A 3D Model of the Distribution and Deuteration of Water in SgrB2(M)

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Deuterium fractionation

- Abundance of deuterated counterpart of a molecular species is enhanced with respect to the cosmic ratio:
- [XD]/[XH] > [D]/[H]
- Important tool to infer physical conditions in molecular clouds:
    - gas-phase fractionation is efficient in cold gas
    - freeze out on dust grains
    - released into gas phase when ices sublimate

—> window onto “fossile" chemistry

Herschel/HIFI observations of Extraordinary Sources:HEXOS

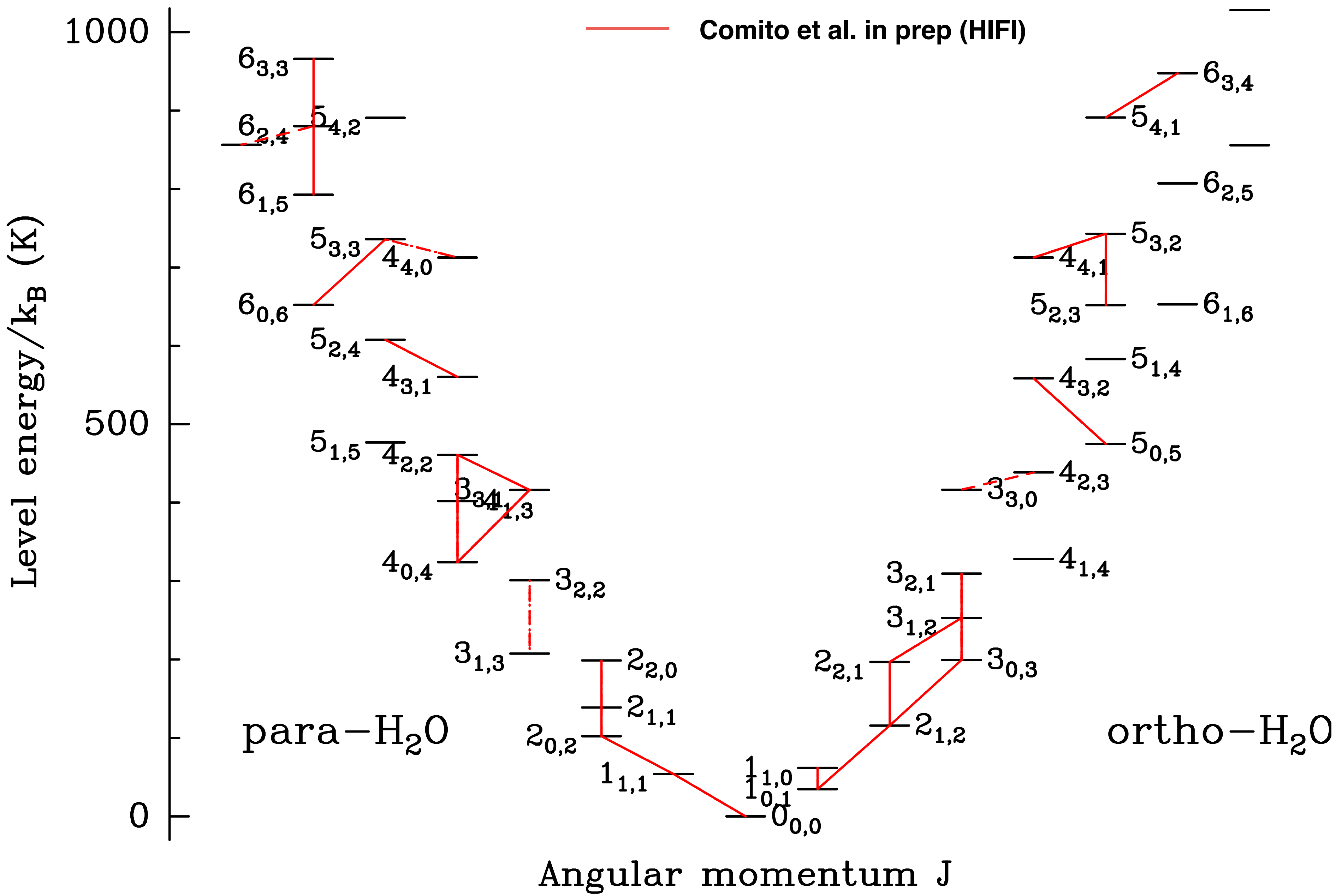
- Herschel GT KP: Unbiased spectral surveys of archetypical molecular clouds Orion and Sgr B2 (Bergin et al. 2010).

- This work is based on the **HIFI SgrB2(M) line survey**. We have detected (or not detected…):

