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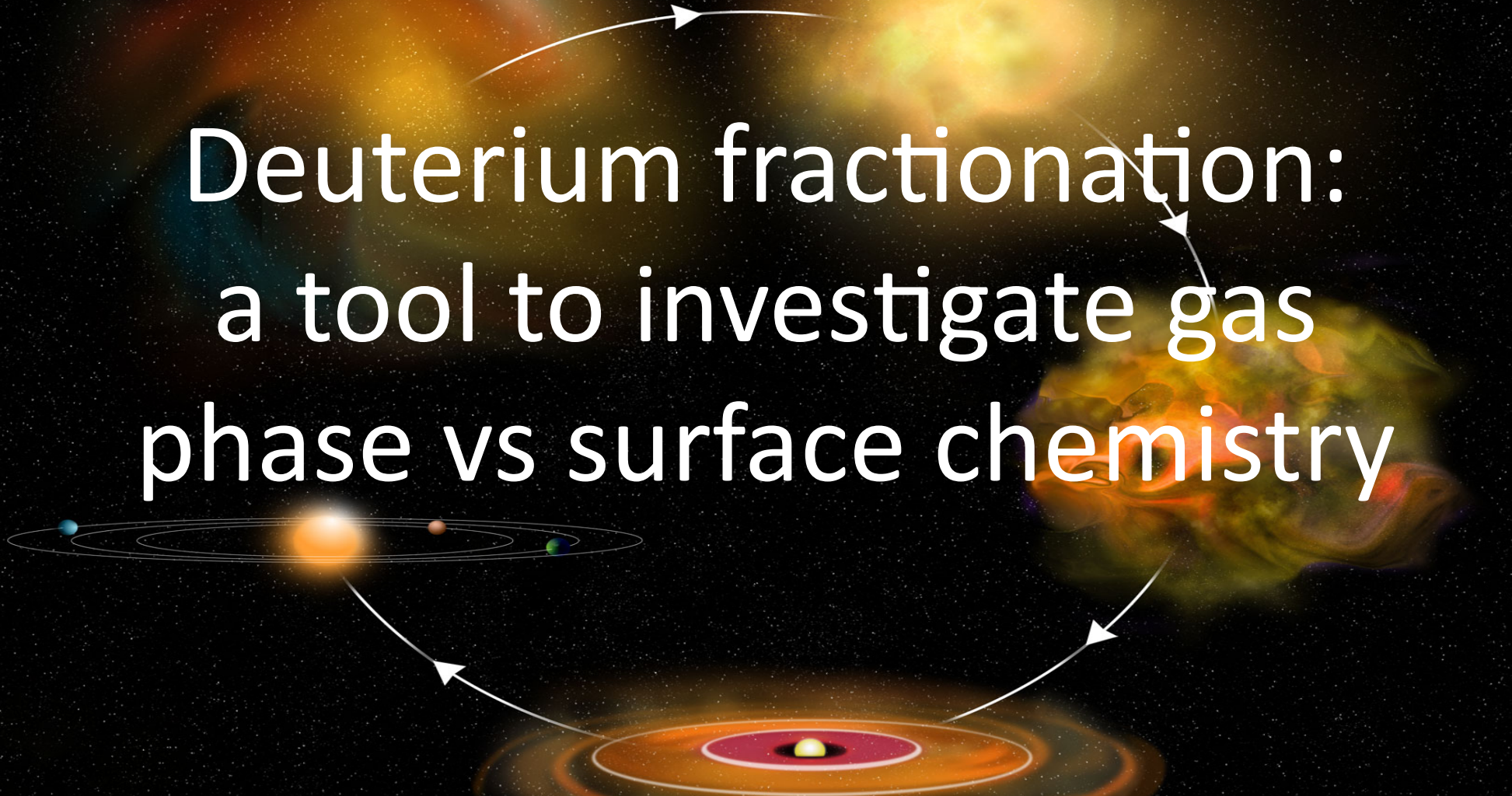
Deuterium fractionation: a tool to investigate gas phase vs surface chemistry



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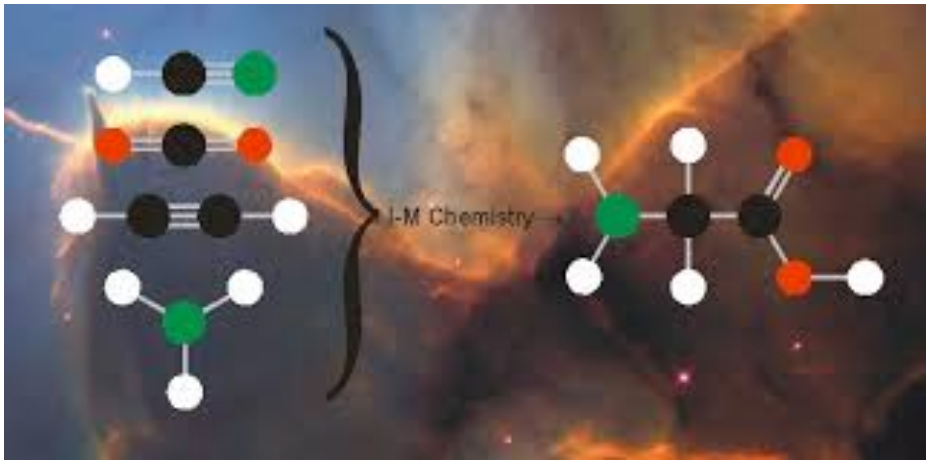
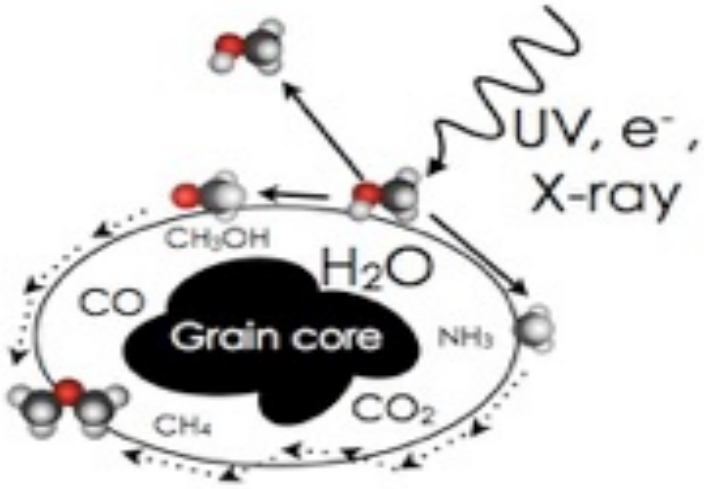
Cecilia Ceccarelli (IPAG); Aina Palau (CRyA); Alvaro Sanchez-Monge (U. of Cologne)
Jonathan Tan (U. of Florida); Marc Audard (U. of Geneva)

