Water and $^{13}C^{17}O$ lines, and multiple ring and gap structures of the protoplanetary disk around HD 163296 observed by ALMA

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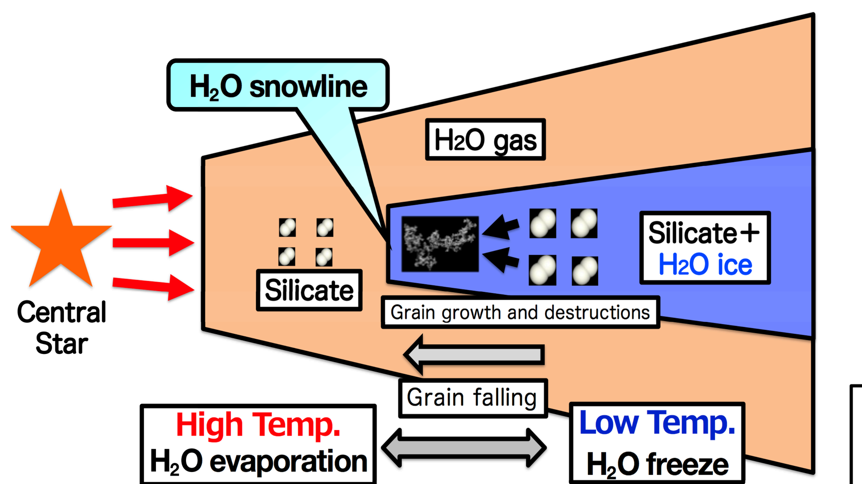
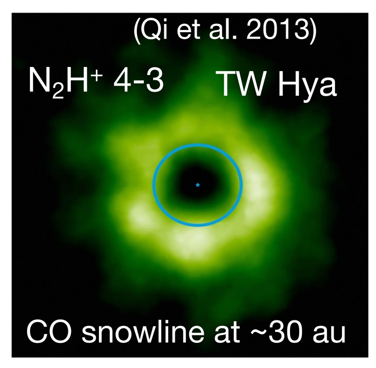
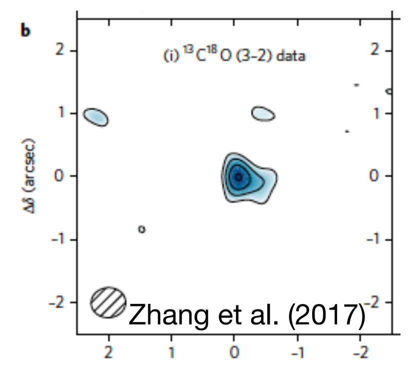
Observationally locating the position of the H_2O snowline (e.g., Hayashi et al. 1981, 1985) in protoplanetary disks is crucial for understanding the dust evolution and planet formation processes, and the origin of water on the Earth. The velocity profiles of emission lines from disks are usually affected by Doppler shift due to Keplerian rotation. Therefore, the line profiles are sensitive to the radial distribution of the line-emitting regions. In our previous works (**Notsu et al. 2016, ApJ, 827, 113; 2017, ApJ, 836, 118; 2018, ApJ, 855, 62**), we calculated the chemical composition of the disks around a T Tauri star and a Herbig Ae star using chemical kinetics and various water line profiles. We found that the water lines with small Einstein A coefficients and relatively high upper state energies are dominated by emission from the hot midplane region inside the H_2O snowline, and therefore through analyzing their line profiles the position of the H_2O snowline can be located. Since the fluxes of these lines from Herbig Ae disks are larger than those from T Tauri disks, the possibility of a successful detection is expected to increase for a Herbig Ae disk. There are several best candidate water lines that trace the position of the H_2O snowline within the coverage of ALMA. Recently, we got the upper limit fluxes of submillimeter ortho-$H_2{}^{16}O$ 321 GHz, para-$H_2{}^{18}O$ 322 GHz, and HDO 335 GHz lines from the disk around the Herbig Ae star HD 163296, using ALMA (**Notsu et al. 2019, ApJ, 875, 96**). These water lines are considered to be the candidate water lines to locate the position of the H_2O snowline, based on our model calculations. We compared the upper limit fluxes with the values calculated by our model calculations with dust emission, and we constrained the line emitting region and the dust opacity from the observations. We also detected multiple ring and gap patterns in the 0.9 mm (ALMA Band 7) dust continuum emission with 15 au spatial resolution, whose positions are consistent with those indicated by other observations (e.g., Isella et al. 2018). Future observations of the submillimeter water lines with longer observation time are required to clarify the position of the H_2O snowline in the disk midplane. In addition, we also detected the rarest stable CO isotopologue, $^{13}C^{17}O$, in a disk for the first time (**Booth et al. 2019, ApJL, 882, L31**). We compared our observation with the existing detections of other CO isotoplogues in the HD163296 disk. We found that this line is optically thin within the CO snowline and will be thus a robust tracer of the bulk disk CO gas mass. We showed that this disk will be 2-6 times more massive than previously estimates.

