Chemical Complexity in Pre-stellar Cores

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COMs: Carbon-based molecules with >6 atoms

(Herbst & van Dishoeck 2009)

- Star forming regions: Hot Cores and Hot Corinos
  (Hollis+2000,2004; Beltran+2009; Belloche+2016; Jorgensen+2012; Lykke+2017)

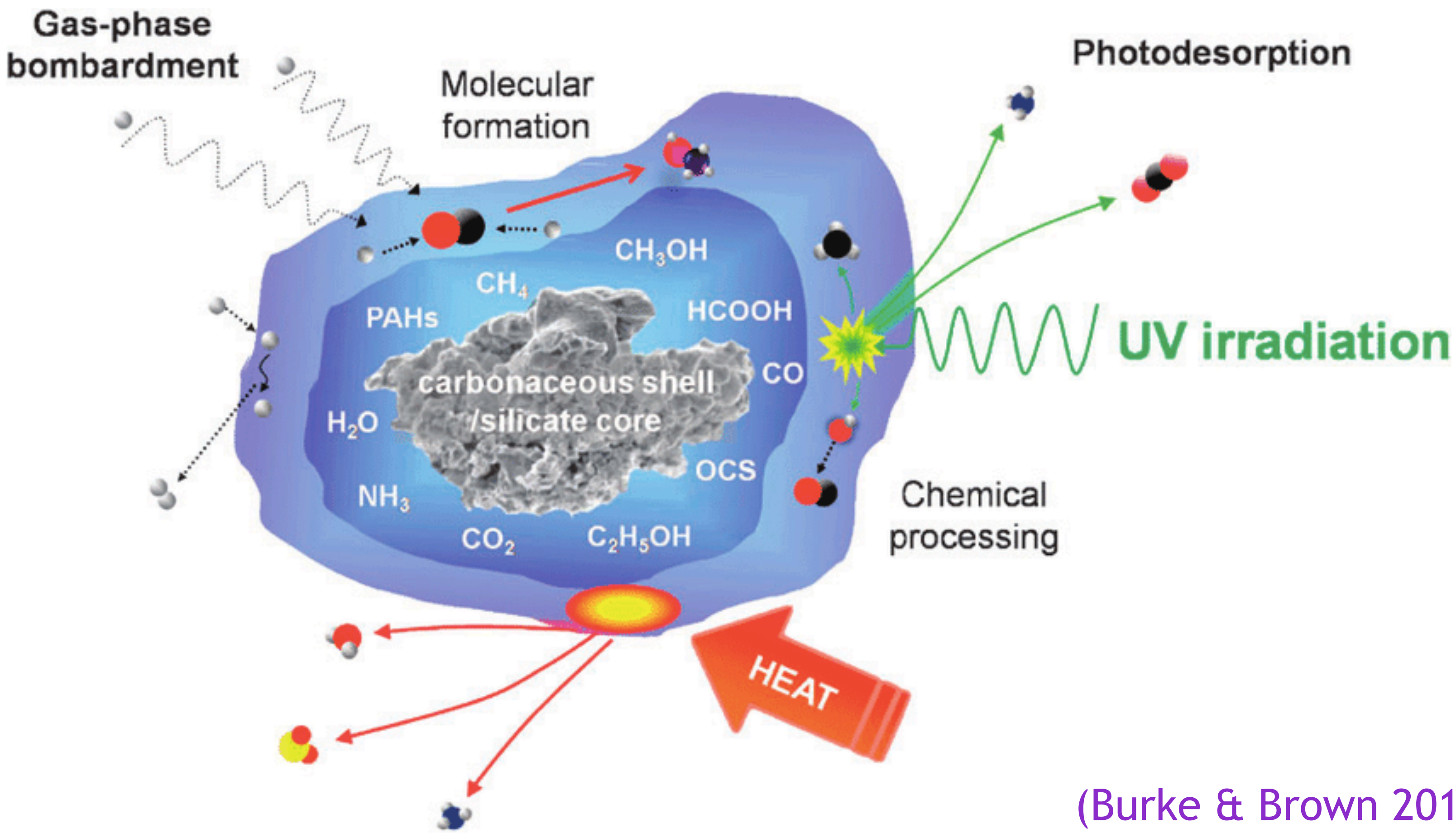
- Galactic Center Giant Molecular Clouds
  (Martin-Pintado+2001;Requena-Torres+2006,2008; Zeng et al. submitted)

- Molecular Outflows
  (Arce+2008; Codella+2015,2017)

COM formation in hot sources

COMs formed mainly via:

1. Hydrogenation (H addition; Charnley et al. 1997, 2001)
2. Radical-radical surface reactions (efficient at T>30 K; Garrod et al. 2008)



(Burke & Brown 2010)

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- Molecular Outflows
  (Arce+2008; Codella+2015,2017)
- Photon-Dominated Regions
  (Guzman+2013; Cuadrado et al. 2017)
- Starless Cores and Pre-stellar Cores
  (Marcelino+2007; Oberg+2010; Bacmann+2012; Cernicharo+2012; Vastel+2014)

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- Starless Cores and Pre-stellar Cores **(T<=10 K)**
  (Marcelino+2007; Oberg+2010; Bacmann+2012; Cernicharo+2012; Vastel+2014)

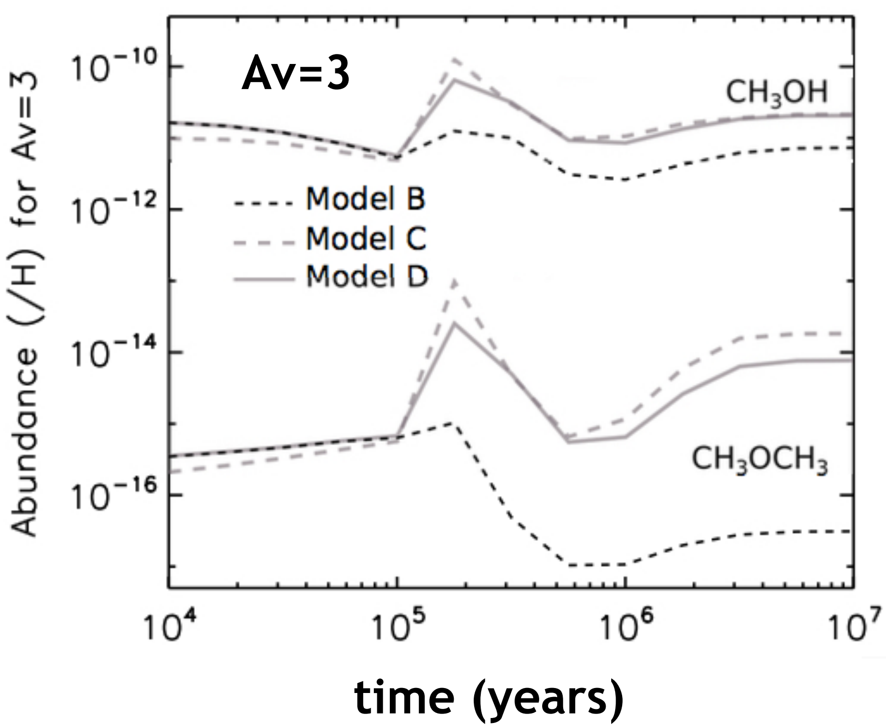
Radical-radical surface formation inefficient at T<30 K

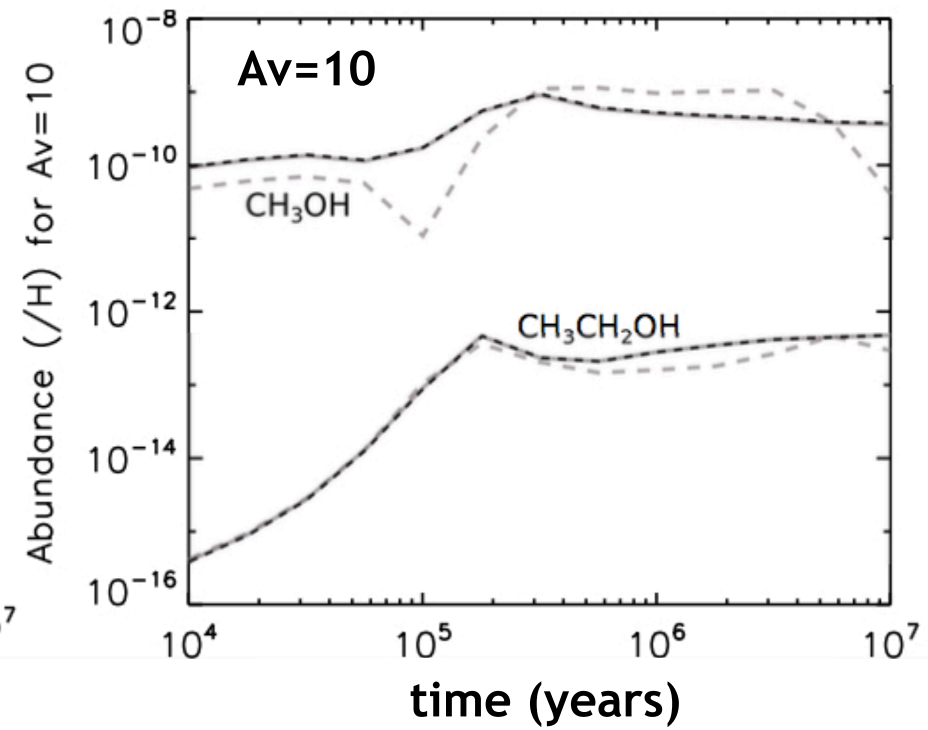
COM formation in cold sources (T=10 K)

