Deuteration and fractionation in prestellar cores and IRDCs from an observational point of view

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Elemental abundances

	Solar system	local ISM
D/H	$1.94\ 10^{-5}$ (a)	$1.6\ 10^{-5}$ (c)
$^{12}C/^{13}C$	89.3 (a)	69±6 (c)
$^{14}N/^{15}N$	441±6 (b)	338±32 (c)
$^{16}O/^{18}O$	499 (a)	557±30 (c)
$^{18}O/^{17}O$	5.4 (a)	3.6±0.2 (c)
$^{32}S/^{34}S$	22.5 (a)	24±5 (d)
$^{34}S/^{33}S$	5.6 (a)	6.3±1.0 (d)
$^{28}Si/^{29}Si$	19.7 (a)	
$^{29}Si/^{30}Si$	1.5 (a)	1.5 (c)

(a) Lodders, ApJ 591, 1220, 2003
(b) Marty et al. 2011, Science 332, 1533
(c) Wilson, 1999 Rep. Progress Phys. 62, 143
(d) Chin et al, 1996, A&A 305, 960

Gradient of $^{12}C/^{13}C$, $^{16}O/^{18}O$, $^{14}N/^{15}N$ as a function of distance from the Galactic Center, D_{GC}

Detected Deuterated species

HD, ND, HDO, D_2O, NH_2D, $^{15}NH_2D$, ND_2H, ND_3, DCN, DNC, C_2D, HDCO, D_2CO, CH_2DOH, CH_3OD, CHD_2OH, CD_3OH, c-C_3HD, c-C_3D_2, CH_3C_2D, CH_2DC_2H, CH_2DCN, HDS, HDCS, D_2CS, C_4D, l-C_4HD, DC_3N, DC_5N

H_2D^+, D_2H^+, DCO^+, $D^{13}CO^+$, CH_2D^+, NH_3D^+, N_2D^+

Detected ^{13}C species

^{13}CO, ^{13}CN, ^{13}CS, $H^{13}CN$, $HN^{13}C$, $H_2{}^{13}CO$, $^{13}CH_3OH$, $H^{13}COOH$, ^{13}CCH, $C^{13}CH$, c-$H^{13}CC_2H$, c-$HCC^{13}CH$, $^{13}CC_3H$, $C^{13}CC_2H$, $C_2{}^{13}CCH$, $C_3{}^{13}CH$, $^{13}CC_2N$, $C^{13}CCN$, $C_2{}^{13}CN$, $H^{13}CC_2N$, $HC^{13}CCN$, $HC_2{}^{13}CN$, $^{13}CH_2NH$, $NH_2{}^{13}CHO$, $H_2{}^{13}CCHCN$, $H_2C^{13}CHCN$, $H_2C_2H^{13}CN$, $^{13}CH_3CN$, $CH_3{}^{13}CN$, $C_2H_5{}^{13}CN$, $^{13}CH_3CH_2CN$, $CH_3{}^{13}CH_2CN$, $H_2{}^{13}CS$, $O^{13}CS$, $C^{13}CCS$, $^{13}CH^+$, $H^{13}CO^+$

Detected ^{15}N species

$C^{15}N$, $HC^{15}N$, $H^{15}NC$, $^{15}NH_3$, $CH_3C^{15}N$, $HC_3{}^{15}N$, $C_2H_5C^{15}N$, $^{15}NNH^+$, $^{15}NNH^+$

Detected ^{18}O species

$C^{18}O$, $^{13}C^{18}O$, ^{18}OH, $H_2{}^{18}O$, $H_2C^{18}O$, $CH_3{}^{18}OH$, $Si^{18}O$, $S^{18}O$, ^{18}OCS, $HC^{18}O^+$

Detected ^{17}O species

$C^{17}O$, $^{13}C^{17}O$, $S^{17}O$, $HC^{17}O^+$

Detected ^{34}S and ^{33}S species

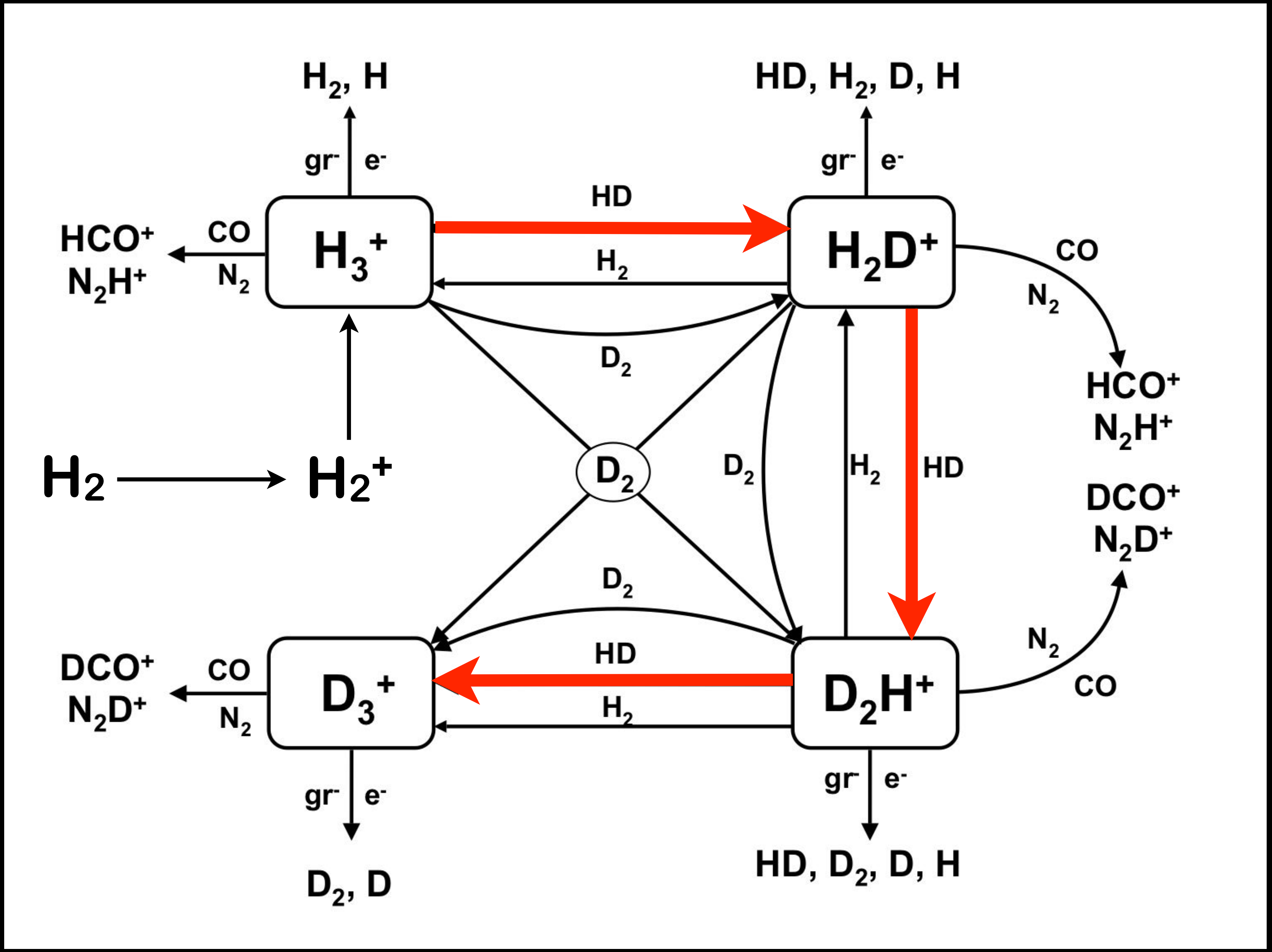
$C^{34}S$, ^{34}SO, $H_2{}^{34}S$, $H_2C^{34}S$, $C_3{}^{34}S$, $^{34}SO_2$, $OC^{34}S$, $Si^{34}S$, $^{30}Si^{34}S$, $^{29}Si^{34}S$, $C^{33}S$, ^{33}SO, $^{33}SO_2$, $H_2{}^{33}S$, $OC^{33}S$, $Si^{33}S$, $H_2C^{33}S$

Detected ^{30}Si and ^{29}Si species

^{30}SiO, $^{30}SiC_2$, ^{30}SiS, ^{29}SiS

Astrochemistry in the dense and cold gas

Deuterated molecules are useful diagnostic tools for studying the cold and dense environments where stars are born.
<u>Low-mass</u>: Caselli+ 2002, Crapsi+ 2007
<u>High-mass</u>: Fontani+ 06,09,11; Pillai+ 07,12



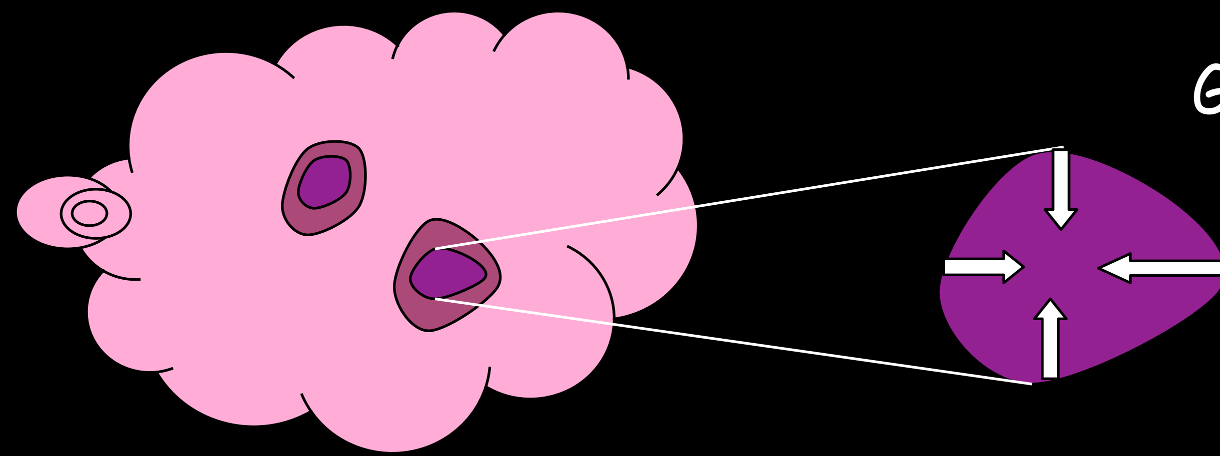
T ≤ 20 K

$H_3^+ + O \longrightarrow H_3O^+ \longrightarrow O, OH, H_2O$

$H_3^+ + N \longrightarrow NH^+ + H_2 \longrightarrow$ highly endothermic! Slower neutral-neutral reactions