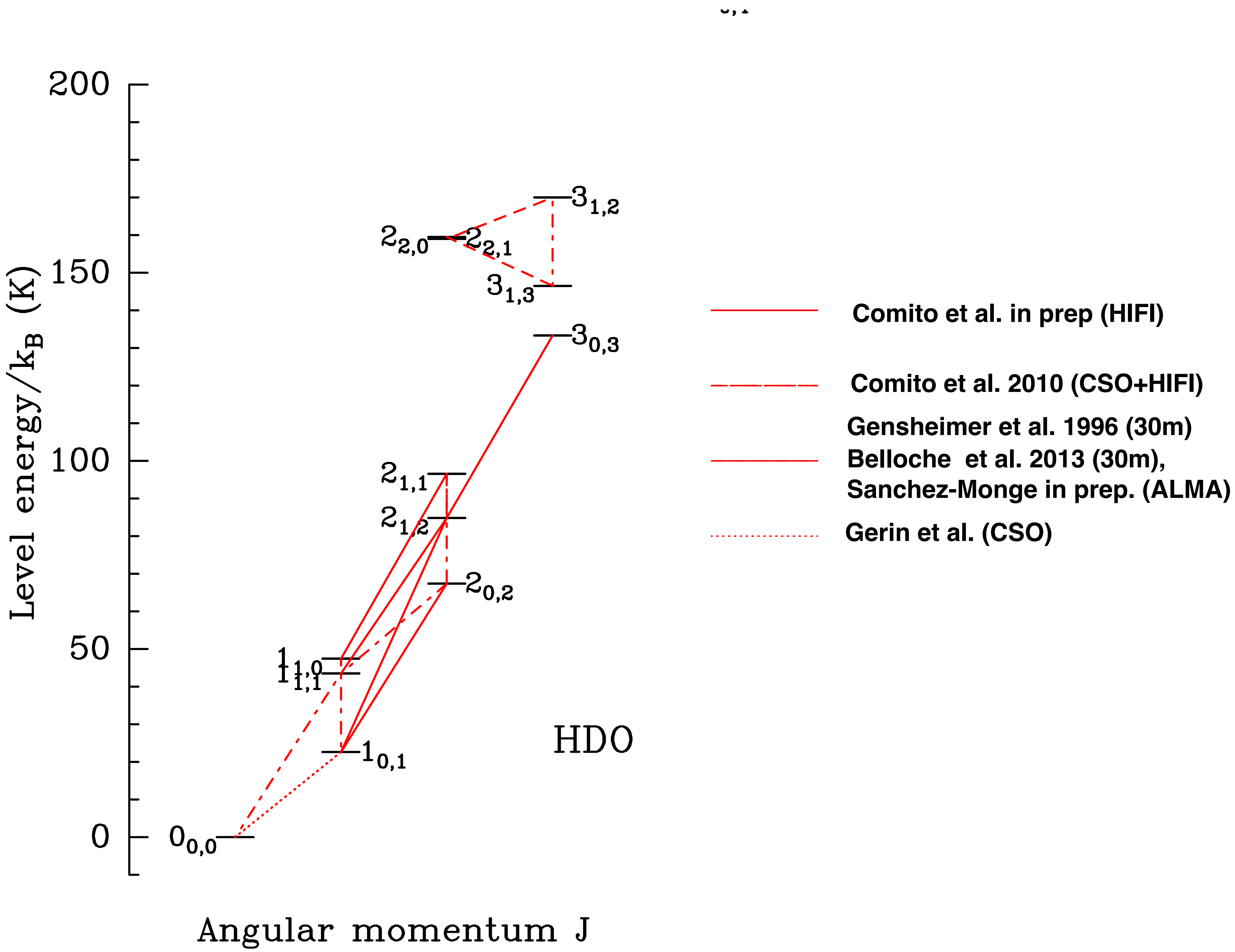
  - **10 HDO transitions**
  - **11 (ortho) + 12 (para) H_2O transitions**
  - **12 (ortho) + 12 (para) $H_2^{18}O$ transitions**
  - **9 (ortho) + 12 (para) $H_2^{17}O$ transitions**

We are attempting to fit **~80 rotational transitions between ~500 and ~1800 GHz simultaneously**.

Non-detections are detections, too!



Comito et al. in prep (HIFI)
1000
500
0
Level energy/k_B (K)
Angular momentum J
para−H2O
ortho−H2O
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
1 1,0
1 0,1
0 0,0
6 3,4
5 4,1
6 2,5
5 3,2
4 4,1
5 2,3
6 1,6
5 1,4
4 3,2
5 0,5
4 2,3
3 3,0
4 1,4
3 2,1
3 1,2
2 2,1
3 0,3
2 1,2



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

The problem

- 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.

