ALMA in Band 2

What type of astrochemistry can we do?

Serena Viti - UCL

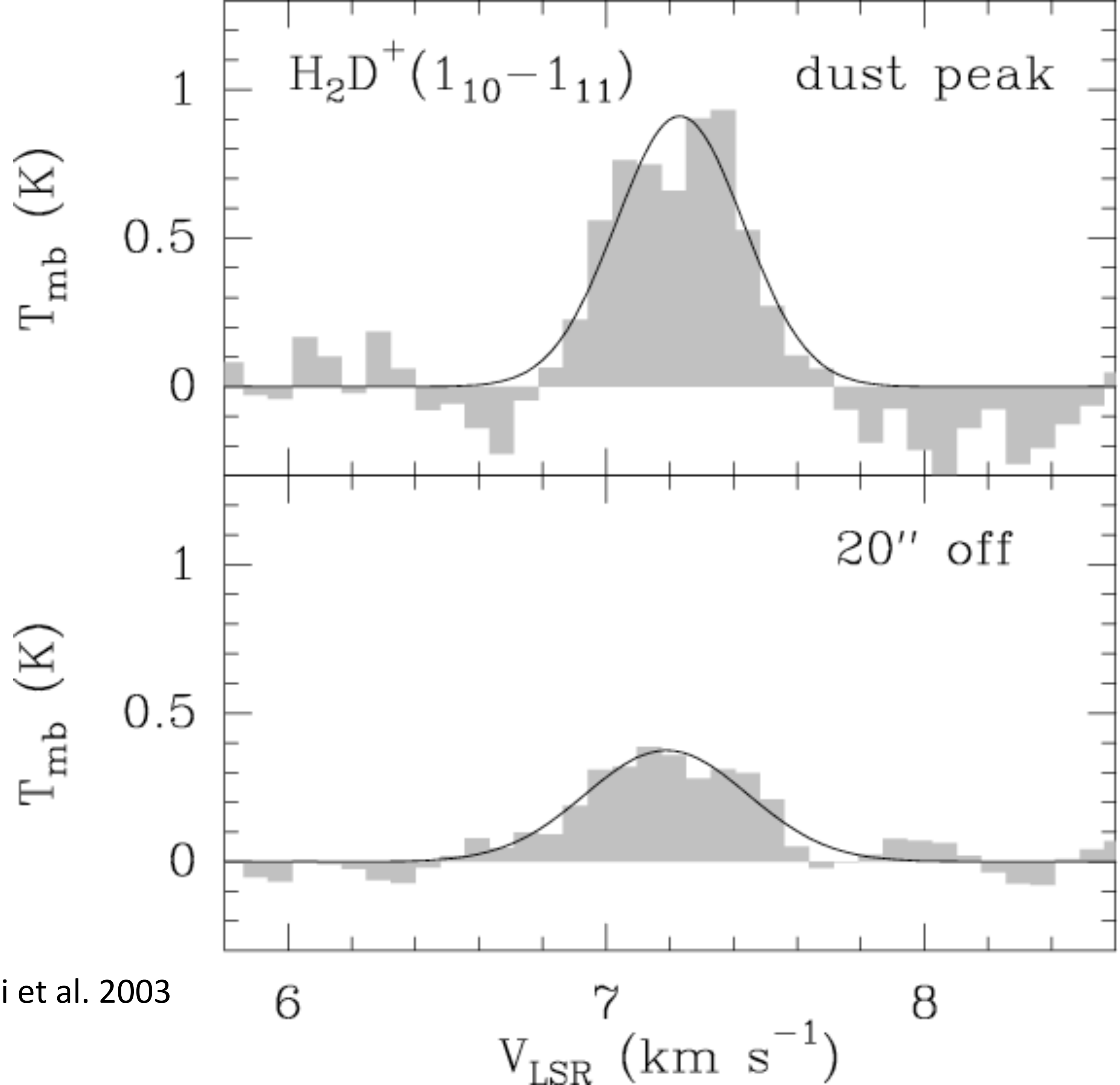
Examples of interesting transitions in Band 2 (mainly for galactic studies)

- HDO 1-1, 7-6
- NH_2D, several low J
- HCN 1-0
- DCN 1-0
- DNC 1-0
- HCO 1-0
- HOC^+ 1-0
- DCO^+ 1-0
- DOC^+ 1-0
- CH_3NH_2
- ……..

Several of these are deuterated species…..

