MILLIMETER AND SUBMILLIMETER WAVE SPECTRA OF THE $HCOO^{13}CH_3$ ISOTOPOLOG OF METHYLFORMATE IN THE GROUND STATE AND IN THE FIRST EXCITED TORSIONAL STATE

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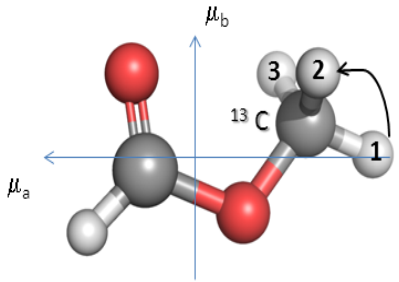
Outline

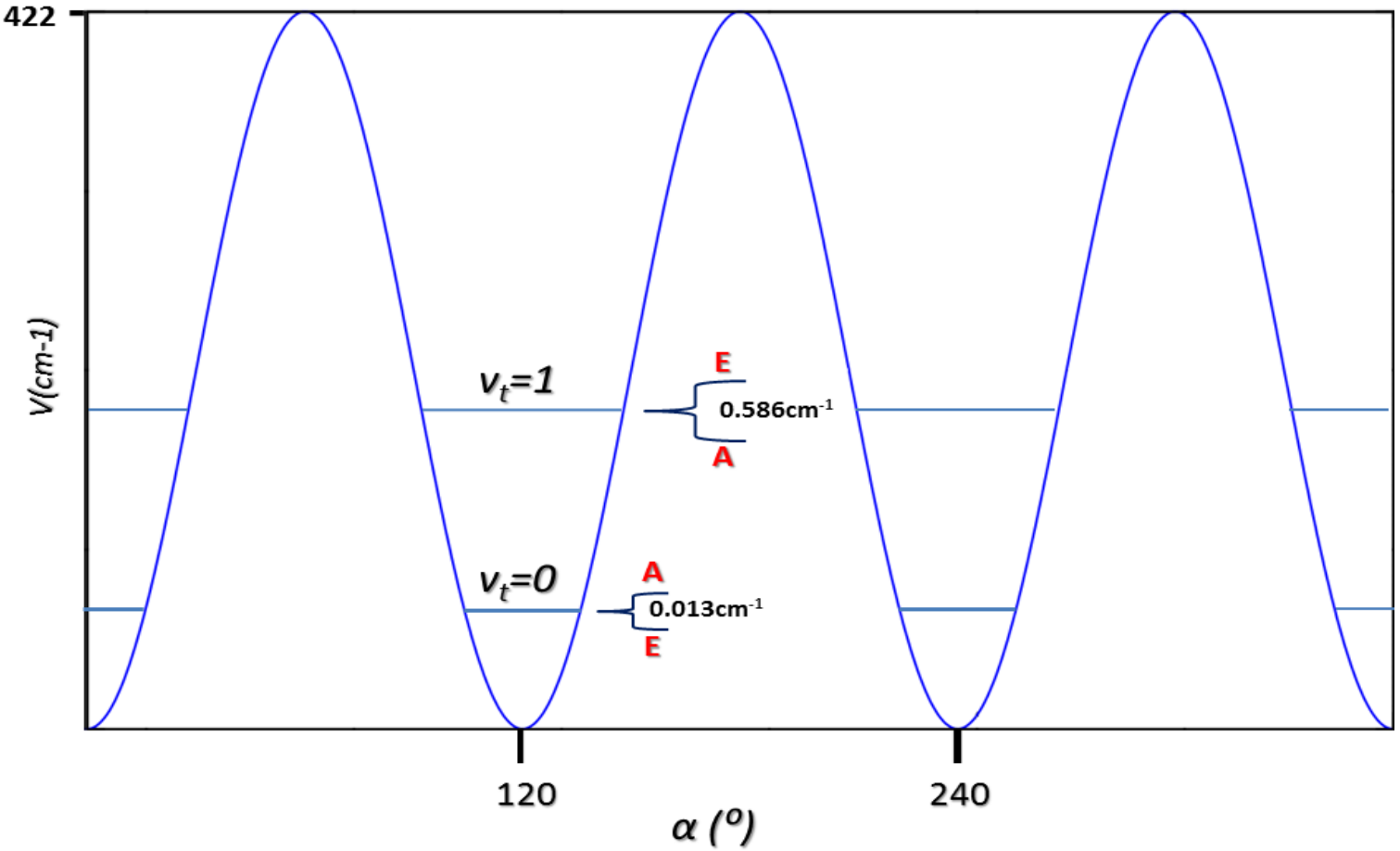
Methylformate in space.

- Is one of the most abundant molecules in Orion KL (Kleinmann-Low infrared nebula).
- More than 900 transitions corresponding to the fundamental state of the parent molecule were detected in different interstellar sources : Orion, W3, W51, IRAS, G34.3+0.15 and Sgr B2.
- In addition to the detection of torsional excited states : ν_t =1 and ν_t = 2 in Orion KL and W51 e2.
- Gaseous roots of formation do not meet the detected abundances of methylformate in space witch leads to wonder about chemical processes on grain surfaces argued by the detection of methyl formate in cold sources.