Radiation transfer in a complex environment

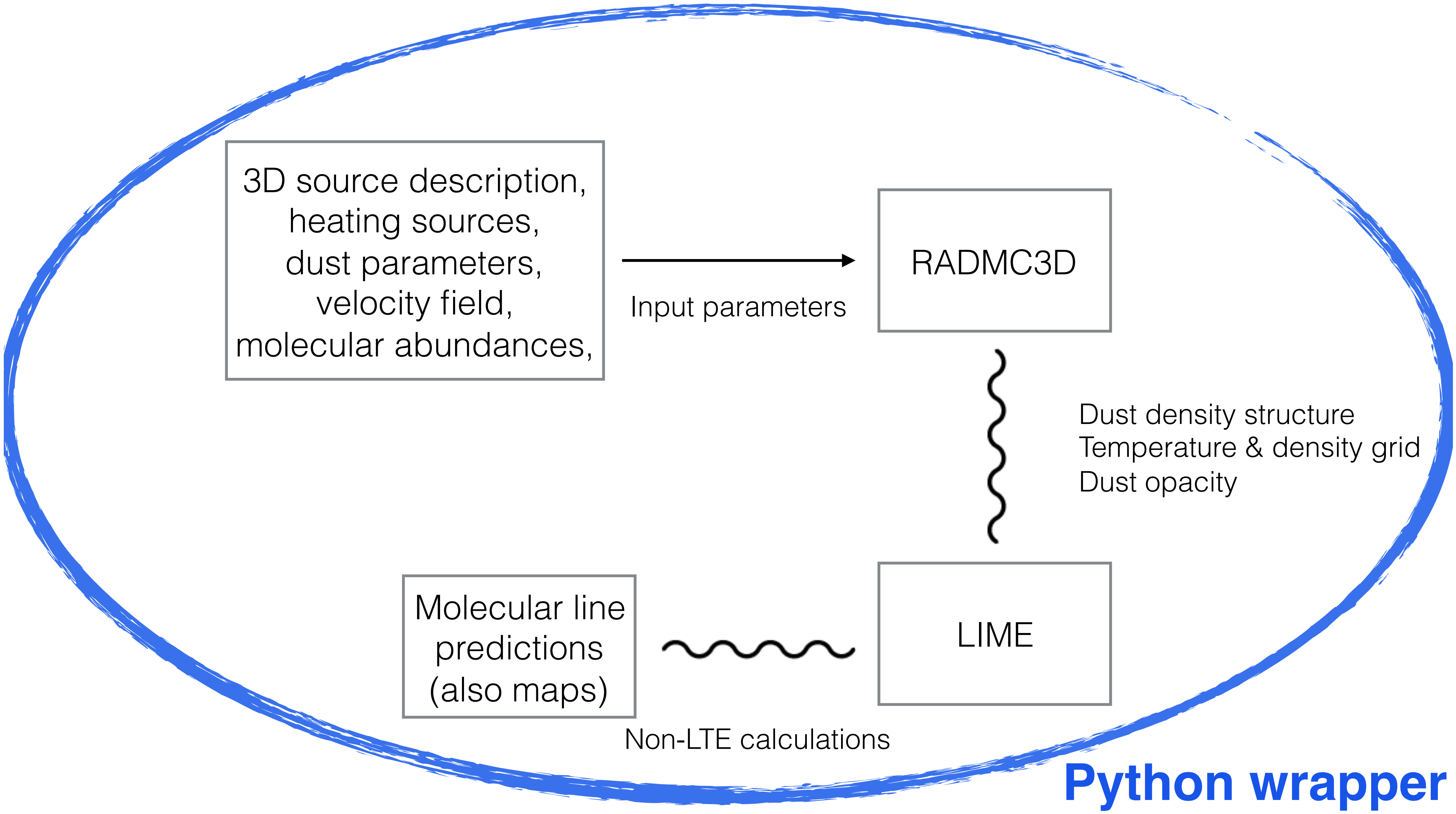
“A photon is emitted, it travels a distance, and then something happens to it.” (Wood et al. 2013)

- We cannot describe the behaviour of single photons as they travel across the medium, but we can describe the **statistical behaviour of N photons —> Monte Carlo method**.

- Continuum emission: **RADMC3D** (Dullemond 2012)

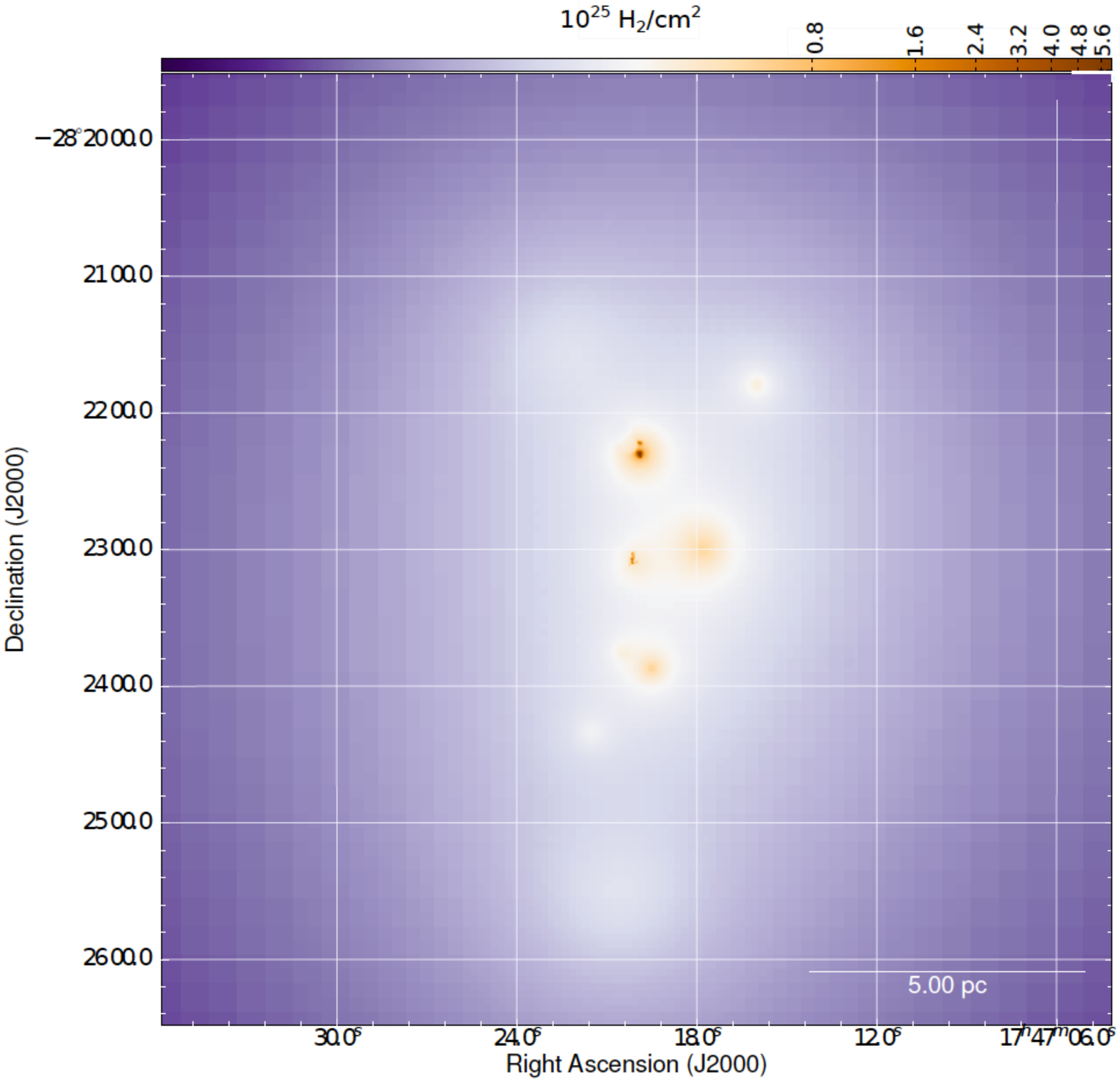
- Molecular lines: **LIME** (Brinch & Hogerheijde 2010)

