CENTRO DE ASTROBIOLOGÍA

STUDY OF CYANOACETYLENE IN ORION KL: DETECTION OF DC_3N

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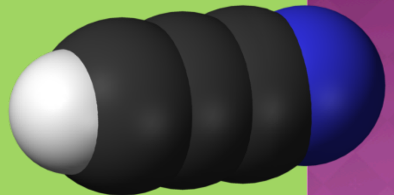
WHY HC_3N?

- Cyanoacetylene has properties making it convenient for deriving physical parameters of molecular clouds.

- Heavy linear molecule with large moment of inertia and small rotational constant *B* ➡ rotational transitions $J \rightarrow J\text{-}1$ are relatively close in frequency.

- Low energy of bending modes ➡ many vibrationally excited states.

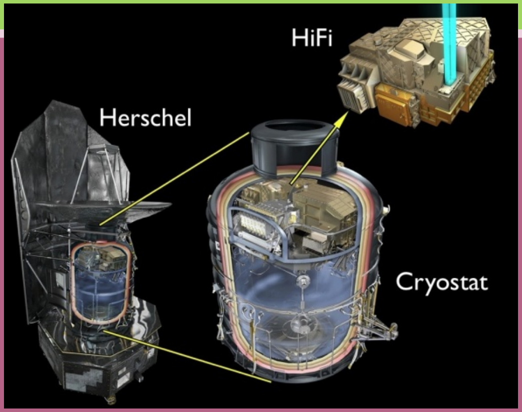
- Excellent tracer of early evolutionary stages of massive stars; hot ($T>150$ K) and dense ($n>10^7$ cm^{-3}) regions affected by high extinction.

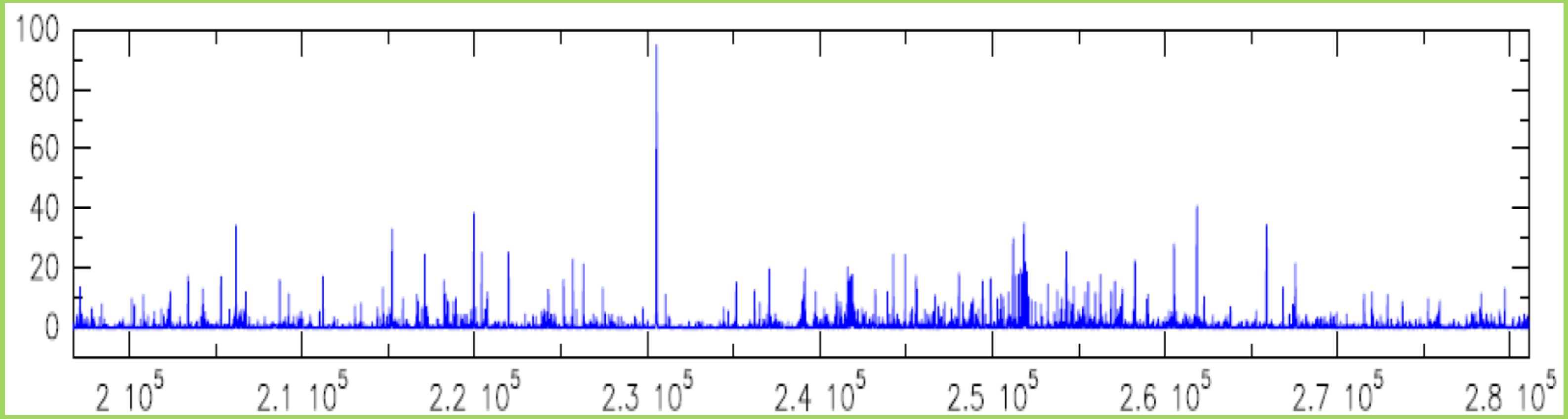


- Two surveys: IRAM+HIFI
- IRAM: 80-280 GHz
- HIFI: 480-1907 GHz
- Detected species:

  * HC_3N ground state (>70 lines) and ^{13}C isotopologues.

