Poster PCMI

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Complex molecules in the Orion Kleinmann-Low nebula

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et al.

We have conducted for several years a spectroscopic study at high spatial resolution (1-2") of the Kleinman-Low (KL) infrared nebula, located in the heart of the Orion Nebula. This study has been undertaken with the IRAM Plateau de Bure Interferometer. Orion KL is one of the regions richest in detected interstellar molecules. Studying the spatial distribution of the molecule we hope to constrain the origin of the molecules and their formation mechanism. In particular, are the molecules produced in the gas-phase, on icy grain mantles, or through a combination of both processes ? Did the recent (< 1000 yr) explosive event play a role in their formation ?

We have studied methyl formate $HCOOCH_3$ (Favre et al 2011), deuterated methanol (both CH_3OD and CH_2DOH ; Peng et al 2012), dimethyl ether CH_3OCH_3 (Brouillet et al, soumis), and are presently working on acetone CH_3COCH_3.

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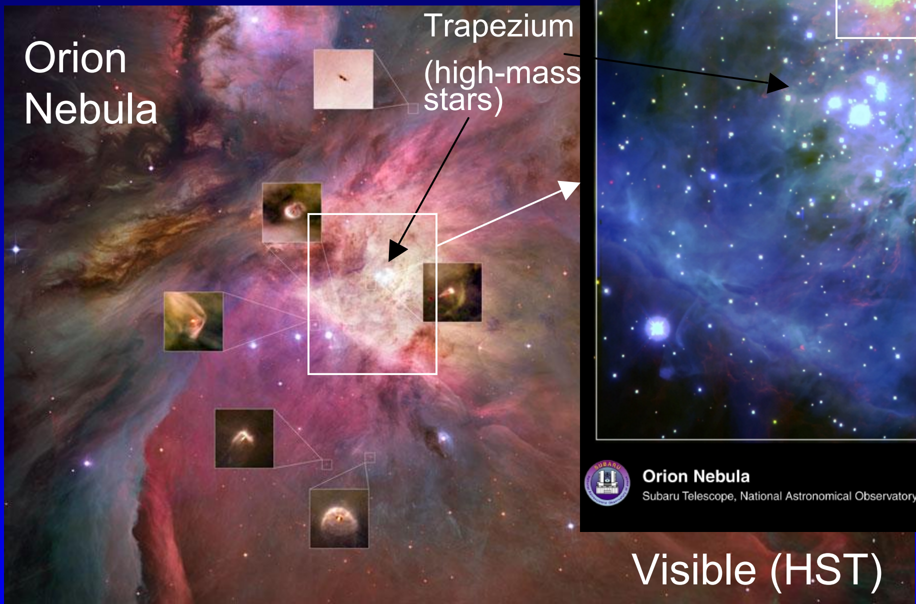
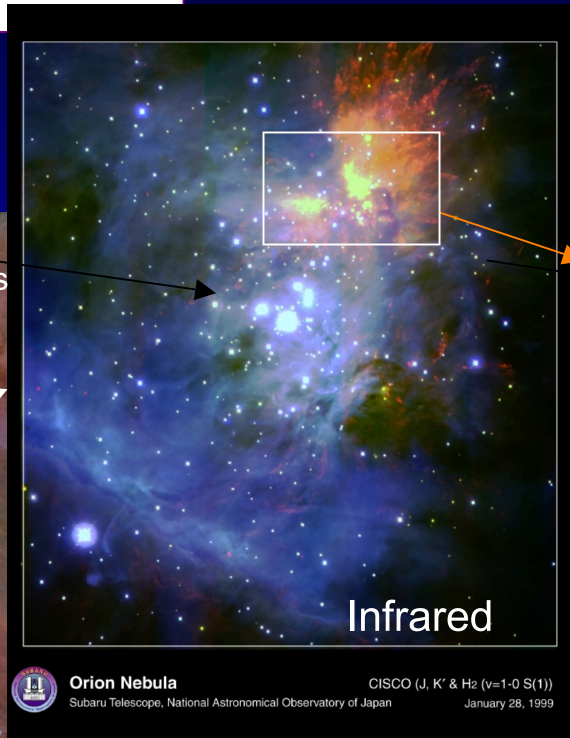
Orion Kleinmann-Low Nebula