Bringing together RADMC3D and LIME:
PANDORA (A. Schmiedeke, PhD Thesis 2016)



SgrB2: Continuum

- Model C from **Schmiedeke et al. 2016**
- 3D Monte Carlo calculations
- Fitting small- and large-scale data, from 140 AU to 45 pc.
- Multi-wavelength dataset, from cm to IR wavelengths.
- Temperature and density distribution of the dust —> starting point for prediction of molecular spectra.
- Figure: Blue: JCMT - SCUBA 850 m, green: CSO –Sharc II 350 m, red: Herschel – PACS 70 m (Schmiedeke et al.2016).



HDO and H_2O model assumptions

- Evaporation of icy grain mantles —> increase in H_2O and HDO abundance in the gas phase. **Two-step abundance increase** (Comito et al. 2010).

- No LTE approximation —> we need **collisional rates.** From the LAMDA database (Schöier et al. 2005):

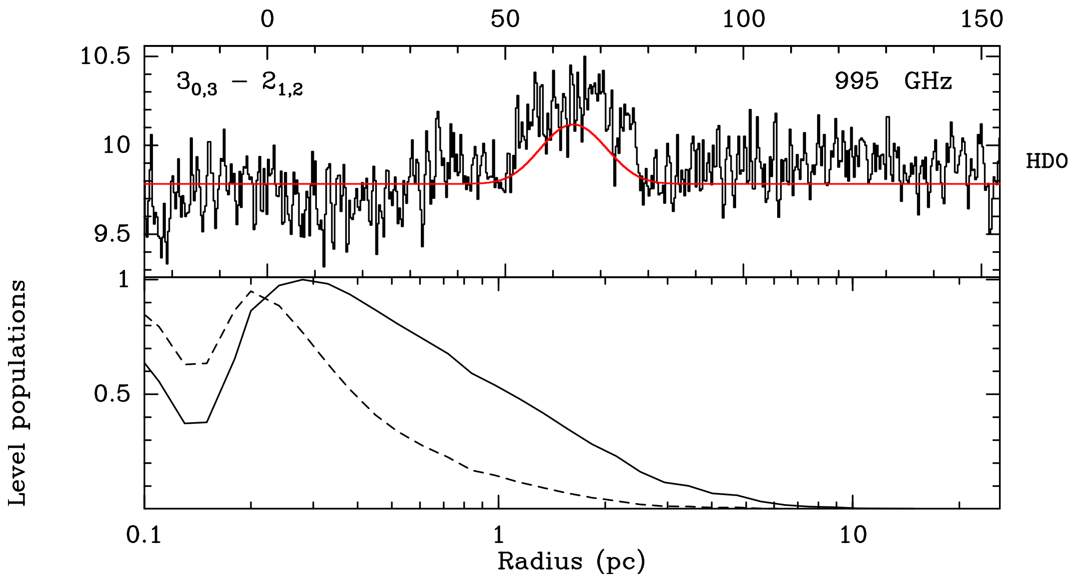
  - HDO (Faure et al. 2012)

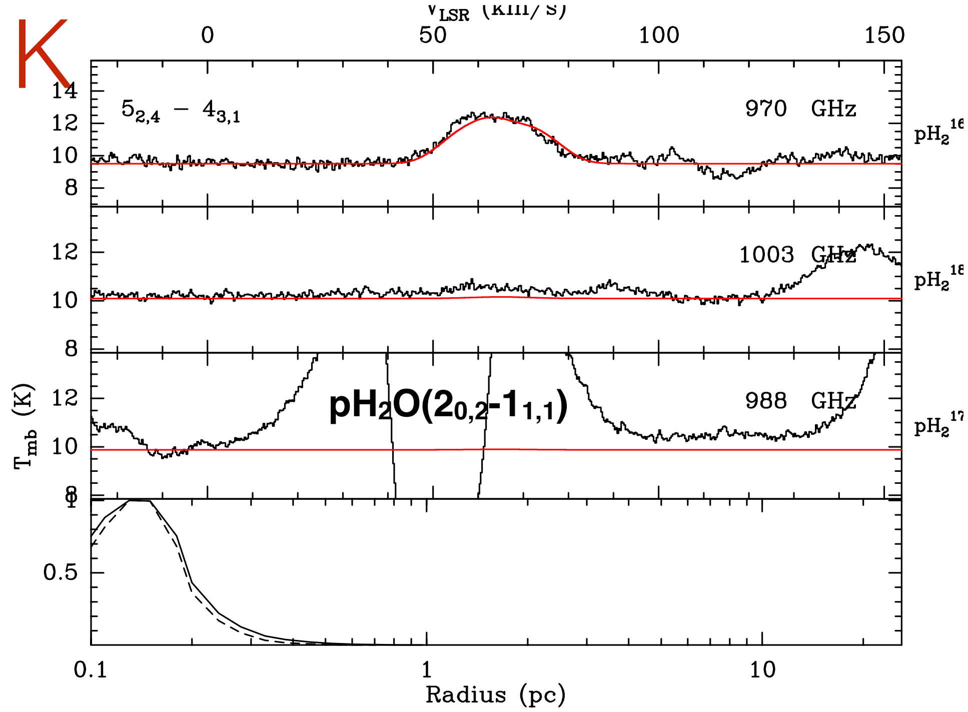
  - o-H_2O, p-H_2O (Barber et al. 2006, Dubernet et al. 2006, Dubernet et al. 2009)