COMs: gas vs grains
We (still) do not know…





D-fractionation: gas or grains
do we (start to) know?

- Cosmic D/H ~ 10^{-5} (e.g. Oliveira et al. 2003, Linsky et al. 2006)
- Measured D/H in molecular cores ~10^{-4} – 10^{-1} (e.g. Crapsi et al. 2005; Emprechtinger et al. 2009, Fontani et al. 2006, 2011, 2015; Pillai et al. 2013)

Formation of D-molecules

GAS

Roberts & Millar 89; Gerlich+02; Asvany+04; Gerlich & Schlemmer 02; Flower+06

If *T* is low

$H_3^+ + HD \longrightarrow H_2D^+ + H_2 + 230K$

If $n(H_2)$ is high

$H_2D^+ + CO \rightarrow DCO^+$

$H_2D^+ + N_2 \rightarrow N_2D^+$

$H_2D^+ + CN \rightarrow \ldots \rightarrow$ **DNC**

$H_2D^+ + NH_3 \rightarrow \ldots \rightarrow NH_2D$

$H_2D^+ + H_2CO \rightarrow \ldots \rightarrow$ **HDCO**

Gas only

GRAINS

Hasegawa et al. 1992; Roueff et al. 2007; Caselli & Ceccarelli 2012; Ceccarelli et al. 2014, PPVI

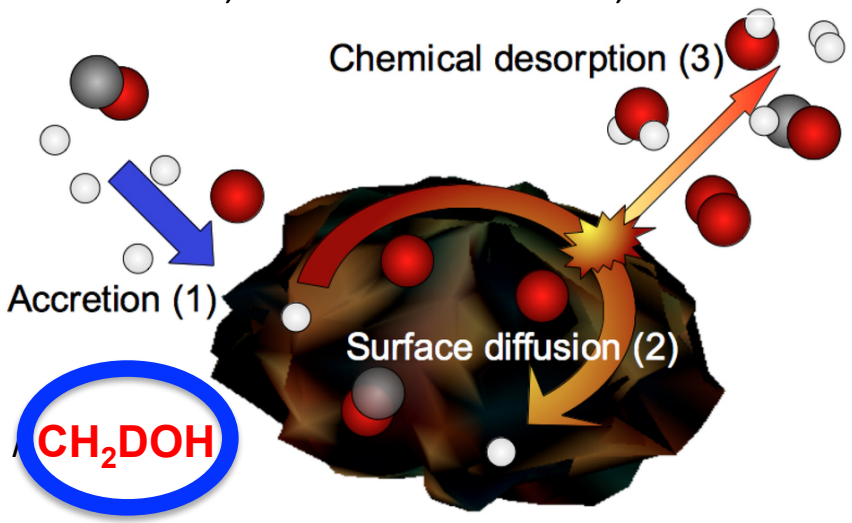
$O \rightarrow OH / OD \rightarrow H_2O /$ **HDO**

$C \rightarrow CH / CD \rightarrow \ldots. \rightarrow CH_4 /$ **CH_3D**

$N \rightarrow NH / ND \rightarrow \ldots. \rightarrow NH_3 /$ **NH_2D**

$CO \rightarrow HCO / DCO \rightarrow H_2CO /$ **HDCO** $\rightarrow \ldots \rightarrow CH_3OH /$ **CH_2DOH**

$CN \rightarrow HNC /$ **DNC**



Grains only

Comparative studies of D-frac in MASSIVE SF cores

Fontani et al. 2011, A&A, 529, L7; Fontani et al. 2014, MNRAS, 440,448; Fontani et al. 2015, A&A, 575, 87

Criteria for species

1) Gas only (N_2D^+);
2) Grains only (CH_2DOH);
3) Gas + grains (NH_2D; DNC)