1. H_2O snowline and CO snowline



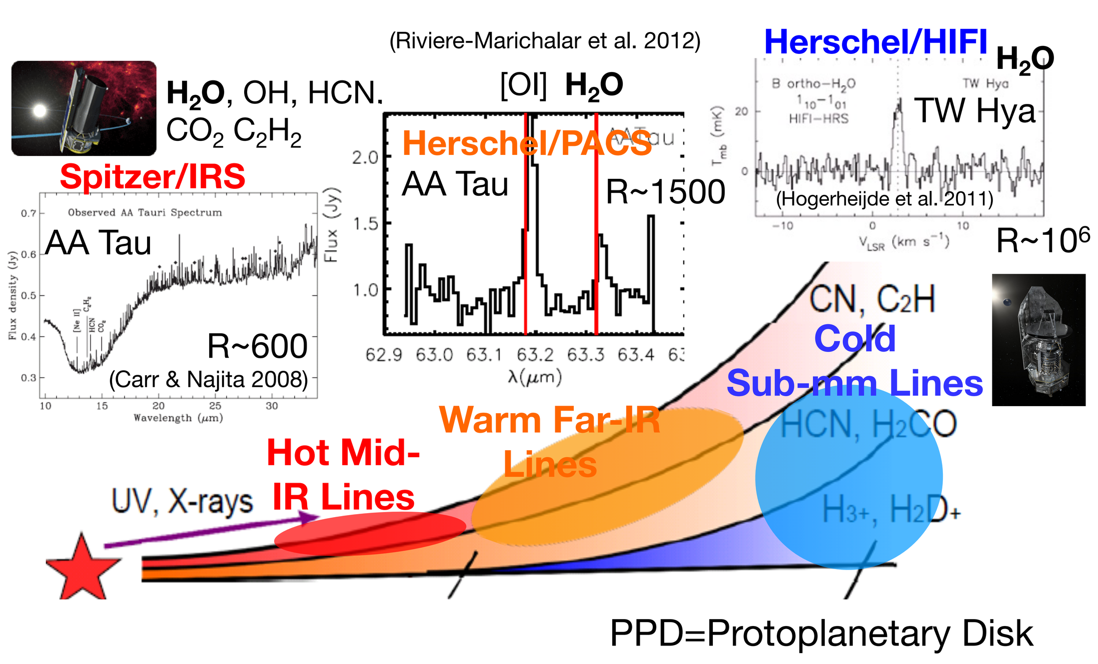


CO snowline at r=20.5 au ($^{13}C^{18}O$ 3-2) TW Hya



Optically thin isotope lines are important for measuring disk gas masses and the snowline positions more precisely.

2. Previous obs. of water lines from PPDs



Previous strong water line observations from PPDs mainly trace the disk surface and the region outside the H_2O snowline, thus they are not good direct tracer of the H_2O snowline.

↓

We want to trace the hot water vapor emission from the inner disk midplane and locate the position of the H_2O snowline.

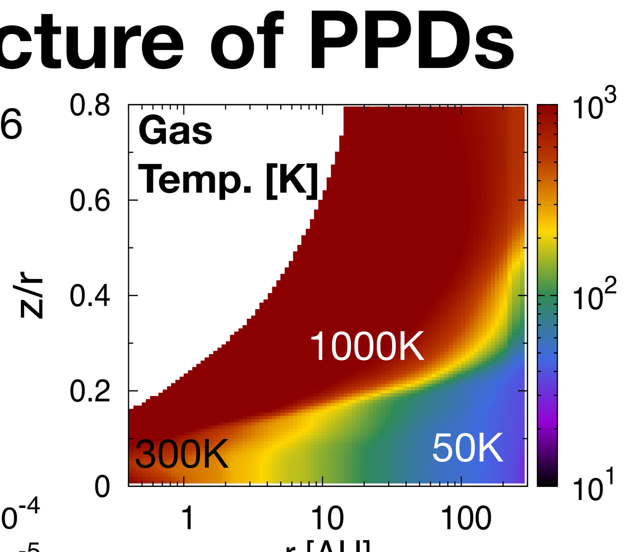
We calculate the chemical structures using chemical kinetics and the profiles of water emission lines of PPDs, and we find the candidate water lines to locate the H_2O snowline through high-dispersion spectroscopic observations.