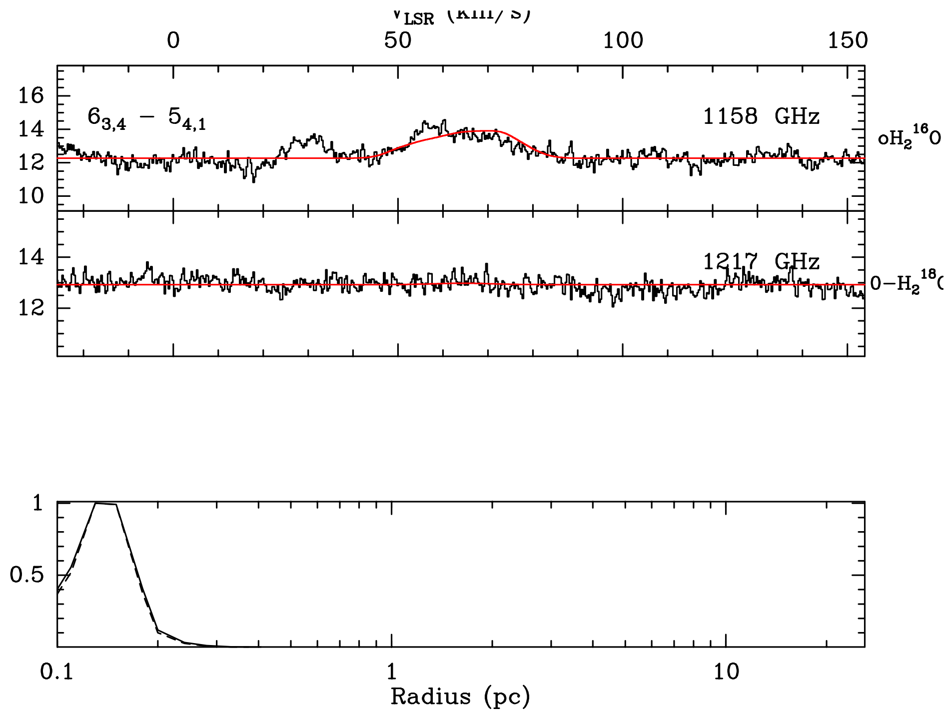
  - o/p-$H_2{}^{18}0$ and o/p-$H_2{}^{17}0$ collisional rates based on o/p-$H_2{}^{16}0$

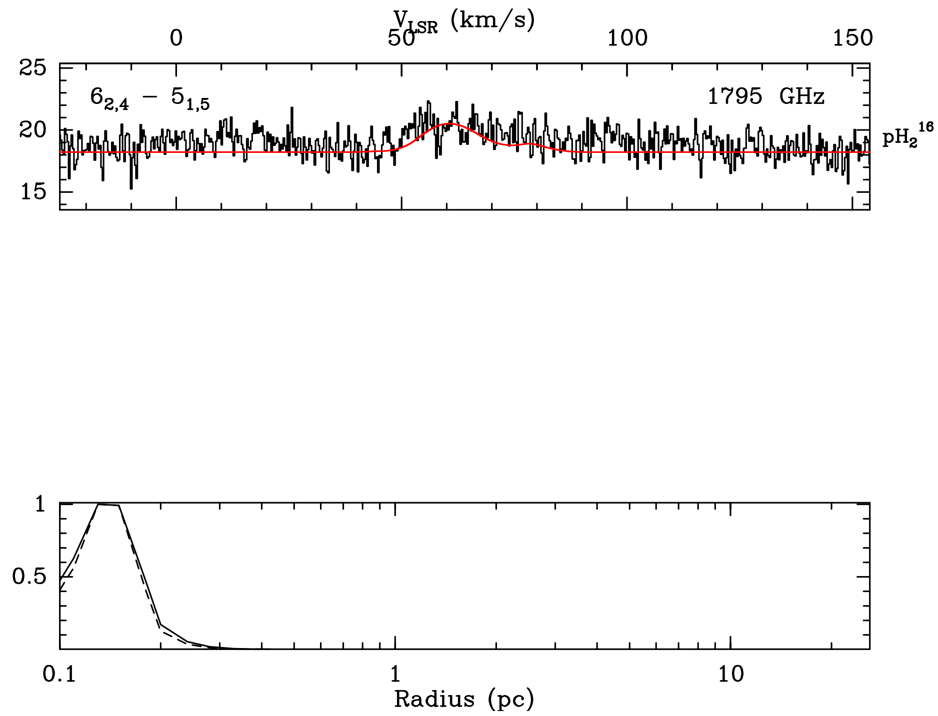
- All data are single-sideband (after **sideband separation**, Comito & Schilke 2002).