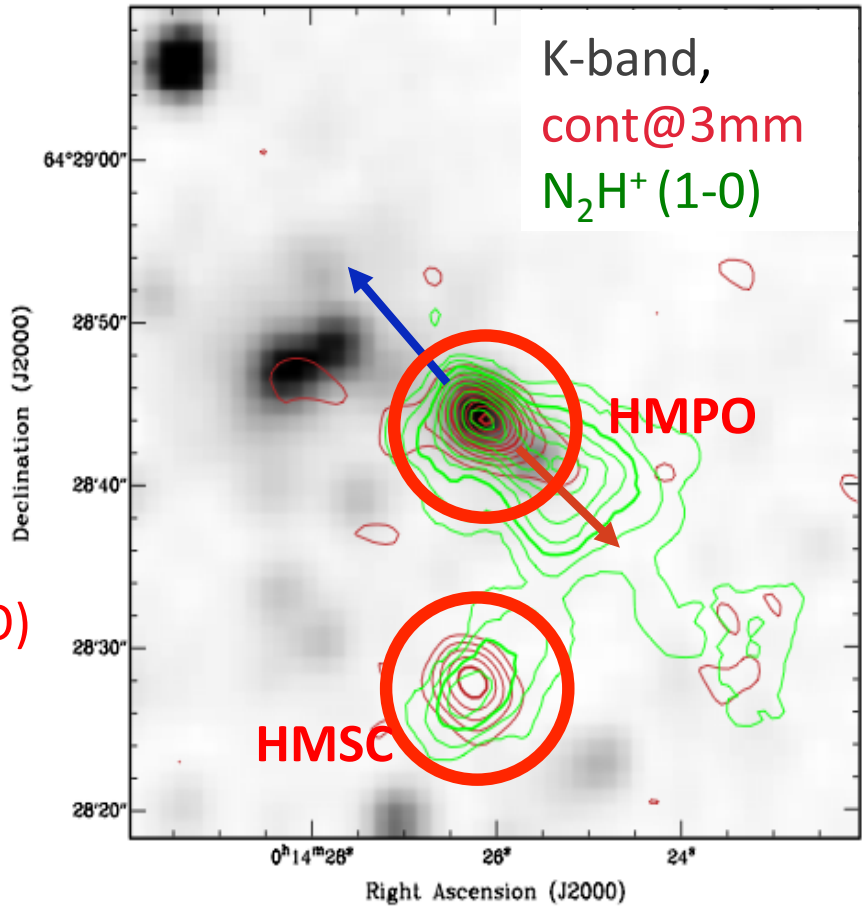
Criteria for cores

i. NO infrared; NO outflows; NO 3.6cm
→ High-Mass Starless Core (HMSC)

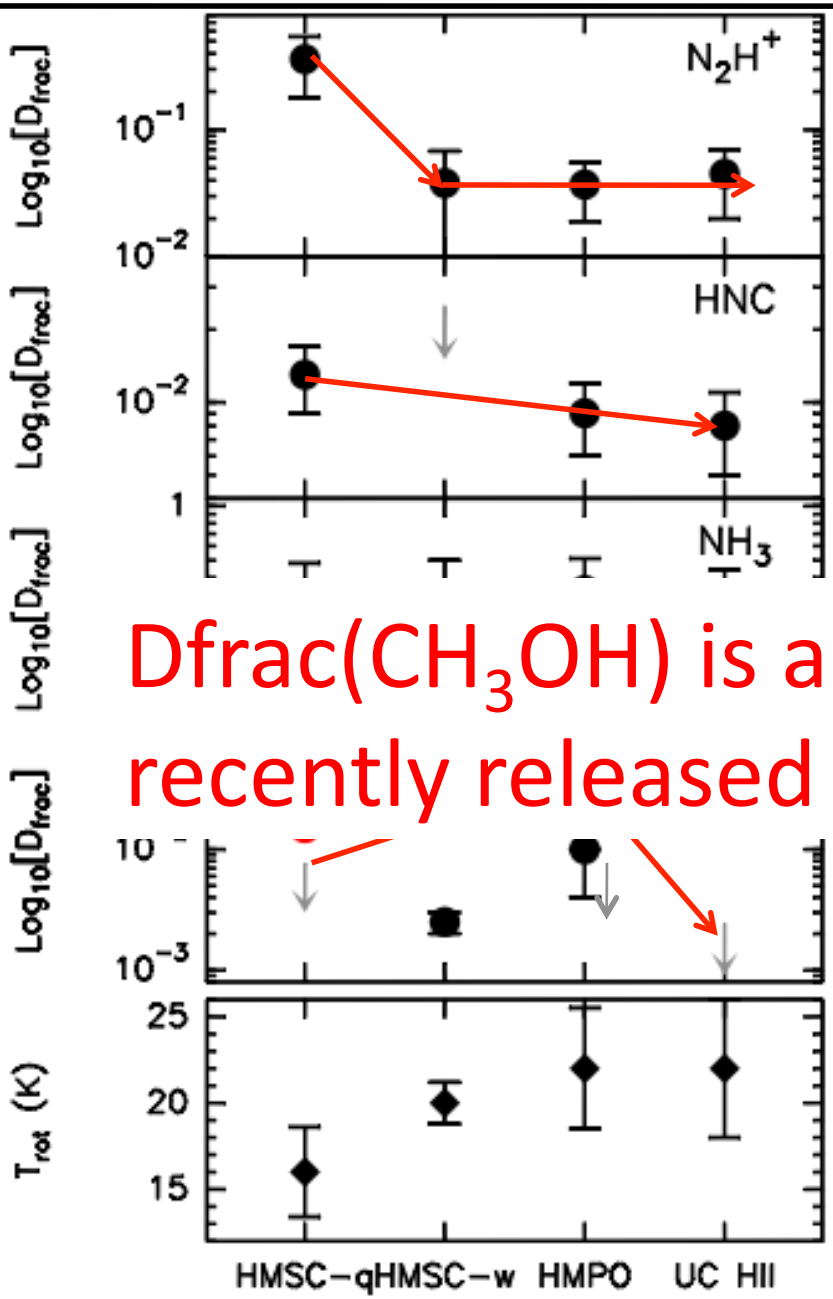
ii. YES infrared; YES outflows; NO 3.6cm
→ High-mass Protostellar Object (HMPO)

iii. YES infrared; YES/NO outflows; YES 3.6cm
→ UltraCompact HII region (UCHII)