Radical-radical surface formation inefficient at T<30 K

New mechanisms proposed:

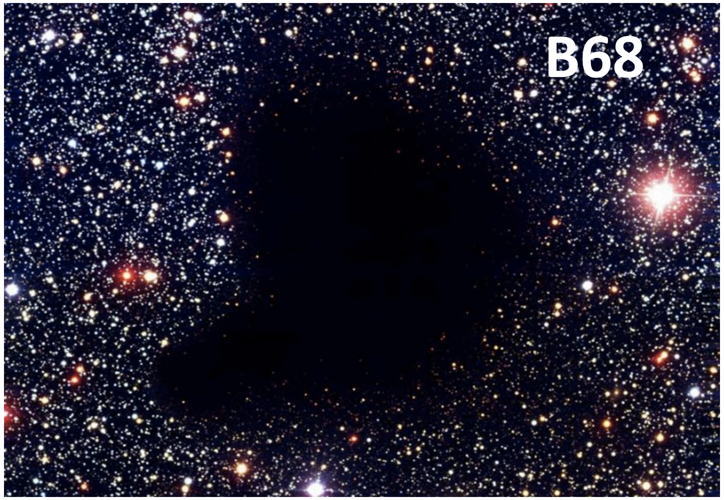
1. Gas phase formation (Vasyunin & Herbst 2013; Balucani+2015; Vasyunin+2017)
2. Non-canonical explosions (Rawlings et al. 2013)
3. Cosmic-ray induced radical diffusion (Reboussin et al. 2014)
4. Impulsive spot heating on grains by CRs (Ivlev et al. 2015)
5. Formation after H atom addition/abstraction on grains (Chuang et al. 2016)

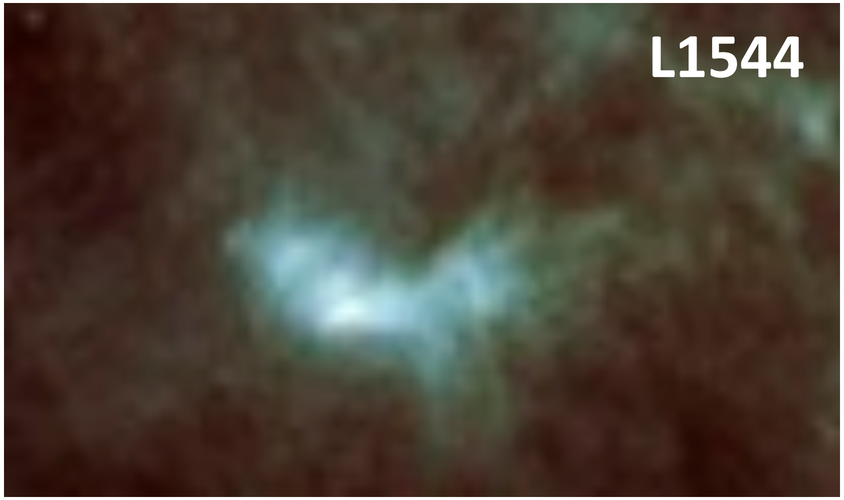




Starless Cores and Pre-stellar Cores

- Low temperatures of the gas: $T_{kin} < 10$ K (e.g. Crapsi et al. 2007)
- Gas densities $n(H_2) > 10^4$ cm^{-3} (e.g. Bacmann+00; Crapsi+05)

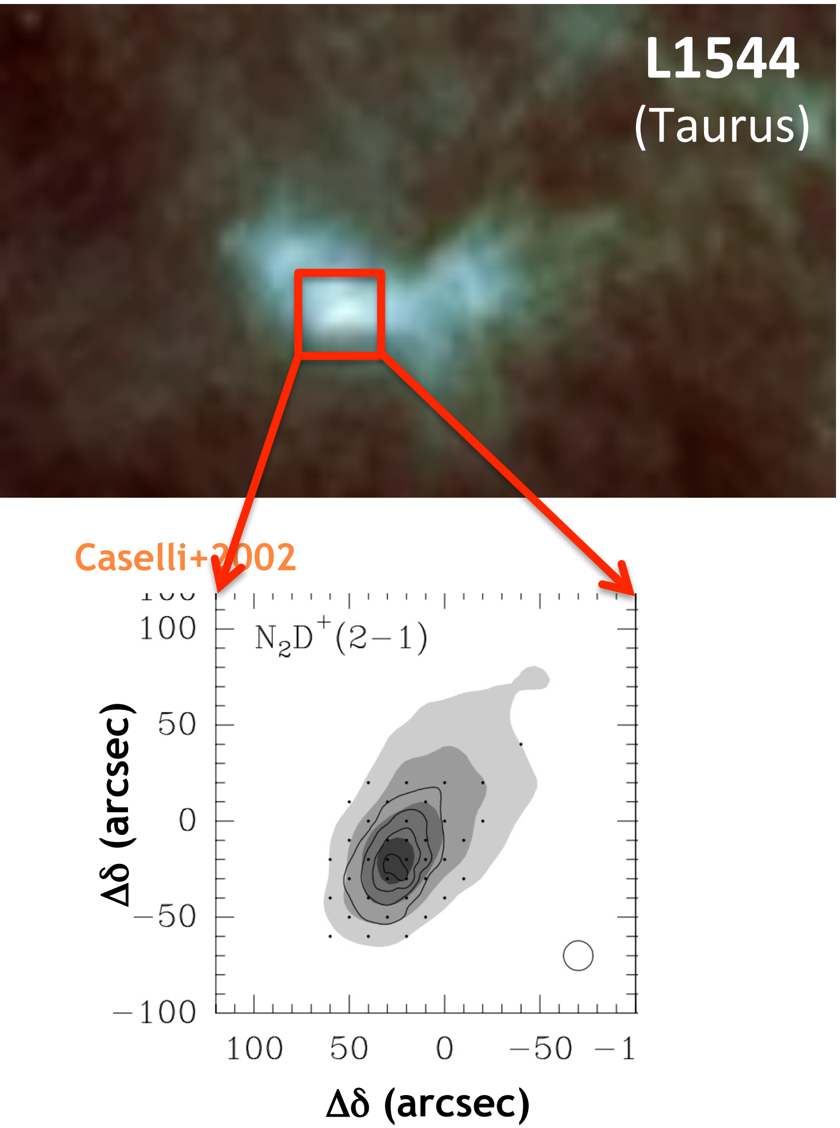




Pre-stellar Cores (Ward-Thompson+99; Crapsi+05)

1) High H_2 column densities ($>10^{22}$ cm^{-2})
2) Compact density profiles at the center of the cores
3) High values of D/H fractions (from e.g. N_2D^+/N2H+)
4) High values of CO depletion
5) Broadening of N_2H^+ lines with infall asymmetry

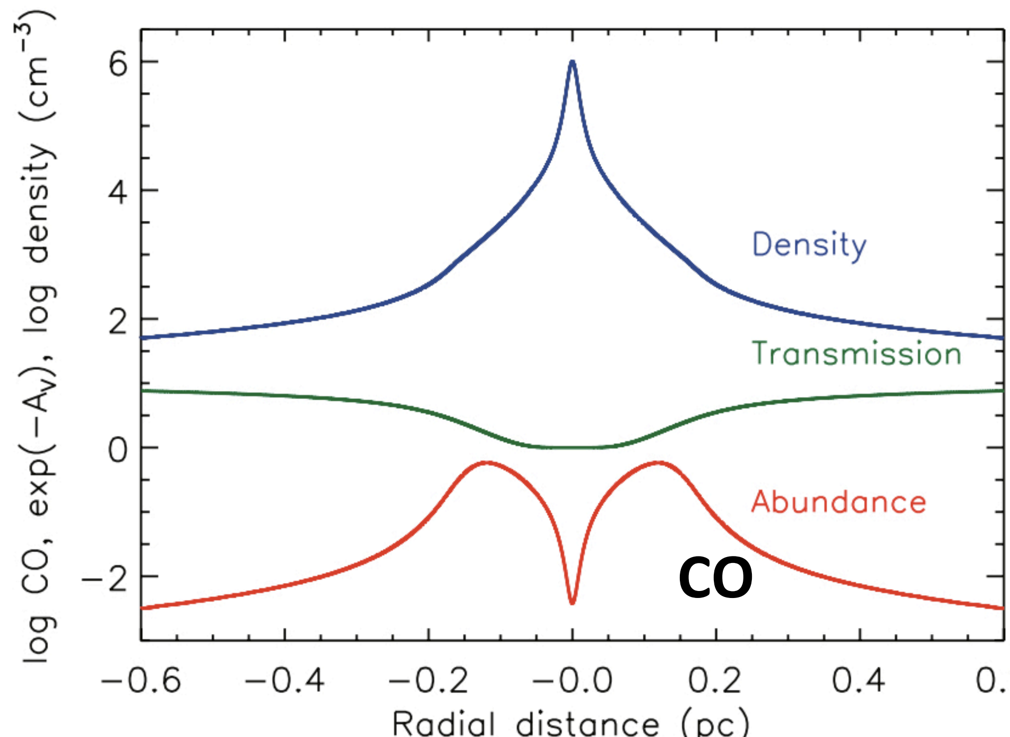
Pre-stellar cores: Precursors of Solar-type systems