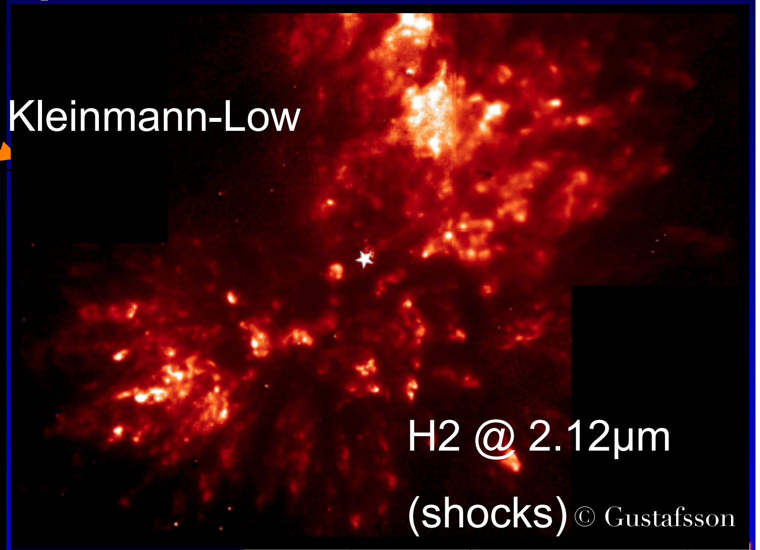
An high-mass star forming region
414 pc from the Sun
(Menten et al. 2007)

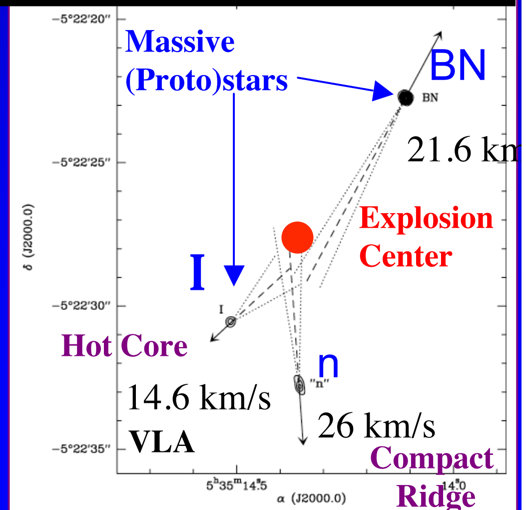
A stellar encounter 500-1000 yr ago !

Bally et al. (2011), Goddi et al. (2011)
Gómez et al. (2005, 2008), Rodríguez et al. (2005)
Zapata et al. (2009)









- Shock waves
- Unique conditions for the study of interstellar chemistry : *recent desorption (< 1000 yr) of molecules from the icy mantles of interstellar grains*

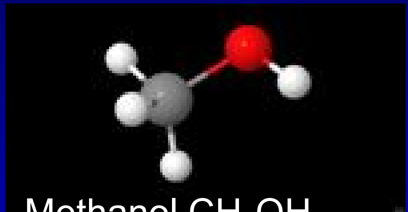
Key Questions

- Here
  - Which molecules are present in the interstellar medium? Which complexity ?
  - Where, when, how did they form ?

- The Origin of Life perspective
  - Complementary studies are required to establish the importance of IS chemistry for the Origin of Life on Earth :
  - Do we find these molecules
    - In the protosolar nebula ?
    - In comets, asteroids, (micro)meteorites?
    - As such or modified ? Inherited from the Interstellar Medium and/or synthesized in the Solar nebula?
  - Did they reach the early Earth?
    - And in sufficient amount to play an important part in prebiotic chemistry ?