Palau et al. 2010



D-fractionation vs evolution



Dfrac(N_2H^+): sharp decrease HMSC → HMPO

Dfrac(HNC): slight decrease HMSC → HMPO

Dfrac(CH_3OH): increase (sharp?) HMSC →HMPO

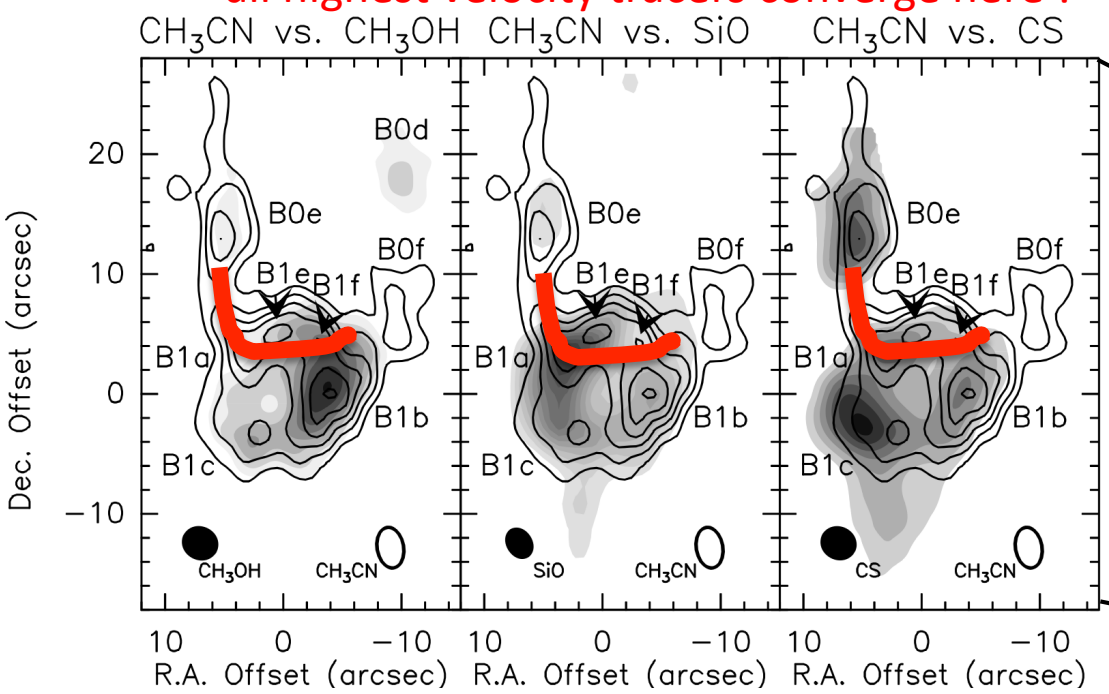
GAS

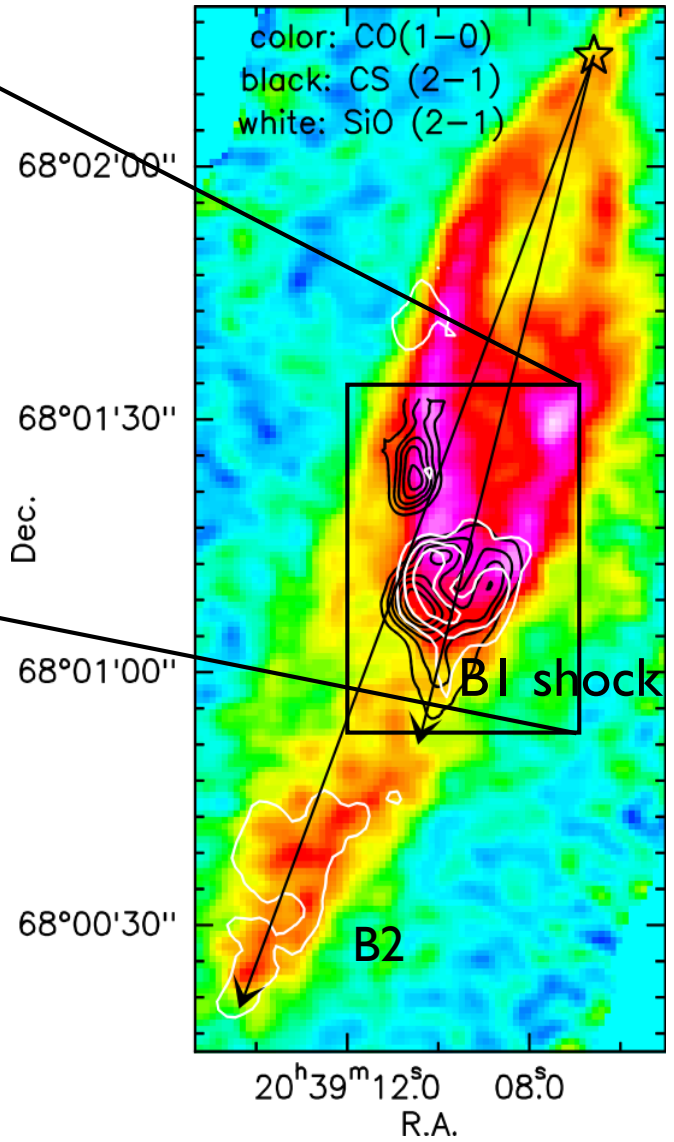
GRAINS

Dfrac(CH_3OH) is a tool to identify material recently released by mantles!

The L1157-B1 young and chemically rich bow-shock

all highest velocity tracers converge here !





Gueth et al. (1998), Benedettini et al. (2007), Codella et al. (2009)

Deuterated molecules in L1157-B1!