Pre-stellar cores:

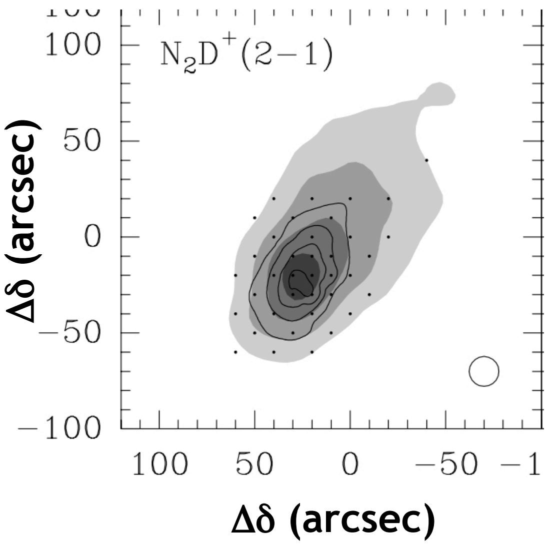
Cold and dense cores on the verge of gravitational collapse (no star inside yet)

Keto & Caselli 2008



L1544 as a testbed

Caselli+2002



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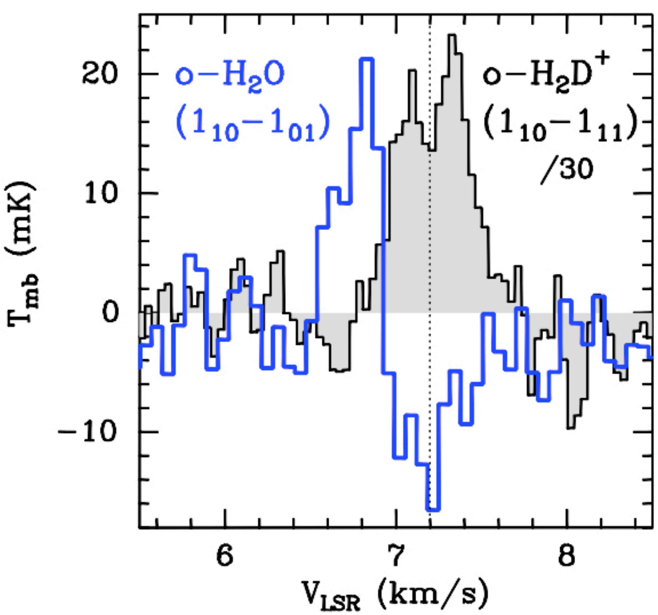

Water vapour in L1544

(Caselli+2012)

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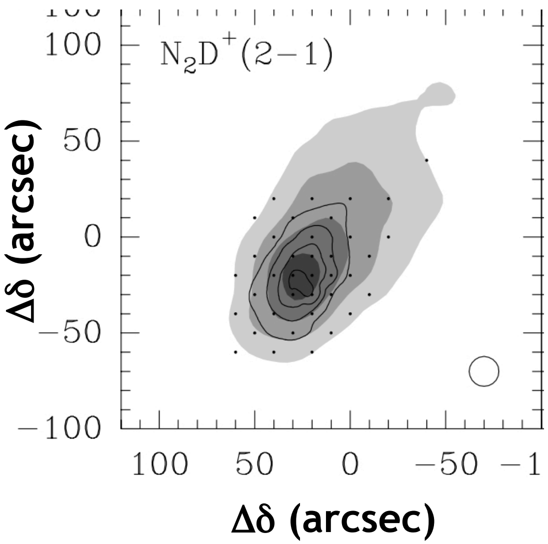

Water vapour in L1544

(Caselli+2012)

COMs(+precursors) released with H_2O

(C_3O, H_2CCO, HCOOH, CH_3CHO)

(Vastel+2014)

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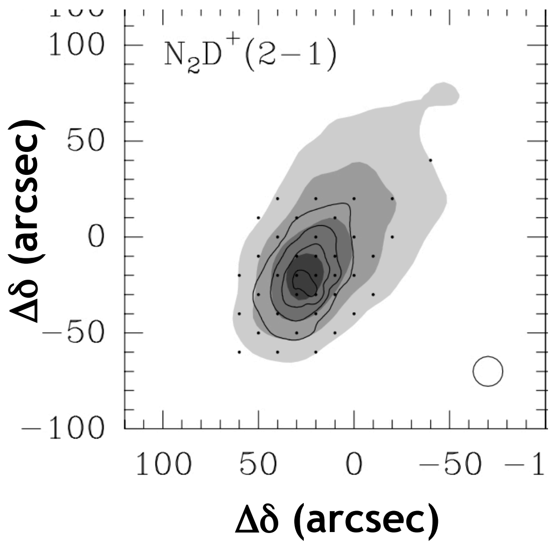

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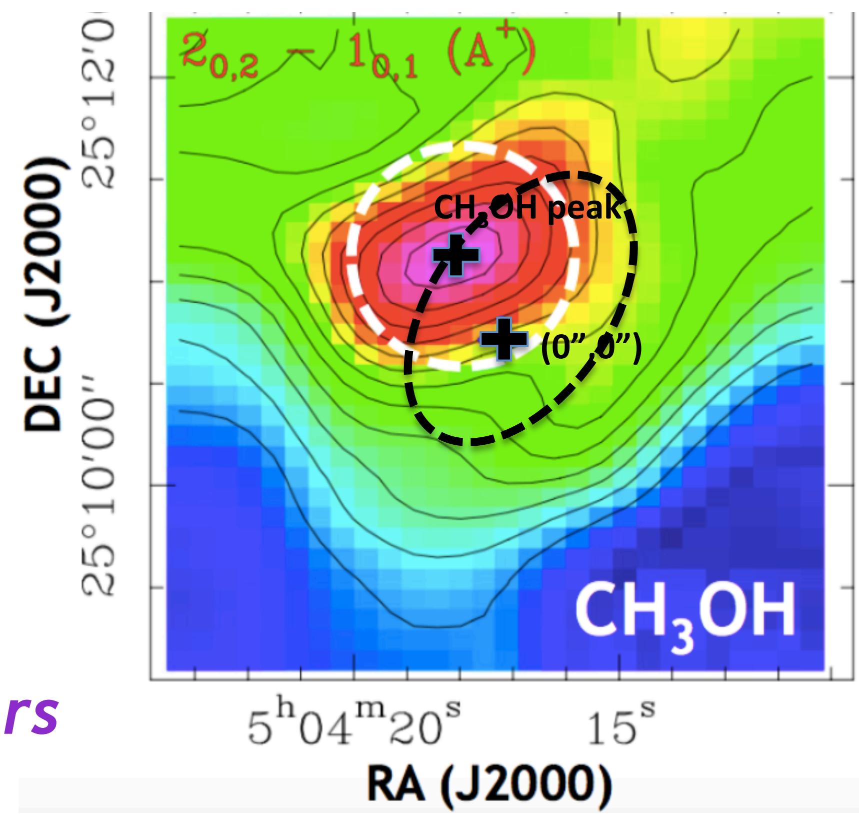
CH_3OH-ring at r~4000 AU