3. Physical and Chemical structure of PPDs

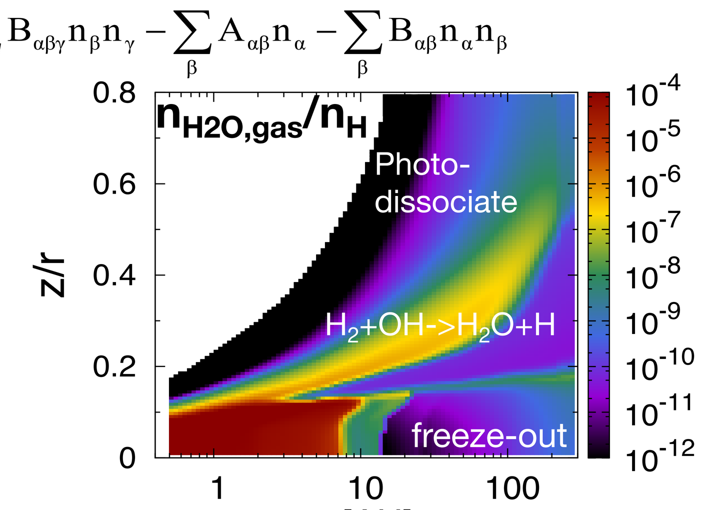
Gas-phase reactions: Woodall et al. (2007), UMIST Rate06
375 molecules, 4346 reactions

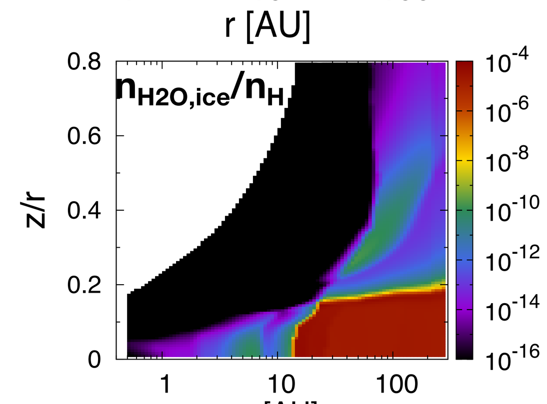
Interactions between gas and dust:
-Freezing out of gas molecules on dust grains.
-Thermal and non-thermal (UV and cosmic ray) desorption from dust grains.

$$\frac{dn_\alpha}{dt}=\sum_\beta A_{\alpha\beta}n_\beta+\sum_{\beta,\gamma}B_{\alpha\beta\gamma}n_\beta n_\gamma-\sum_\beta A_{\alpha\beta}n_\alpha-\sum_\beta B_{\alpha\beta}n_\alpha n_\beta$$



Herbig Ae disk
$t_{total}\sim 10^6$ yr





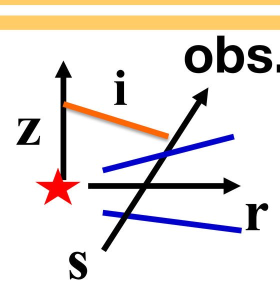
e.g., Woodall et al. (2007)
Walsh et al. (2010, 2012, 2015)
Notsu et al. (2016, 2017, 2018)

4. Calculations of water line profiles

Rybicki & Lightman (1986), Notsu et al. (2016, 2017, 2018)

E_{up} n_u
A_{ul}
E_{low} n_l

A_{ul}: Einstein A coefficient [s^{-1}]
E_{up}: Energy in upper state [K]