Prestellar cores

Gravitational collapse

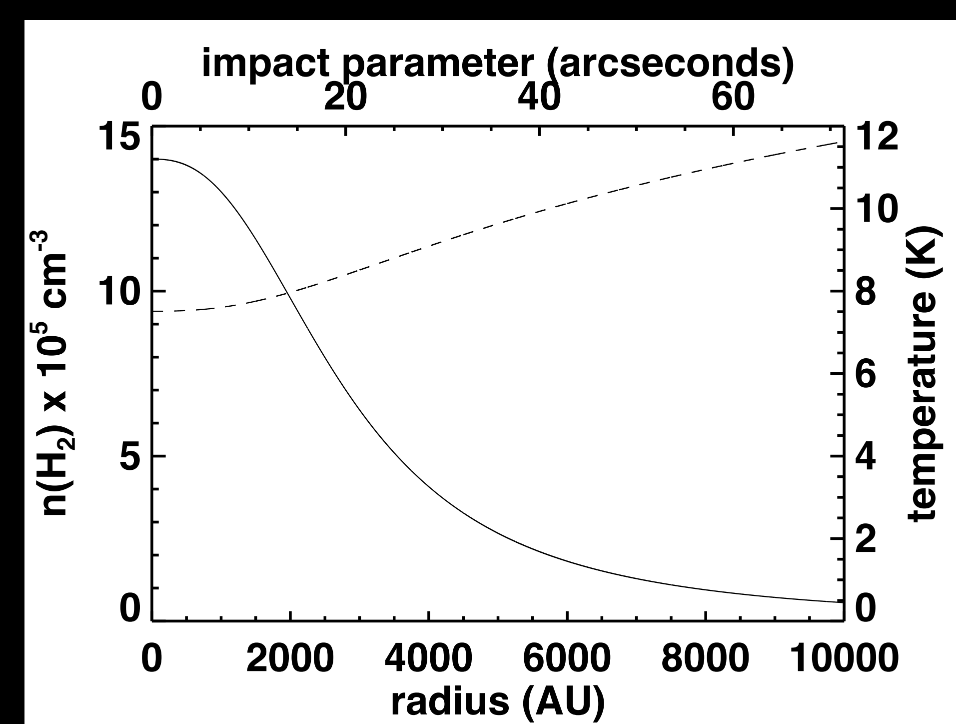


Molecular cloud

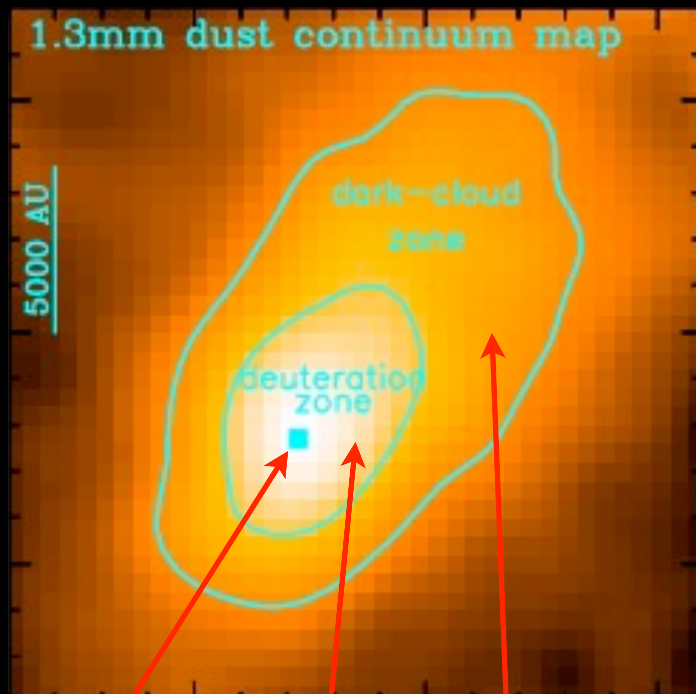
Prestellar core → **protostar phase**

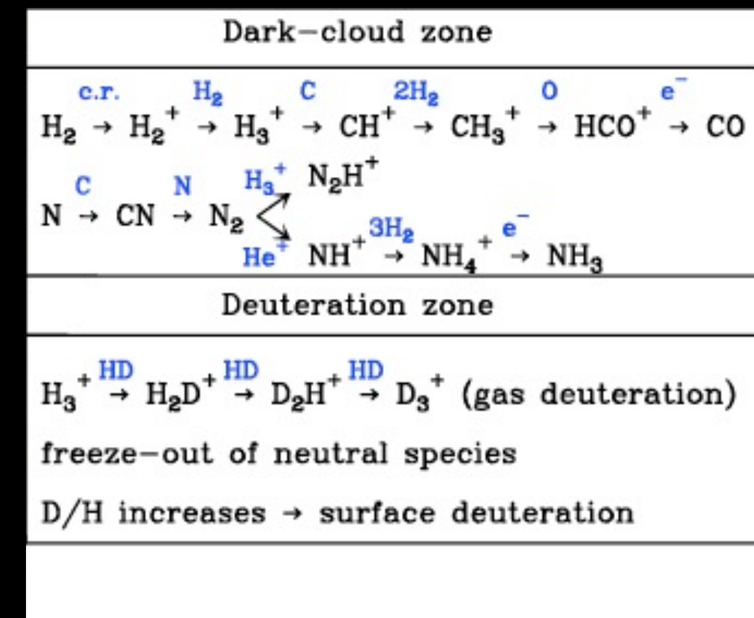
Prestellar cores provide the original reservoir of material from which future planetary systems are built

- Low T_{gas} and T_{dust} (< 10 K)
- High density (≥10^5 cm^{-3})
- Typical lifetime ~ 10^5 years
- Strong mm emissivity; absorption NIR, MIR
- High deuterium fractionation