intermediate density shell

interesting chemistry appears



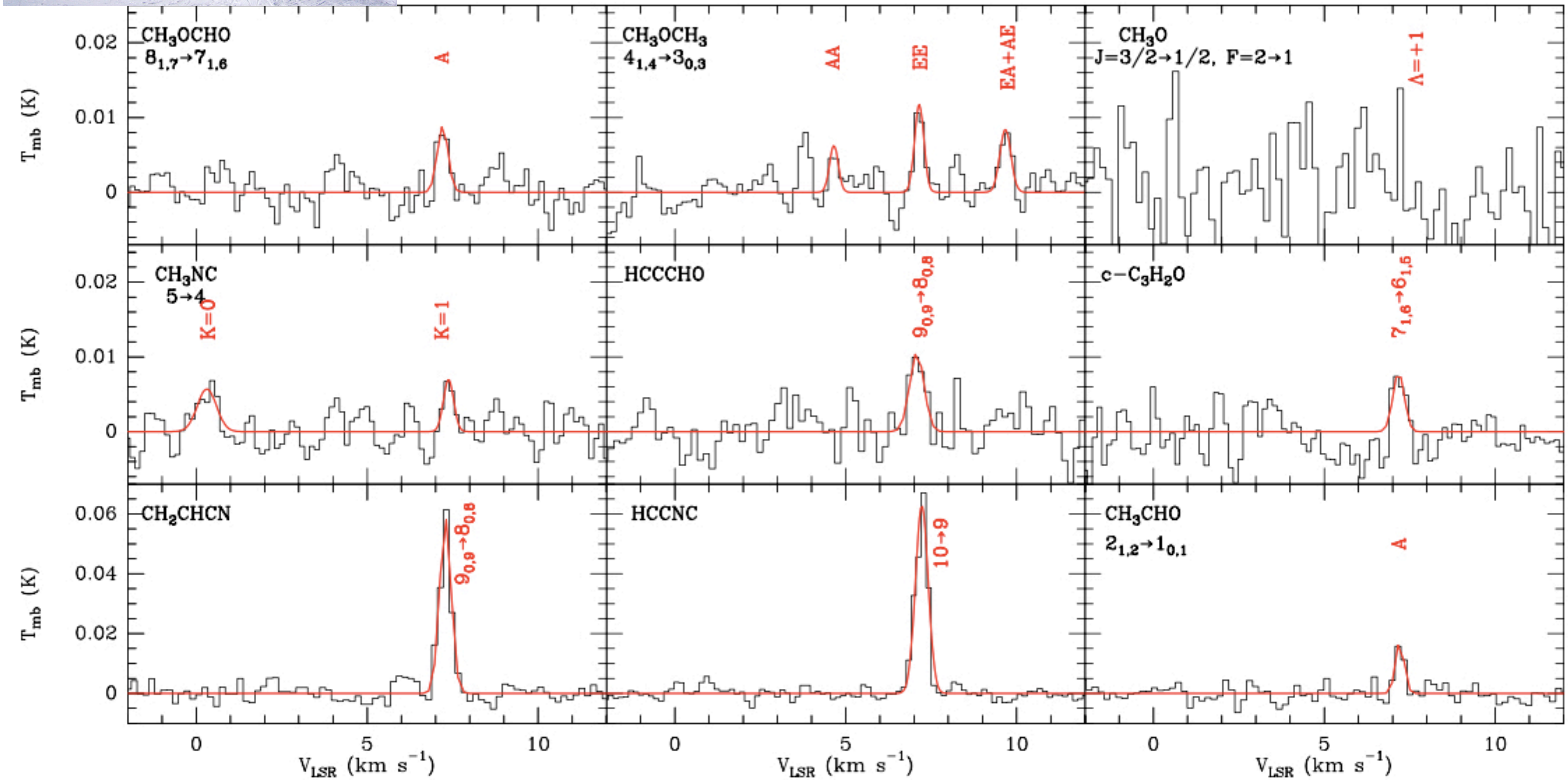
Bizzocchi et al. 2014

Detection of large COMs in L1544

CH_3OCHO, CH_3OCH_3, CH_3CHO, c-C_3H_2O, CH_2CHCN, CH_3NC, HCCNC, HCCCHO

(0,0)

Jimenez-Serra et al. (2016)



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CH_3OH peak

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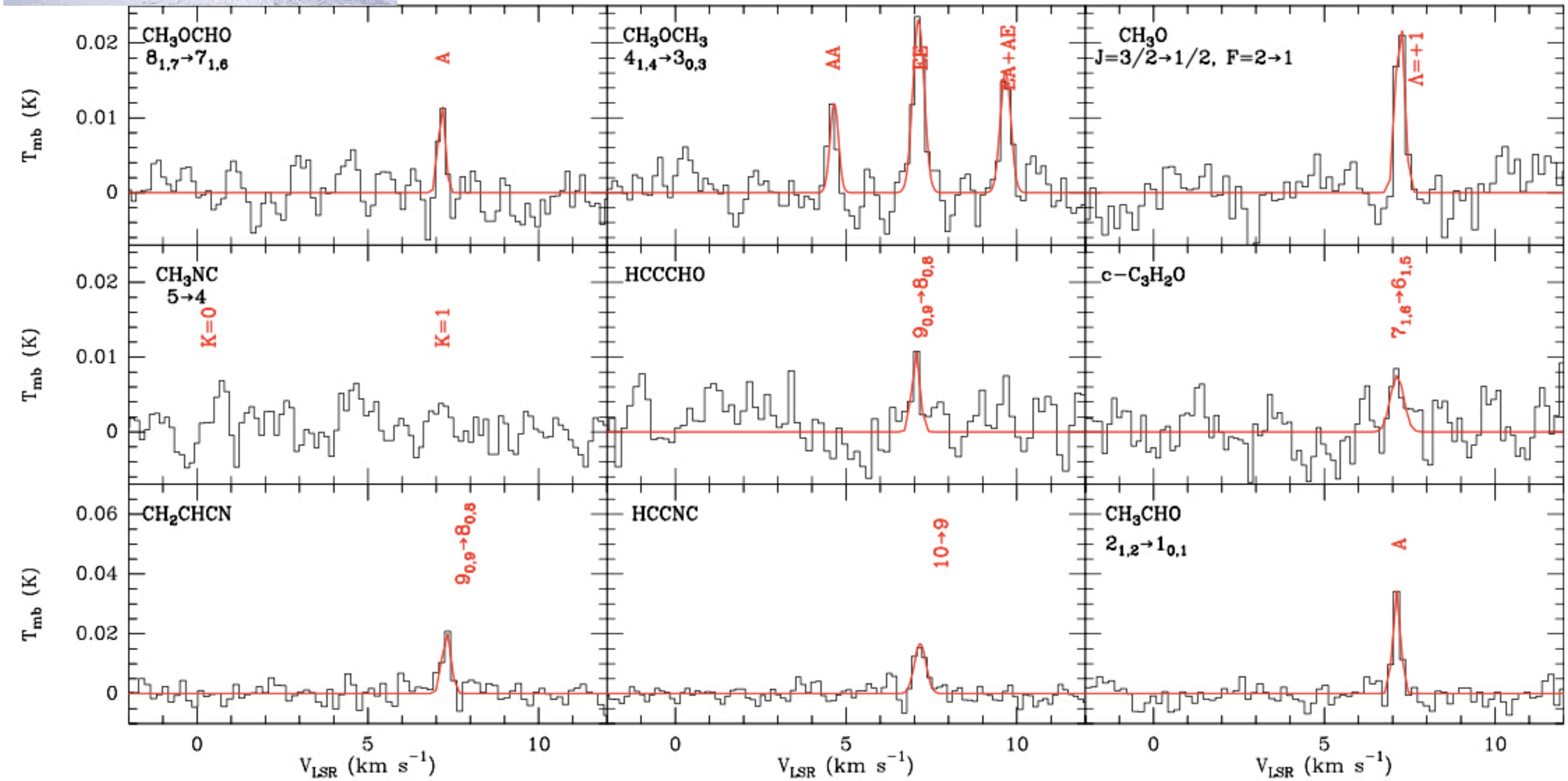
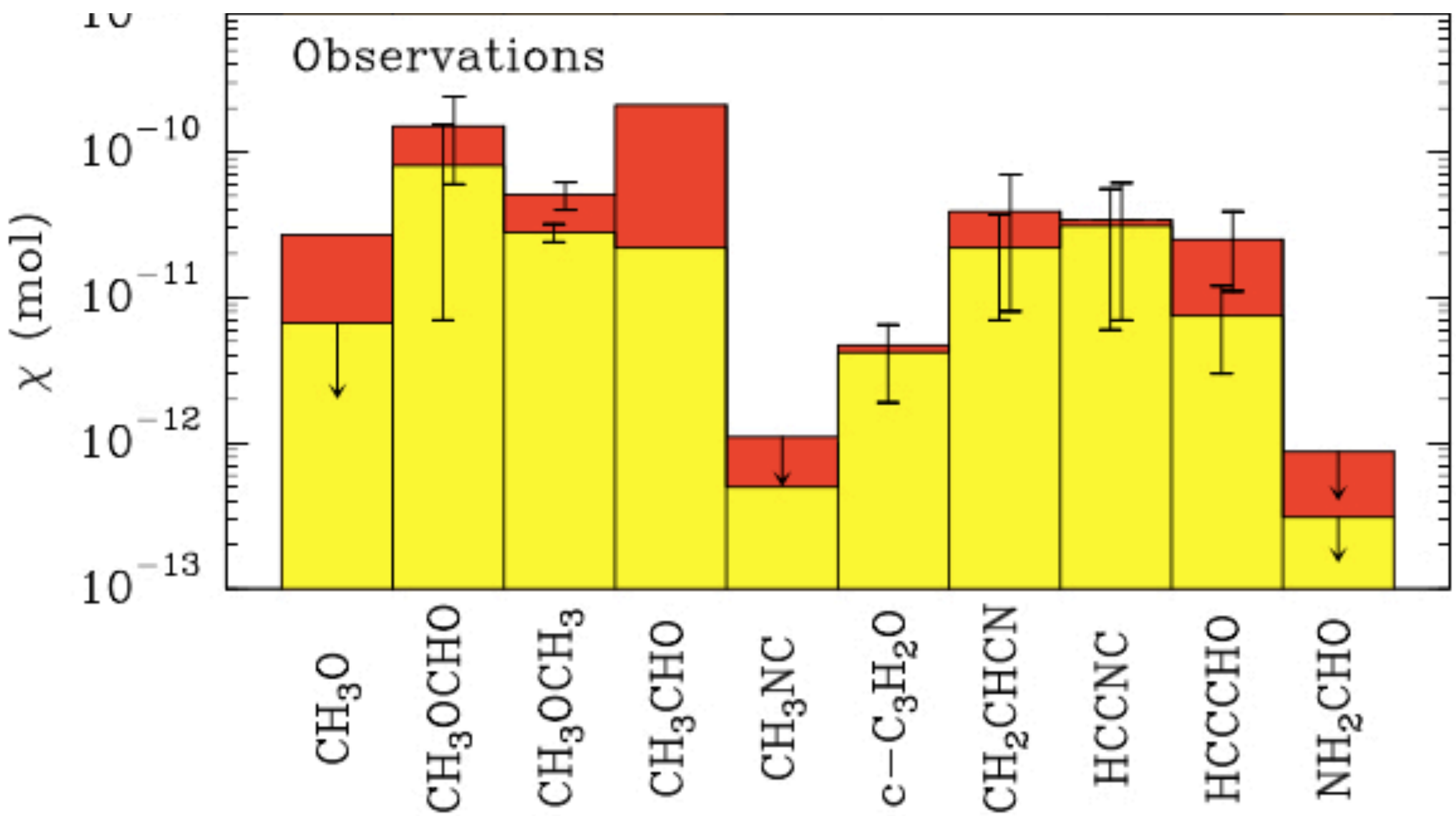