Potential function of the methyl torsion



$$V(\alpha) = \frac{V_3}{2}(1 - cos3\alpha) + \frac{V_6}{2}(1 - cos6\alpha) + \ldots$$



The RAM Hamiltonian implemented in BELGI program

The RAM Hamiltonian is divided into four distinct Hamiltonians :

$$H_{RAM} = H_r + H_{cent} + H_t + H_{rt}$$

The rotational Hamiltonian is given by :

$$H_r = A_{RAM}J_a^2 + B_{RAM}J_b^2 + C_{RAM}J_c^2 + D_{ab}(J_aJ_b + J_bJ_a)$$

The torsional Hamiltonian is given by :

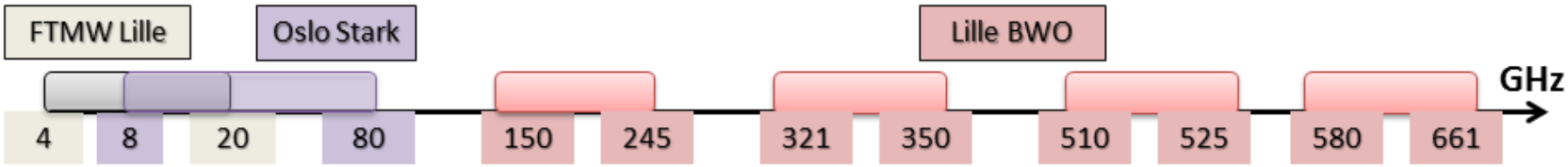
$$H_t = F(p_\alpha - \rho J_z)^2 + V(\alpha)$$

Where,

- $\mathrm{F} = \dfrac{\hbar^2}{2\mathrm{I}_{\mathrm{CH_3}}}$
- $\rho = \dfrac{\lambda \mathrm{I}_{\mathrm{CH_3}}}{\mathrm{I_z}}$

The rotation-torsion Hamiltonian H_{rt} is constructed by the product of the rotational and torsional operators

Isotopolog $HCOO^{13}CH_3$



Previous achievements :

- Spectra recorded in different frequency ranges [a].
- 936 lines, including both A and E symmetries, for ν_t=0 up to J=63 and K_a = 34 quantum numbers[a].
- Fit with the BELGI [b] program based on Rho-Axis Method (RAM)[a].
- 28 determined parameters with the barrier height V_3 = 407.1549(147)[a].
- High correlations prevented the determination of the parameters V_6 and F [a].

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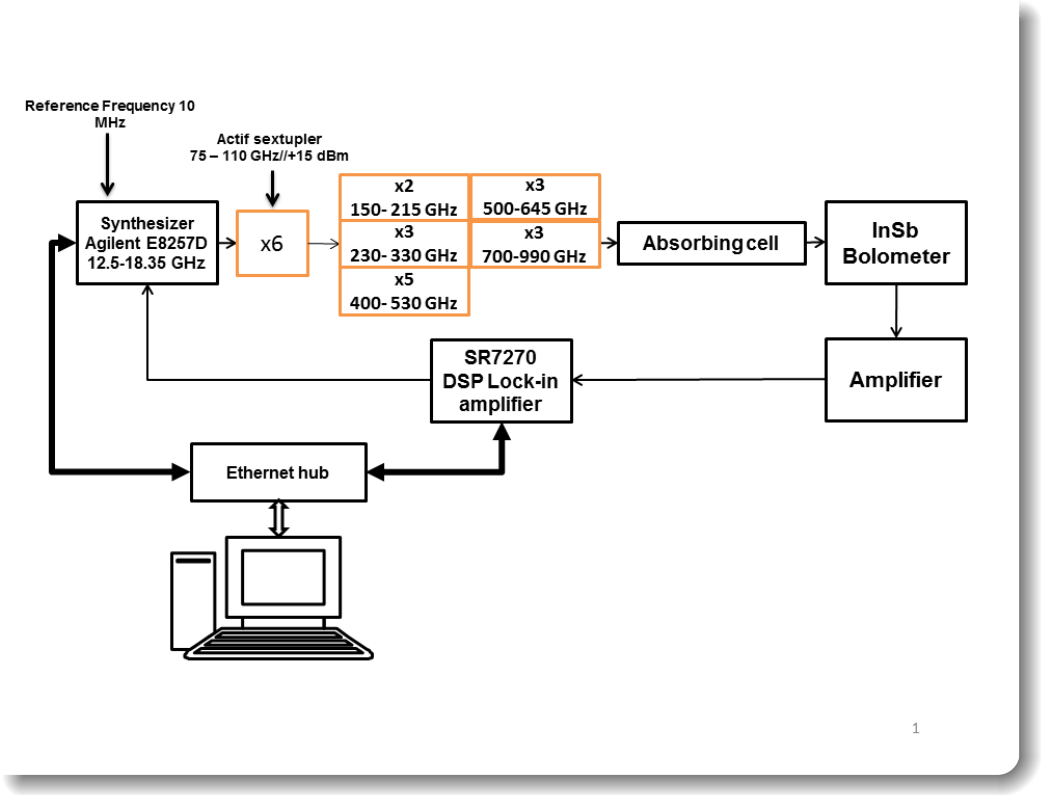
a. Carvajal et al. *A&A*, **500**, 1109, (2009)