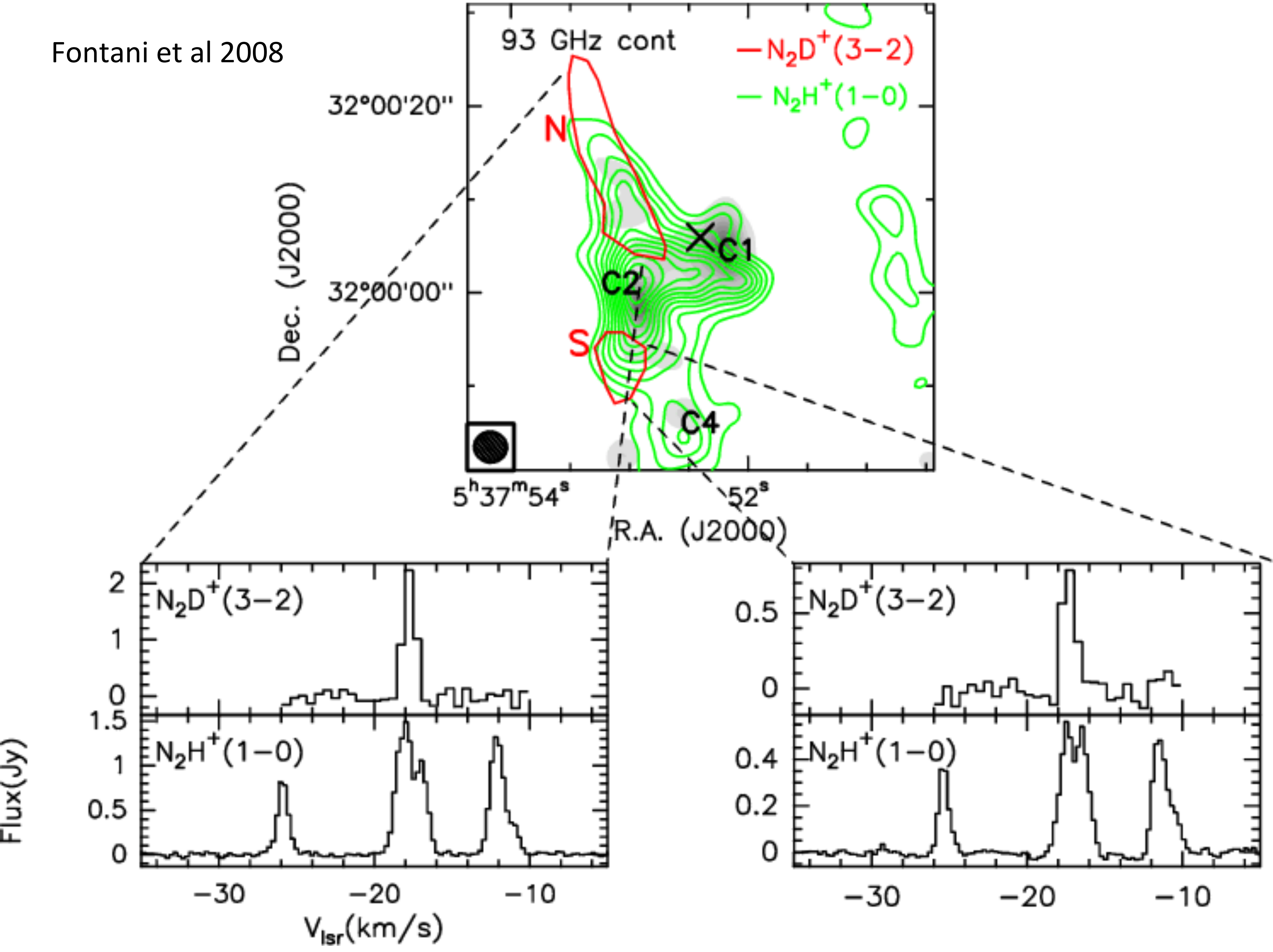
Deuterated molecules

- Deuterium form during the Big Bang and destroyed in the interiors of stars
- Observations along different lines of sights give D/H ~ 10^{-5}
- Yet, in the ISM deuteration is enhanced for many molecules more than a factor of 10^5 w.r.t. above ratio
- In particular, multiply deuterated species