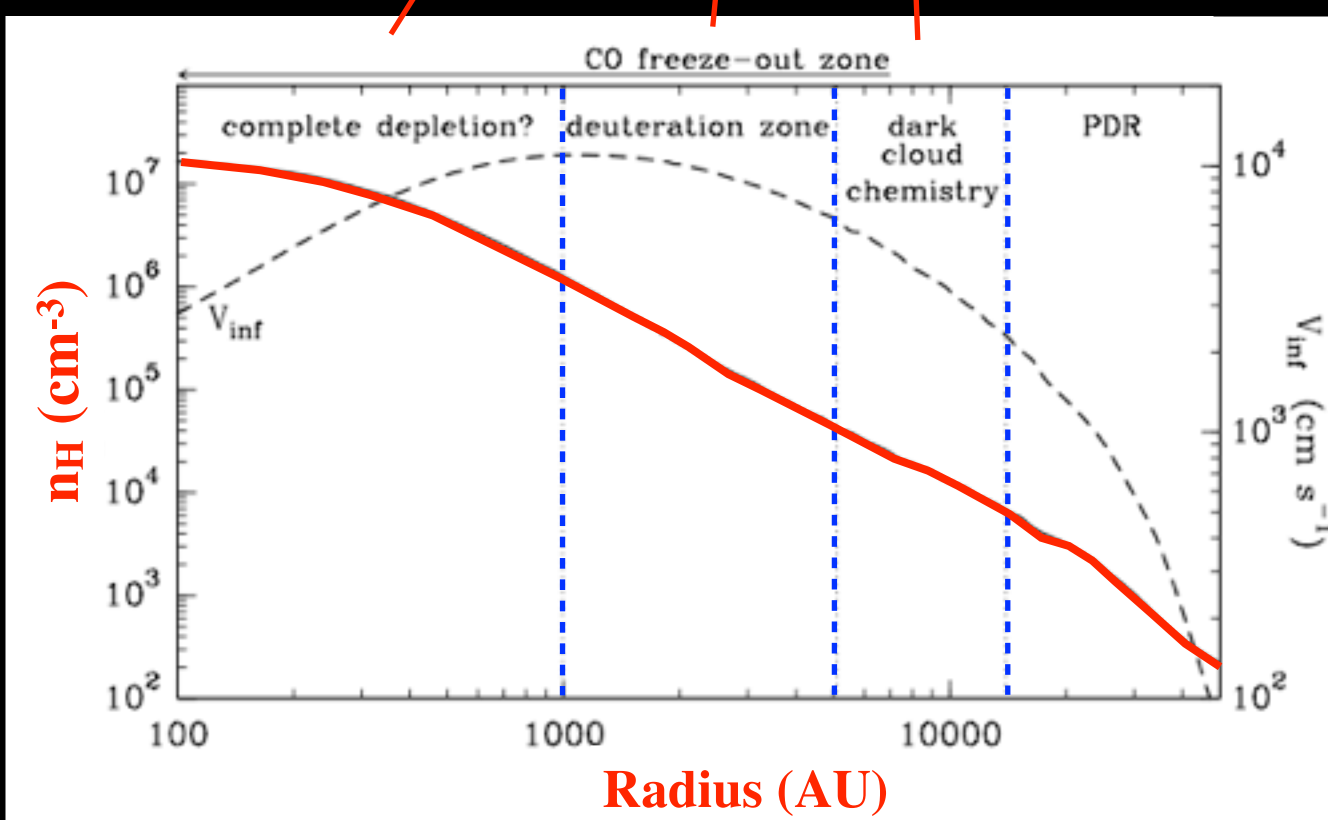


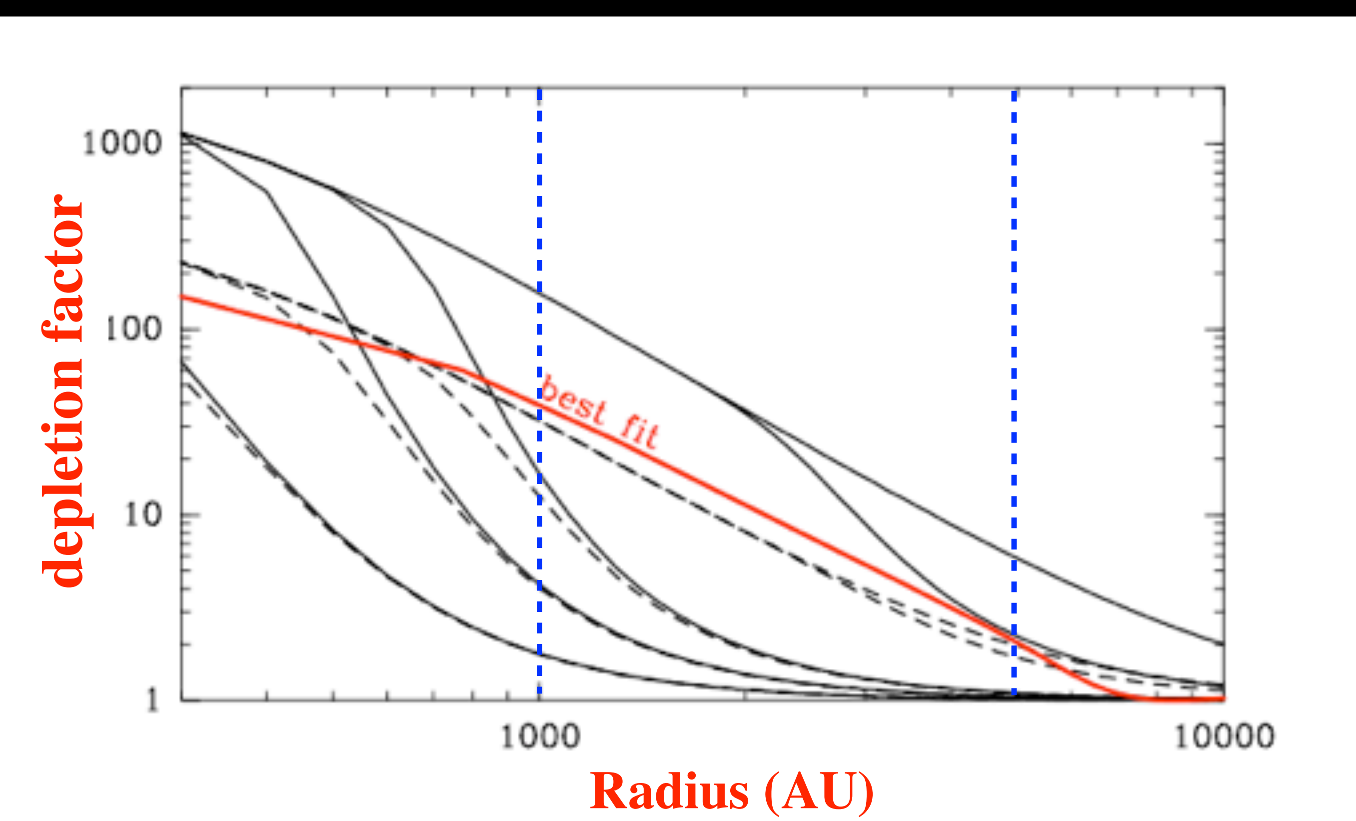
Prestellar cores



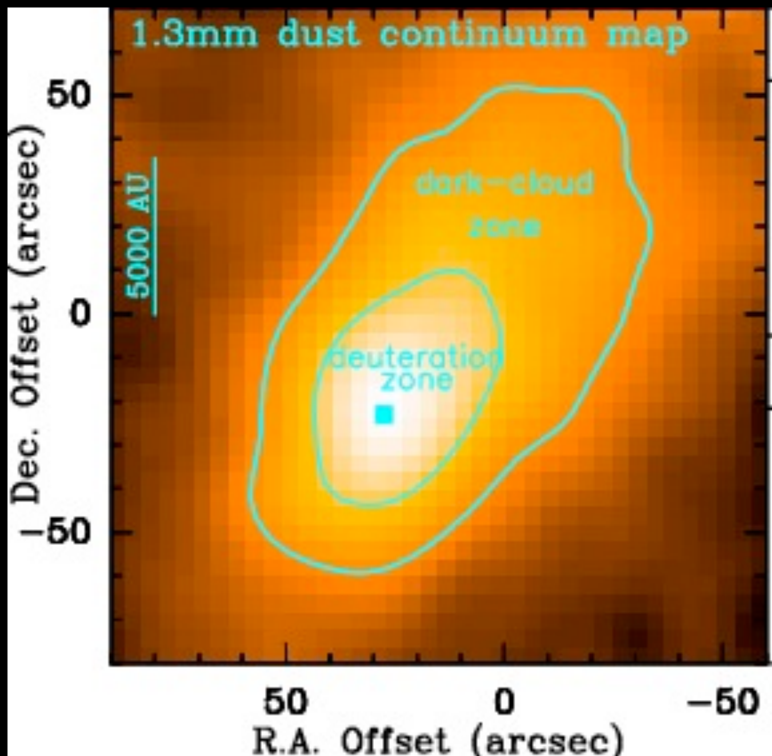


Caselli et al. 2011, Keto & Caselli 2010



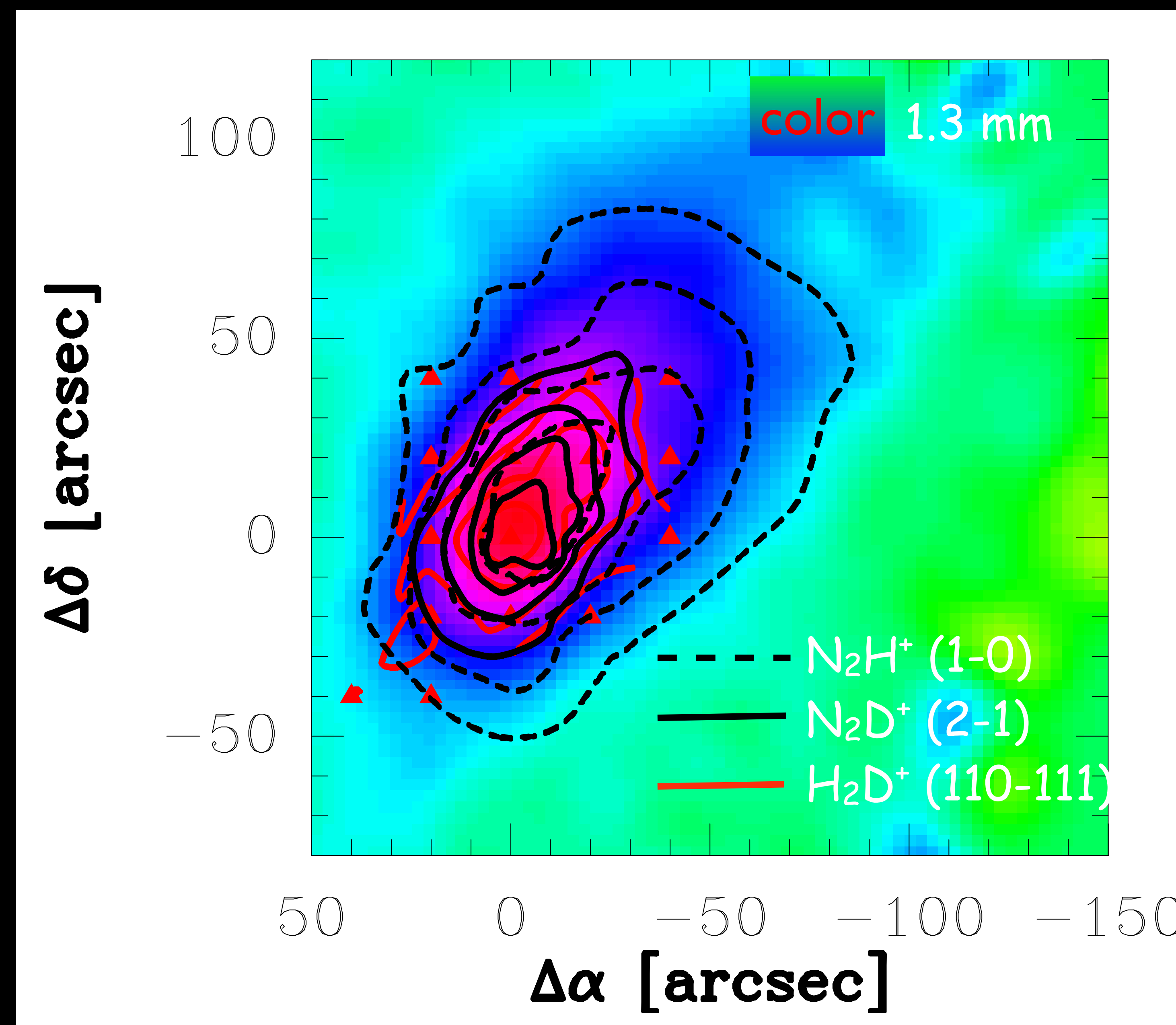


L1544: a prototypical isolated prestellar core



<u>Many first detections:</u>

- H_2D^+ (Caselli et al. 2004)
- H_2O (Caselli et al. 2010, 2012)
- c-C_3D_2 (Spezzano et al. 2013)
- HDCCC (Spezzano et al. 2016)



Deuteration as a chemical clock?

$D_{frac}(N_2H^+) = 0.2$

3-5 10^5 years (6-10 x t_{ff})

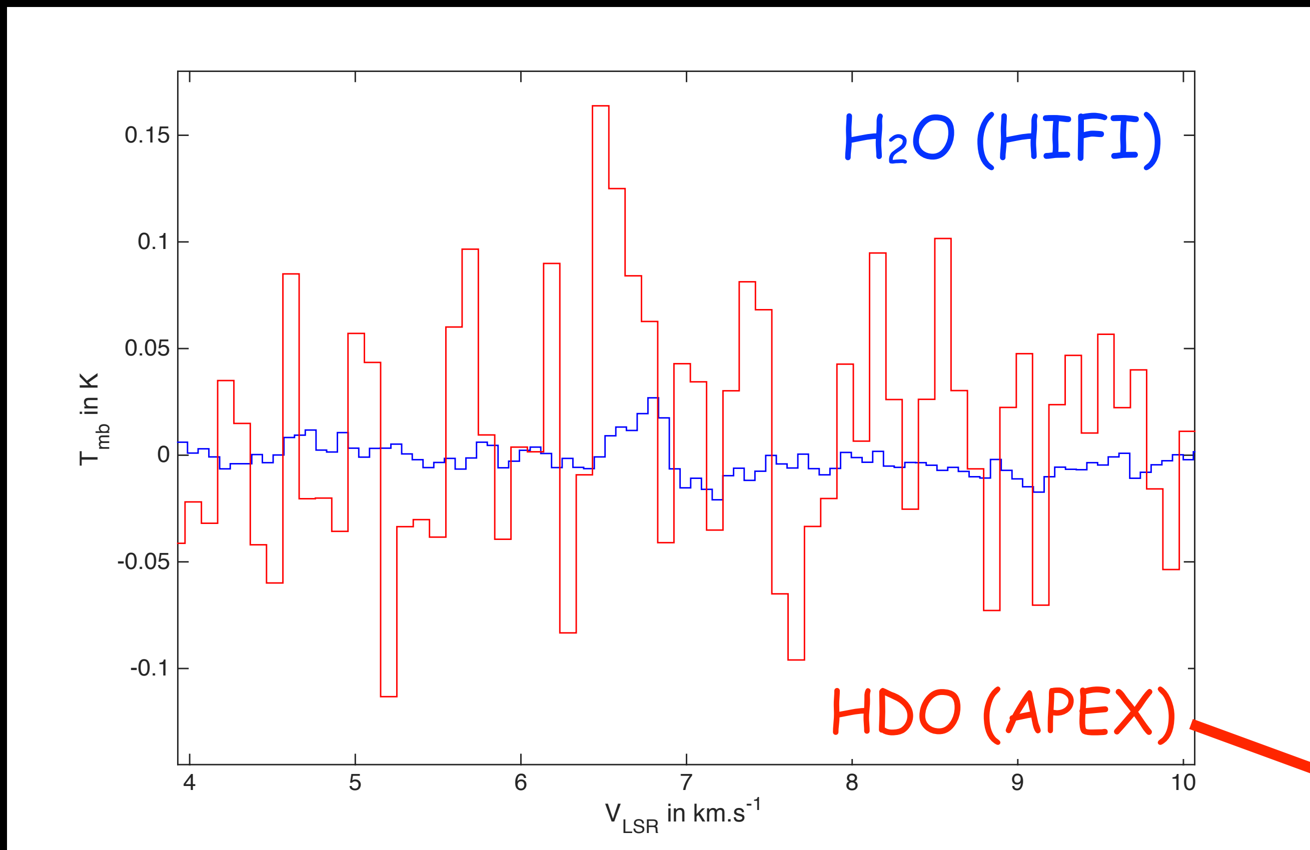
(depending on H_2 OPR)

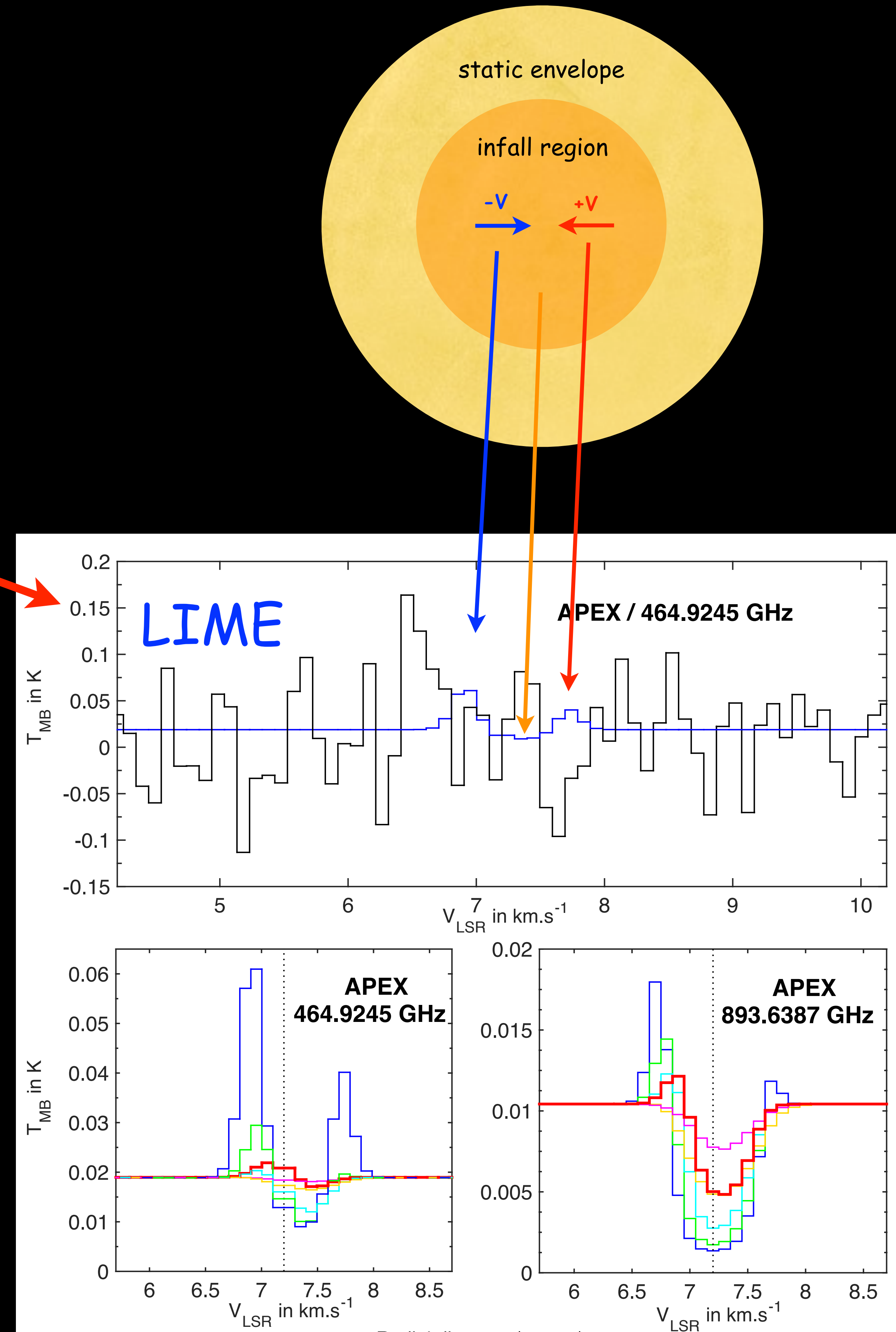
Very slow contraction

(ambipolar diffusion)