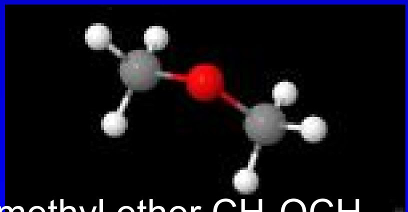
Main molecules under study

- **Small organic molecules**

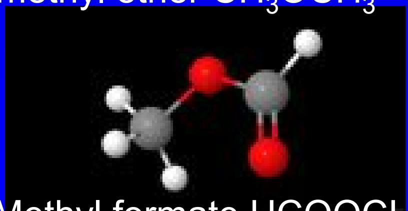


Methanol CH_3OH

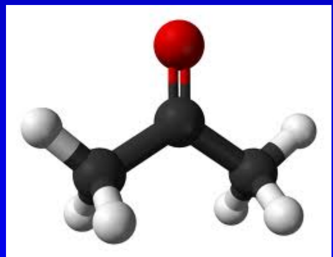
Acetaldehyde CH_3CHO



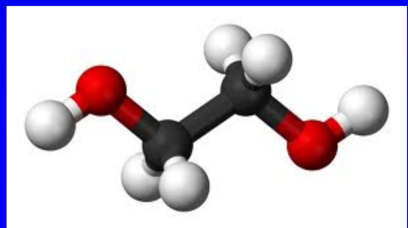
Dimethyl ether CH_3OCH_3



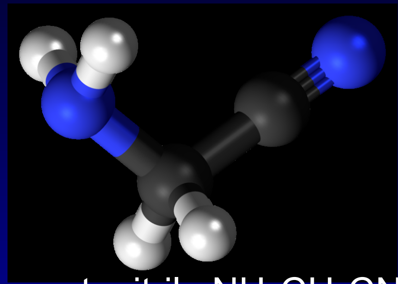
Methyl formate $HCOOCH_3$



Acetone CH_3COCH_3

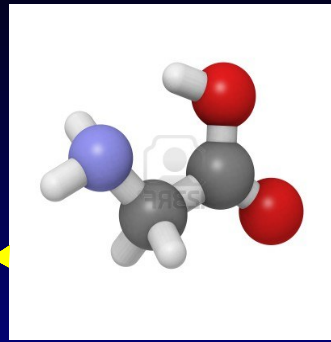


Ethylene glycol CH_2OHCH_2OH



Aminoacetonitrile NH_2CH_2CN

H_2O (liq.)

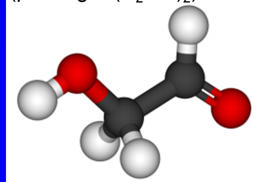


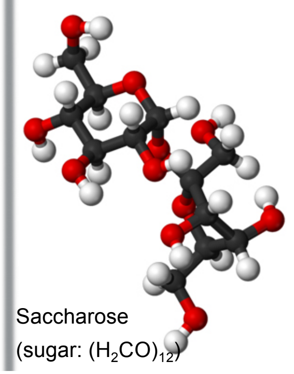
Glycine NH_2CH_2COOH (amino acid)

- **Search for molecules of interest for prebiotic chemistry : upper limits in Orion KL**
  - CH_2OHCHO (glycolaldehyde), a pre-sugar
  - aminoacetonitrile NH_2CH_2CN , a glycine precursor
  - glycine NH_2CH_2COOH itself, the simplest aminoacid

  have been searched for but only upper limits have been obtained in Orion KL (e.g. Favre et al 2011)
- NB: the discovery of glycolaldehyde in the low-mass protostar IRAS16293 has been announced recently (Jorgensen et al. 2012)
- Aminoacetonitrile and glycolaldehyde have been observed in the galactic center Sgr B2 (Belloche et al 2009; Hollis et al 2002)

Glycolaldehyde
CH_2OHCHO
(pre-sugar $(H_2CO)_2$)



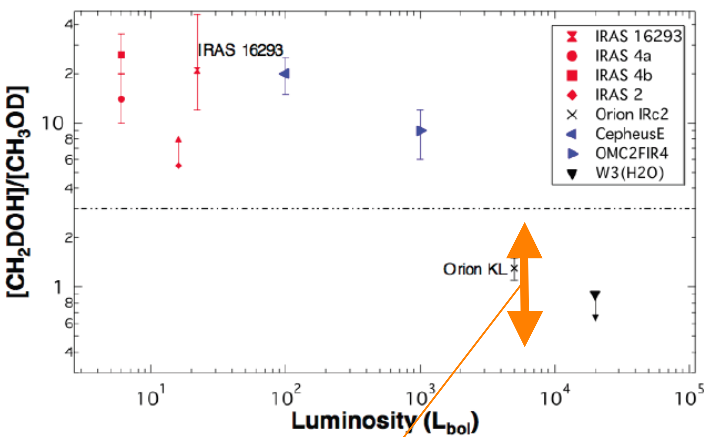


Saccharose
(sugar: $(H_2CO)_{12}$)

Deuterated methanol : CH_3OD vs CH_2DOH Sublimation of ancient ices?

– The study of deuterated methanol has shown that the ratio CH_2DOH/CH_3OD is relatively constant in Orion KL; this constancy, which contrasts with the present variety of physical conditions in the region, suggests deuterated methanol formed in ice mantles, at a time the interstellar matter in the region was more homogenous. The value we find, <1 in average, confirms the strong difference between Orion KL et the surroundings of low-mass protostars (e.g. IRAS16293) found by Rataczack et al 2011.