INNER CORE(S), T > 200 K



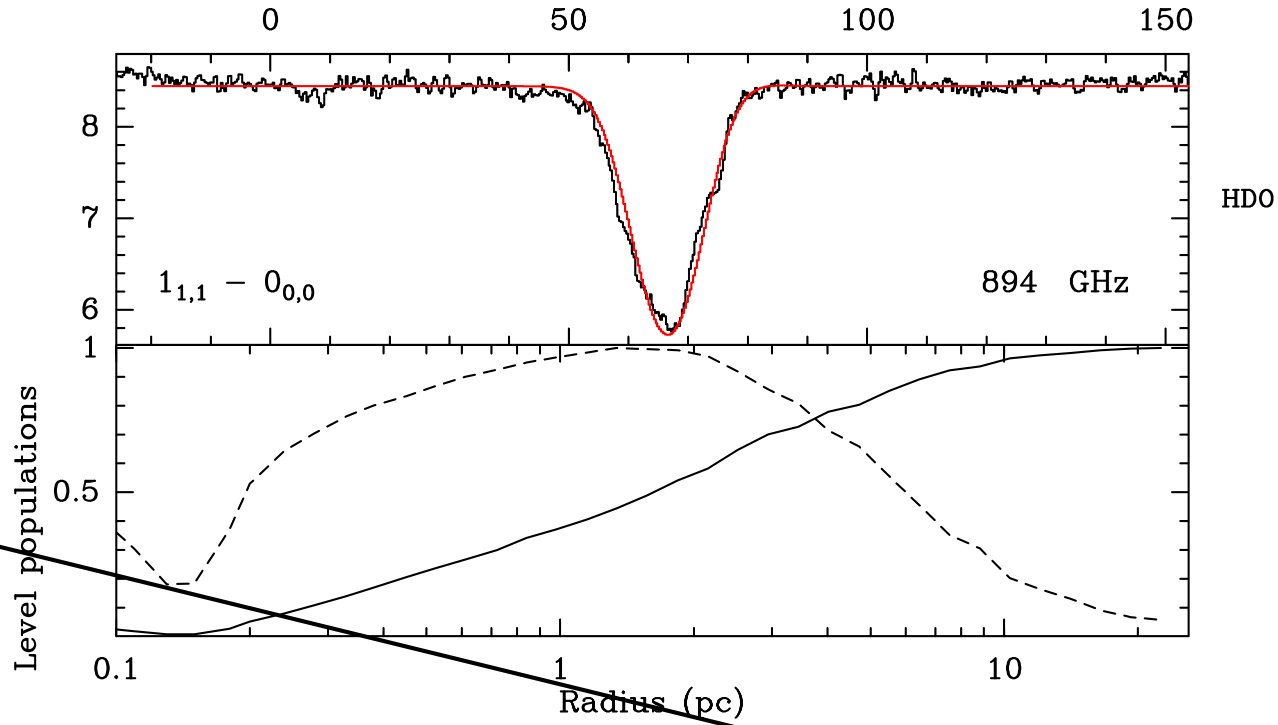


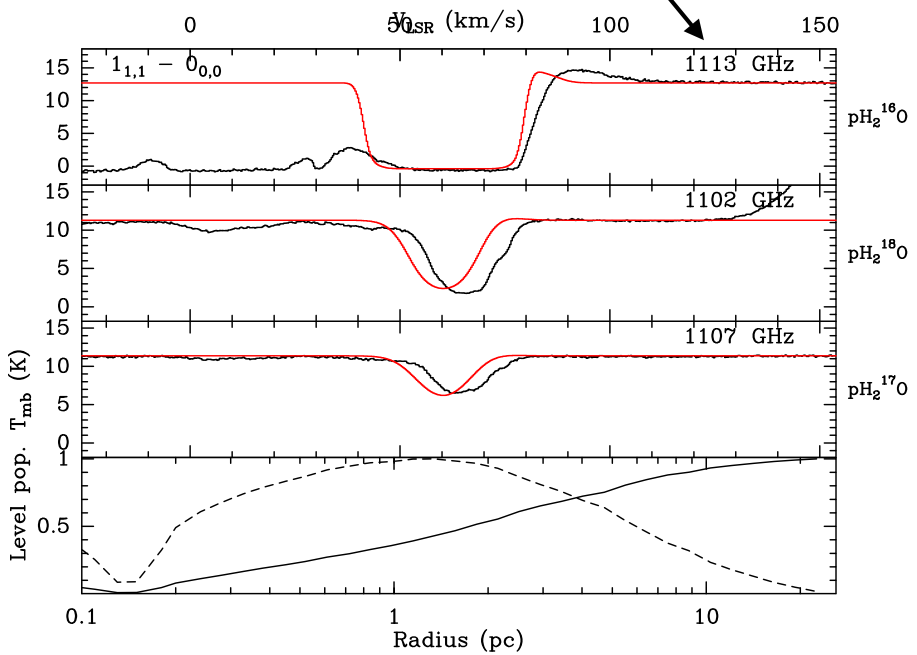