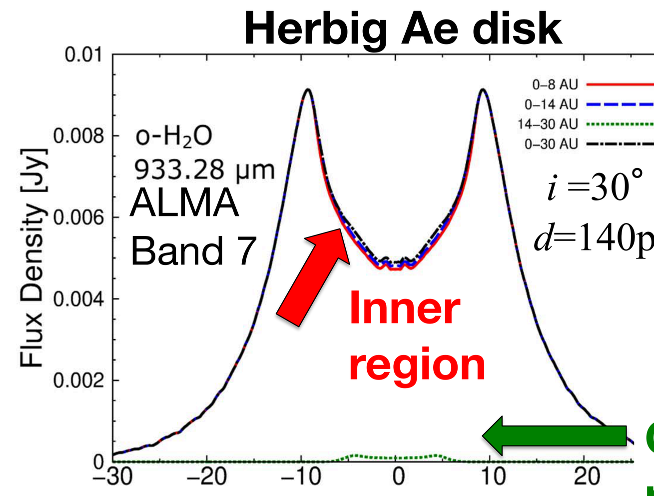
n_u & n_l : LTE distribution (snowline tracer: OK)
$\Phi(\nu)$: emission profile (**Kepler** & thermal velocity)
τ_{ul} : optical depth (H_2O gas and dust absorption)
Line data : LAMDA ($H_2{}^{16}O$) & HITRAN ($H_2{}^{18}O$)

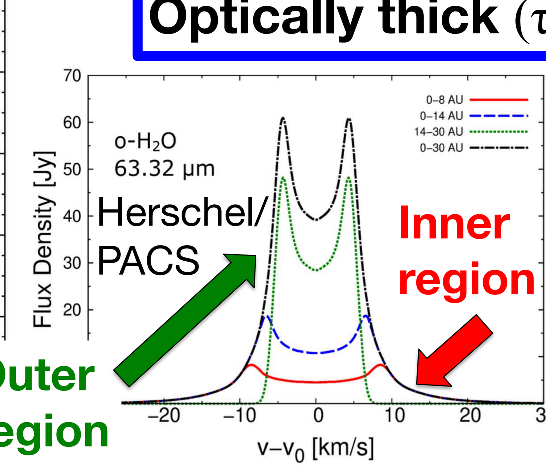
$$\nu_K=\frac{\nu_{ul}}{c}\sqrt{\frac{GM_*}{r}}\sin\phi\sin i,$$

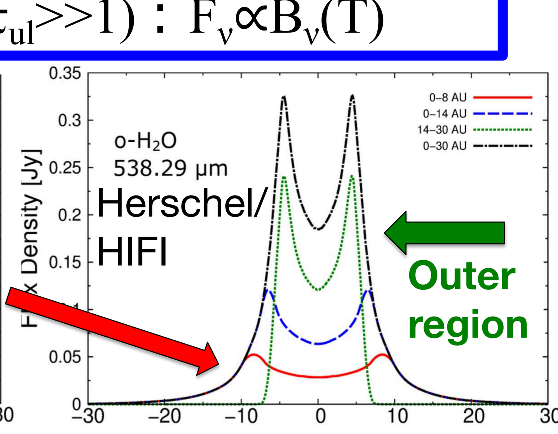
$$F_{ul}(r,\nu)=\int_{-s_\infty}^{s_\infty}n_u A_{ul}\frac{h\nu_{ul}}{4\pi}\varphi(\nu)\exp(-\tau_{ul})ds$$

Optically thin (τ_{ul}<<1) : $F_\nu \propto n_u(E_{up})A_{ul}$
Optically thick (τ_{ul}>>1) : $F_\nu \propto B_\nu(T)$

Herbig Ae disk







ortho-$H_2{}^{16}O$ 933.28μm (321.23GHz)	ortho-$H_2{}^{16}O$ 63.32μm(4.73THz)	ortho-$H_2{}^{16}O$ 538.29μm (556.94GHz)
A_{ul}= 6.165×10^{-6} s^{-1} E_{up}=1861.2K	A_{ul}= 1.772 s^{-1} E_{up}=1070.6K	A_{ul}= 3.497×10^{-3} s^{-1} E_{up}=61K

If A_{ul} is small and E_{up} is relatively large, the contribution from the optically thick hot midplane region within the H_2O snowline becomes large compared with those from the optically thin surface layer and the photodesorption region of the outer disk .
→We can locate the position of the H_2O snowline by analyzing the profiles of water emission lines that have small A_{ul} (10^{-6}~10^{-3} s^{-1}) and relatively large E_{up}.