Kong+2015

Deuterated water in prestellar cores

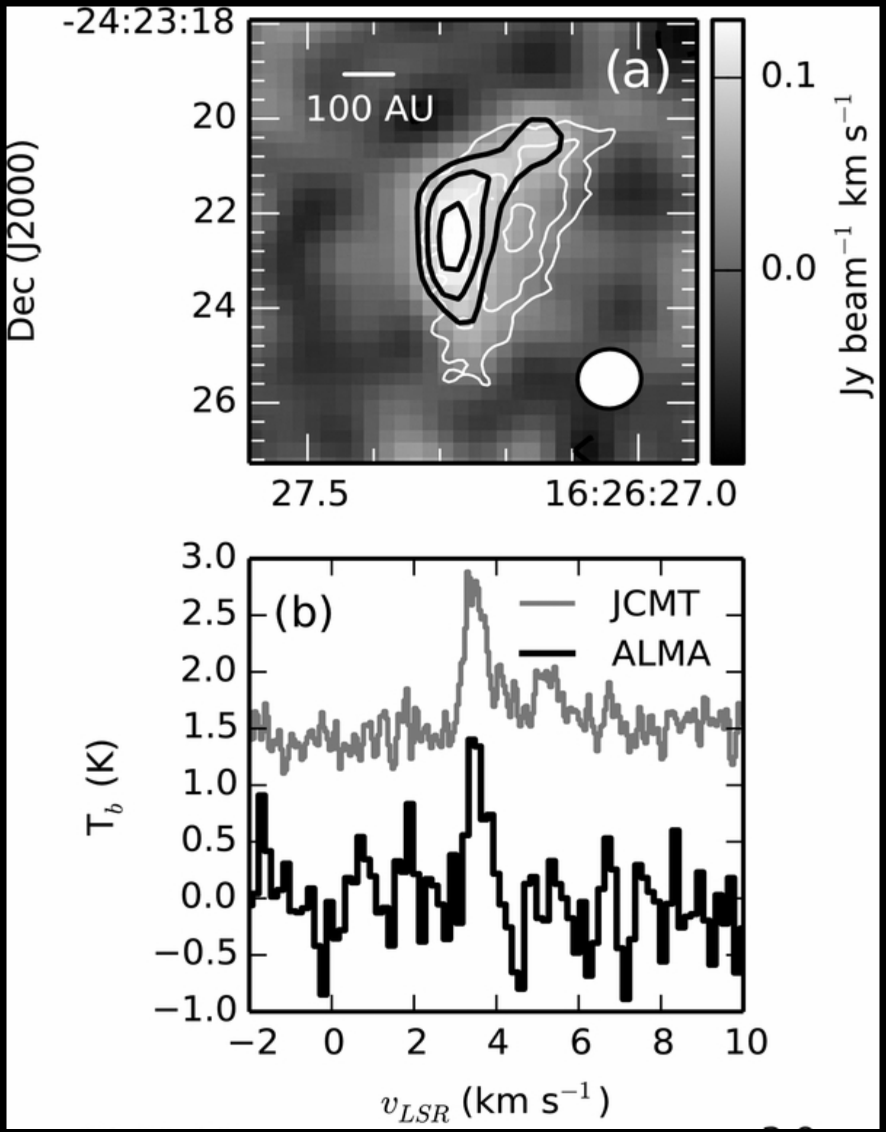




- Detection limits!
- ALMA: extended emission
- Need of a detailed benchmark among different radiative transfer codes for this particular problem of water in pre-stellar cores.

Quénard, Taquet, Vastel et al. 2016

High spatial resolution of H_2D^+



Friesen et al. 2014:

Integrated H_2D^+ 1_{10}–1_{11} intensity (black contours) toward the SM1N core (grayscale) at 1.3"(FWHM) resolution. White contours show the continuum emission

ALMA (black) and JCMT (gray) H_2D^+ spectra toward SM1N.

These data observationally reveal the earliest stages of the formation of circumstellar accretion regions and agree with theoretical predictions that disk formation can occur very early in the star formation process, coeval with or just after the formation of a first hydrostatic core or protostar.

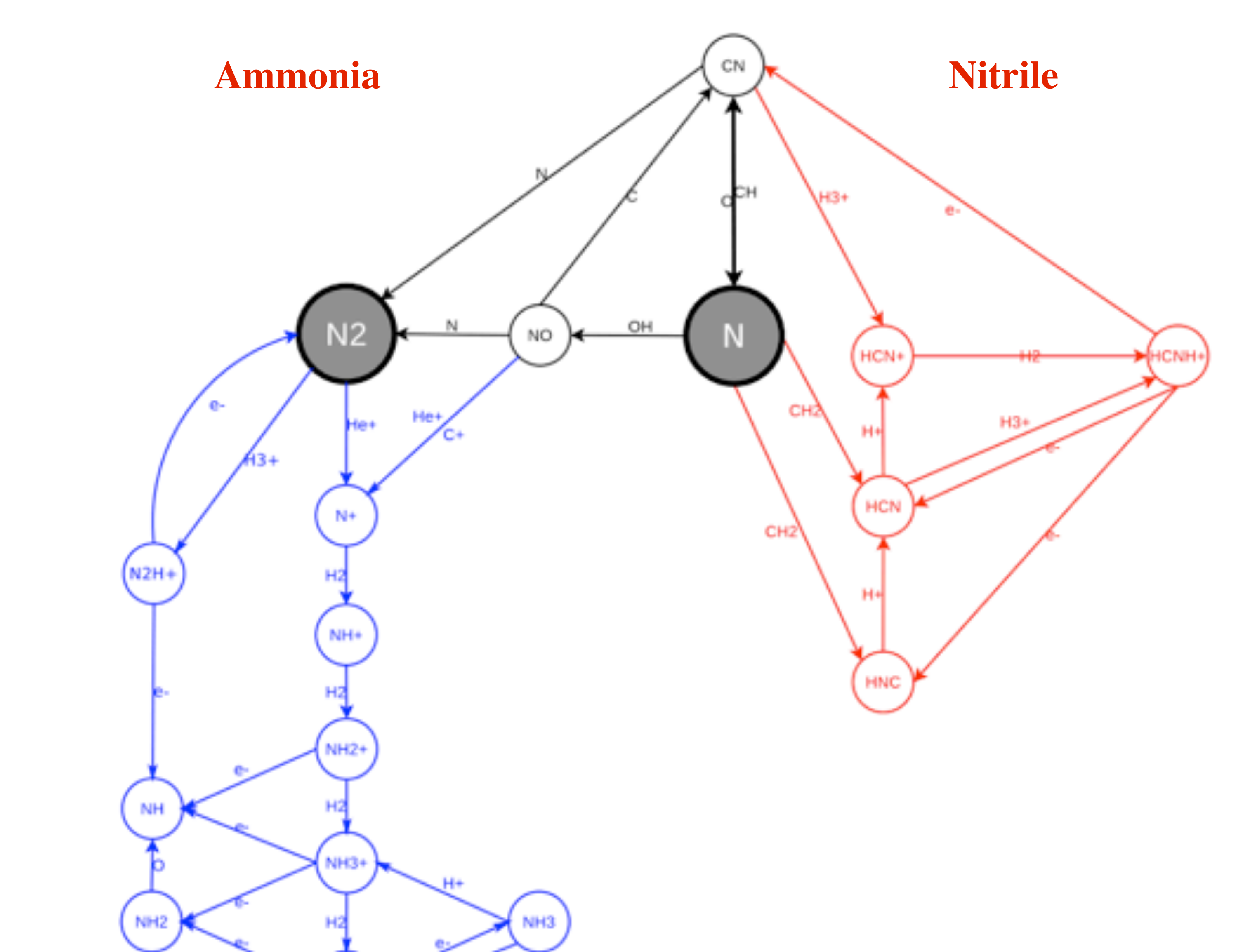
Nitrogen fractionation in L1544

Nitrile-bearing species (molecule carrying the –CN group or its isomer) have been found to be considerably enriched in ^{15}N (Ikeda+2002; Milam & Charnley 2012; Hily-Blant+2013):

Low $^{14}N/^{15}N \sim 260$ (HCN)

whereas ammonia derivatives show no ^{15}N enhancements or even a substantial depletion:

High $^{14}N/^{15}N > 700$ (NH_2D: Gérin+09; N_2H^+: Bizzocchi+2013)



Hily-Blant et al. 2013

Nitriles derive from atomic nitrogen, while ammonia is formed via N^+, which in turns come from N_2. The chemical networks responsible for their ^{15}N enrichment are thus well separated.

Nitrogen fractionation in L1544

^{15}N-enrichment of ammonia is highly sensitive to the H_2 ortho-to-para (OPR) ratio, while the fractionation evolution of nitriles is not significantly affected (Wirstrom+12).

The production of NH_3 is initiated by the ion-neutral reaction:

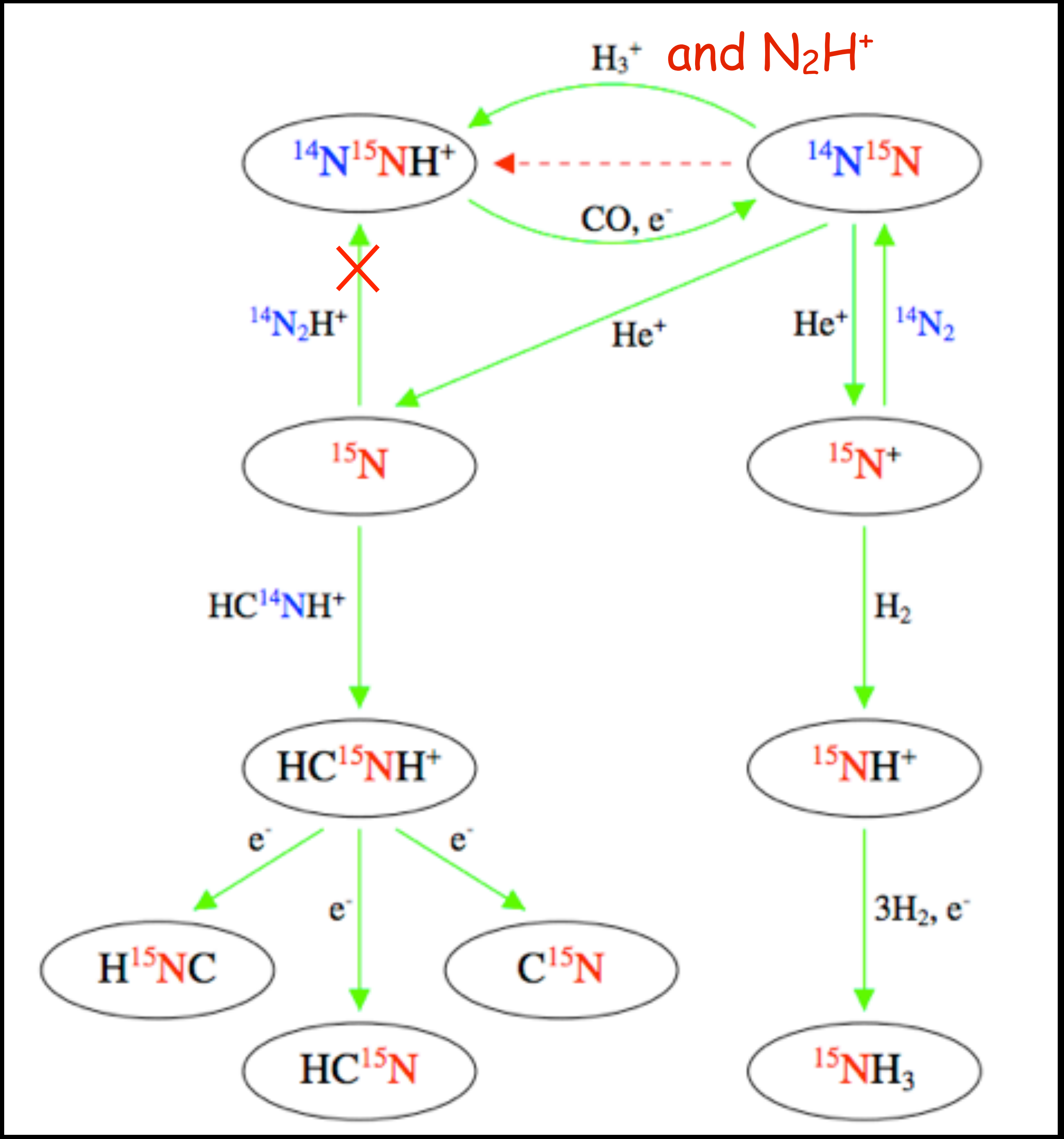
$$N^+ + H_2 \rightarrow NH^+ + H$$

whose activation energy barrier of ~200 K can be efficiently overcome by the o-H_2 internal energy.

