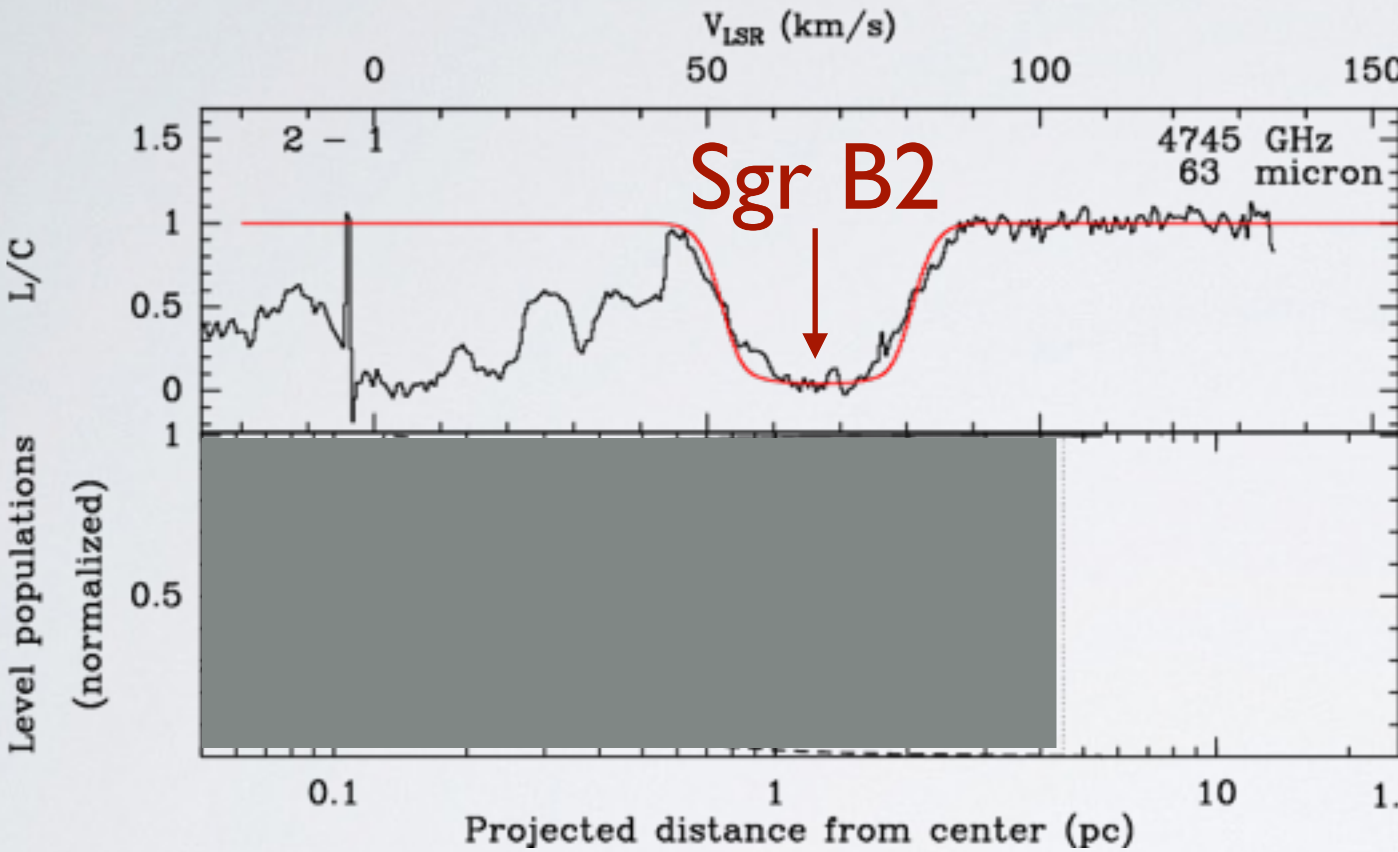
- [HDO]/[H_2]:
  - **3.4×10^{-11}, 8.2×10^{-10}, 8.2×10^{-10}**
- [HDO]/[H_2O]:
  - **3×10^{-4}, 3×10^{-4}, 2×10^{-4}** respectively.
    - Up to 150 times larger than [D]/[H] in the Galactic Center? Lubowich et al. 2000.
    - cf. Neill+ 2013 in Orion-KL. Coutens+ 2014 in G34.26+0.15: [HDO]/[H_2O] in absorbing gas 10x lower than in hot core.