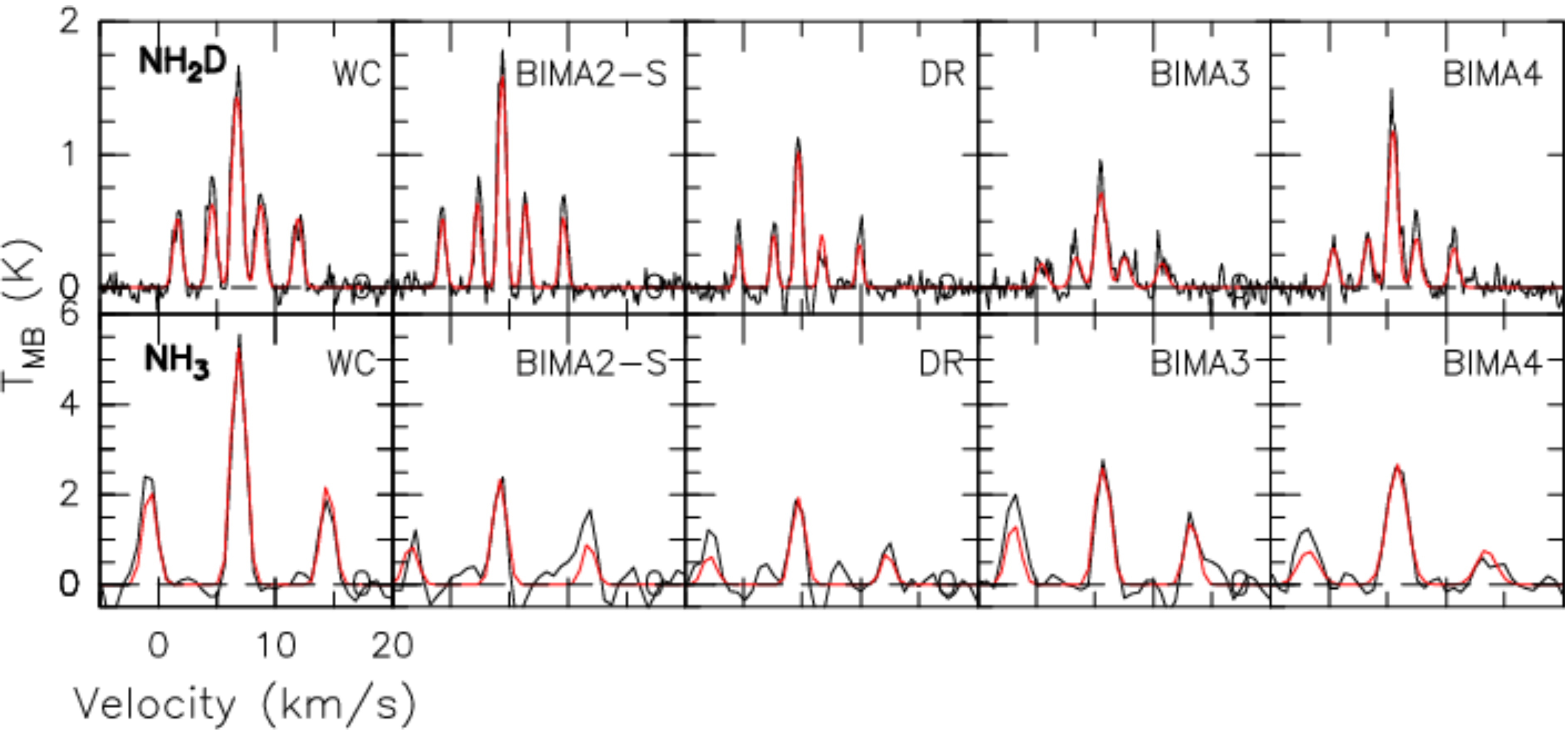


Caselli et al. 2003

Fontani et al 2008



Busquet et al. 2010



We know why....

- Start from HD (~10^{-5})
  - $H_3^+ + HD \rightarrow H_2D^+ + H_2$ (reverse is endothermic)
  - H_2D^+ + any other H-molecule → D-molecule
- In clouds, the main removal agent of H_3^+ is CO; but in a very cold dense cloud, CO is (partially) depleted on the surface of the grains → i.e in pre-stellar cores highest levels of deuteration, also 'left' in later phases.

- This is confirmed by several species:
  - D_2CO/H_2CO
  - $HDCO/H_2CO$
  - CD_3OH/CH_3OH
  - ND_3/NH_3
  - etc

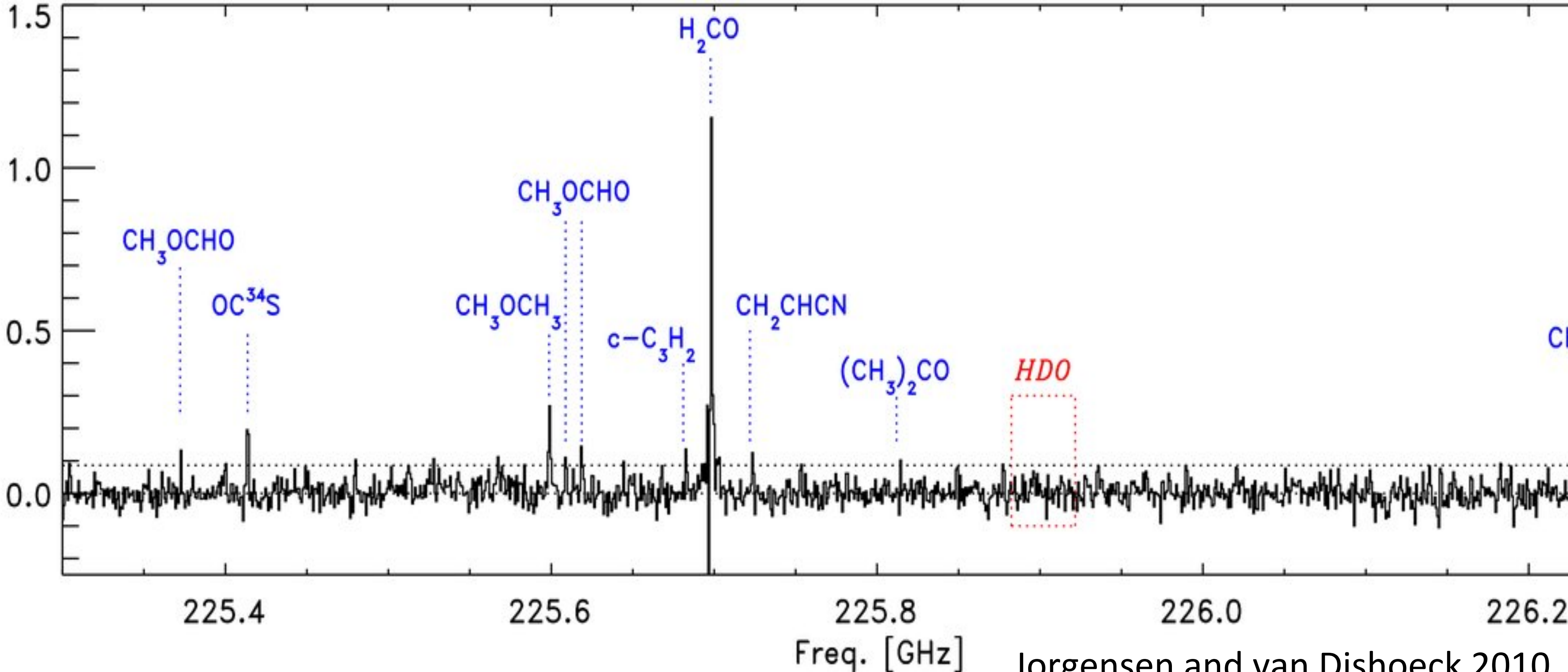
- However, water (via observations of hot corinos for example) constitutes a puzzle…
  - $HDO/H_2O < 0.2\%$ in the outer envelope (cold as in pre-stellar cores)
  - $HDO/H_2O \sim 3\%$ the inner envelope (ices evaporates, warm)