COM abundance profile in L1544



Jimenez-Serra et al. (2016)

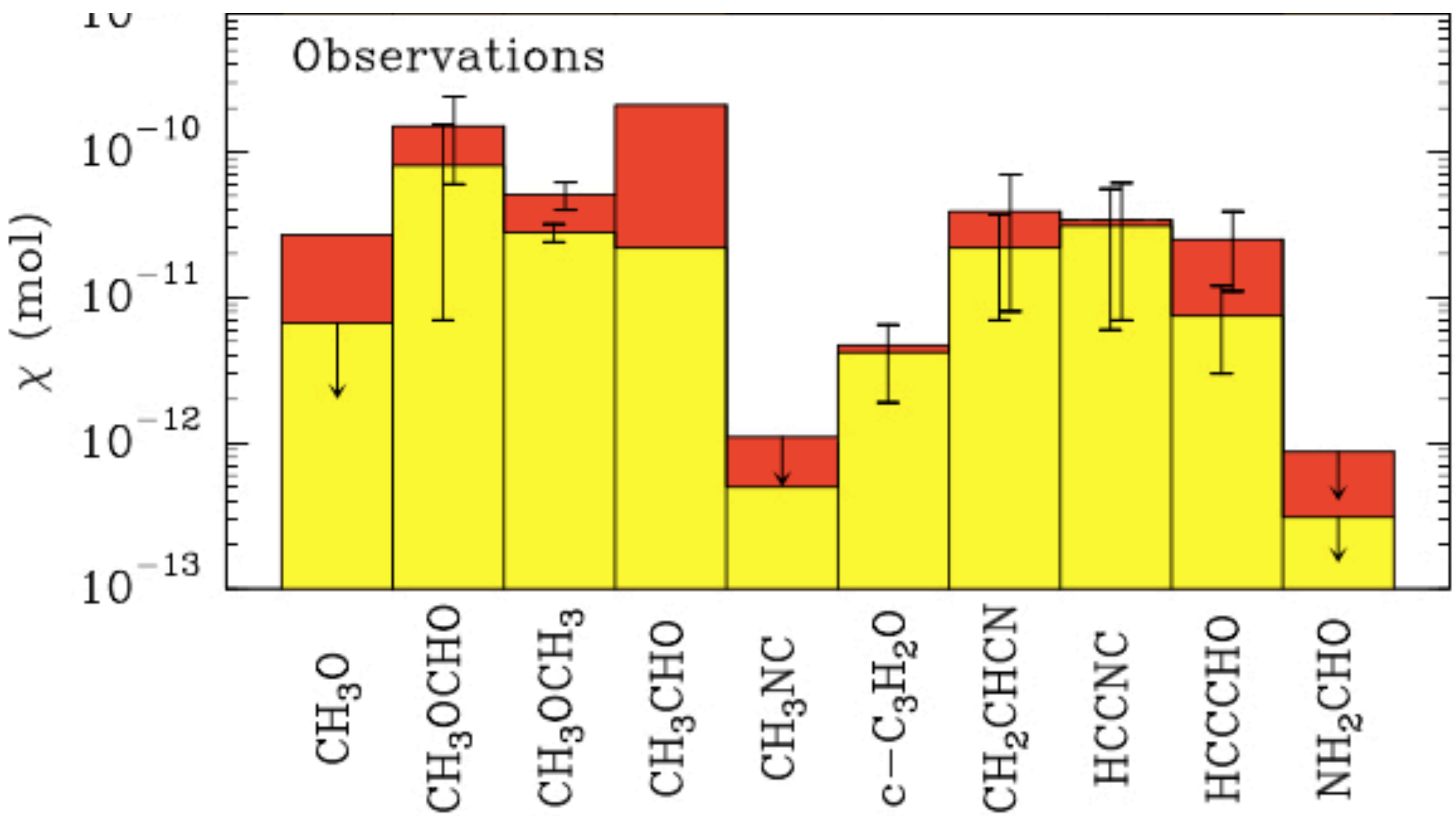
CH_3O, CH_3CHO:

>6-10 x more abundant at r~4000 AU

CH_3OCH_3, CH_3OCHO and N-bearing COMs:

~2-3 x more abundant at r~4000 AU

COM abundance profile in L1544



Jimenez-Serra et al. (2016)

Non-detections:

X [Glycine] < 10^{-10}

X [NH_2CHO] < 10^{-12} (Lopez-Sepulcre+2014)

X [CH_3NCO] < 10^{-12} (Cernicharo+2016)

O-bearing COM chemical modelling in L1544

Gas-grain chemical code of Vasyunin & Herbst (2013)

Considers the complex structure of the ices (active surface + inert bulk)

Includes chemical reactive desorption (RD; Minissale+2016)

Neutral-neutral reactions (Shannon+13,14; Balucani+15)

$OH + CH_3OH \rightarrow CH_3O + H_2O$

$OH + CH_3OCH_3 \rightarrow CH_3OCH_2 + H_2O$

$F + CH_3OCH_3 \rightarrow CH_3OCH_2 + HF$

$Cl + CH_3OCH_3 \rightarrow CH_3OCH_2 + HCl$

$CH_3OCH_2 + O \rightarrow HCOOCH_3 + H$

$CH_3O + CH_3 \rightarrow CH_3OCH_3 + h\nu$

$CH + CH_3OH \rightarrow CH_3CHO + H$

$CH + CH_3OH \rightarrow CH_3 + H_2CO$

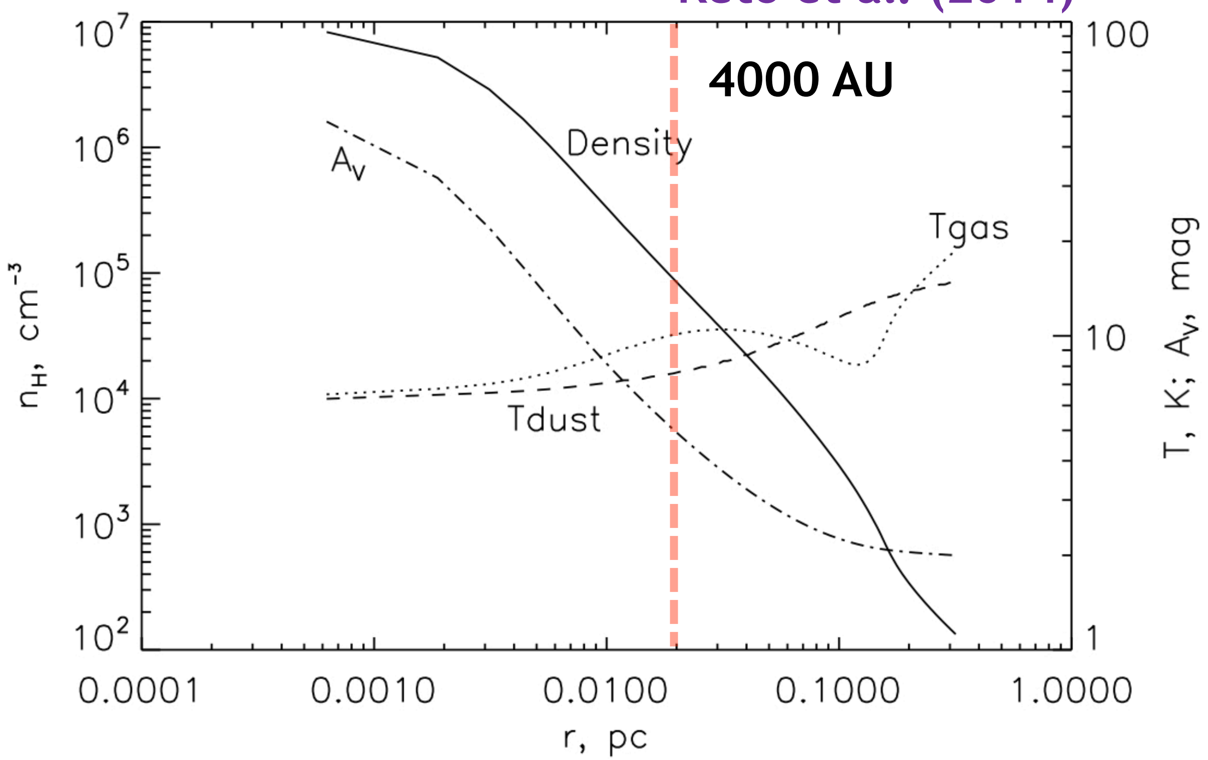
$C + CH_3CHO \rightarrow C_2H_4 + CO$

$C + H_2CO \rightarrow CO + CH_2$

$CH_3 + HCO \rightarrow CH_3CHO + h\nu$

$NH_2 + H_2CO \rightarrow NH_2CHO + H$

Keto et al. (2014)