On the other hand, ammonia fractionation gets much less efficient as the OPR decreases, and then an increasing quantity of $^{15}N^+$ is circulated back into molecular nitrogen by the equilibrium:

$$^{15}N^+ + {}^{14}N_2 \rightleftarrows {}^{14}N^+ + {}^{15}N^{14}N$$

Interdependence of C and N chemistries



Wirstrom+2012
Roueff+2015

Nitrogen fractionation in L1544

Bizzocchi+10: $^{14}N/^{15}N \sim 446 \pm 71$
($N^{15}NH^+$, LTE)

Bizzocchi+13: $^{14}N/^{15}N \sim 1000 \pm 200$
($^{15}N_2H^+$, non LTE)
Gérin+09: $^{14}N/^{15}N > 700$
(NH_2D)

Common fractionation pathway for the two molecules: not consistent with chemical models, which predicted small or no ^{15}N fractionation of N_2H^+.
Depletion?

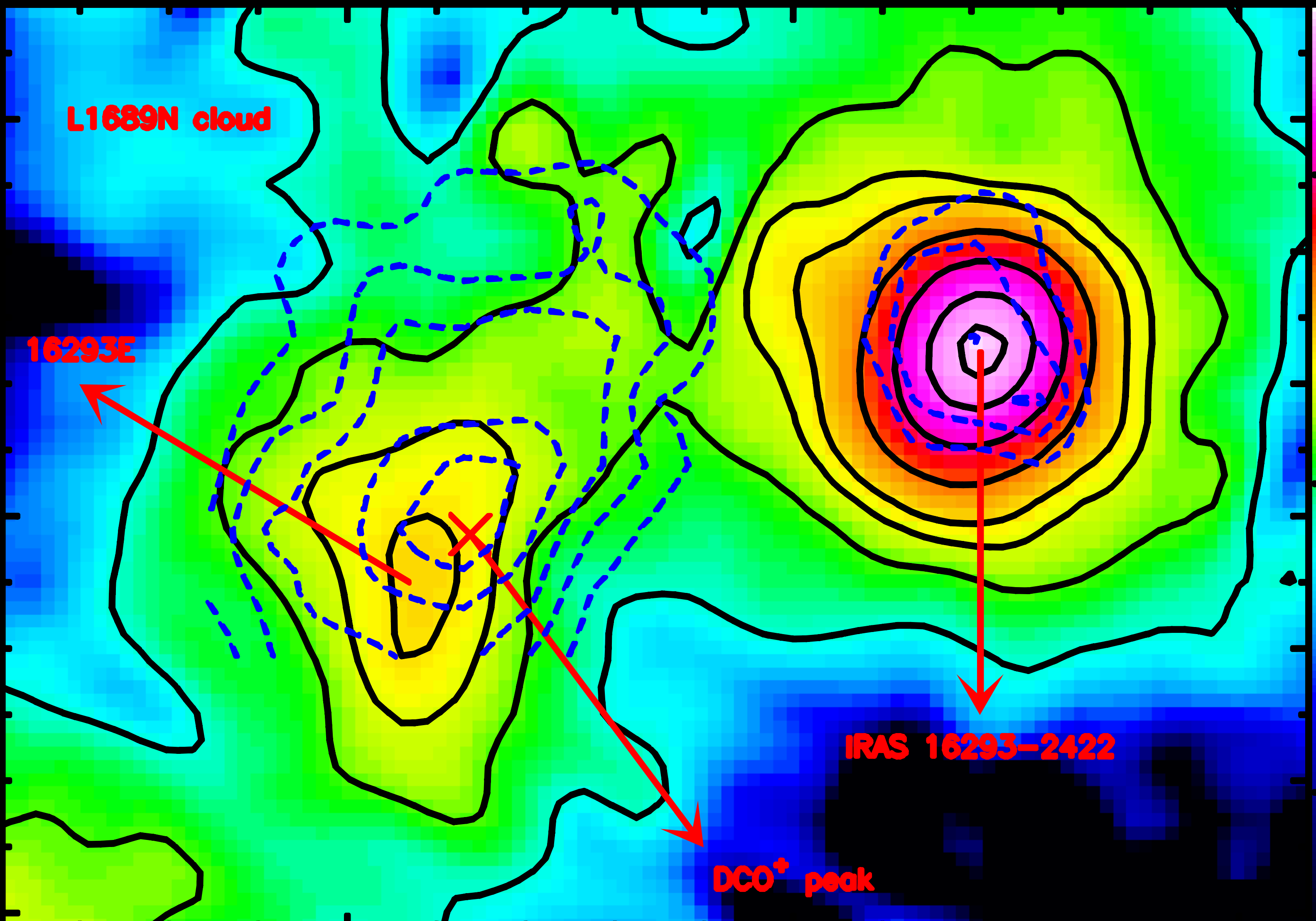
N_2H^+: $N_2 + H_3^+ \rightarrow N_2H^+ + H_2$

NH_3: $N^+ + H_2 \rightarrow NH^+ + H$

depends on the H_2 OPR

A way to reconcile our observational results with chemical modelling is to allow <u>selective freeze-out of ^{15}N</u> in some molecular form (possibly $^{15}N^{14}N$) on the surface of dust grains, something that needs to be tested in future models that include ^{15}N-bearing species and surface chemistry, as well with <u>laboratory work</u>.

Influence of the environment: 16293E



<u>D-ammonia</u>:
Lis+ 2002, 2006, Roueff+ 2015
<u>H_2D^+, D_2H^+</u>:
Vastel+ 2004, 2012
<u>ND</u>:
Bacman+ 2016
<u>Interferometric ND_3, N_2D^+</u>:
Lis+ 2016

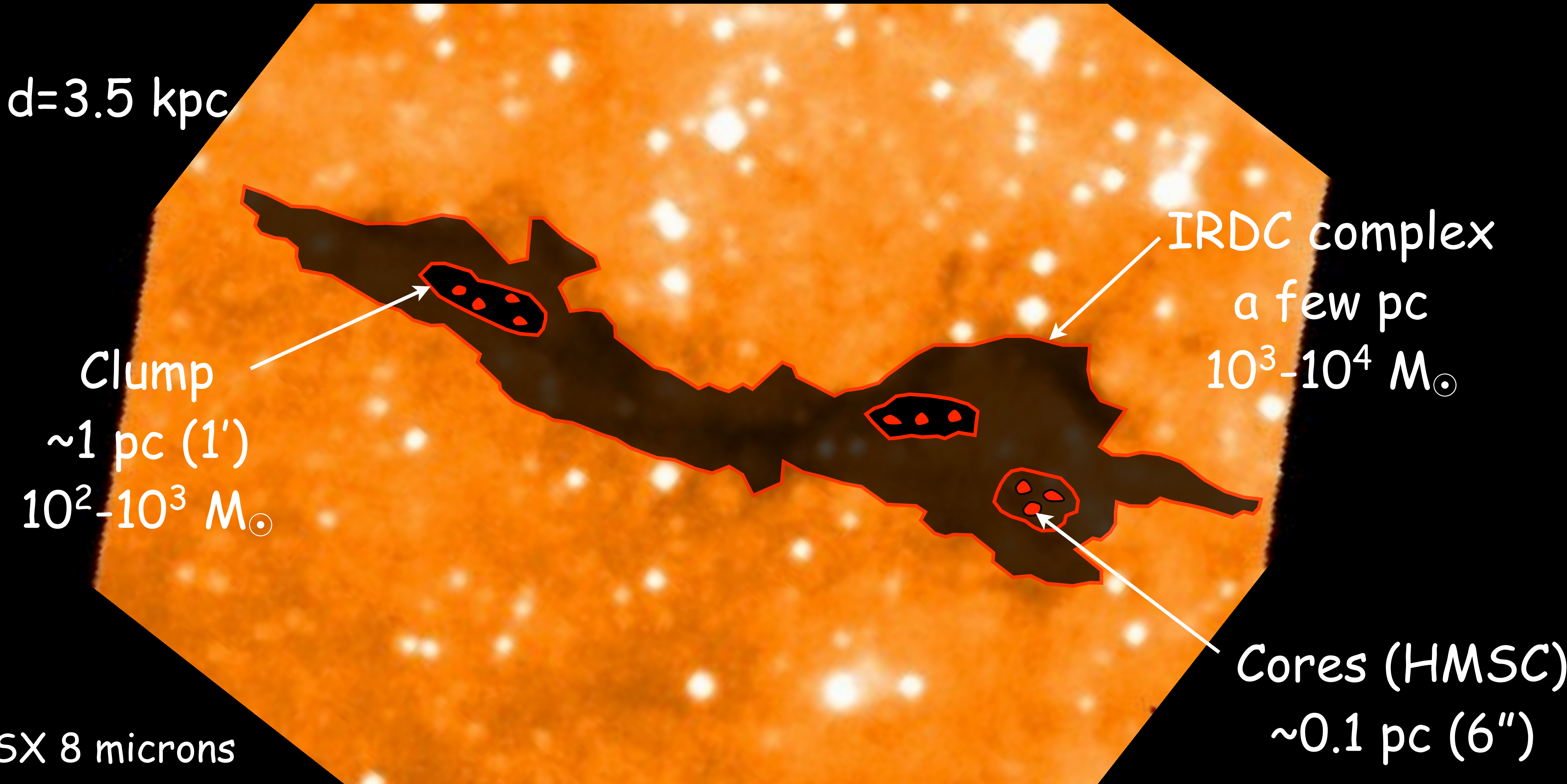
Daniel+ 16: N_2H^+ / $N^{15}NH^+$ ~ 330 comparable to the elemental isotope ratio inferred for the local ISM : no chemical fractionation.
Indeed, the most recent gas-phase network of Roueff+ 15 suggests that the fractionation reaction of ^{15}N with N_2H^+ is inefficient due to the presence of an activation barrier. However, cannot explain the L1544 observations.

⚠ Temperature dependance?

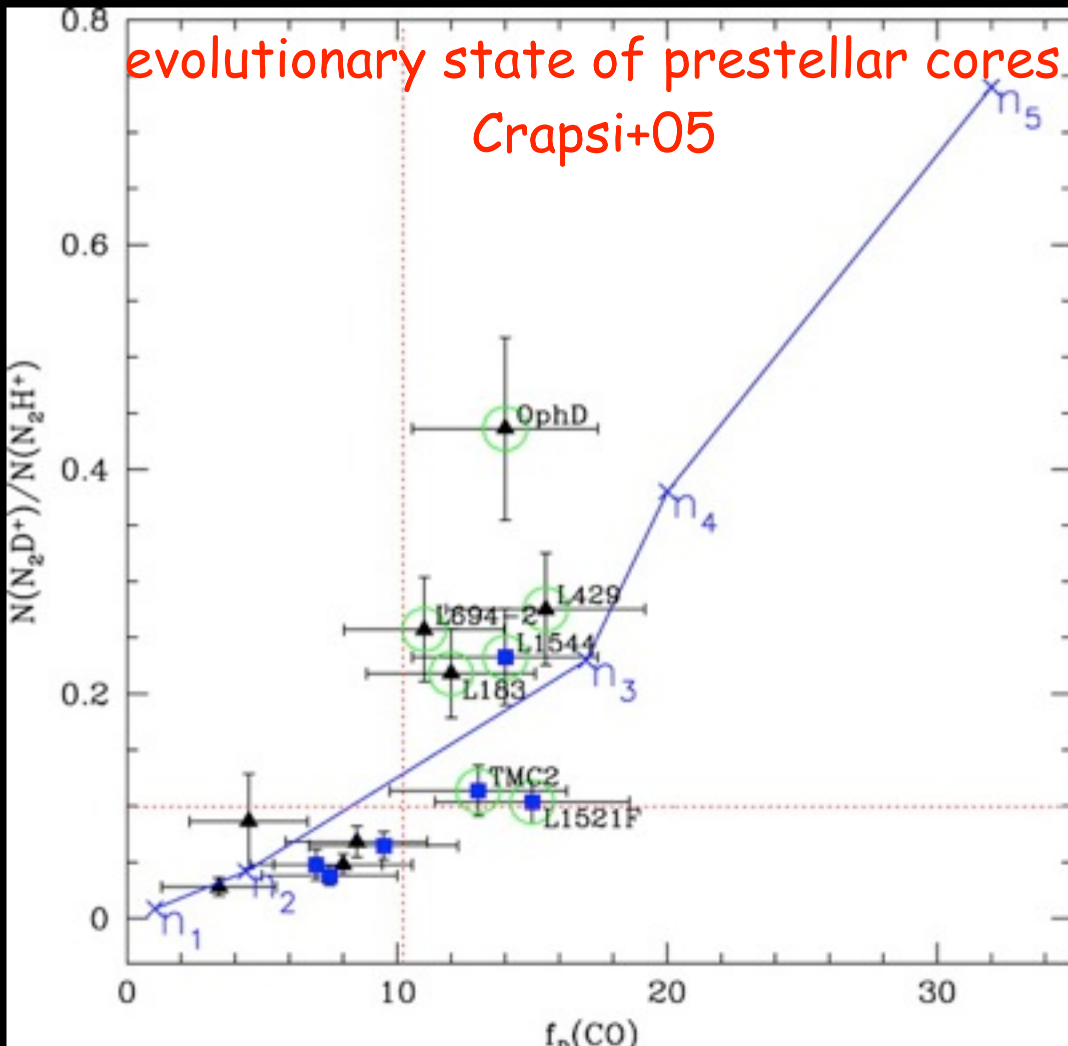
Massive vs low-mass prestellar core?