Cazaux et al 2011

Table 1
Deuterium Fractionation of Formaldehyde and Water Observed in Different Environments

Environment	Hot Corinos	Hot Cores	Compact Ridges	Comets
Densities (cm^{-3})	$\sim 10^{8}$ [a]	10^{9}–10^{10} [b]	10^{6} [c]	10^{10} [d]
$HDCO/H_2CO$	0.07–0.22 [e]	0.01–0.03 [e]	0.09–0.26 [f]	⩽0.05 [g] 0.28 [h]
D_2CO/H_2CO	0.01–0.03 [e]	⩽0.01 [e]	0.016–0.03 [f]	
HDO/H_2O	⩽$6\ 10^{-4}$ [i]	6×10^{-5}–5×10^{-4} [j]		3×10^{-4}–4×10^{-4} [k]
	⩾0.01 [l]			
	0.007–0.027 [m]			

Notes.
[a] Ceccarelli (2005).
[b] Roberts & Millar (2007).
[c] Charnley (1997).
[d] Woitke et al. (2009).
[e] Roberts & Millar (2007), Parise et al. (2006).
[f] Turner (1990).
[g] Crovisier et al. (2004) Hale-Bopp.
[h] Kuan et al. (2008) C/2002 T7.
[i] Liu et al. (2011) NGC1333-IRAS2A.
[j] Gensheimer et al. (1996).
[k] Meier et al. (1998), Villanueva et al. (2009).
[l] Jørgensen & van Dishoeck (2010) NGC 1333-IRAS4B.
[m] Hershel results IRAS16293−2422 (A. Coutens et al., in preparation).



Jorgensen and van Dishoeck 2010

- HDO/H_2O: key diagnostic for water evolution during star and planet formation
- It's enhanced in comets and on Earth w.r.t cosmic
- When does the enhancement happen?
- Observations of low mass protostars show that, in the inner 50 AU at least, it must be after the formation of the star
- Ultimately HDO detections are tentative!

HDO with ALMA (galactic)

- Maps of HDO (low J vs high J) covering the evolutionary sequence of low to high mass protostars, from pre-stellar to hot corinos/hot cores
- Objective would be to determine the spatial distribution of the water fractionation
- One of the main aims could be determination of the water abundance (HDO seems to be the same in ices, so removes the unknown factor of depletion)

NH_2D with ALMA

- $[NH_2D]/[NH_3]$: large (0.025--0.18), which is among the highest deuterium fractionation so far observed in massive pre-protostellar cores (Busquet et al. 2010)
- This could be indicative of evolution (because NH_2D abundance is high for starless cores, but low for YSOs) , but outflow interactions and UV could play a role.