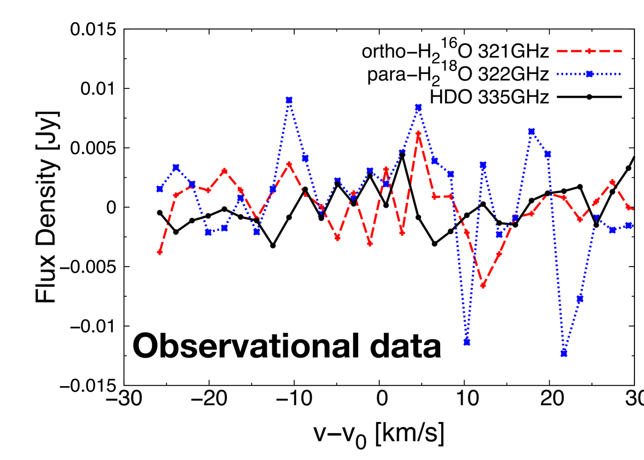
5. ALMA Band 7 water line observation

Notsu et al. (2019)

Our target
Herbig Ae star HD163296
d=101.5pc (GAIA DR2)
i=42° M_{star}~2.4M_{sun}

Detailed setup of our observation
P.I. Shota Notsu ID:2015.1.01259.S (ALMA Cycle 3)
Observational date: Sep. 16th, 2016
On source time : 43.35 min. (~**20%** of our requested time)

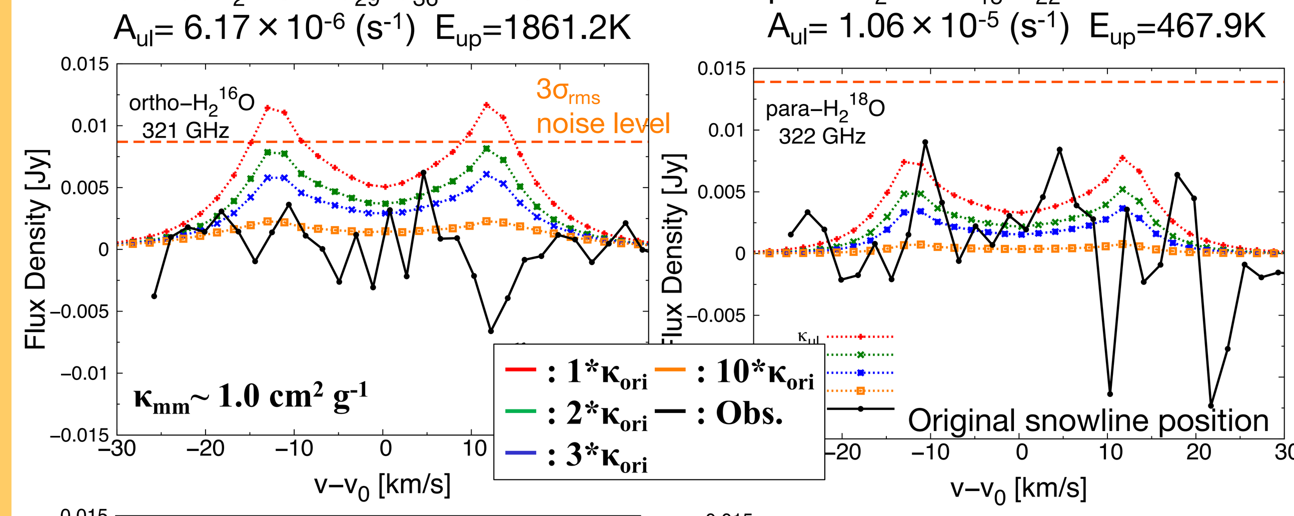
Band 7 water lines (Δv~1.9km/s)
-ortho-$H_2{}^{16}O$ 321GHz, para-$H_2{}^{18}O$ 322GHz, HDO 335GHz lines
-We avoided 325GHz strong telluric water absorption.
Band 7 (0.9 mm) continuum (7.5GHz bandwidth in total)
-We added ACA data (2016.1.00884.S) to avoid the missing flux.
Band 7 $^{13}C^{17}O$ J=3-2 line 321.85GHz



Non detection because of the shortage of observation time.