  * vibrational states v_7, $2v_7$, $3v_7$, v_5, v_6, v_6+v_7 (>200 lines)





ANALYSIS:

- Fit line profiles using an LVG code (line-widths due to the existence of large velocity gradients across the cloud).
- Components of the cloud:

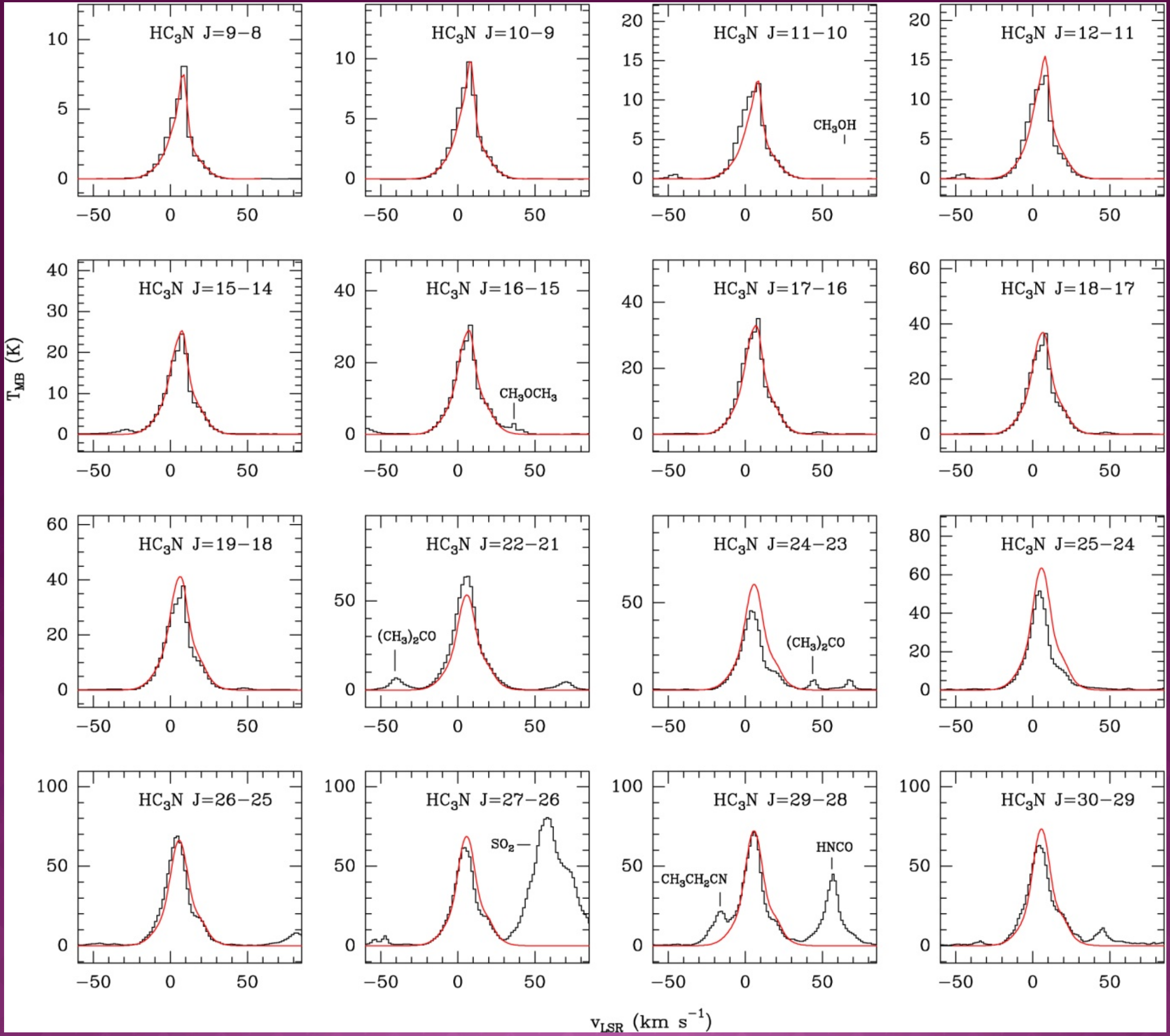
Component	Source diameter ($''$)	Offset (IRc2) ($''$)	$n(H_2)$ cm^{-3}	T_K (K)	Δv_{FWHM} ($km\ s^{-1}$)	v_{LSR} ($km\ s^{-1}$)
Extended ridge (ER)	120	0	10^5	60	4	8.5
Compact ridge (CR)	15	3	10^6	110	3	8
High velocity plateau (HP)	30	0	10^6	100	30	11
Plateau (PL)	20	2	$5x10^6$	150	25	6
Outer hot core (HC1)	10	3	$1.5x10^7$	180	10	5.5
Hot core (HC2)	7	3	$5x10^7$	250	7	5.5
20.5 $km\ s^{-1}$ component	5	2	$5x10^6$	90	7.5	20.5