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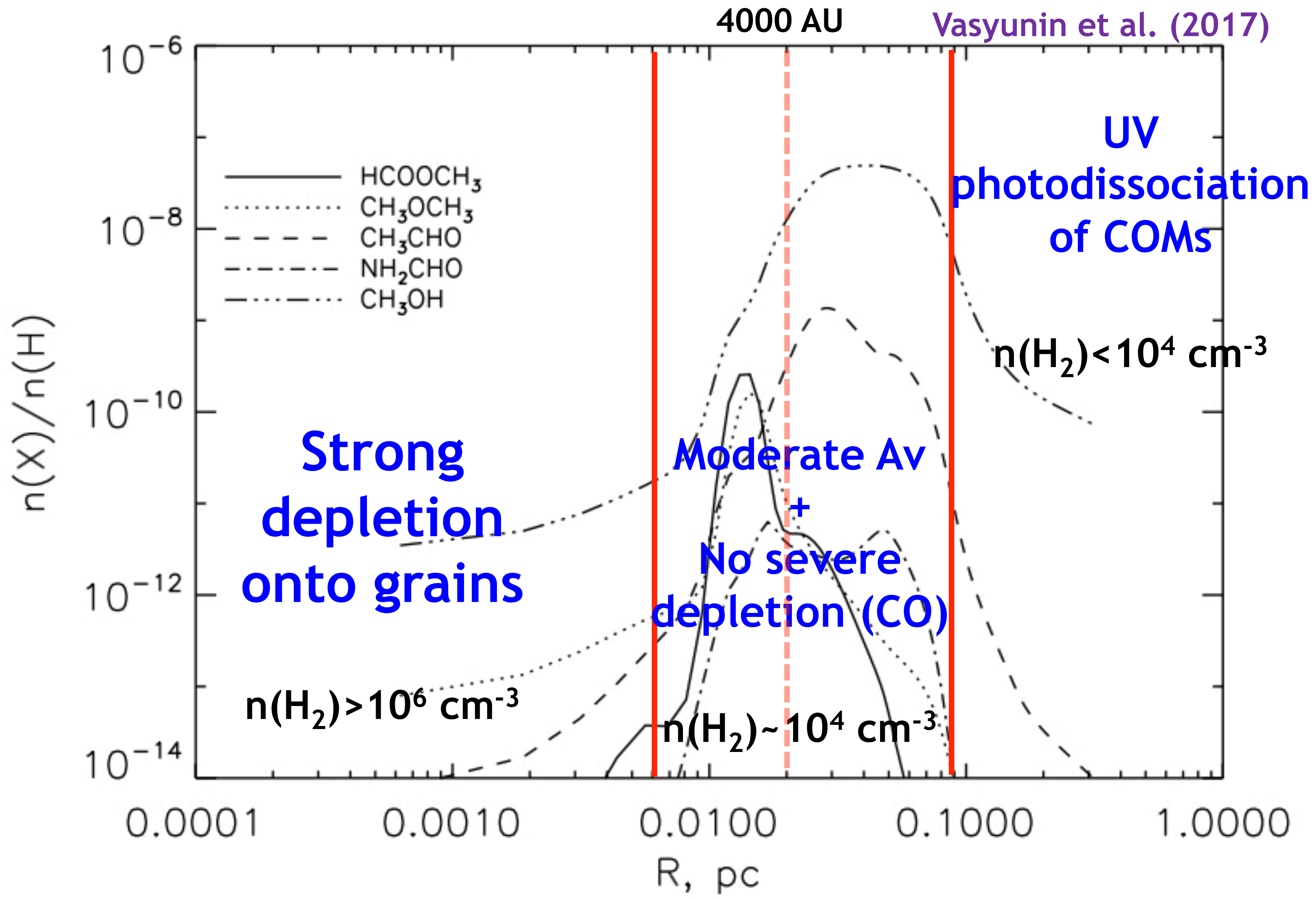
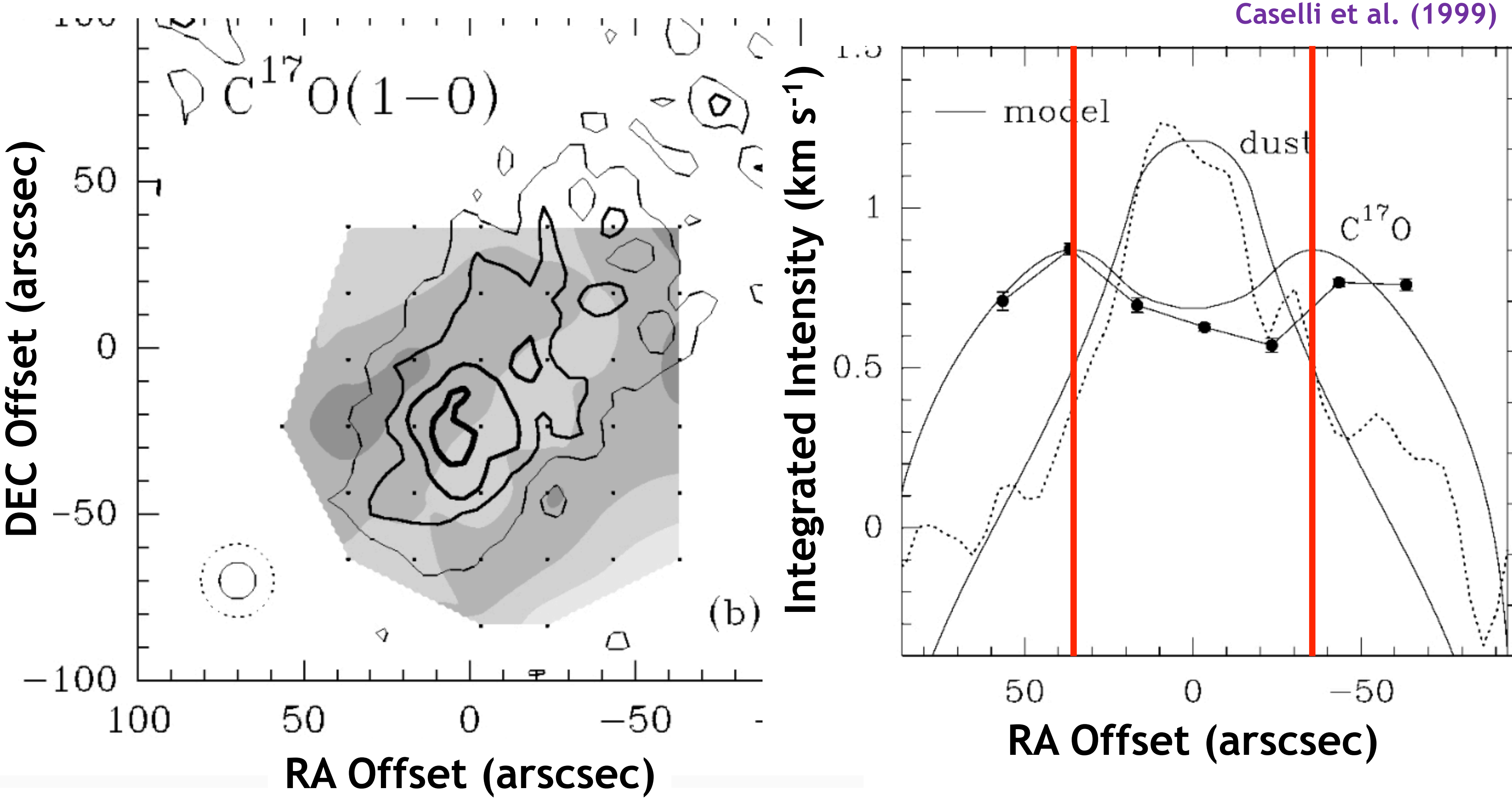


Where does CO depletion occur?