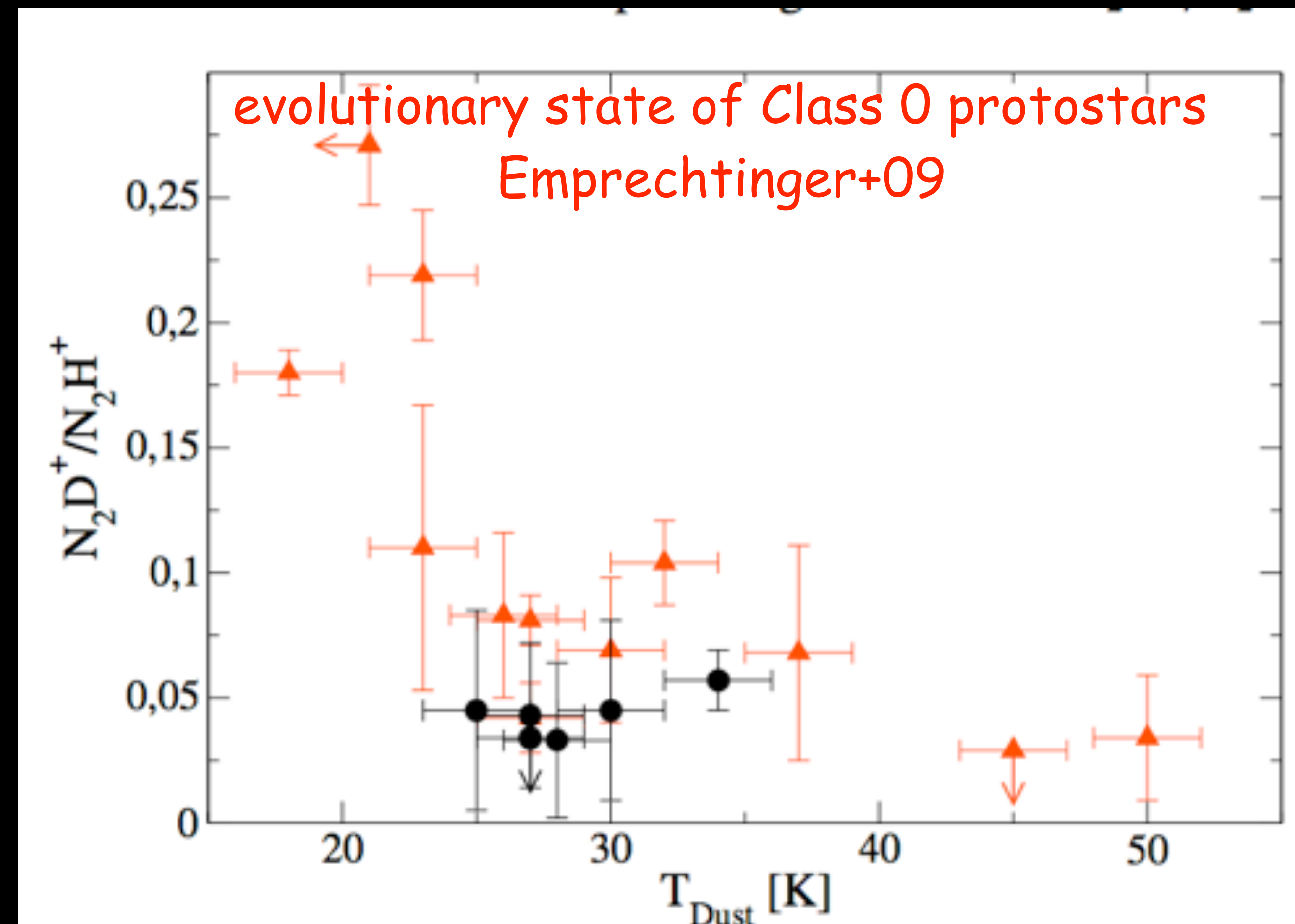
The sites of initial conditions of massive star birth are difficult to study.
Infrared dark clouds (IRDCs) are dense (n_{H_2}~10^5 cm^{-3}), cold molecular clouds (T<20K) , with masses 100-1000 $M_\odot$, seen in silhouette against 8μm Galactic plane emission.

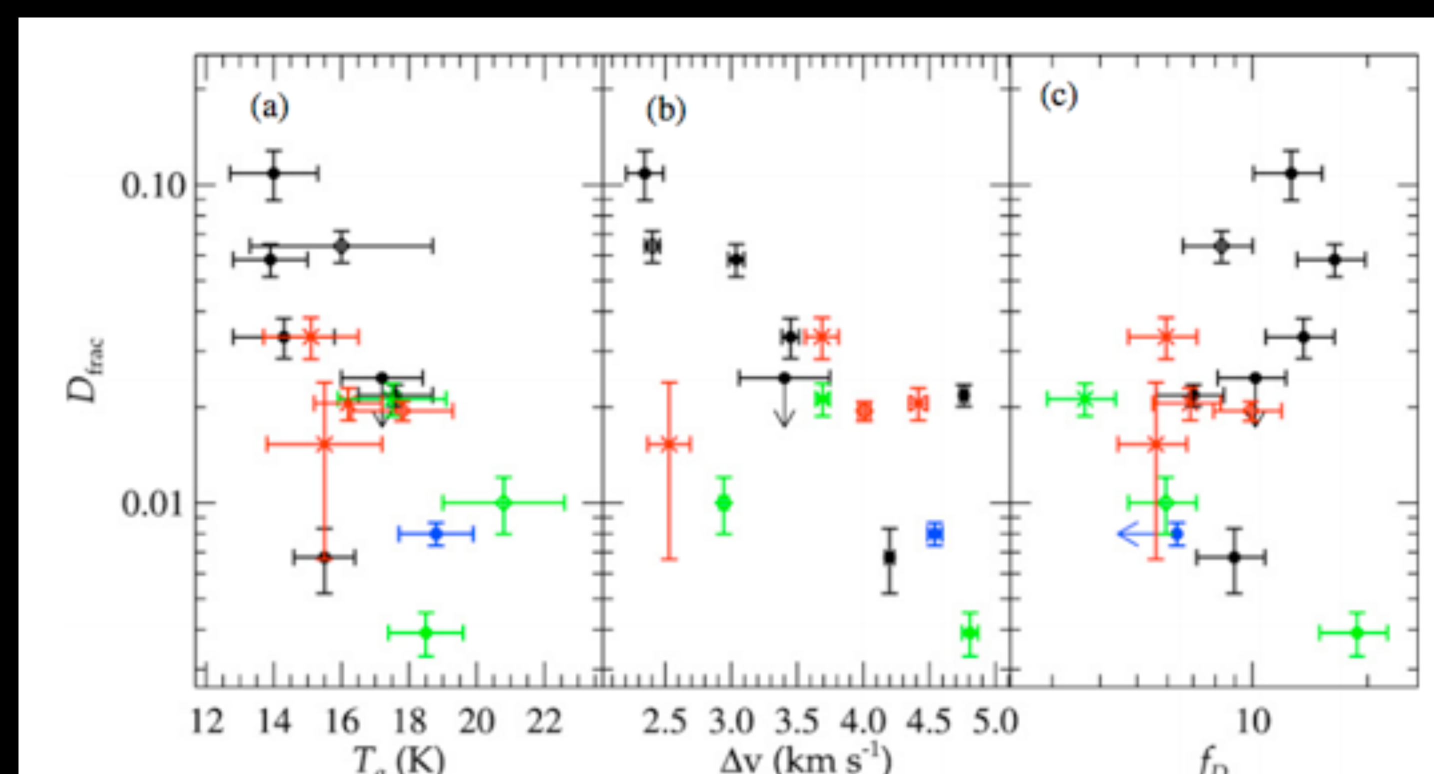
Pillai et al. (2007) detected high deuteration in IRDC clumps, evidence of very low temperatures.



D_{frac}^{N2H+} as an evolutionary indicator in the low and high-mass star formation process?





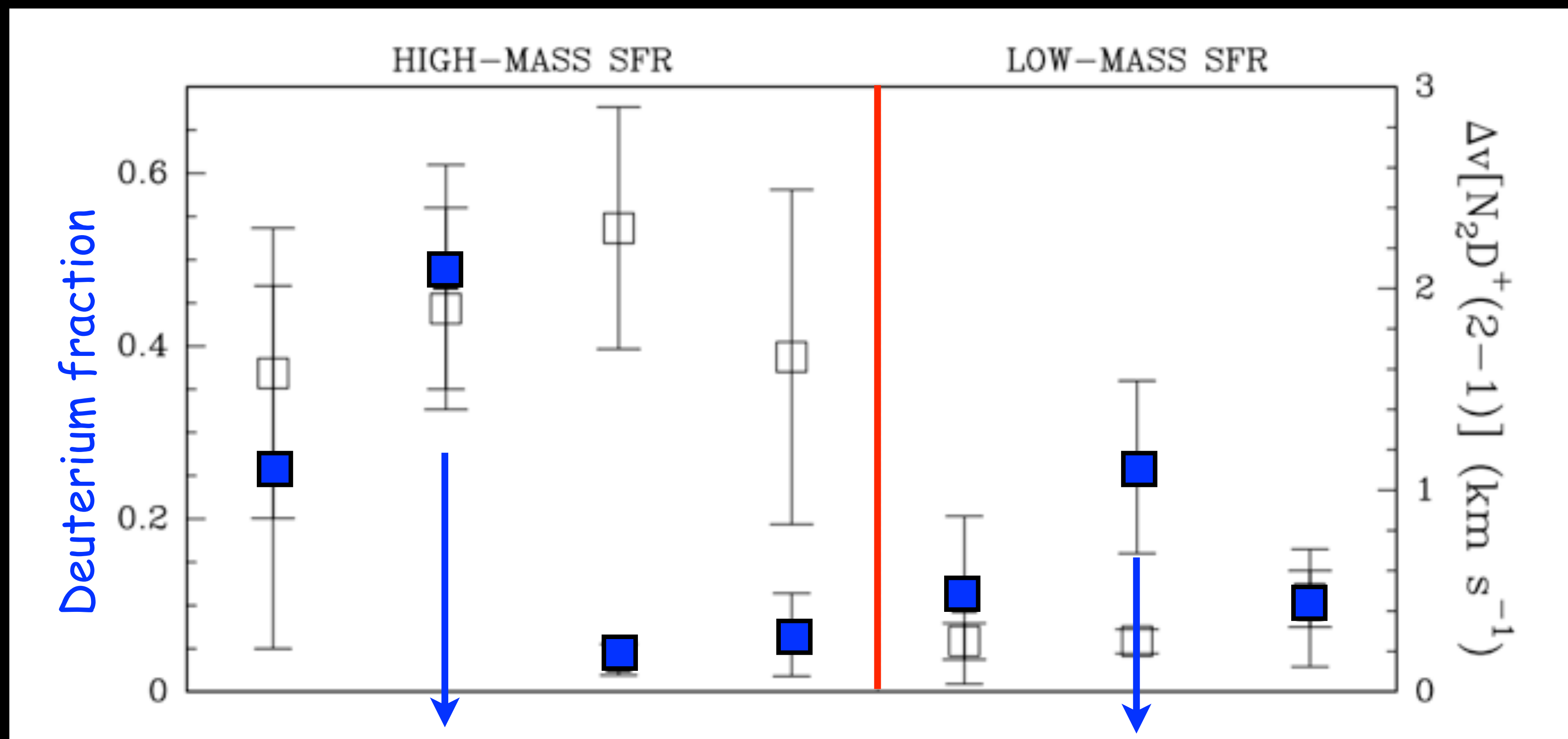


evolutionary state for high-mass star forming regions

Chen+11

Massive vs low-mass prestellar core?