- We fix all the above parameters, leaving only as a free parameter the column density.
- Obtain physical parameters (column densities and abundances).

IRAM

- 80-280 GHz
- $19<E_{up}<203$ K
- $8<J<30$
- Excellent tracer of cold gas from extended ridge (3 mm).
- The hot core dominates (2-1.3 mm) with:

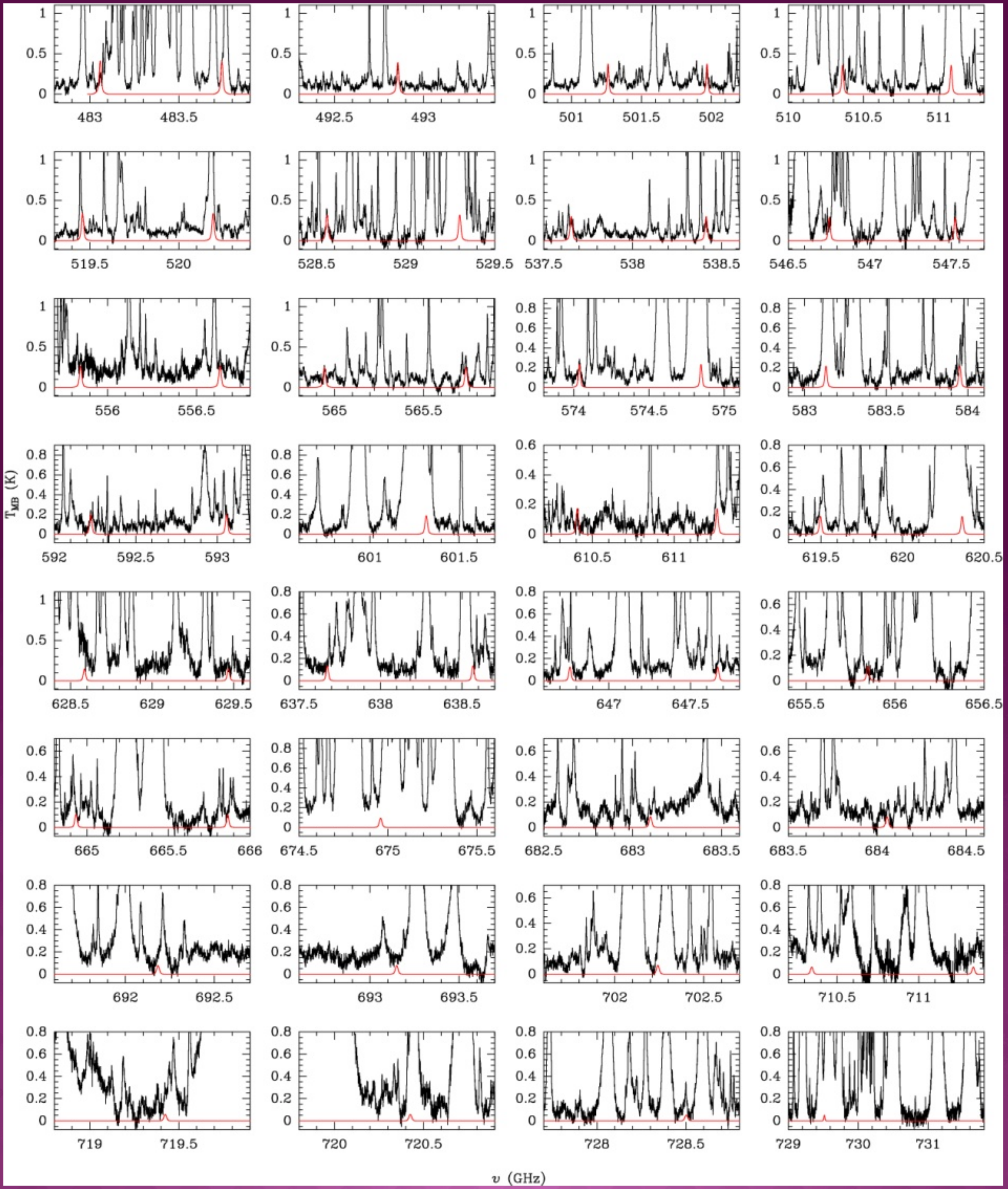
$N_{HC3N}=1.0\pm0.2\times10^{15}cm^{-2}$
$N_{HC3N\ v5}=1.5\pm0.3\times10^{14}cm^{-2}$
$N_{HC3N\ v6}=3.0\pm0.6\times10^{14}cm^{-2}$
$N_{HC3N\ v7}=1.2\pm0.4\times10^{15}cm^{-2}$