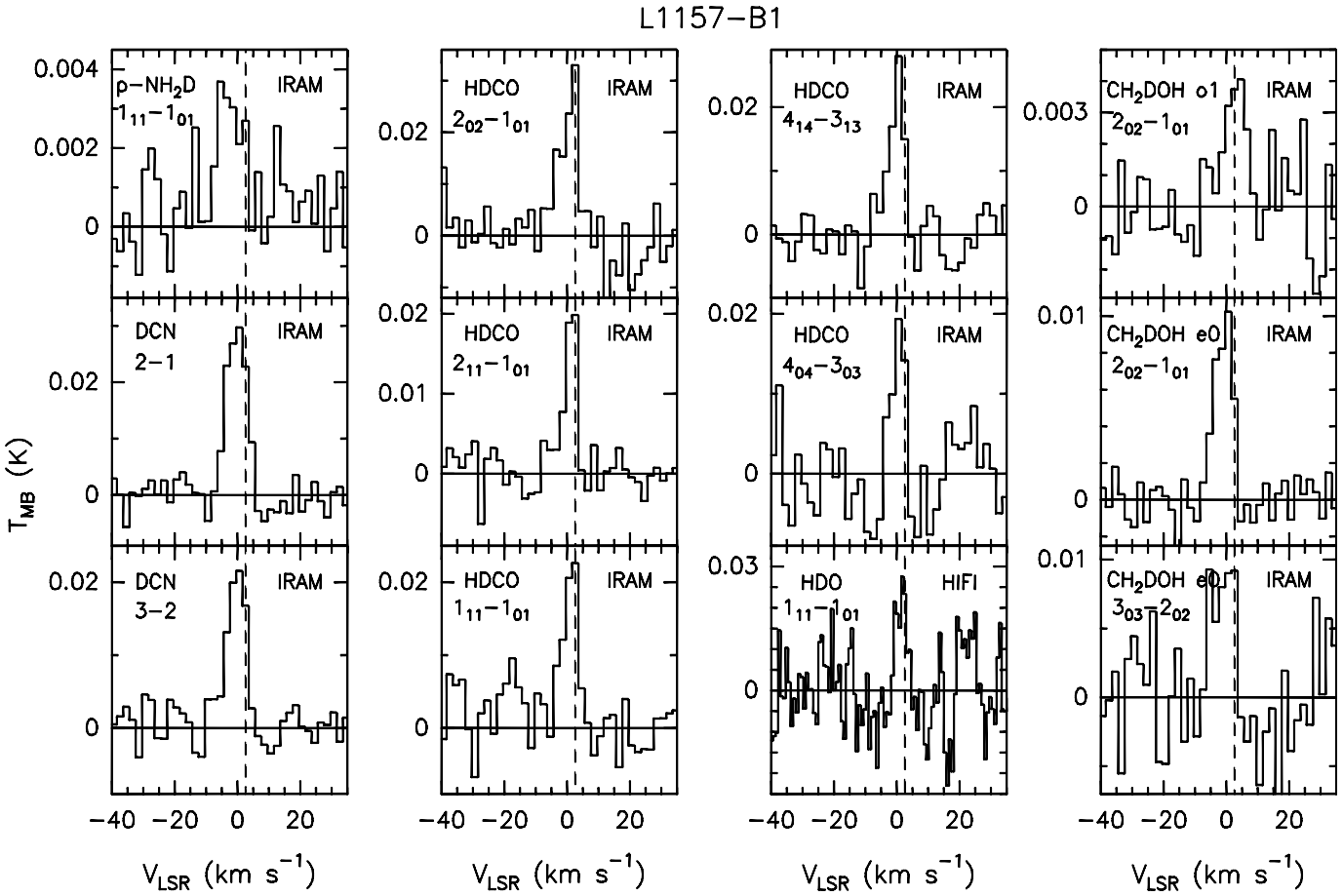
Codella+12, ApJ, 757, L9

- L1157-B1 surveyed as part of the Herschel/CHESS and IRAM-30m/ASAI Large Programmes (Ceccarelli+10, http://www.oan.es/asai) in:

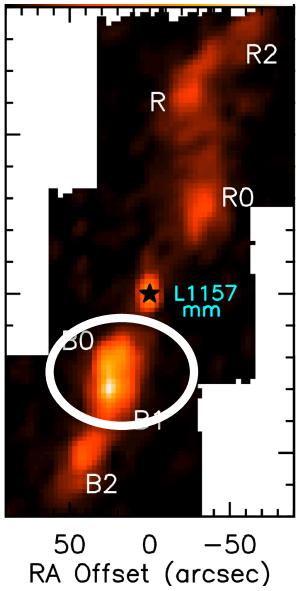
  78 – 350 GHz (IRAM-30m)

  500 – 2000 GHz (Herschel)

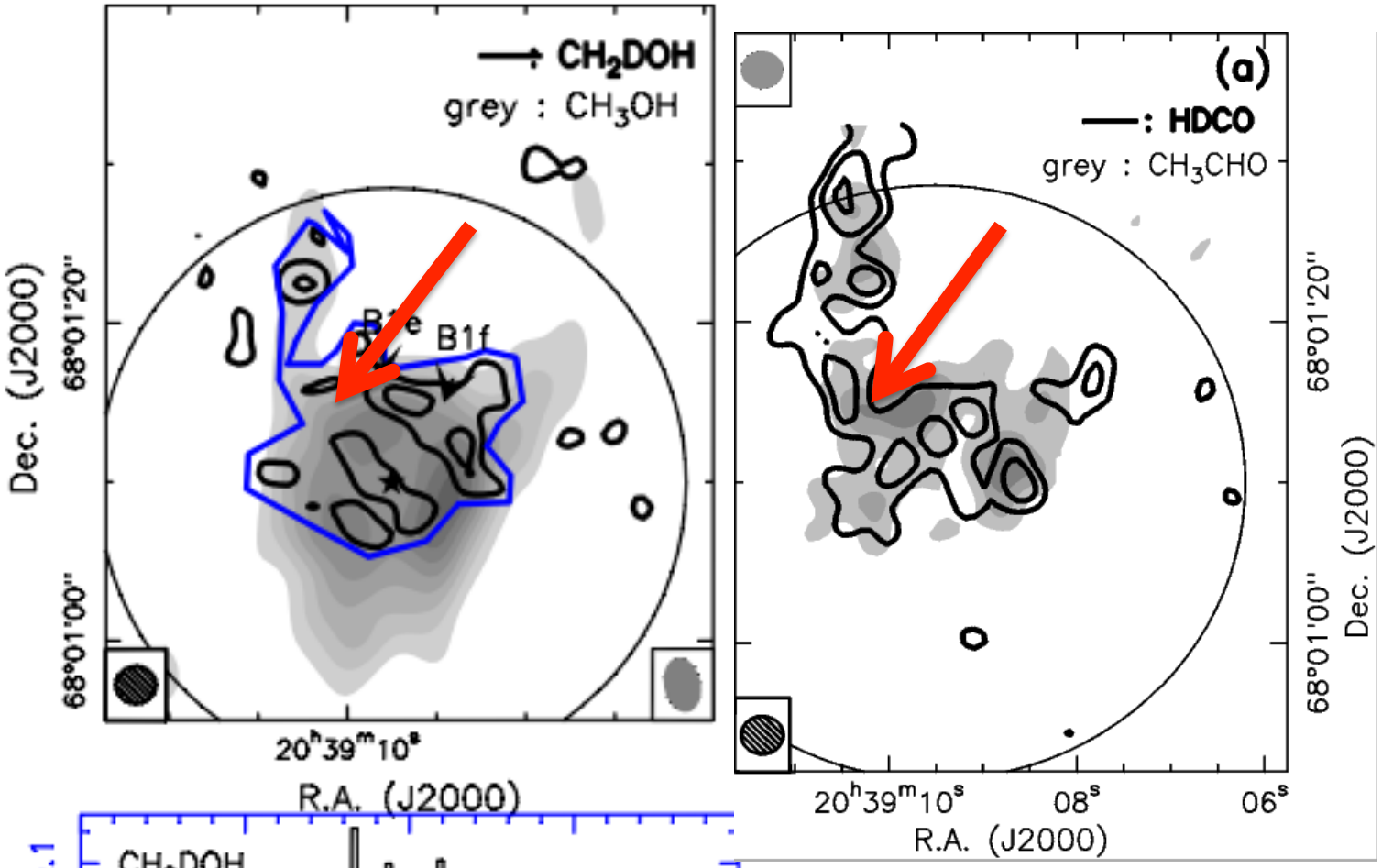
- 12 lines of deuterated molecules detected