Figure 1: CH_2DOH/CH_3OD (d1/d2) ratios adopted from (Ratajczak et al., 2011). A simple model would give a statistical ratio of 3 (dot dashed line). CH_2DOH appears overabundant in low-mass star forming regions and less abundant in high-mass star forming regions.



Range of values of CH_2DOH/CH_3OD in our map (Fig 2 b; Peng et al 2012)

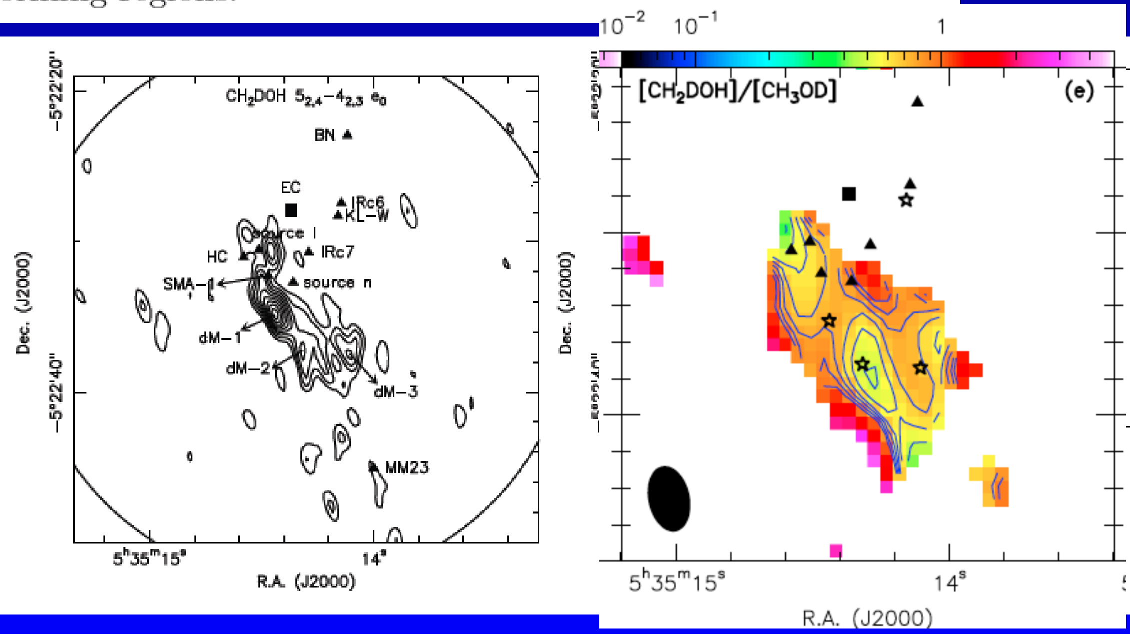


Fig 2: map **a)** of CH_2DOH emission and **b)** of the ratio CH_2DOH/CH_3OD in Orion KL

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Astronomy & Astrophysics

Deuterated methanol in Orion BN/KL ⋆

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ABSTRACT

Aims. Deuterated molecules have been detected and studied toward Orion BN/KL in the past decades, mostly with single-dish telescopes. However, high angular resolution data are critical not only to interpret the spatial distribution of the deuteration ratio but also to understand this complex region in terms of cloud evolution involving star-forming activities and stellar feedbacks. Therefore, it is important to investigate the deuterated ratio of methanol, one of the most abundant grain-surface species, on a few arcseconds scale to better understand the physical conditions related to deuteration in Orion BN/KL.

Methods. Orion BN/KL was extensively observed with the IRAM Plateau de Bure Interferometer from 1999 to 2007 in the 1 to 3 mm range. The angular resolution varies from $1''.8 \times 0''.8$ to $3''.6 \times 2''.3$ and the spectral resolution varies from 0.4 to 1.9 km s^{-1}. Deuterated methanol CH_2DOH and CH_3OD and CH_3OH lines were searched for within our 3 mm and 1.3 mm data sets.