HERSCHEL-HIFI

- 480-1907 GHz
- 53<J<73
- 300<E_{up}<1700 K

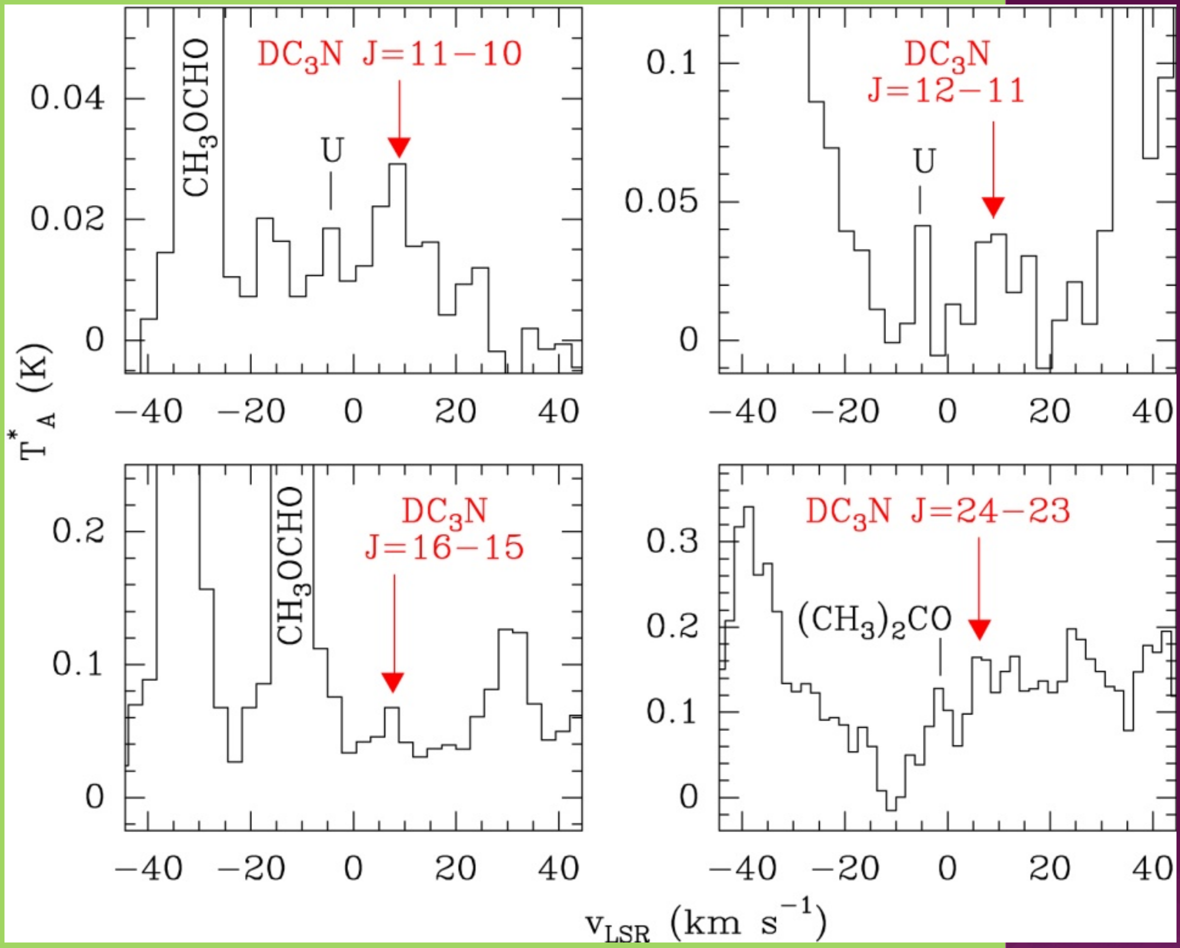
- Gradient within the hot core: hotter (T=250 K) and inner component (HC2).
- Column densities in HC2 are between 1-5 times larger than in HC1.
- With higher energies, weaker lines and more overlapping.