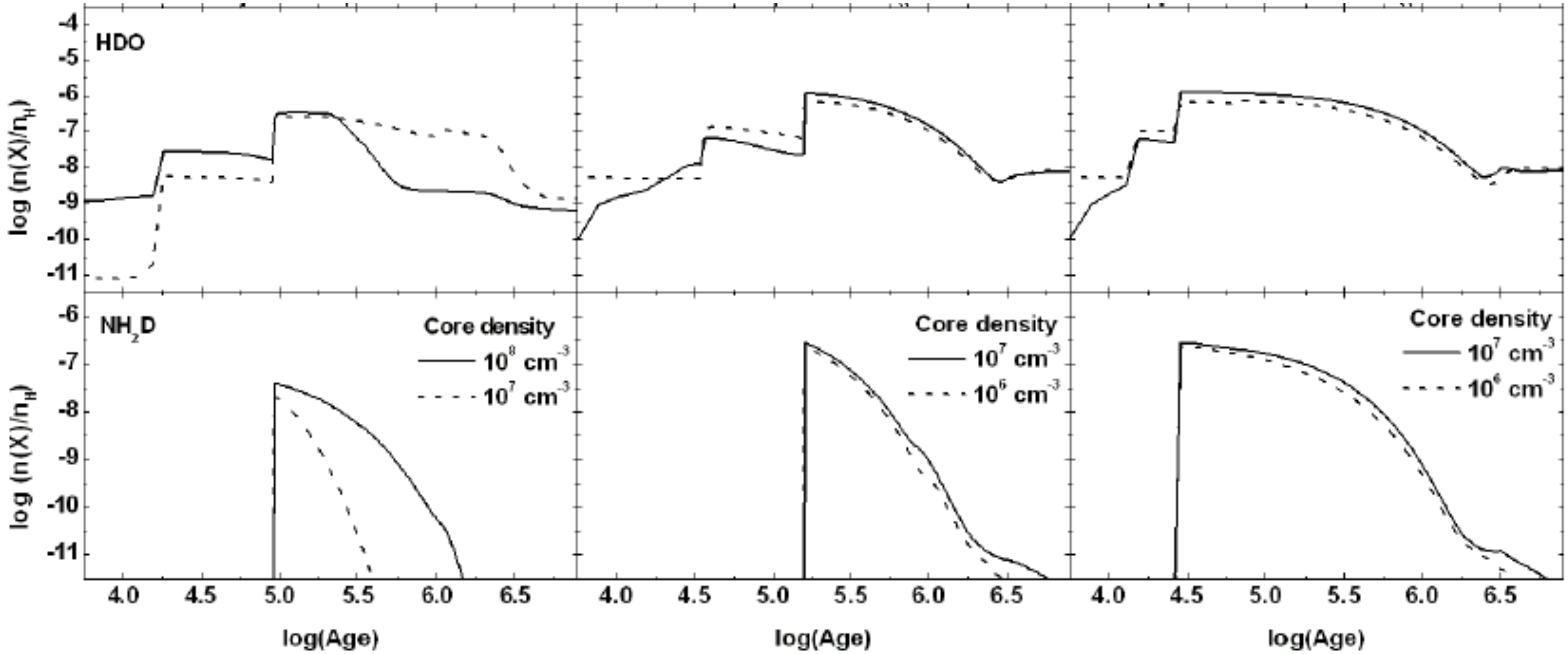


Figure 1. The chemical evolution (from top to bottom) of HDCS, HDS, HDO, and NH_2D in warm cores (column a: 1 $M_\odot$) and hot cores (column b: 5 $M_\odot$, and column c: 25 $M_\odot$) as a function of time. The different curves compare the evolution of the species at two different final densities for the collapsing cloud (see key, bottom plots).

Chemical models indeed confirm that NH_2D^+ varies with time – mapping could exclude variations due to UV or outflowing material (in general very little mapping work in high mass stars clusters has been done for deuterated species)

Awad, Viti, Williams, 2010

Nearby galaxies: Non deuterated molecules of interest

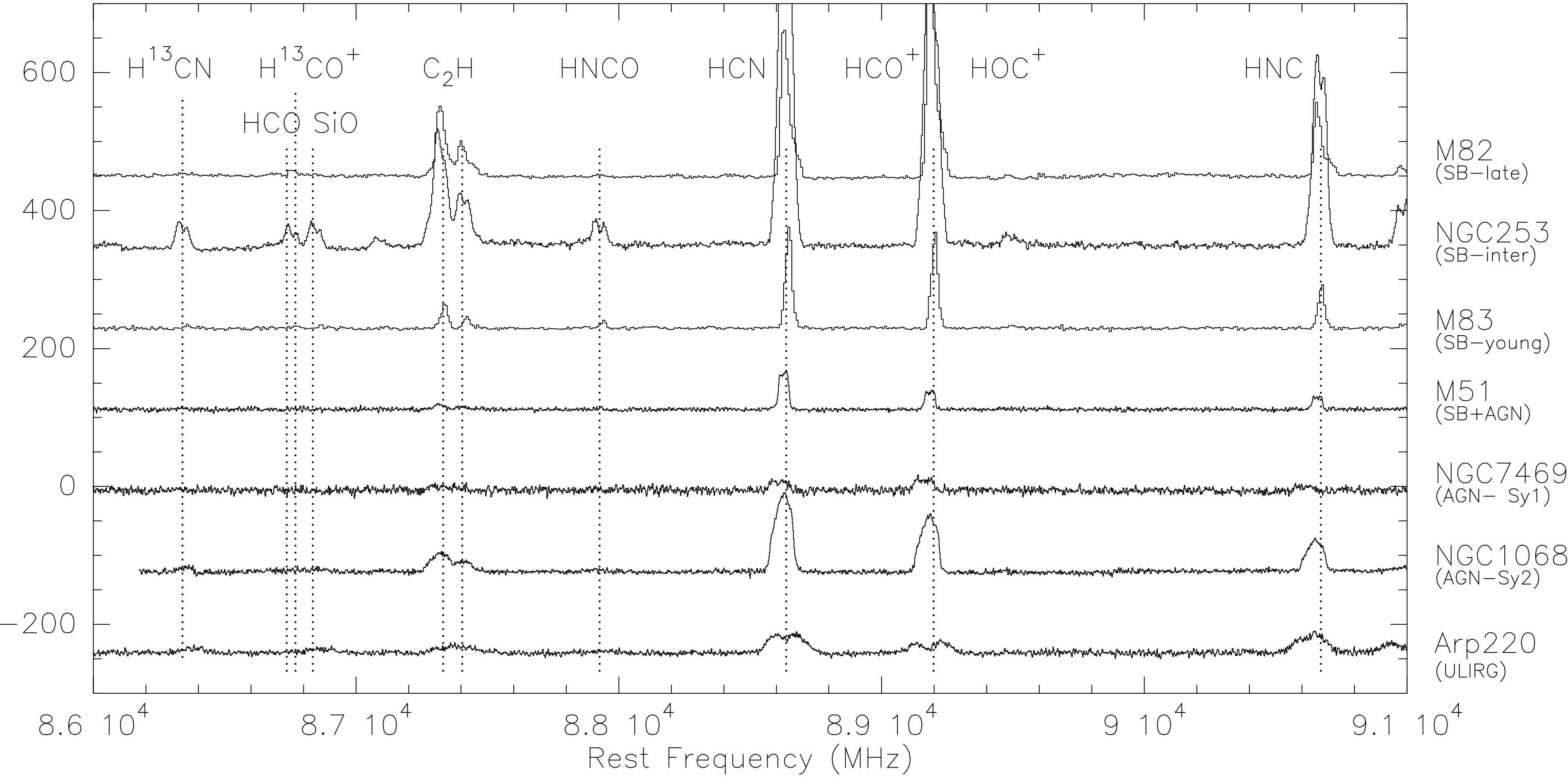
Already detected (Aladro et al. in prep)