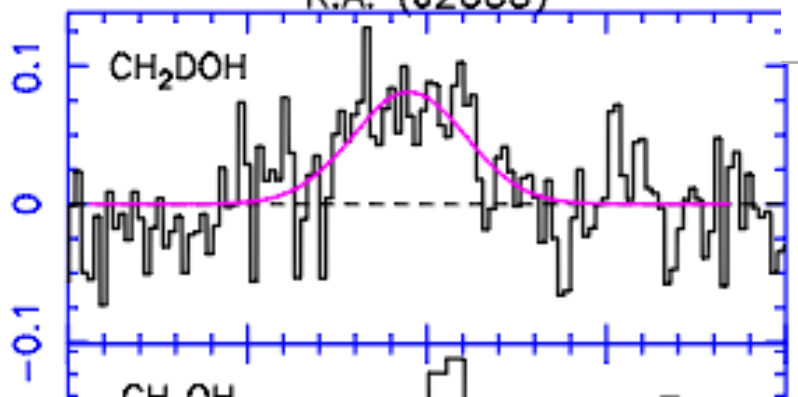


CH_2DOH and HDCO in L1157-B1

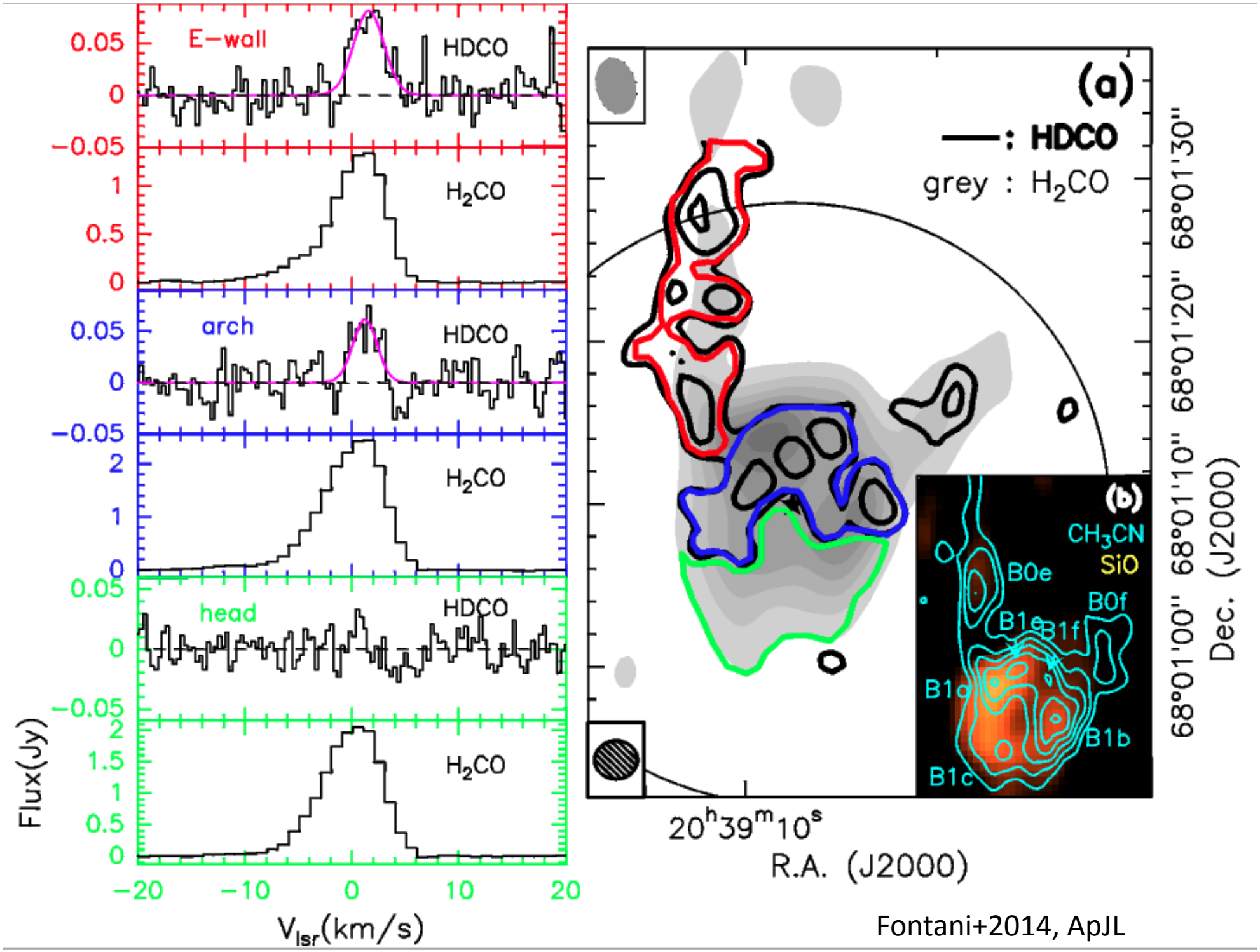


Herschel-PACS
H_2O@179 μm
(Nisini et al. 2010)