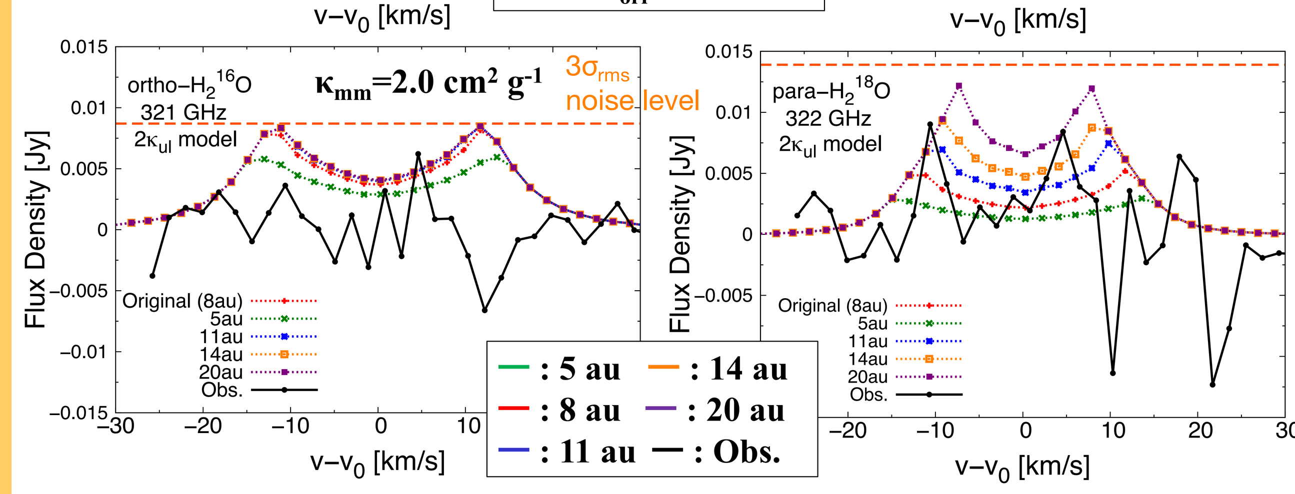
ortho-$H_2{}^{16}O$ 10_{29}-9_{36} 321GHz
A_{ul}= 6.17×10^{-6} (s^{-1}) E_{up}=1861.2K

para-$H_2{}^{18}O$ 5_{15}-4_{22} 322GHz
A_{ul}= 1.06×10^{-5} (s^{-1}) E_{up}=467.9K



Observed vs Calculated water line profiles with different dust opacity

The mm dust opacity κ_{mm} will be larger than 2.0 cm^2 g^{-1}, if the position of the water snowline is outer than 8 au.



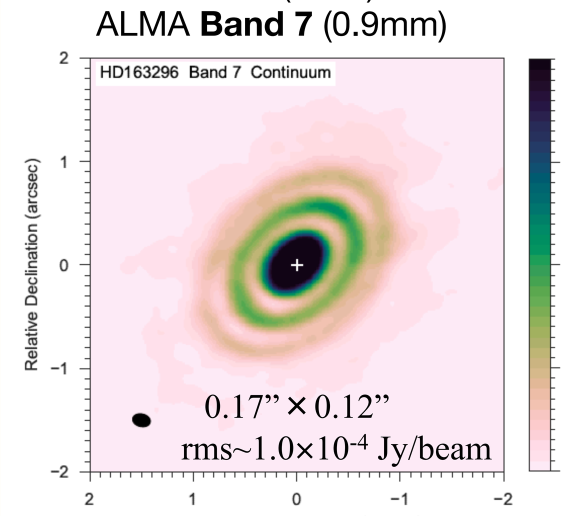
Observed vs Calculated water line profiles with different position of the water snowline

The position of the water snowline will be inside 20 au, if κ_{mm} is 2.0 cm^2 g^{-1} (=estimated from our dust continuum observation).