Caselli et al. (1999)



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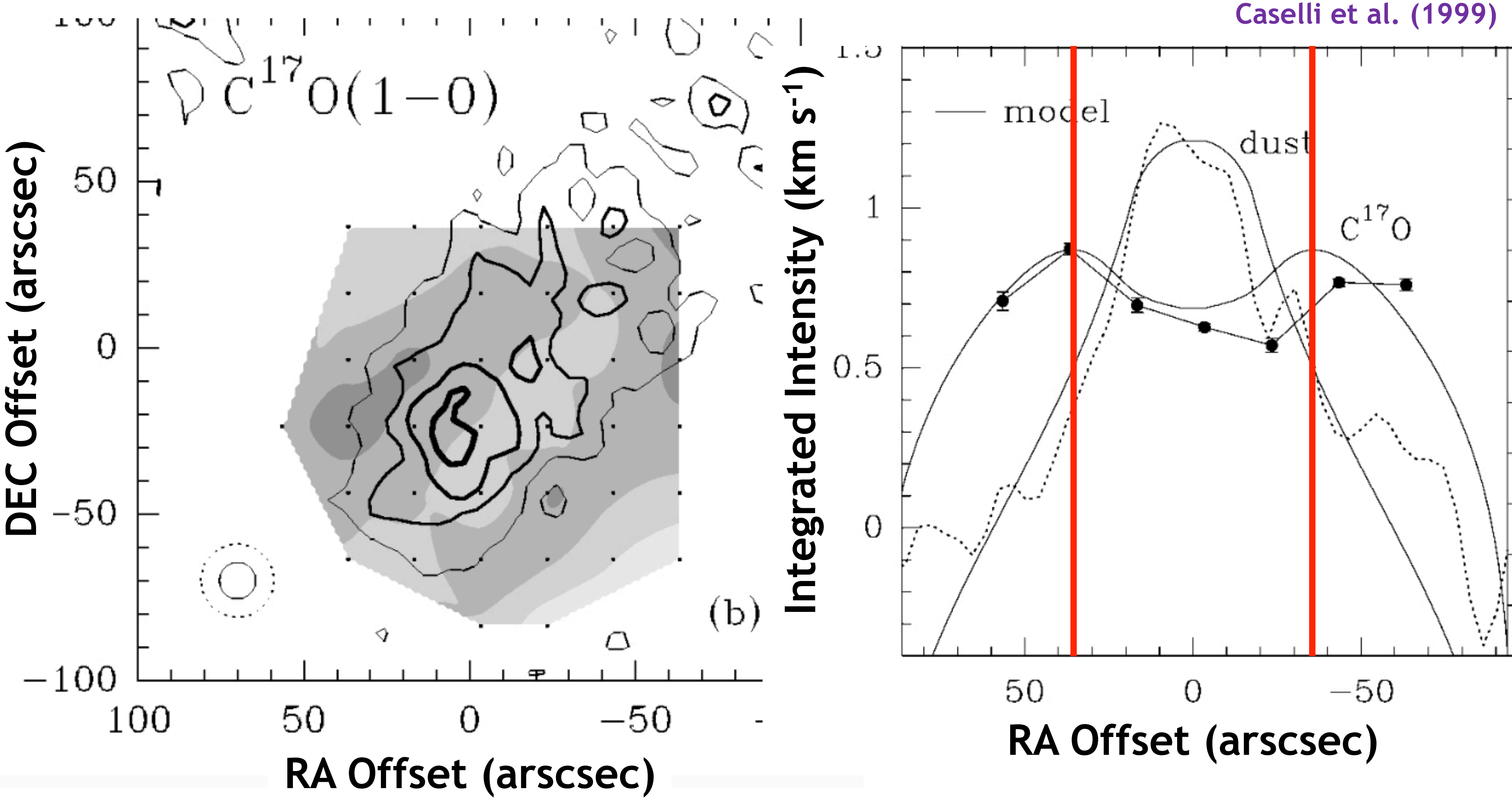

Catastrophic depletion of CO ➔

CO snow-line in pre-stellar cores

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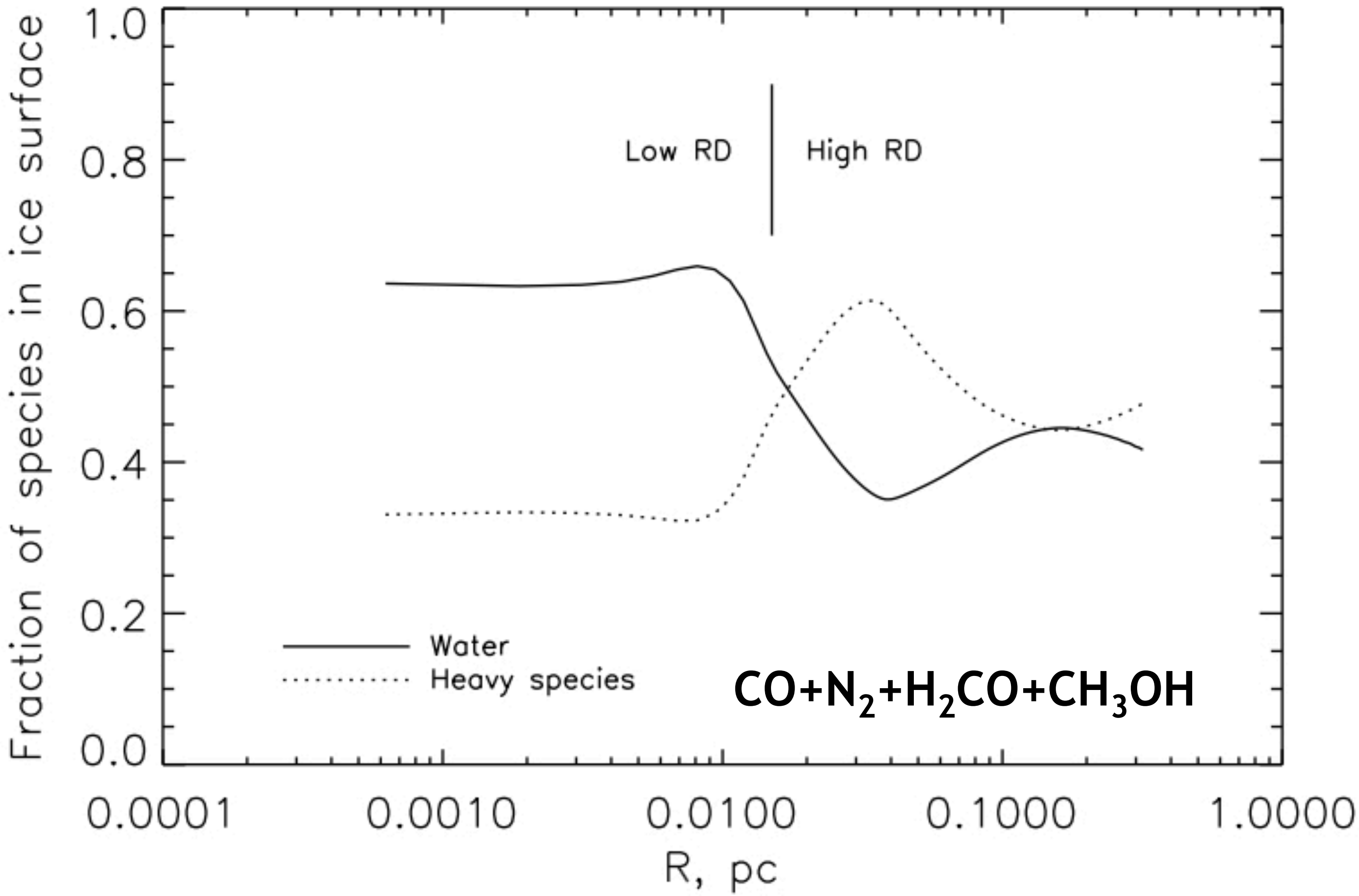
Vasyunin et al. (2017)