Fontani, Codella, Ceccarelli, LeFloch, Viti & Benedettini 2014, ApJL, 788, 43



Fontani+2014, ApJL

Deuterated fractions in L1157-B1

Table 1. Line parameters of HDCO, H_2CO, CH_2DOH and CH_3OH derived in the three regions identified in Fig. 1 (E-wall, arch, and head), and from spectra integrated over the whole emission of both HDCO (Tot HDCO) and CH_2DOH (Tot CH_2DOH), as explained in Sect. 3. The uncertainties given between parentheses include only the statistical errors. The (range of) excitation temperatures 10 – 70 K used to derive τ, N and D_{frac} have been assumed equal to the rotation temperatures derived in Codella et al. (2012) and Lefloch et al. (2012).

	Δv (km s^{-1})	$\int T_{MB} dV$ (K km s^{-1})	V_{LSR} (km s^{-1})	FWHM (km s^{-1})	τ 10K - 70K	N ($\times 10^{14}$cm^{-2}) 10K - 70K	D_{frac} 10K - 70K
E-wall							
HDCO($2_{1,1} - 1_{0,1}$)	–1.5; +3	0.23(0.02)	1.6(0.15)	3.3(0.3)		0.026(0.003) - 0.10(0.01)	
H_2CO($2_{0,2} - 1_{0,1}$)	–1.5; +3	3.56(0.02)			0.15 - 0.01	0.163(0.002) - 0.71(0.01)	0.16(0.02) - 0.14(0.02)
Arch							
HDCO($2_{1,1} - 1_{0,1}$)	–1.5; +3	0.19(0.02)	1.2(0.2)	2.7(0.3)		0.021(0.003) - 0.08(0.01)	
H_2CO($2_{0,2} - 1_{0,1}$)	–1.5; +3	11.02(0.02)			0.55 - 0.04	0.506(0.002) - 2.20(0.01)	0.041(0.007) - 0.035(0.006)
Head							
HDCO($2_{1,1} - 1_{0,1}$)	–	≤0.05	–	1.2[a]		≤0.006 - ≤ 0.02	
H_2CO($2_{0,2} - 1_{0,1}$)	–1.5; +3	7.2			0.32 - 0.03	0.330(0.001) - 1.439(0.006)	≤0.017 - 0.015
Tot HDCO							
HDCO($2_{1,1} - 1_{0,1}$)	–1.5; +3	0.18(0.01)	1.5(0.1)	2.9(0.2)		0.021(0.002) - 0.077(0.009)	
H_2CO($2_{0,2} - 1_{0,1}$)	–1.5; +3	6.30(0.02)			0.29 - 0.02	0.289(0.002) - 1.259(0.006)	0.071(0.008) - 0.061(0.007)
Tot CH_2DOH							
HDCO($2_{1,1} - 1_{0,1}$)	–1.5; +3	0.10(0.02)	1.4(0.2)	2.7(0.3)		0.011(0.002) - 0.04(0.01)	
H_2CO($2_{0,2} - 1_{0,1}$)	–1.5; +3	5.74(0.02)			0.25 - 0.05	0.26(0.03) - 1.13(0.07)	0.042(0.009) - 0.035(0.009)
CH_2DOH($3_{0,3}$–$2_{0,2}$)	–5; +3	0.15(0.02)	–0.9(0.4)	7.2(0.9)		0.18(0.06) - 2.2(0.7)	
CH_3OH($3_{0,3}$–$2_{0,2}$)	–5; +3	16.89(0.06)			0.64 - 0.05	7.0(0.2) - 69(2)	0.03(0.01) - 0.026(0.009)

[a]assumed equal to the line width detected in "arch".

WALL

ARCH

HEAD

N(HDCO)/N(H_2CO) = 0.15 in WALL → = 0.04 in ARCH → < 0.016 in HEAD

DEUTERATION CHANGES BY AN ORDER OF MAGNITUDE

HDCO: gas or grains?

✓ grain surface reactions: Dfrac(H_2CO) up to 0.1 or more

e.g. Hidaka et al. 2009, Taquet et al. 2011, 2014

✓ gas-phase reactions?

e.g. Loren & Wootten (1984), Roueff et al. (2007)