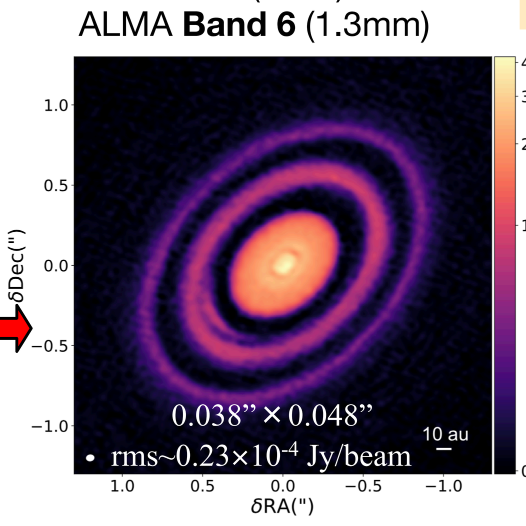
6. ALMA Band 7 dust continuum emission

Notsu et al. (2019)

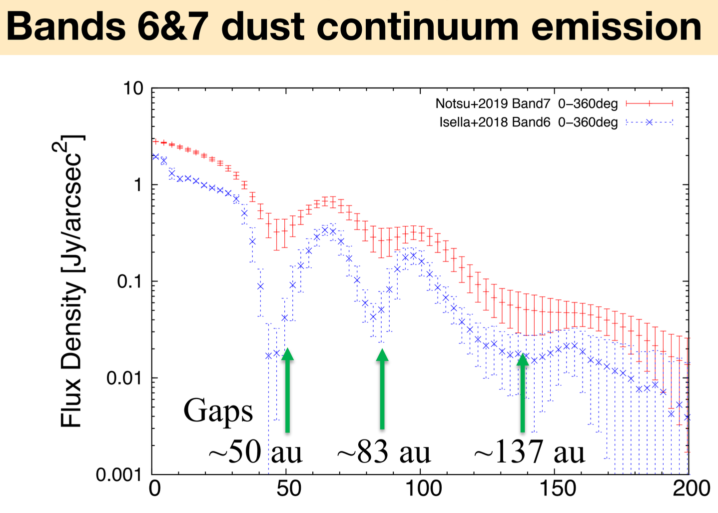
Notsu et al. (2019)
ALMA **Band 7** (0.9mm)



Isella et al. (2018)
ALMA **Band 6** (1.3mm)



Similar multiple ring and gap patterns in Bands 6&7 dust continuum emission



Gap formation mechanism in PPDs
- Planet-disk interactions (e.g., Kanagawa et al. 2015&2016&2018, Pinte et al. 2016)
- Efficient grain-growth around the snowlines (e.g., Banzatti et al. 2015, Okuzumi et al. 2016)
- Gas instability (e.g., Takahashi & Inutsuka 2014&2016, Tominaga et al. 2018)
- Dust accumulation around the deadzone (e.g., Flock et al. 2015) etc.