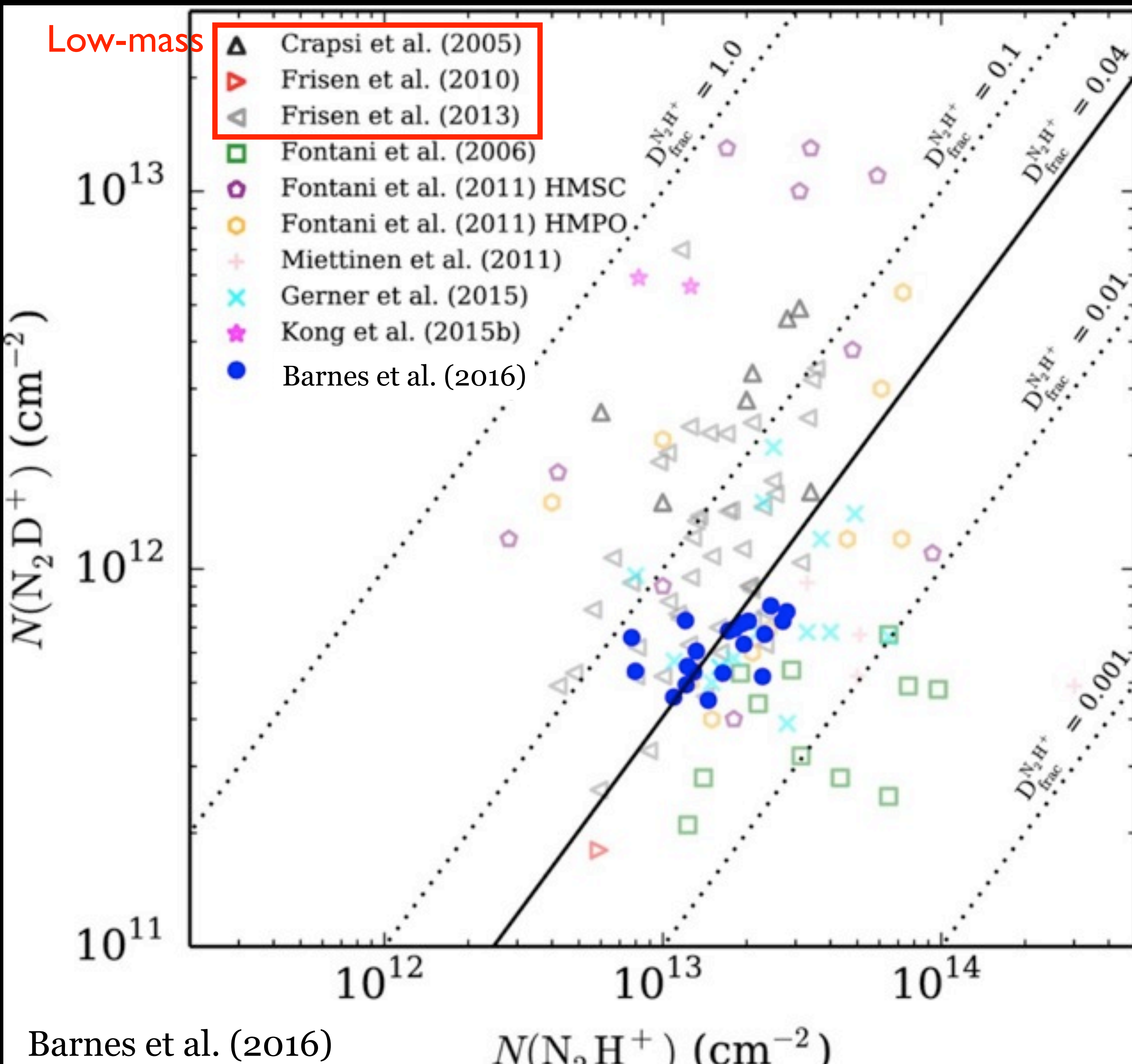
Differences: widespread NH_3 and N_2H^+ emission, presence of large scale SiO emission (shocks across the whole length of filament), higher pressure (larger line widths). But high deuteration.



Caselli 2014
Fontani+11,15
Crapsi+2005

high-mass starless cores in warm IRDCs
high-mass starless cores in cold IRDCs
high-mass protostellar objects
Ultra Compact HII regions
Low-mass starless cores
Low-mass pre-stellar cores
Class 0 sources

D_{frac}^{N2H+} as an evolutionary indicator in the low and high-mass star formation process?

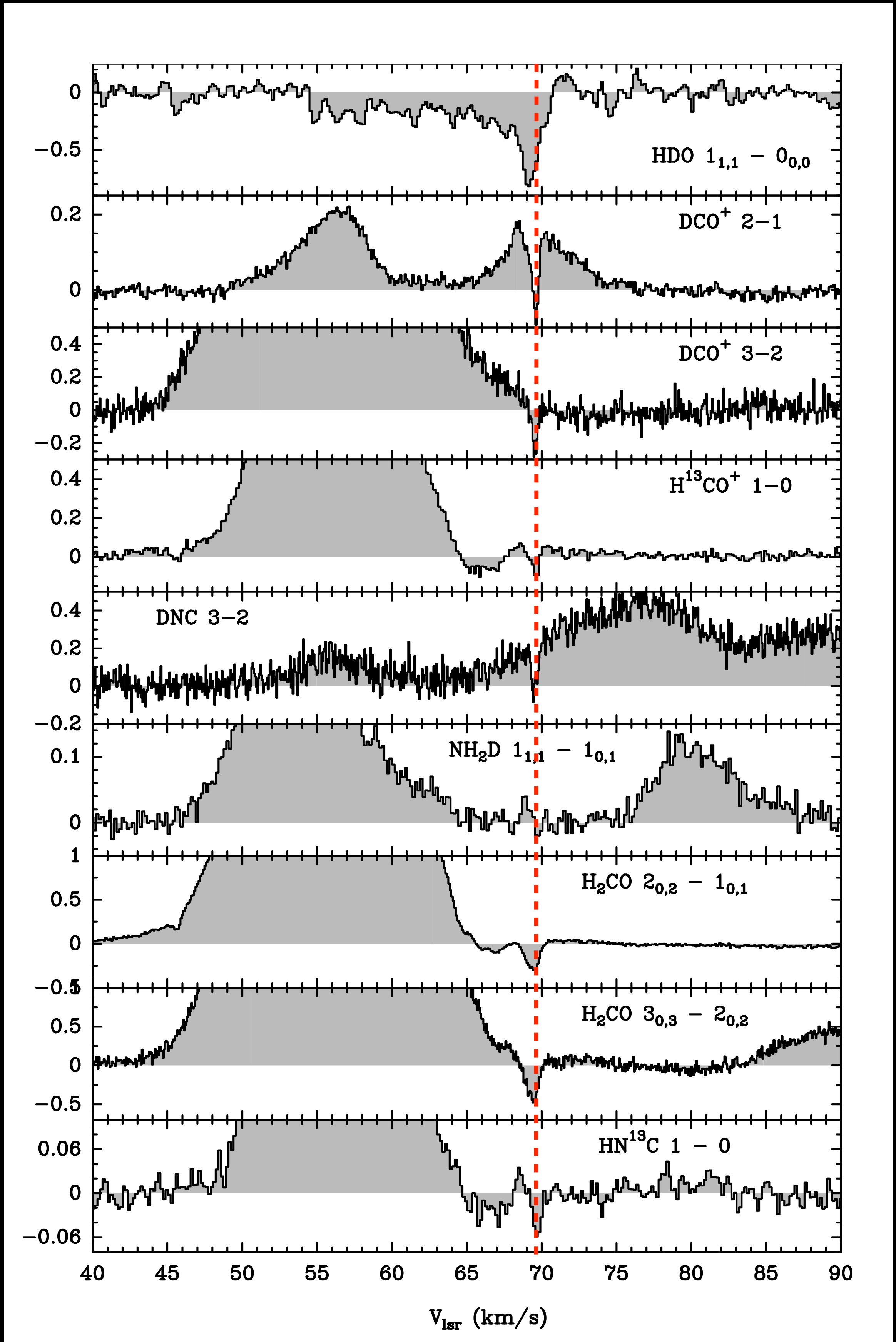


1) Some low D-frac found in some IRDCs (Gerner+15, Barnes+16) might be due to some <u>unresolved evolved object</u> (24 μm sources) since the average D-frac to similar to the values observed towards HMPO candidates (0.04; Fontani+11).

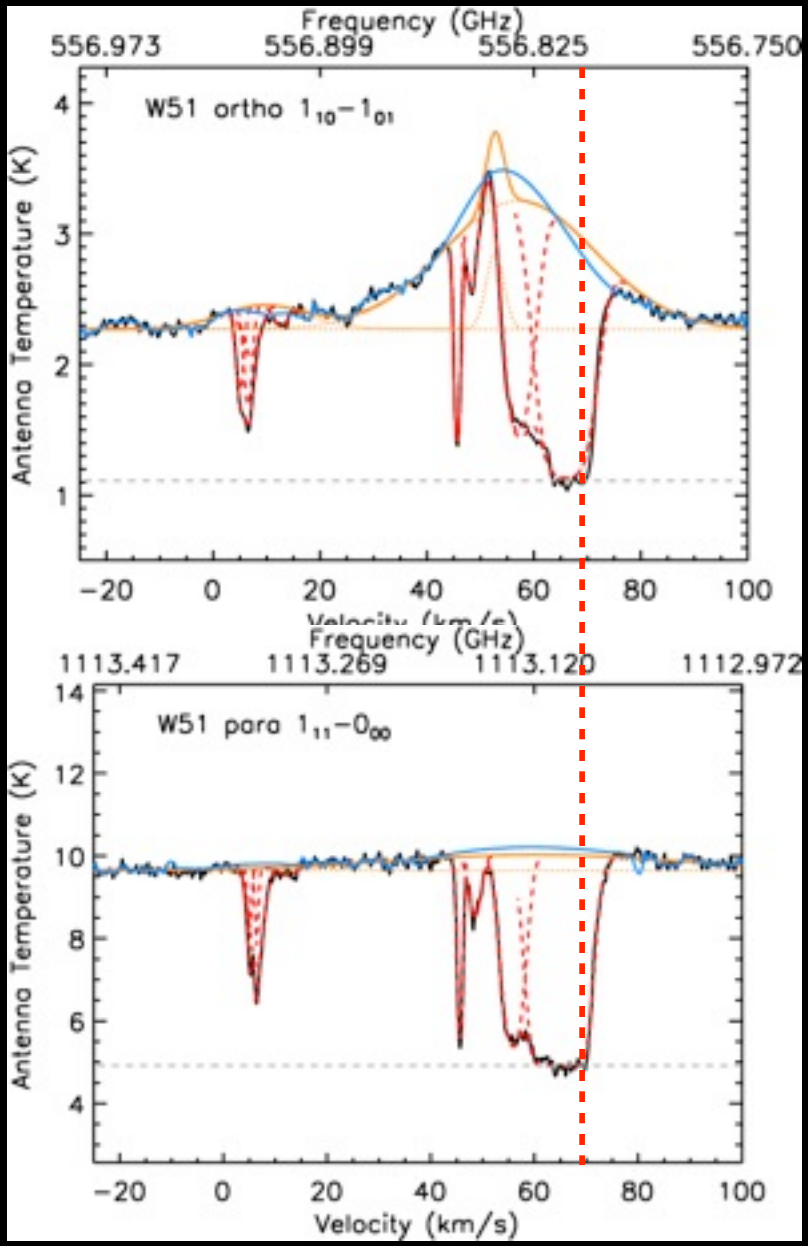
2) N_2D^+ more spatially concentrated in cores than N_2H^+ which is also present in the clump envelope. Therefore, measurement of the D-frac in massive star forming region could be limited by low spatial resolution (<u>beam dilution</u>).

Need for high spatial resolution of N_2H^+, N_2D^+ and H_2D^+ observations

A distant dark cloud?