Results. We present here the first high angular resolution ($1''.8 \times 0''.8$) images of deuterated methanol CH_2DOH in Orion BN/KL. Six CH_2DOH lines were detected around 105.8, 223.5, and 225.9 GHz. In addition, three E-type methanol lines around 101–102 GHz were detected and were used to derive the corresponding CH_3OH rotational temperatures and column densities toward different regions across Orion BN/KL. The strongest CH_2DOH and CH_3OH emissions come from the Hot Core southwest region with a velocity which is typical of the Compact Ridge ($V_{LSR} \approx 8$ km s^{-1}). We derive $[CH_2DOH]/[CH_3OH]$ abundance ratios of $\lesssim 1 \times 10^{-3}$ toward the CH_2DOH emission peaks. A new transition of CH_3OD was detected at 226.2 GHz, **first time in the interstellar medium**. Its distribution is similar to that of CH_2DOH. Besides, we find that the $[CH_2DOH]/[CH_3OD]$ abundance ratios are smaller than unity in the central part of BN/KL. Furthermore, one HDO line at 225.9 GHz was detected and its emission distribution shows a few arcseconds shift with respect to the deuterated methanol emission, which likely results from different excitation effects. The deuteration ratios derived along Orion BN/KL are not markedly different from one clump to another. However, various processes such as slow heating due to ongoing star formation, heating by luminous infrared sources, or heating by shocks could be competing to explain some local differences observed for these ratios.

Similarity of dimethyl ether CH_3OCH_3 and methyl formate $HCOOCH_3$ spatial distributions : A common precursor ?

- The comparison of CH_3OCH_3 with $HCOOCH_3$ has shown a striking correlation of the spatial distribution of both species. Such a tight correlation is not found with ethanol CH_3CH_2OH, nor with formic acid HCOOH - which in the opposite appears anticorrelated.

- The simplest explanation seems to be a common precursor for both species. Two main models have been proposed to form these species

- If the formation occurs on grains (Bisschop et al 2007, Oberg et al 2010), the common precursor would be the $CH_3O\bullet$ radical :
  - $CH_3O\bullet + CH_3\bullet \Rightarrow CH_3OCH_3$
  - $CH_3O\bullet + HCO\bullet \Rightarrow HCOOCH_3$

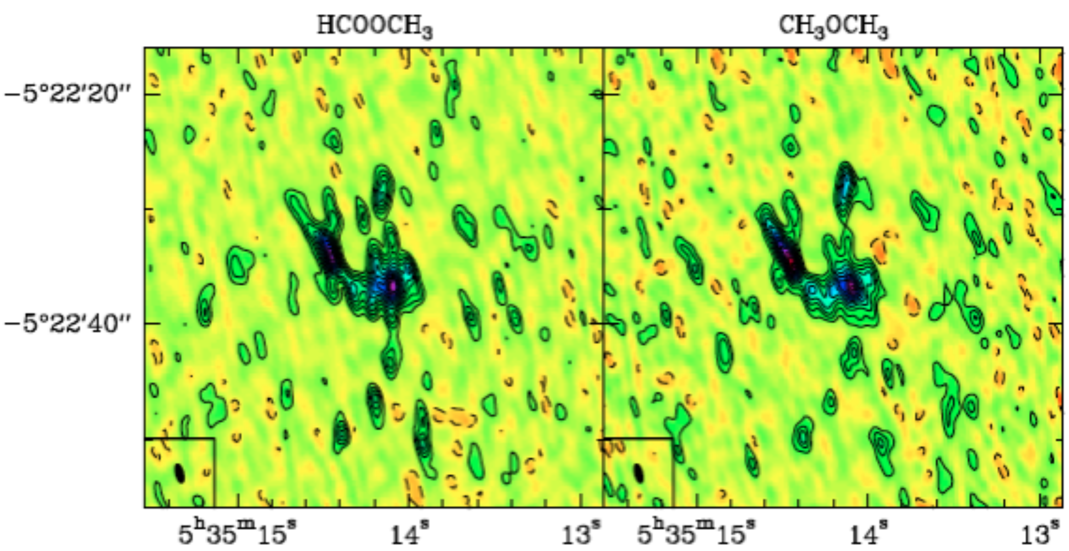
- If the formation takes place in the gas phase, protonated methanol $CH_3OH_2^+$ would be the common precursor (Neill et al 2010) of the related protonated species
  - $CH_3OH_2^+ + CH_3OH \Rightarrow (CH_3OCH_3)H^+ + H_2O$
  - $CH_3OH_2^+ + HCOOH \Rightarrow (HCOOCH_3)H^+ + H_2O$

- An electronic dissociative recombination of the latter would complete the process. The presence of protonated methanol is linked to methanol injection into the gas phase from icy grain mantles.

- Another reaction, producing $HCOOCH_3$ from H_2CO has been considered (Blake et al 1988),but suffers from a too high barrier (128 $kJ.mol^{-1}$ ~ 15000 K ~ 1.2 eV ; Horn et al. 2004).