$H_3^+ + HD \rightarrow H_2D^+ + H_2 + 230K$

$H_2D^+ + H_2CO \rightarrow H_2$

$H_2DCO^+ + e^- \rightarrow HD$

$CH_3^+ + HD \rightarrow CH_2D$

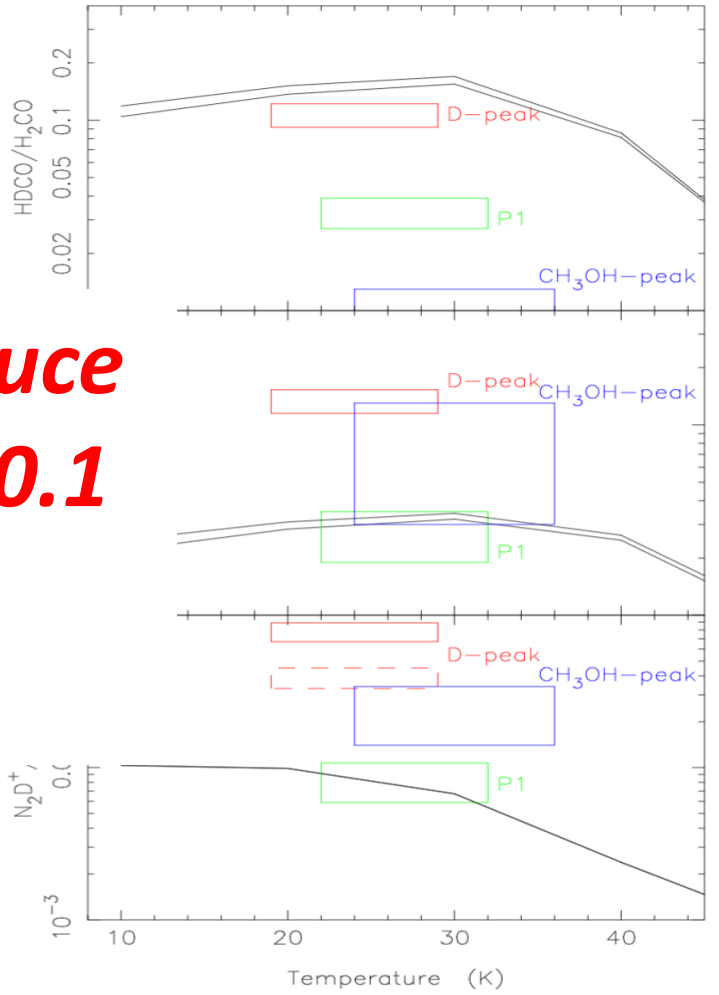
$CH_2D^+ + H_2 \rightarrow CH_4$

$CH_4D^+ + e^- \rightarrow CH_2D + H_2$

$CH_2D + O \rightarrow HDCO + H$

Cannot reproduce $HDCO/H_2CO = 0.1$ in warm gas → grains!!

Roueff et al. (2007)



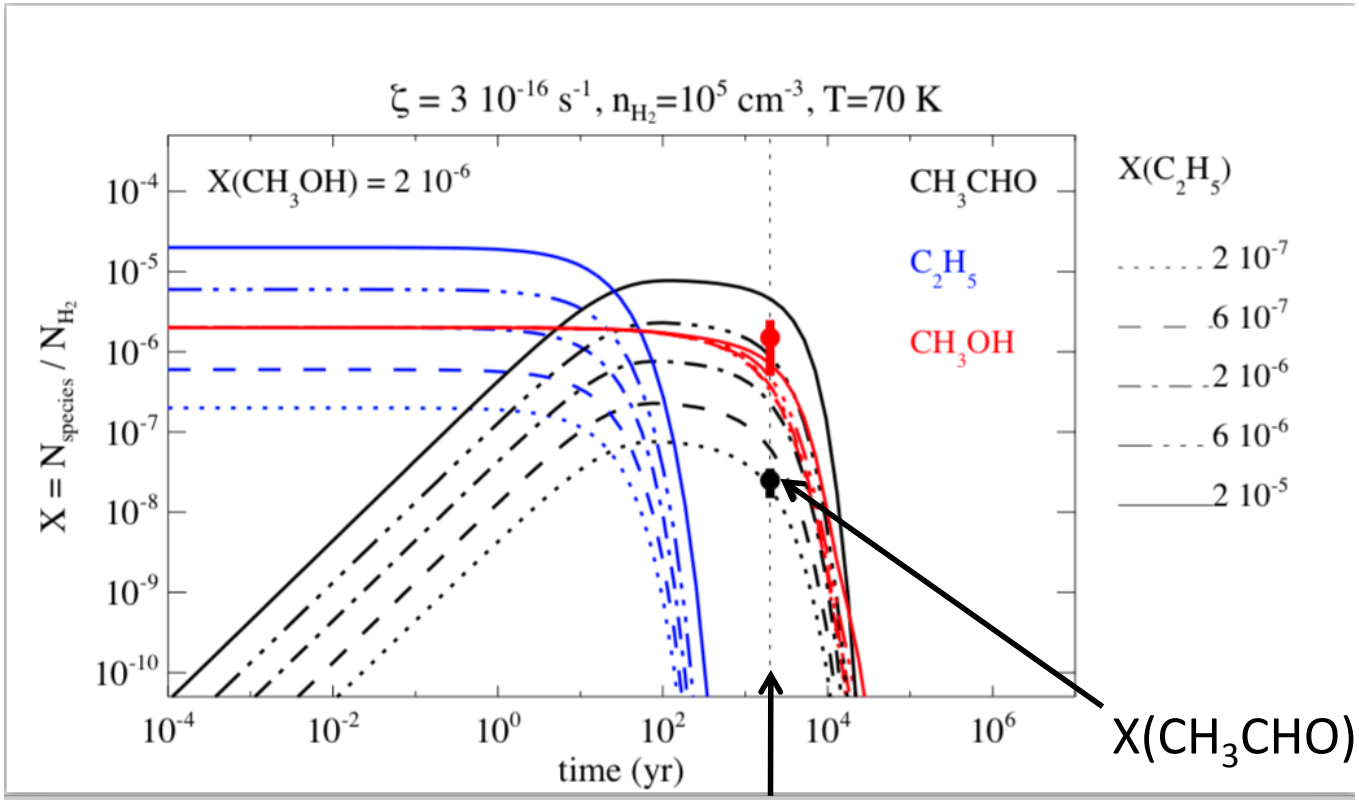
Acetaldehyde: gas or grains?

Codella+15, MNRAS, 449, L11

Unique plausible gas-phase route (Charnley 2004):

$C_2H_4 \rightarrow \ldots \rightarrow C_2H_5 \xrightarrow{O} CH_3CHO$

ASTROCHEM
http://smaret.github.com/astrochem



X(CH_3CHO) measured ≈ 2-3 10^{-8}

2000 yrs = Shock age!
Gueth+1996

Summary and conclusions

1) D-fractionation: gas or grains? We start to know!

2) CH_2DOH and HDCO traces material recently released from dust grains

3) Acetaldehyde and HDCO in L1157-B1 have same morphology: both produced on grains (?)