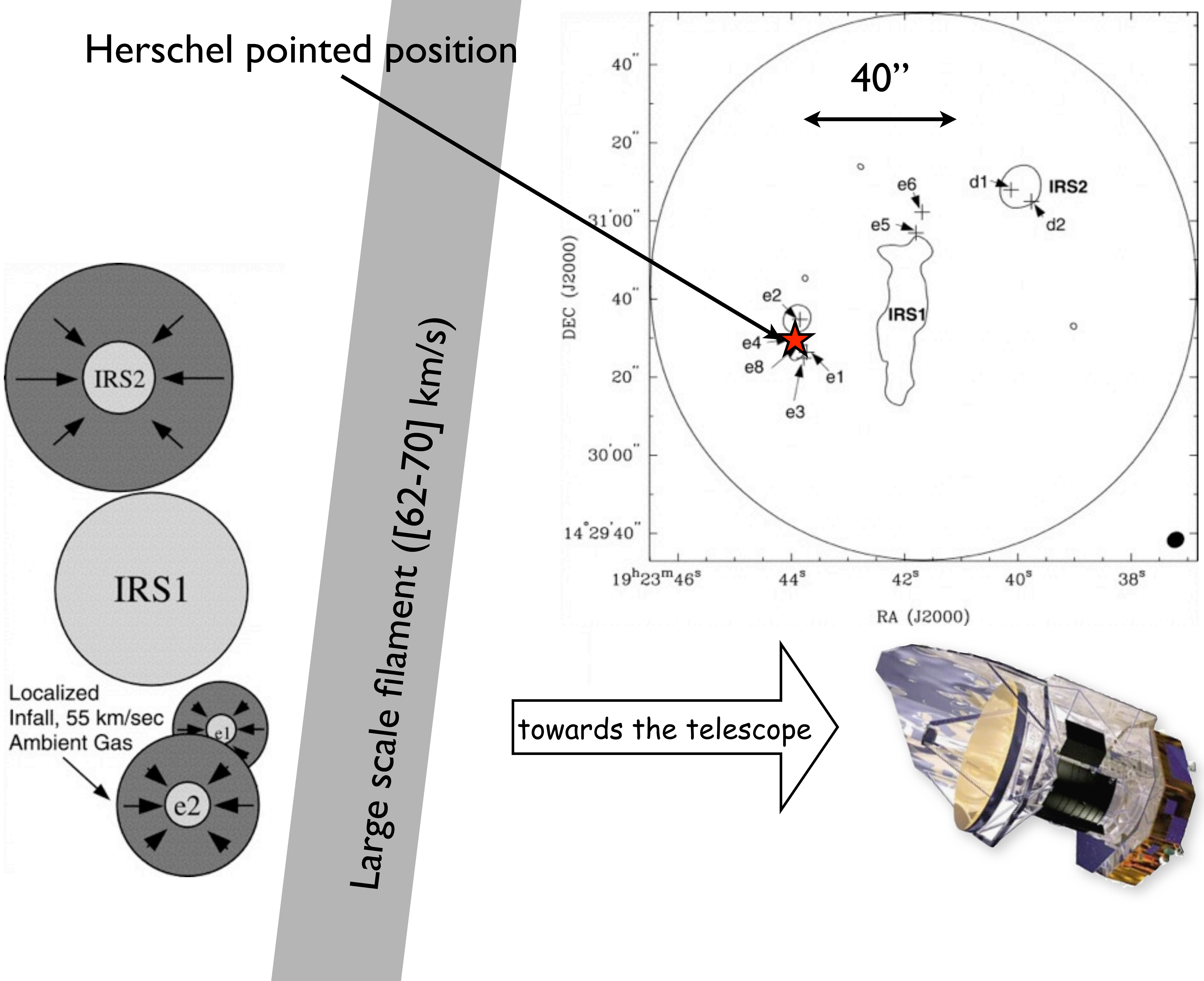


W51
d~5 kpc



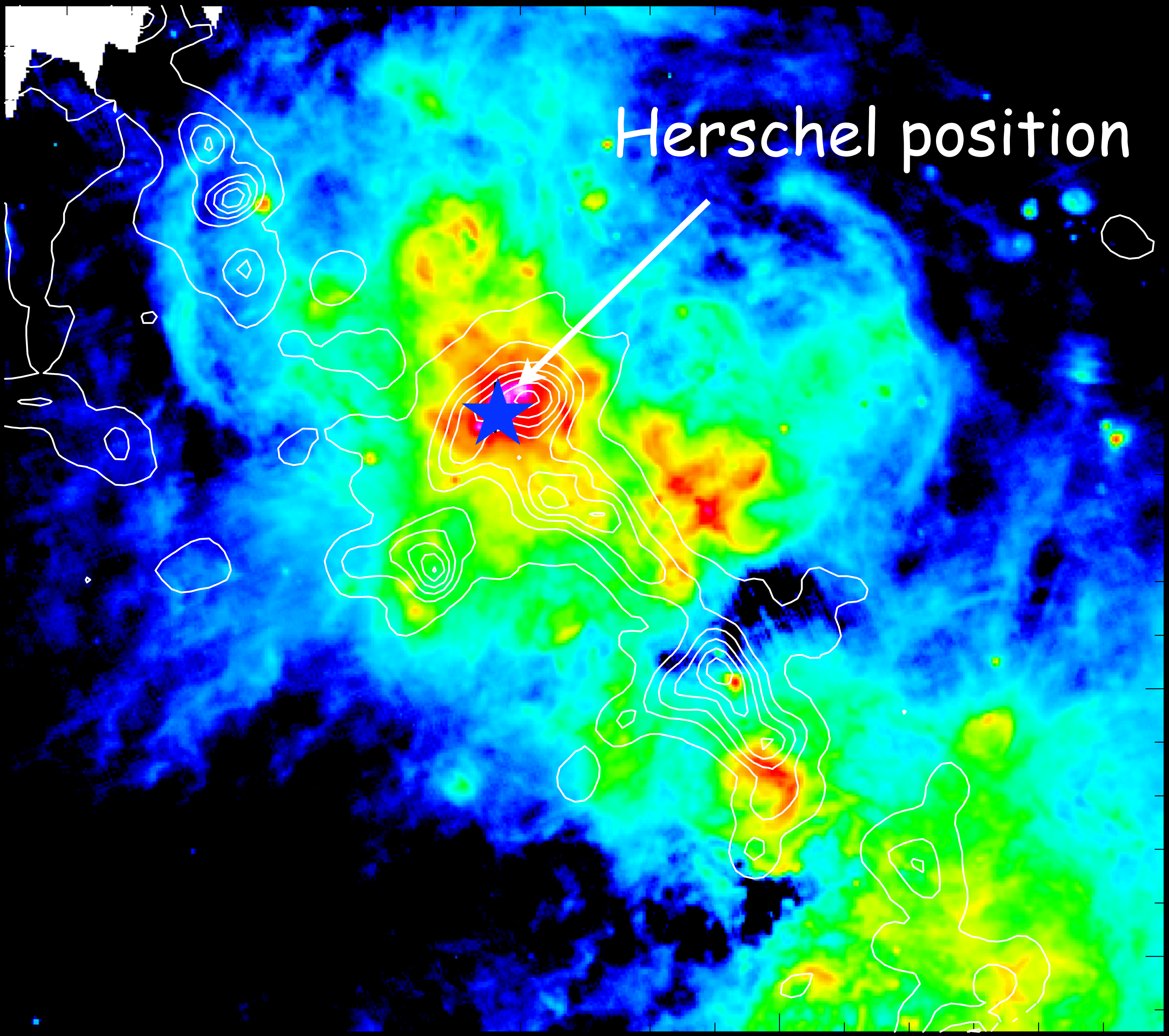
Flagey+2013

Mookerjea+2013
Vastel+2016



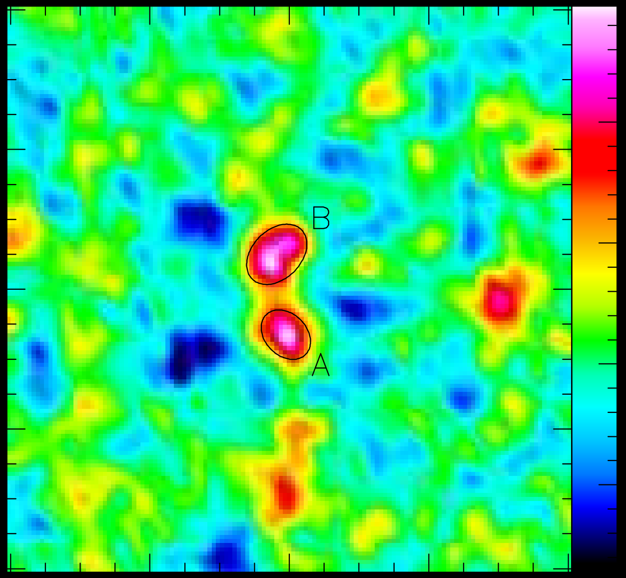
Herschel pointed position
40''
Large scale filament ([62-70] km/s)
IRS2
IRS1
Localized
Infall, 55 km/sec
Ambient Gas
e1
e2
d1
d2
e6
e5
e4
e8
e3
DEC (J2000)
RA (J2000)
40''
20''
31'00''
40''
20''
30'00''
14°29'40''
19h23m46s
44s
42s
40s
38s
towards the telescope

A distant dark cloud?



$HDO/H_2O=0.001$
$DCO^+/HCO^+=0.2$
$DNC/HNC=0.14$
$T\sim10K$
$n_{H_2}\sim2.5\ 10^4\ cm^{-3}$

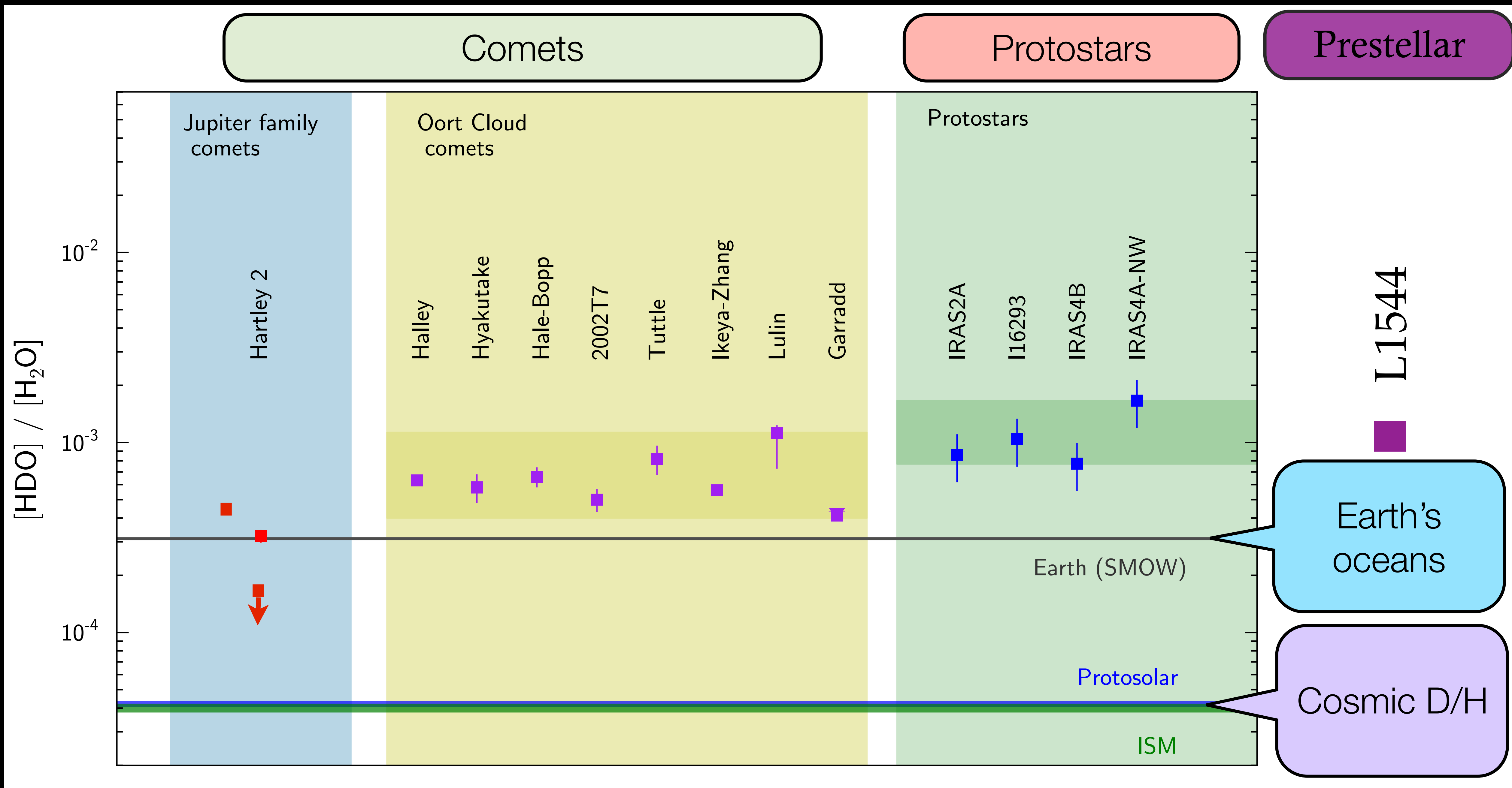
Dark cloud conditions (TMC1)



Vastel+2016

Result from the collision of the filament with W51

From prestellar, to protostar and planet



Thanks for your attention!