  Could the supplement of (kinetic) energy in the shock help overcome this barrier ?

Methyl formate vs Dimethyl ether



Spatial distribution (spatial resolution 1" ~ 400 AU)

Pixel to pixel correlations

Fig. 6. Comparison of the methyl formate map (left) at 223.534 GHz (E_u=305 K) and the dimethyl ether map (right) at 223.41 GHz (E_u=330 K). The transitions are from the same data cube and the 1.79″ × 0.79″ beam is plotted in the bottom left corner.

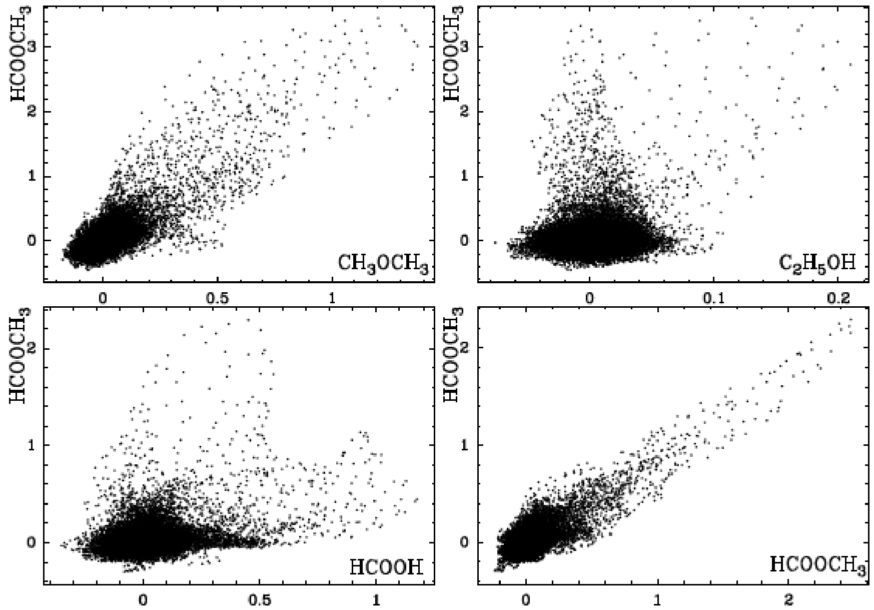


Fig. 7. Intensity of the pixel in the methyl formate maps versus the intensity of the same pixels in the dimethyl ether (top left), ethanol (top right), formic acid (bottom left) **and methyl formate (bottom right)** maps. Dimethyl ether shows clearly the tightest spatial correlation with methyl formate. Care has been taken to use transitions with similar E_u energies. **See Sect. 5.1.1 for details.**

CH_3OCH_3 in Orion-KL: a striking similarity with $HCOOCH_3$ ⋆

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Submitted to A&A

ABSTRACT

Context. Orion-KL is a remarkable nearby star forming region where a recent explosive event has generated shocks which could have produced the release of complex molecules from the grain mantles.
Aims. Comparison of the distribution of the different complex molecules will help to understand their formation and constrain the chemical models.
Methods. We used several data sets from the Plateau de Bure Interferometer to map the dimethyl ether emission with different spatial resolutions and different energy levels (from E_{up}=18 to 330 K) to compare with our previous methyl formate maps.
Results. Our data show a remarkable similarity even at small scale (1.8″×0.8″ or ~ 500 AU) between the dimethyl ether, CH_3OCH_3, and methyl formate, $HCOOCH_3$, distributions. This long suspected similarity from both observational and theoretical arguments is demonstrated with unprecedented confidence, with a correlation coefficient of maps ~ 0.8.
Conclusions. A common precursor is the simplest explanation of our correlation. Comparison with previous laboratory work and chemical models suggests a major role of grain surface chemistry, and a recent release, probably with little processing, of mantle molecules by shocks. In this case the CH_3O radical produced from methanol ice would be the common precursor (whereas ethanol, C_2H_5OH, is produced from the radical CH_2OH). The alternative gas phase scheme, with protonated methanol $CH_3OH_2^+$ as the common precursor through reactions with HCOOH and CH_3OH to produce methyl formate and dimethyl ether is also compatible with our data. Our observations cannot yet definitely allow a choice between the different chemical processes, but the tight correlation between the distributions of $HCOOCH_3$ and CH_3OCH_3 is **in strong contrast** with the different behavior we observe for the distributions of ethanol and formic acid and provides a very significant constraint on models.

Methyl formate $HCOOCH_3$: A link with shocks ?