DC_3N:

* Deuterated species are produced mainly in molecular environments characterised by low temperatures (T≤20 K), typical of low-mass pre-stellar cores.

* We detect four lines in the IRAM line survey.



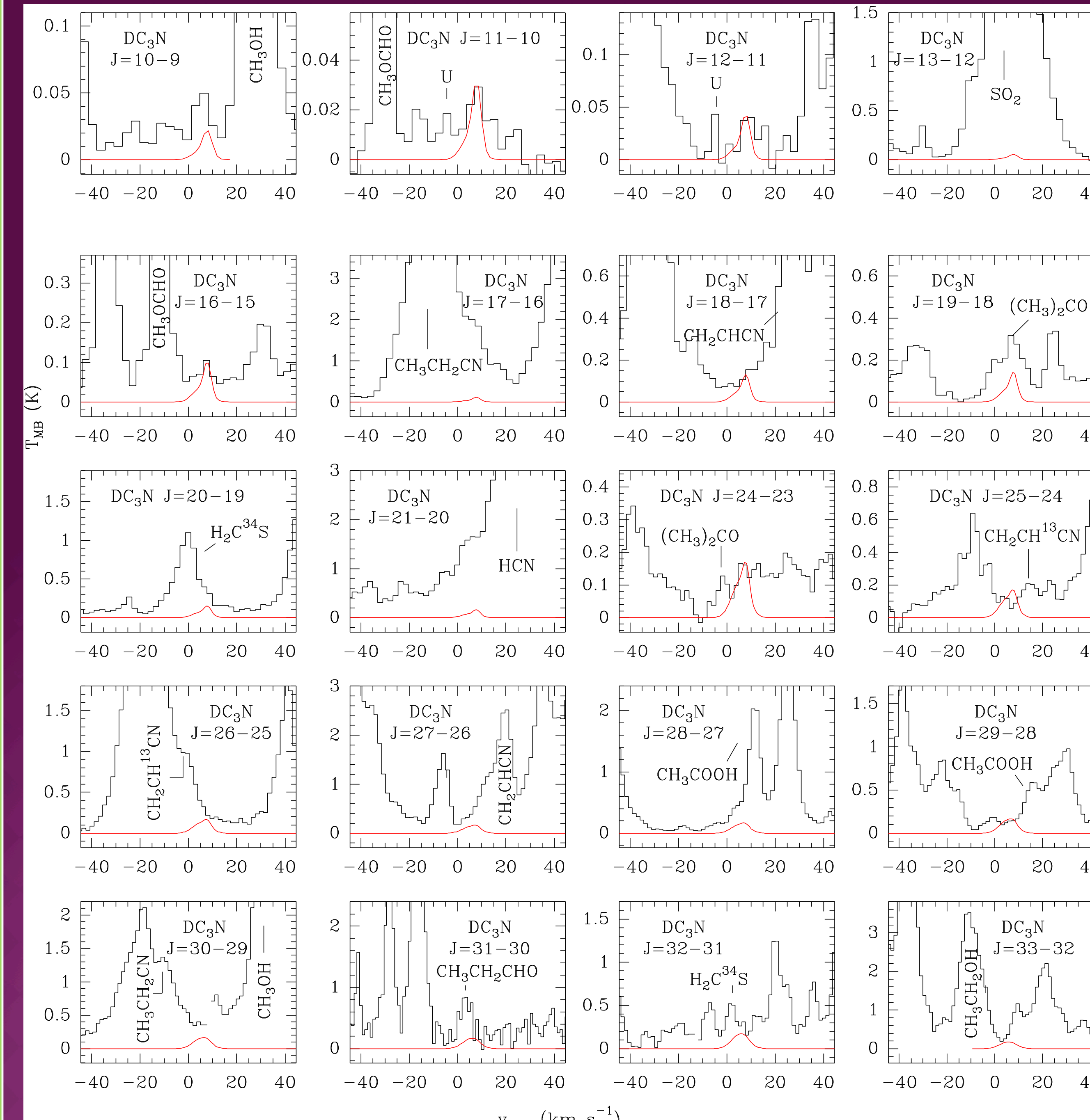
Species	Transition	Frequency (MHz)	E_{up} (K)
DC_3N	11-10	92872.37	26.7
DC_3N	12-11	101314.82	31.6
DC_3N	16-15	135083.18	55.1
DC_3N	24-23	202610.90	121.6