- H13CN (1-0) @ 86.339
- HN13C(1-0) @ 87.090
- HCO+(1-0) @ 89.188
- H13CO+ (1-0) @ 86.754
- SiO (2-1) @ 86.846

Not observed so far

- CH3OH @ 68.366
- CH3CCH (4K-3K) @ 85.457
- CH3CCH (5K-4K) @ 73.590
- CH3CN (4K-3K) @73.590
- NS(2_1-1_1) @69-69.4(faint)
- SO (2_2-1_1) @86.093 (faint)
- HC3N (8-7) @ 72.783
- HC3N (9-8) @81.881
- OCS (6-5) @ 72.976 (faint)
- OCS (7-6) @ 85.139 (faint)

Aladro et al. in prep



- IRAM bands: > 80 GHz (in reality >85 GHz)
- CH_3CCH: heaviest molecule so far observed in external galaxies
- **H_2CO, CH_3CCH, CH_3CN: lines available for Band 2 complementary to transitions already observed → constrain excitation and column density**
- Note: for extragalactic environments, determining the excitation and density structure is essential to 'disentangle' degenerate solutions of chemical models and hence to determine the dominant energetic process(es)

Unexplored territory.....

- Bayet et al. (2010) have explored a large parameter space of physical conditions ‘covering’ different extragalactic environments
- Guide to observations of deuterated tracers of dense star forming gas in external galaxies

Bayet, Awad, Viti, 2010, ApJ

Table 3
Input Parameters for the UCL_Chem Models (See Section 2)

Model	n_f (cm^{-3})	Size (pc)	Metallicity[a] ($z_\odot$)	Gas-to-dust mass ratio	Ini. Elem. Abund. ratios	ζ[b] ($\zeta_\odot$)	Temp. T_2 (K)	I ($I_\odot$)	Comb. parameters
Normal spiral									
NS_1	10^5	1.00	1	100	ST	1	300	1	CB-A
NS_2	10^6	0.15	1	100	ST	1	300	1	CB-B
NS_3	10^7	0.03	1	100	ST	1	300	1	ST
Starburst									
SB_1	10^5	1.00	1	100	ST	1	500	10^3	CB-C
SB_2	10^6	0.15	1	100	ST	1	500	10^3	CB-D
SB_3	10^7	0.03	1	100	ST	1	500	10^3	CB-E
Cosmic-rays Enhanced									
SB_1+	10^5	1.00	1	100	ST	100	300	1	CB-A
SB_2+	10^6	0.15	1	100	ST	100	300	1	CB-B
SB_3+	10^7	0.03	1	100	ST	100	300	1	ST
Low metallicity									
Low-met_1	10^5	1.00	1/5	500	ST/5	1	500	10^3	CB-F
Low-met_2	10^6	0.15	1/5	500	ST/5	1	500	10^3	CB-G
Low-met_3	10^7	0.03	1/5	500	ST/5	1	500	10^3	CB-H
High redshift									
High-z_1	10^5	1.00	1/5	500	ST/5	100	500	10^3	CB-F
High-z_2	10^6	0.15	1/5	500	ST/5	100	500	10^3	CB-G
High-z_3	10^7	0.03	1/5	500	ST/5	100	500	10^3	CB-H

Notes. The abbreviation "ST" represents the standard values listed in Tables 1 and 2. The abbreviation "CB-A, -B, -C, -D, -E" correspond to the values listed in Table 4.

[a] $z_\odot = 1$ corresponds to solar values of the elemental abundances ratios.

[b] Expressed in units of $\zeta_\odot = 1.3 \times 10^{-17}\ s^{-1}$.

Bayet, Awad, Viti, 2010, ApJ

Table 5

Deuterated Molecules Detectable in Extragalactic Star Forming Regions and their Corresponding D/H Ratios (at a time = 10^6 yr) for Five Models Representative of Five Types of Galaxies (See Section 2)