- The study of $HCOOCH_3$ has shown some spatial association between this molecule and the peaks of the 2.12 µm excited H_2 emission, which traces shocks.

Contours : $HCOOCH_3$

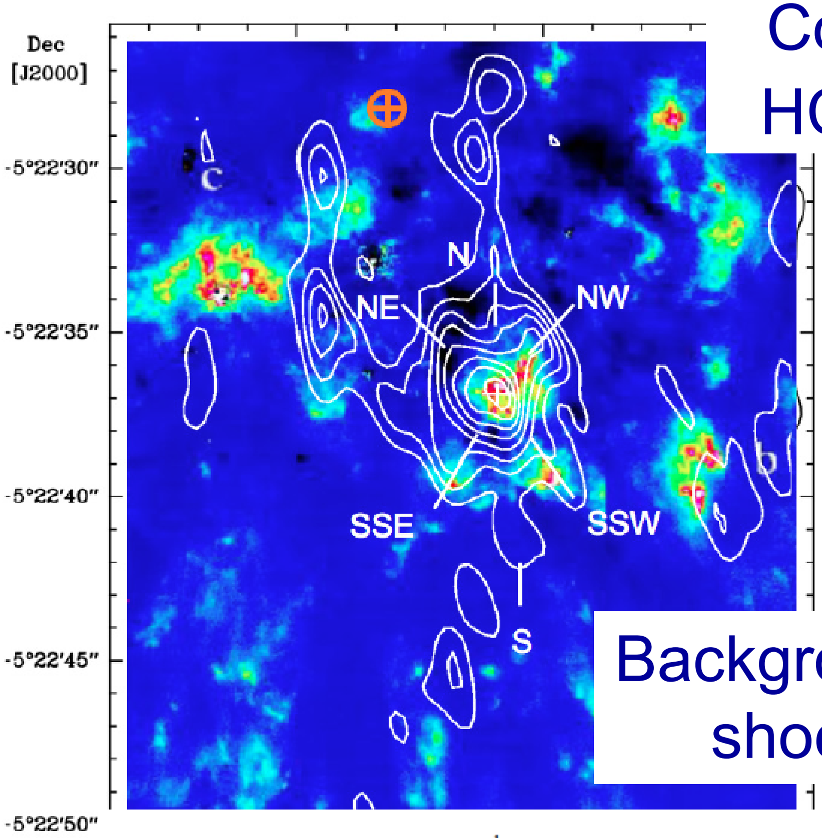

Fig. 20. Methyl formate 8.7 km s^{-1} channel map contours overlaid over Lacombe et al. (2004) 2.12 μm excited H_2 emission showing a good correlation of both tracers toward MF1 (white cross) and around (northwest (NW), south-southwest (SSW) and south-southeast (SSE)). The northeast (NE) region analysis is hampered by the subtraction of strong 2 μm continuum from IRc4 (see Fig. 17) – which results in an artefact (the zone in black). The red circled cross marks the proper motion center where the sources n, I, and BN were located 500 years ago (Gómez et al. 2005, 2008; Rodríguez et al. 2005).