IRAM

DC_3N

- Column densities:
  - Hot core HC1: $N=1.1\pm0.3\times10^{13}$ cm^{-2}
  - Compact ridge: $N=2.7\pm0.8\times10^{12}$ cm^{-2}
- $(DC3N/HC3N)_{OrionKL}$ $=0.011\pm0.006$
- $(DC3N/HC3N)_{TMC1}$ $=0.02-0.08$

What is the origin of this DC_3N??



ABOUT THE ORIGIN OF DC_3N:

- To obtain large ratios of D/H, low temperatures and high density ($n>10^4$ cm^{-3}) are required.

- 1. A plausible mechanism is that DC_3N is formed prior to the gas-phase (on grain surfaces) and then evaporated.

- But HC_3N is mainly formed during the gas-phase.

- Deuterium is mainly locked into HD and transfered to other species by exothermic ion-molecule reactions.

$$H_3^+ + HD \rightarrow H_2D^+ + H_2 \qquad C_2H_2^+ + HD \rightarrow C_2HD^+ + H_2$$

$$CH_3^+ + HD \rightarrow CH_2D^+ + H_2$$

- 2. DC_3N could be formed subsequently through deuterated ions reacting with HC_3N:

$$H_2D^+ + HC_3N \rightarrow HDC_3N^+ + H_2$$

CHEMICAL MODEL

- A time-dependent chemical model for the hot core of Orion KL.

- Two phases:

* Phase I: chemical evolution during the cloud's gravitational collapse, until the formation of a dense core. (Cold phase where molecules are adsorbed onto the dust grains).
* Phase II: after the molecular gas is evaporated from grain surfaces (when the central star is formed) up to now.