OPEN ISSUES

- HDO/H_2O steady across the Sgr B2(M) envelope: age? Compare to Sgr B2(N), chemical models.
- **mm lines** (Gensheimer+ 1990, Belloche+ 2013, Sanchez-Monge in prep.) **underestimated** → model description of inner cores needs to be improved (IRAM 30m, ALMA)
- "Where's the oxygen??" (thanks Cecilia Ceccarelli!)

ATOMIC OXYGEN

Comito, Ceccarelli+ in prep.



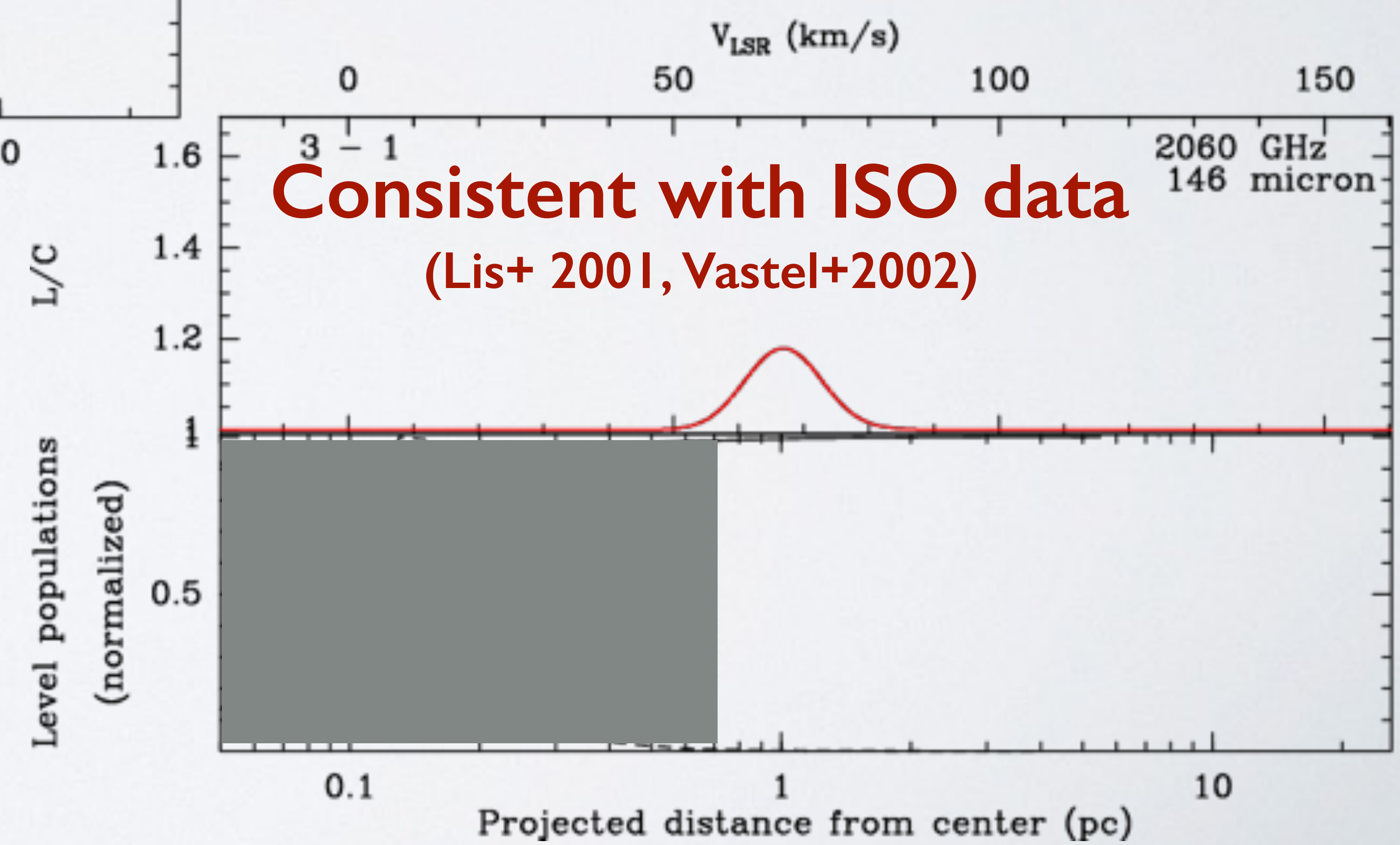
best fit:

$[O]/[H_2] = 5x10^{-5}$

(constant)

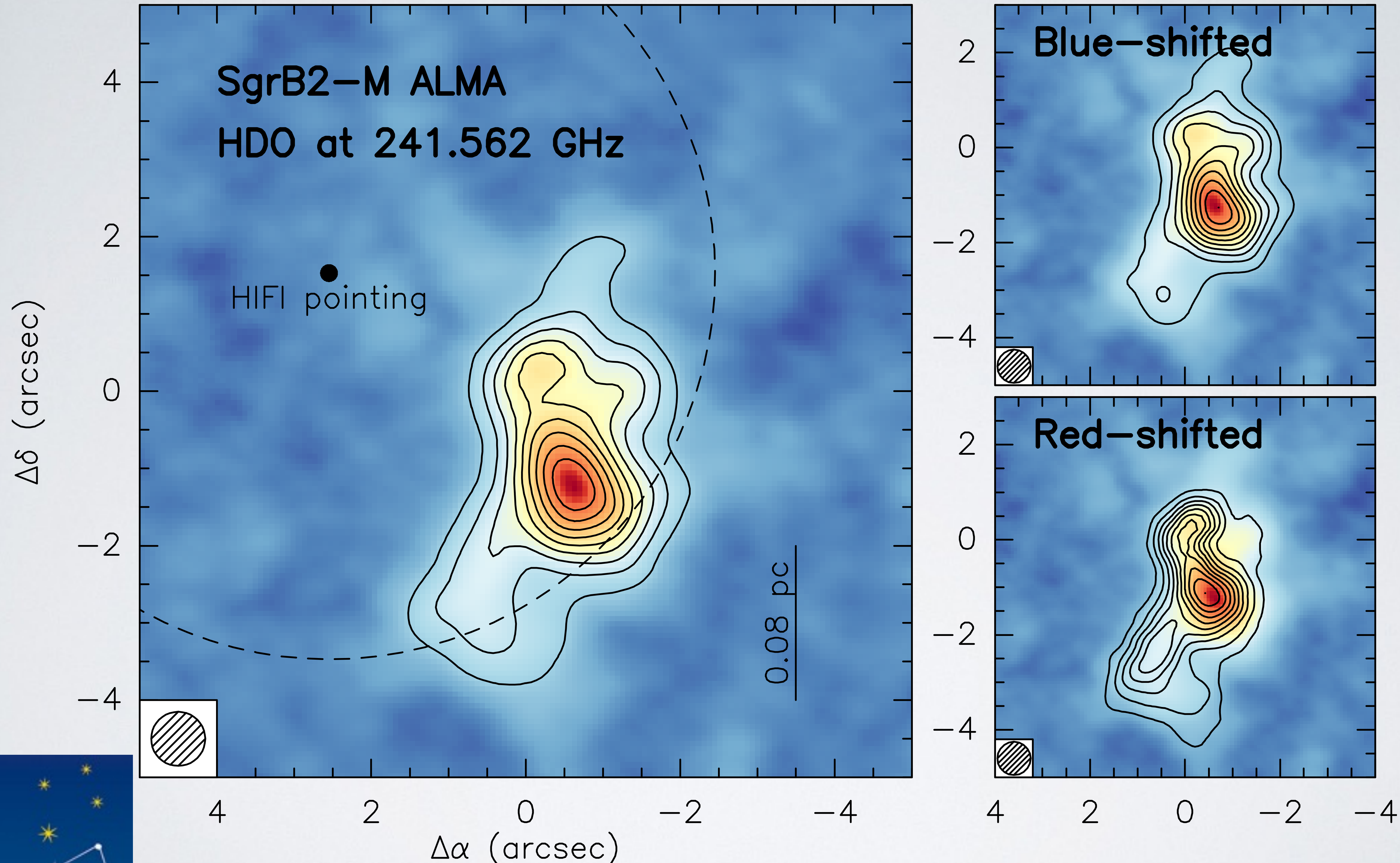
Consistent with ISO data

(Lis+ 2001, Vastel+2002)



Beware of dust opacity!

It's a 3D model! From single-point spectra to maps (ALMA)



Sanchez-Monge+, Comito+ in prep.