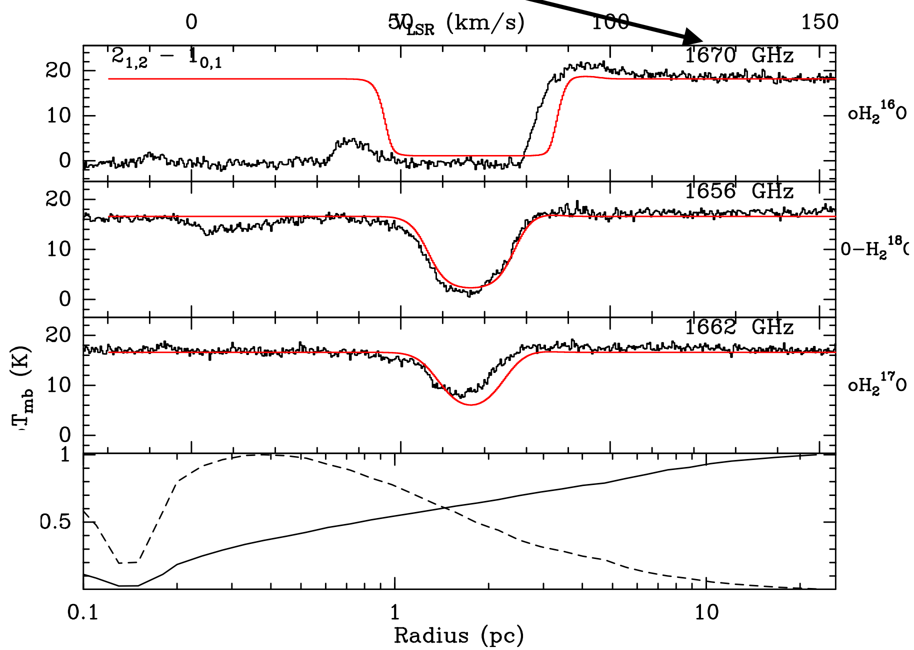


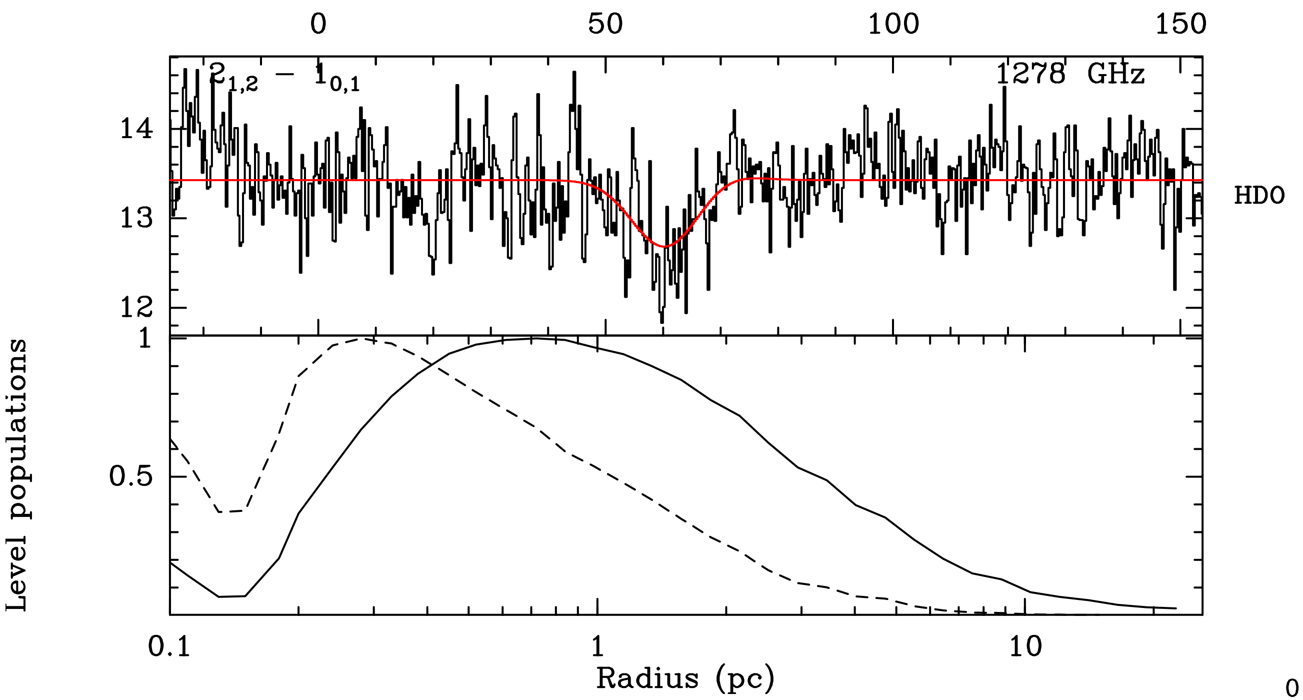
OUTER ENVELOPE
T < 100 K

Beware of dust opacity!