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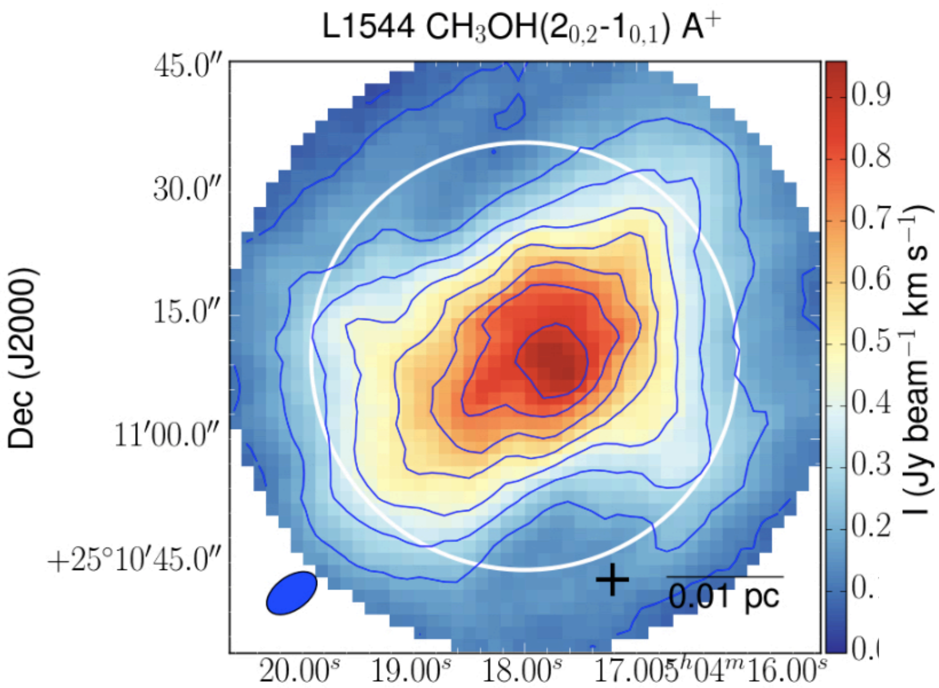
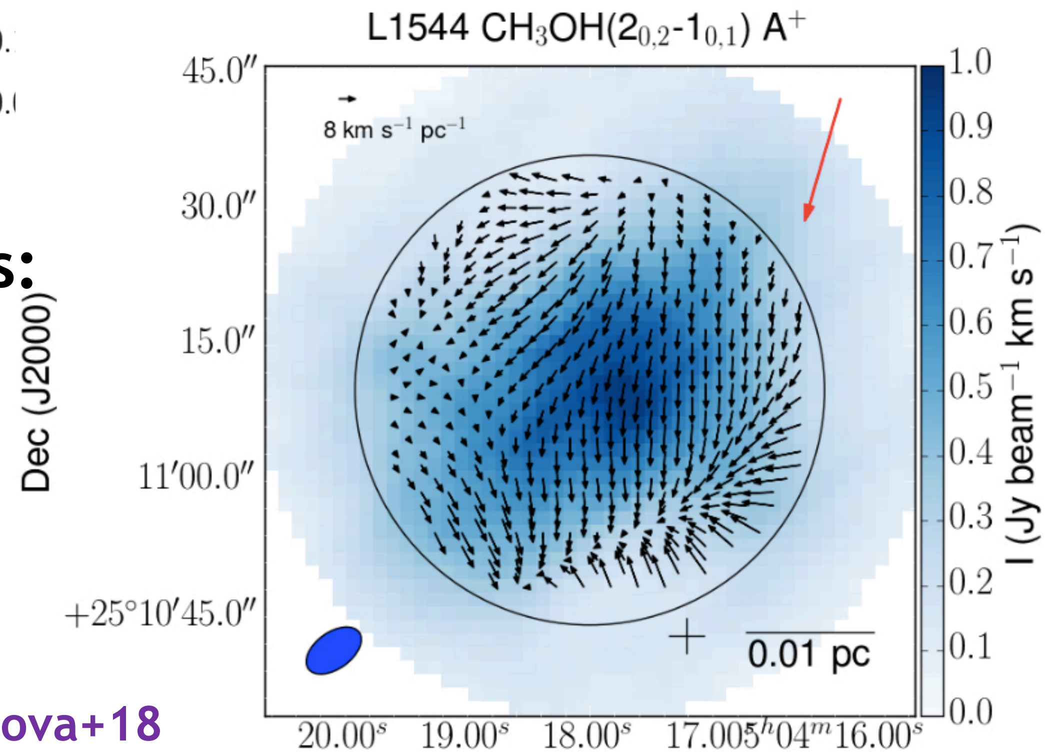
Surface Chemistry contribution to COM formation

Vasyunin et al. (2017)

Species	Surface contribution, %	RD efficiency
CH_3O	45	3.4(-5)
OH	10	4.5(-2)
HCO	20	2.1(-3)
CH_3	3	6.2(-1)
C_2H_4	98	6.0(-2)
NH_2	5	2.5(-1)
H_2CO	75	5.4(-2)
CH_3OH	99	6.4(-3)

Small-scale structure of the CH_3OH peak





CH_3OH shows inward motions:

Gas accretion…?

Punanova+18

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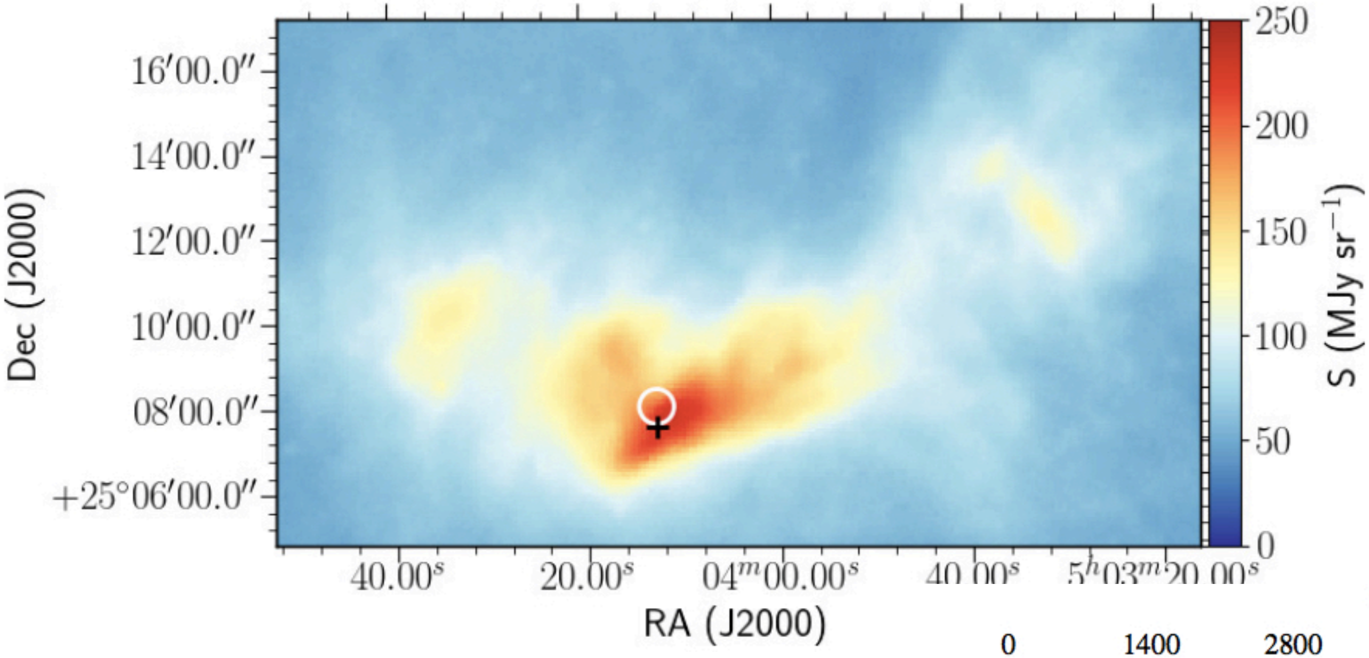

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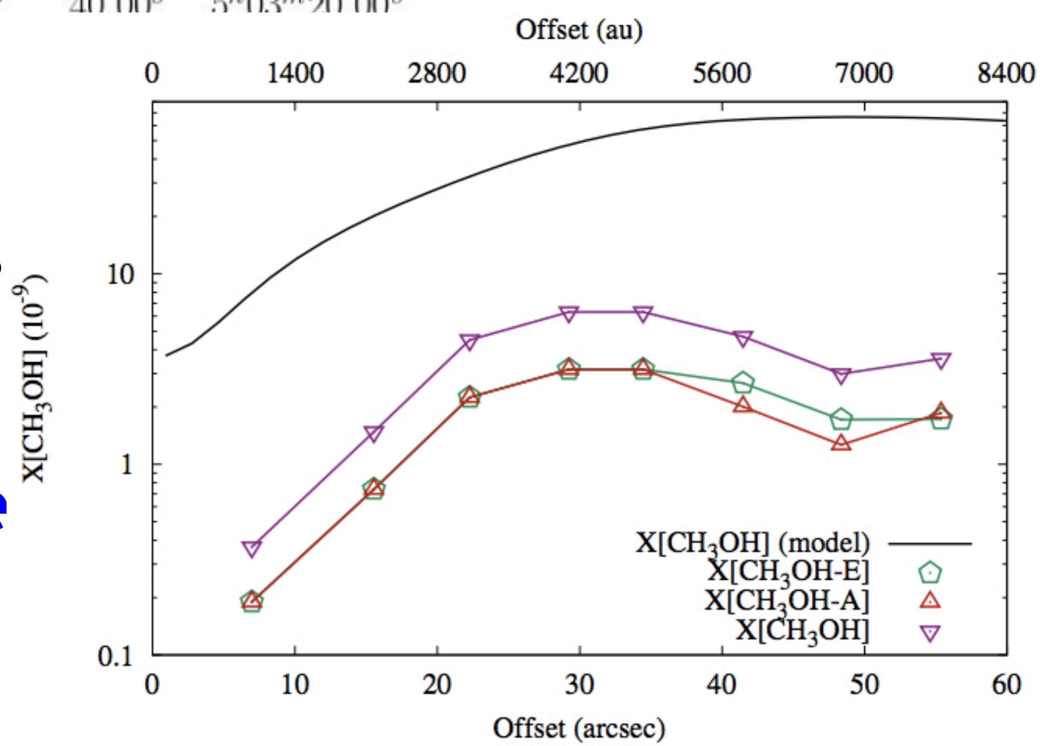

CH_3OH shows inward motions

…Or merging of filaments?

Gas dynamics need to be considered

Conclusions

- COMs are ubiquitous in the ISM. Large COMs even detected in Pre-stellar Cores (PSCs).

- COM abundance profile predicted by chemical modelling -> Outer, intermediate-Av shells in PSCs may represent the main O-bearing COM reservoir.

- Chemical complexity may increase with core evolution