Molecule	Normal Spiral			Starburst			Cosmic- rays Enhanced			Low metallicity			High redshift		
	NS_1	NS_2	NS_3	SB_1	SB_2	SB_3	SB_1+	SB_2+	SB_3+	Low-met_1	Low-met_2	Low-met_3	High-z_1	High-z_2	High-z_3
HDCO	++	++	++	++	++	++	+	+	+	+	+	+	+	+	++
D_2CO	+	+	+	+	+	+	-	-	-	-	-	-	-	-	-
DCN	++	+	+	++	+	+	++	++	++	++	++	+	++	++	++
DNC	+	+	-	-	-	-	-	-	-	-	-	-	-	-	-
DC_3N	-	-	-	+	-	-	-	-	-	-	-	-	-	-	-
DCO^+	-	-	-	-	-	-	+	-	-	-	-	-	-	-	-
H_2D^+	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HDO	++	++	++	++	++	++	++	++	++	++	++	++	++	++	++
C_2D	++	++	++	++	++	++	-	-	-	++	++	++	++	++	++
HDCS	++	++	++	++	++	++	-	-	-	++	++	++	+	+	+
HDS	+	+	+	-	-	+	-	-	+	-	-	-	-	-	-
NH_2D	++	++	++	++	++	++	+	-	-	+	+	-	-	-	-
N_2D^+	-	-	-	-	-	-	-	-	+	-	-	-	-	-	-
CH_3OD	+	+	+	+	+	+	-	-	-	-	-	-	-	-	-
CH_2DOH	+	+	+	+	+	+	-	-	-	+	-	-	-	-	-
CH_2DCN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
D_2CO/H_2CO	5.1×10^{-6}	8.8×10^{-7}	6.2×10^{-6}	2.8×10^{-5}	1.6×10^{-6}	4.0×10^{-5}	1.2×10^{-4}	4.2×10^{-4}	2.7×10^{-5}	3.1×10^{-6}	8.8×10^{-6}	3.7×10^{-6}	5.5×10^{-7}	3.8×10^{-6}	2.6×10^{-6}
DCN/HCN	1.4×10^{-4}	7.2×10^{-5}	2.0×10^{-4}	3.1×10^{-4}	7.6×10^{-4}	4.2×10^{-3}	1.6×10^{-3}	8.7×10^{-3}	2.0×10^{-3}	6.0×10^{-4}	3.5×10^{-3}	3.1×10^{-3}	6.3×10^{-4}	2.6×10^{-3}	8.2×10^{-3}
DNC/HNC	4.8×10^{-5}	2.4×10^{-5}	2.8×10^{-5}	6.5×10^{-6}	6.5×10^{-6}	2.2×10^{-5}	3.3×10^{-10}	2.3×10^{-11}	5.4×10^{-11}	1.9×10^{-7}	5.9×10^{-8}	8.8×10^{-8}	9.6×10^{-9}	3.2×10^{-9}	2.6×10^{-10}
NH_2D/NH_3	2.7×10^{-5}	1.3×10^{-5}	1.4×10^{-5}	3.3×10^{-5}	2.4×10^{-5}	2.6×10^{-5}	5.0×10^{-5}	1.5×10^{-5}	3.0×10^{-5}	1.3×10^{-6}	1.5×10^{-6}	1.8×10^{-6}	1.8×10^{-6}	1.6×10^{-6}	2.1×10^{-6}
DCO^+/HCO^+	3.9×10^{-4}	2.0×10^{-4}	2.1×10^{-4}	3.0×10^{-4}	2.4×10^{-4}	4.2×10^{-4}	6.5×10^{-3}	2.2×10^{-3}	2.9×10^{-4}	8.2×10^{-5}	1.5×10^{-4}	2.4×10^{-4}	7.1×10^{-4}	5.6×10^{-4}	5.4×10^{-4}
$HDCO/H_2CO$	1.0×10^{-3}	5.7×10^{-4}	5.0×10^{-4}	3.3×10^{-3}	9.2×10^{-4}	2.5×10^{-4}	1.7×10^{-2}	3.3×10^{-2}	2.5×10^{-1}	6.2×10^{-3}	9.5×10^{-3}	1.4×10^{-3}	7.5×10^{-3}	6.7×10^{-2}	1.4×10^{-1}
CH_3OD/CH_3OH	1.1×10^{-3}	7.2×10^{-4}	7.3×10^{-4}	9.3×10^{-4}	5.8×10^{-4}	6.4×10^{-4}	1.5×10^{-2}	1.2×10^{-2}	3.6×10^{-3}	8.0×10^{-3}	6.7×10^{-3}	9.1×10^{-3}	4.6×10^{-3}	9.0×10^{-3}	8.3×10^{-2}
CH_2DOH/CH_3OH	1.5×10^{-3}	1.2×10^{-3}	1.1×10^{-3}	1.5×10^{-3}	8.7×10^{-4}	5.8×10^{-4}	1.9×10^{-2}	1.5×10^{-2}	1.3×10^{-2}	9.5×10^{-2}	6.6×10^{-2}	2.4×10^{-2}	7.5×10^{-3}	3.0×10^{-2}	3.3×10^{-1}
CH_2DCN/CH_3CN	7.2×10^{-4}	1.4×10^{-3}	5.4×10^{-4}	6.1×10^{-3}	1.0×10^{-3}	1.1×10^{-4}	3.1×10^{-5}	2.9×10^{-5}	3.8×10^{-5}	4.1×10^{-3}	3.9×10^{-3}	4.2×10^{-4}	7.2×10^{-3}	6.8×10^{-2}	5.3×10^{-2}
H_2D^+/H_3^+	7.5×10^{-5}	7.6×10^{-5}	7.6×10^{-5}	5.6×10^{-5}	5.6×10^{-5}	5.3×10^{-6}	6.6×10^{-5}	6.1×10^{-5}	5.6×10^{-5}	1.8×10^{-5}	1.7×10^{-5}	1.7×10^{-5}	1.9×10^{-5}	1.1×10^{-5}	4.7×10^{-6}
N_2D^+/N_2H^+	5.2×10^{-4}	2.1×10^{-4}	2.4×10^{-4}	5.3×10^{-4}	5.4×10^{-4}	1.4×10^{-3}	1.2×10^{-3}	9.4×10^{-4}	1.9×10^{-4}	2.9×10^{-4}	4.8×10^{-4}	8.1×10^{-4}	7.1×10^{-4}	1.1×10^{-3}	1.5×10^{-3}

Notes. The limit of detectability has been taken to be $[n(X)/n_H] = 1 \times 10^{-12}$, as is typical for dense gas in the Milky Way. Below this limit, we assumed the species as not detectable (symbol "-"). Otherwise, they are marked with the symbol "+." When the fractional abundance of a deuterated species is above $[n(X)/n_H] = 1 \times 10^{-10}$, the symbol "++" is used.