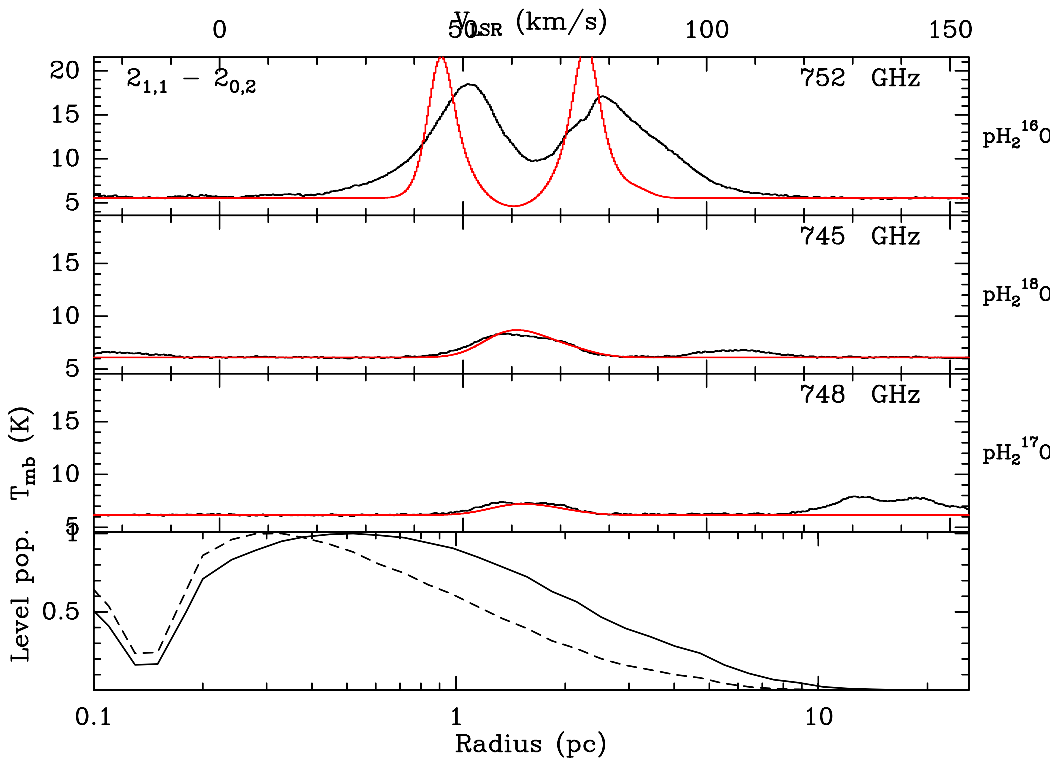








INTERMEDIATE REGION
100 < T < 200 K



RESULTS

- We have achieved a simultaneous fit of ~ 80 H_2O and HDO transitions between 500 and 1800 GHz, and of the continuum emission, towards SgrB2(M).
- Total H_2O abundance, **$[H_2O]/[H_2]$:**
  - **1.25×10^{-7} when $T < 100$ K**
  - **2.5×10^{-6} when $100 < T < 200$ K**
  - **3.5×10^{-6} when $T > 200$ K**
- **$[HDO]/[H_2O]$:**
  - **3×10^{-4}**, **1×10^{-4}**, **5×10^{-4}** respectively. Factor of ~2 less than in Comito et al. 2003 (based on 2 lines!). Up to 250 times larger than [D]/[H] in the Galactic Center? Lubowich et al. 2000.
- Continuum fit within 15% of observations over HIFI range
- Ortho/para = 3, standard isotopic ratios OK.

Homework

- mm-wavelength lines are underestimated —> improve hot-core description.

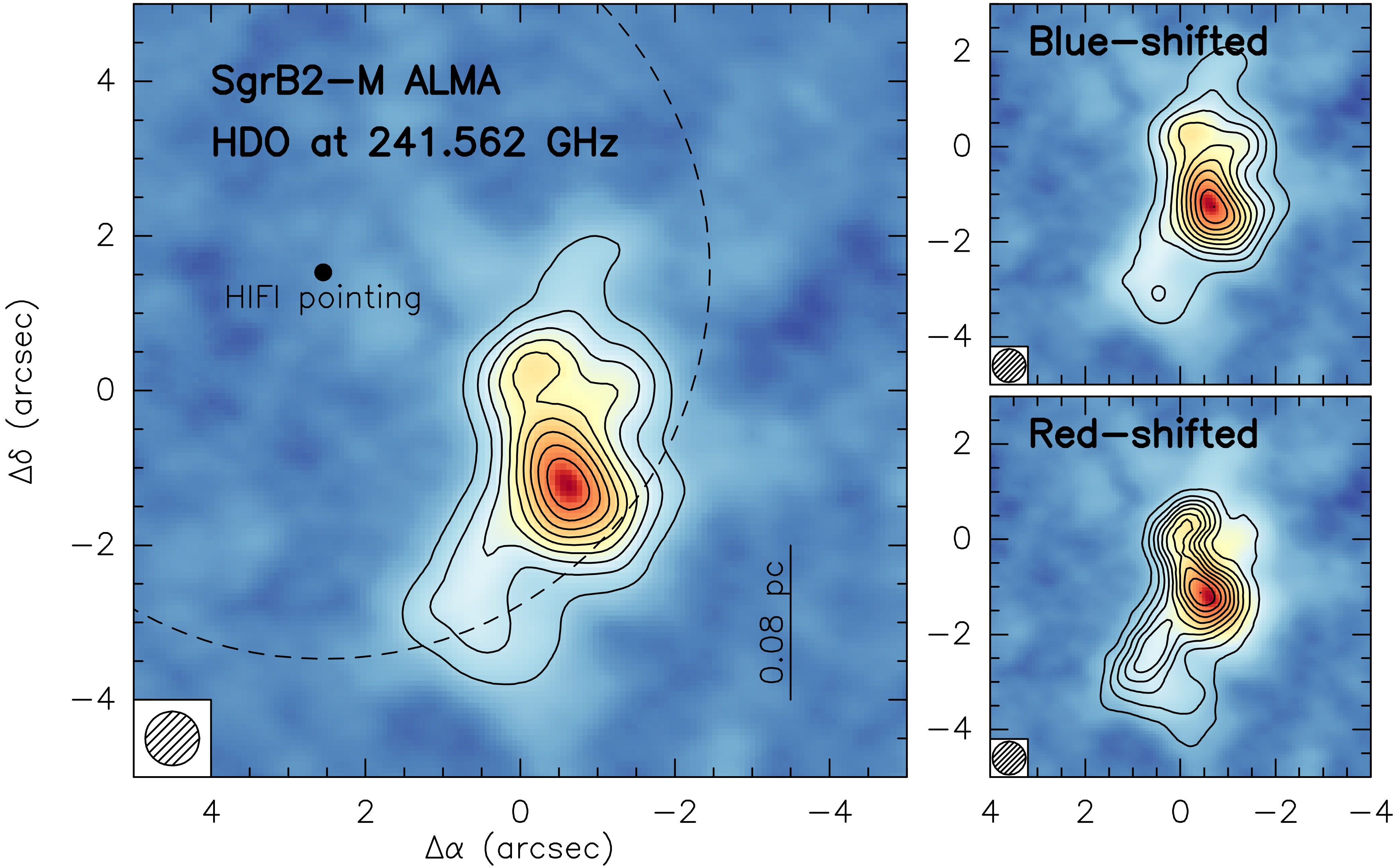
- Improve velocity field

- Parametrize H_2O, HDO abundances vs. T_{gas} —> plug in chemical models

- From eye-balling to chi^2…

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

THANK YOU!



Sanchez-Monge et al., Comito et al., in prep.