Background image: shocked gas

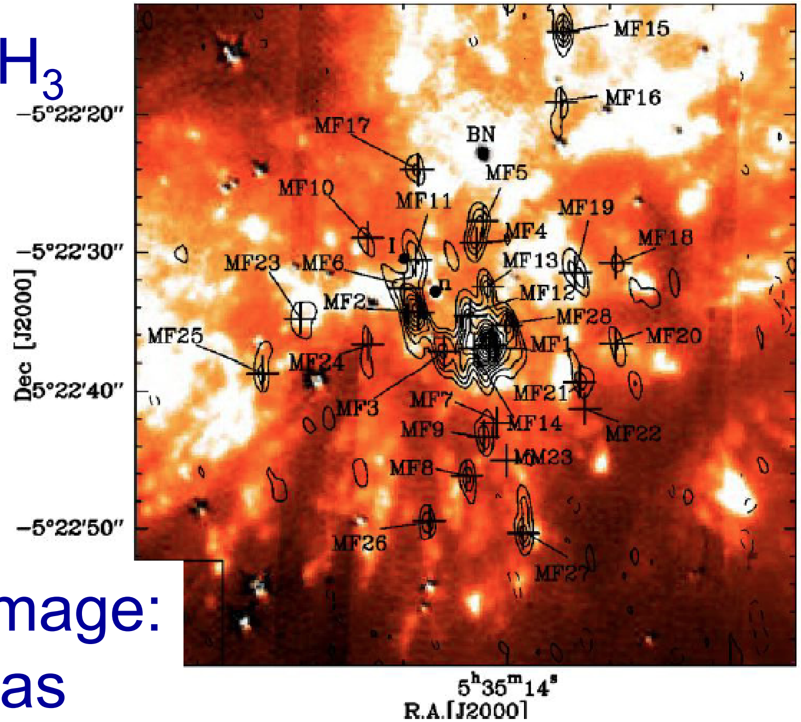

Fig. 21. Map of the integrated methyl formate emission (cf. Fig. 4) overlaid over a Subaru Observatory image of H_2 at 2.12 μm emission (© Subaru Telescope, NAOJ. All rights reserved).

Favre et al 2011

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Astronomy & Astrophysics

$HCOOCH_3$ as a probe of temperature and structure in Orion-KL★,★★,★★★

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ABSTRACT

Context. The Orion Kleinmann-Low nebula (Orion-KL) is a complex region of star formation. Whereas its proximity allows studies on a scale of a few hundred AU, spectral confusion makes it difficult to identify molecules with low abundances.

Aims. We studied an important oxygenated molecule, $HCOOCH_3$, to characterize the physical conditions, temperature, and density of the different molecular source components. Methyl formate presents strong close rotational transitions covering a wide range of energy, and its emission in Orion-KL is not contaminated by the emission of N-bearing molecules. This study will help in the future 1) to constrain chemical models for the formation of methyl formate in gas phase or on grain mantles and 2) to search for more complex or prebiotic molecules.

Methods. We used high-resolution observations from the IRAM Plateau de Bure Interferometer to reduce spectral confusion and to better isolate the molecular emission regions. We used twelve data sets with a spatial resolution down to $1.8'' \times 0.8''$. Continuum emission was subtracted by selecting apparently line-free channels.

Results. We identify 28 methyl formate emission peaks throughout the 50″ field of observations. The two strongest peaks, named MF1 and MF2, are in the Compact Ridge and in the southwest of the Hot Core, respectively. From a comparison with single-dish observations, we estimate that we miss less than 15% of the flux and that spectral confusion is still prevailing as half of the expected transitions are blended over the region. Assuming that the transitions are thermalized, we derive the temperature at the five main emission peaks. At the MF1 position in the Compact Ridge we find a temperature of 80 K in a $1.8'' \times 0.8''$ beam size and 120 K on a larger scale ($3.6'' \times 2.2''$), suggesting an external source of heating, whereas the temperature is about 130 K at the MF2 position on both scales. Transitions of methyl formate in its first torsionally excited state are detected as well, and the good agreement of the positions on the rotational diagrams between the ground state and the $v_t = 1$ transitions suggests a similar temperature. The LSR velocity of the gas is between 7.5 and 8.0 km s^{-1} depending on the positions and column density peaks vary from 1.6×10^{16} to 1.6×10^{17} cm^{-2}. A second velocity component is observed around 9–10 km s^{-1} in a north-south structure stretching from the Compact Ridge up to the BN object, and this component is warmer at the MF1 peak. The two other $C_2H_4O_2$ isomers are not detected, and the derived upper limit for the column density is $\leq 3 \times 10^{14}$ cm^{-2} for glycolaldehyde and $\leq 2 \times 10^{15}$ cm^{-2} for acetic acid. From the 223 GHz continuum map, we identify several dust clumps with associated gas masses in the range 0.8 to 5.8 $M_\odot$. Assuming that the methyl formate is spatially distributed as the dust is, we find relative abundances of methyl formate in the range $\leq 0.1 \times 10^{-8}$ to 5.2×10^{-8}. We suggest a relation between the methyl formate distribution and shocks as traced by 2.12 μm H_2 emission.

Some missing knowledge

- Is the $CH_3OH_2^+$ +H_2CO reaction to form methyl formate $HCOOCH_3$ possible if protonated methanol is accelerated in a shock?
  - Horn et al 2004 showed there is a barrier preventing this reaction under standard ISM conditions (low T)
- What is the millimeter spectrum of $CH_3OH_2^+$?
- What favours the production of the CH_3O• radical over CH_2OH• ?
- Could the dimethyl ether CH_3OCH_3 to $HCOOCH_3$ ratio converge to a constant value at long times, without a common precursor ?
- What are the possible reactions to form acetone CH_3COCH_3 ?
  - The distribution of acetone in Orion KL is definitely distinct from other O-bearing species (e.g. CH_3OCH_3)