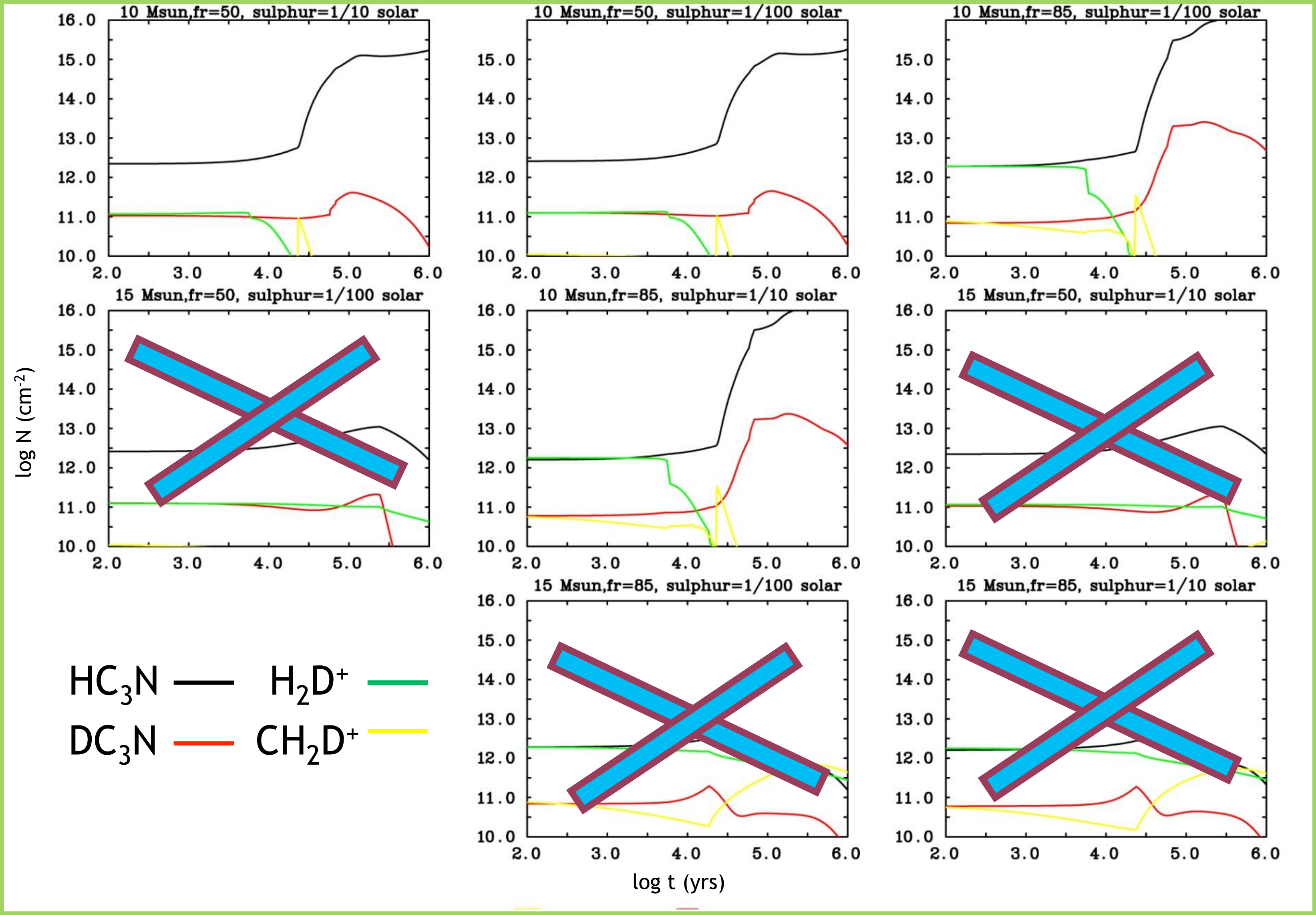
- Different masses for the central star formed, initial abundances and freeze out efficiencies.

- Output parameter: column densities as a function of time.

- Comparison with observations.

CHEMICAL MODEL

$N(HC_3N)_{HC1}$=1.0x10^{15} cm^{-2}
$N(DC_3N)_{HC1}$=1.1x10^{13} cm^{-2}



CONCLUSIONS

- HC_3N is an excellent hot and dense gas tracer with column densities up to two orders of magnitude larger in the hot core than in the other components.
- The large number of detected lines (ground and vibrational states), especially at very high frequencies and energies (HIFI), demonstrates the necessity of considering a stratification of the hot core.
- Detection of DC_3N for first time in a giant molecular cloud.
- DC_3N is formed during the gas-phase

$t_{hot\ core}$~60,000 years.

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