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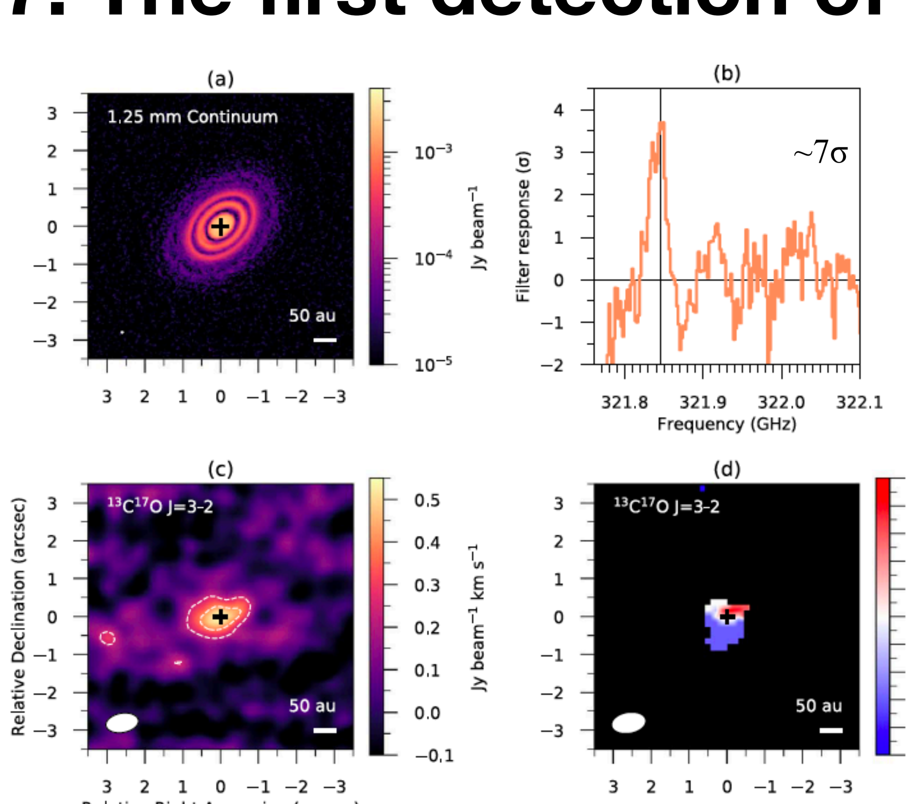
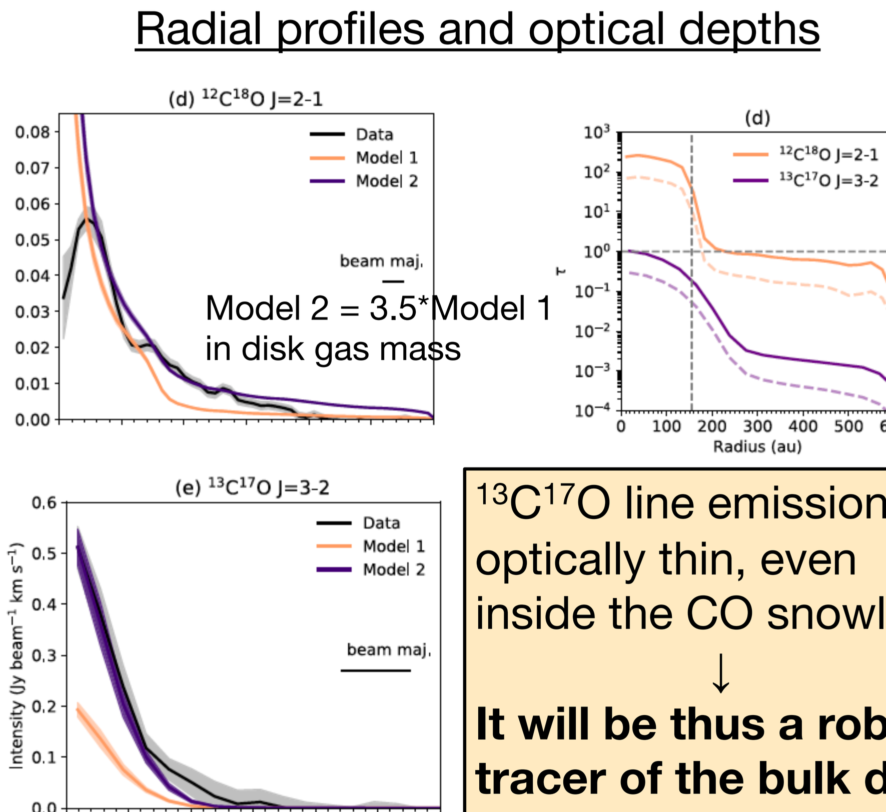
7. The first detection of $^{13}C^{17}O$ line in a disk

Booth et al. (2019)

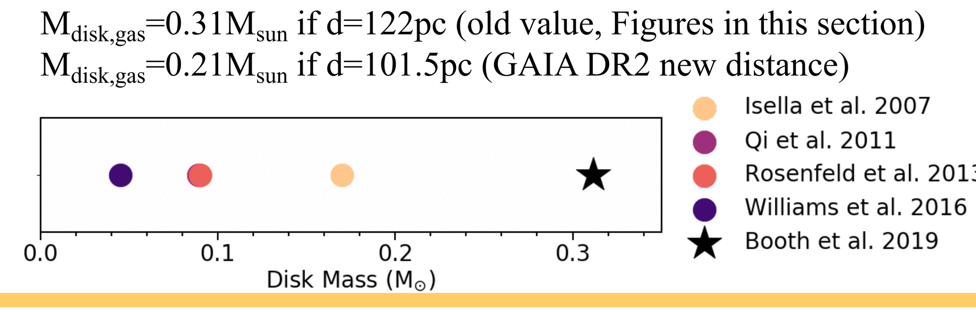


Radial profiles and optical depths



$^{13}C^{17}O$ line emission is optically thin, even inside the CO snowline.
↓
It will be thus a robust tracer of the bulk disk CO gas mass.

$M_{disk,gas}$=0.31M_{sun} if d=122pc (old value, Figures in this section)
$M_{disk,gas}$=0.21M_{sun} if d=101.5pc (GAIA DR2 new distance)



Disk gas mass is around 2-6 times larger than previous estimates in this disk.