Model predictions: of particular interest for extragalactic studies for ALMA band 2….

- HDO, DCN: very abundant regardless of the environments
- DCO^+: tracer of cosmic-ray enhanced galaxies, with a strong high density gas component
- DCN: abundant only in spirals with a strong high density gas component

Deuteration in nearby galaxies

- Few detections of deuterated species (e.g. Mauersberger et al. 1995; 2mm survey by Martin et al. 2006)
- As D/H depends on degree of processing of the gas → give clues on the evolution of the galaxy

Martin et al. 2006)

TABLE 4

PARAMETERS OF SELECTED DEUTERATED SPECIES

Molecule	Transition $J-J'$	ν (MHz)	rms[a] (mK)	$\int T_{MB}\,dv$[b] ($K\ km\ s^{-1}$)	[DX]/[HX]
DCO^+	2–1	144077.3	1.9	<0.30	$<4 \times 10^{-3}$[c]
DCN	2–1	144827.9	1.1	<0.18	$<1 \times 10^{-3}$[c]
DNC	2–1	152609.7	3.1	0.49	$\leq 1 \times 10^{-2}$[c]
N_2D^+	2–1	154217.0	2.8	0.57	$\leq 1.4 \times 10^{-3}$[d]

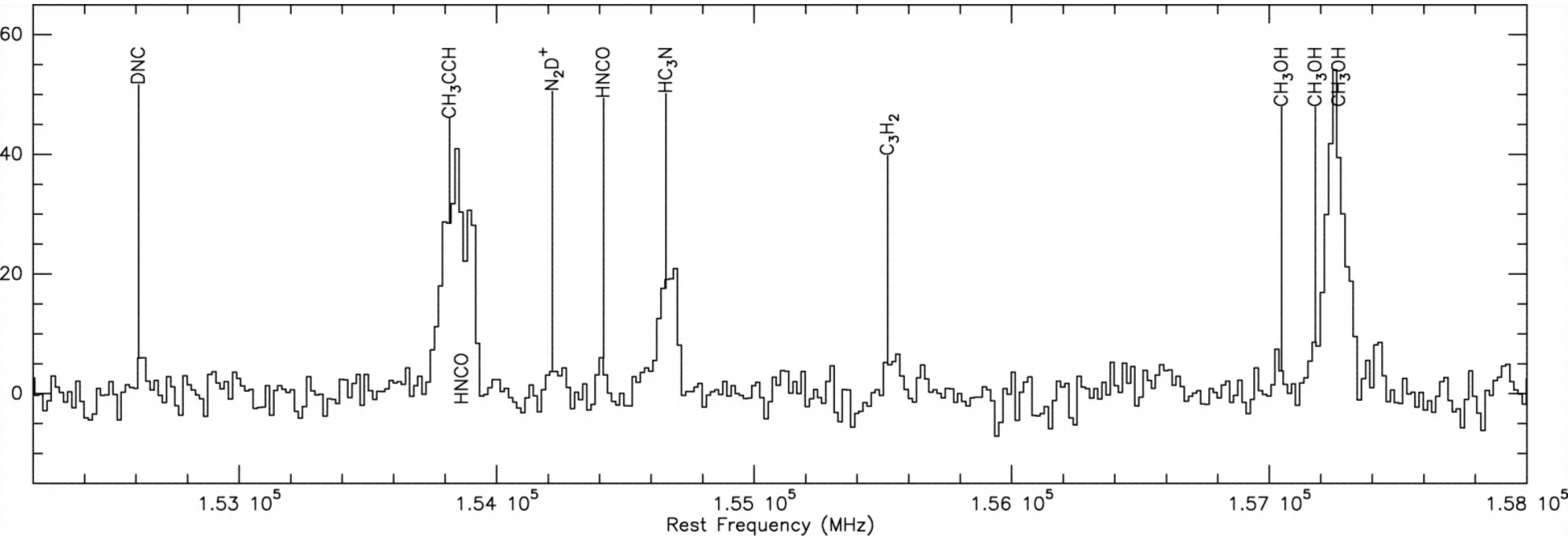
NOTE.—See § 4.2 for details.

[a] rms computed for 20 km s^{-1} wide channels.

[b] 3 σ limit to the integrated intensity assuming a line width of 150 km s^{-1}. DNC and N_2D^+ detections are tentative.

[c] Using the ^{13}C bearing species measured in this survey and assuming $^{12}C/^{13}C \sim 40$ (Henkel et al. 1993).

[d] Using the $J = 1-0$ N_2H^+ transition from Mauersberger & Henkel (1991).



Martin et al. 2006