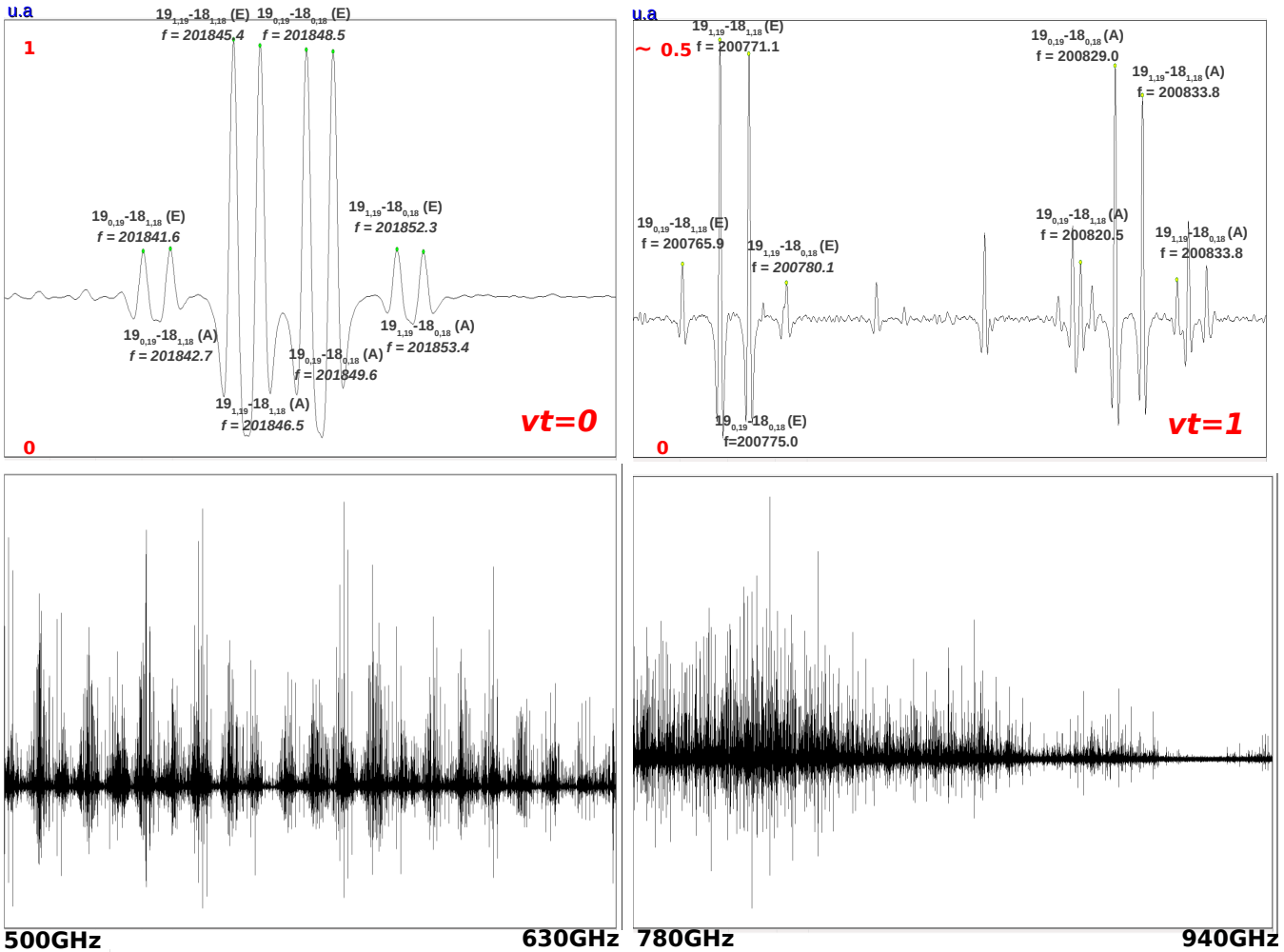
b. I. Kleiner *J. Mol. Spectr.*, **260**, 1, (2010)

Millimeter- and submillimeter- wave spectrometer in Lille



- The 75-990 GHz spectral range shown here was recently extended up to 1.6 THz in a recent improving of the Mm- and Submm- wave spectrometer in Lille.
- The accuracy of an isolated line is better than 30 kHz up to 630 GHz and 50 kHz above.
- The resolution is limited by the Doppler width of the line profile.

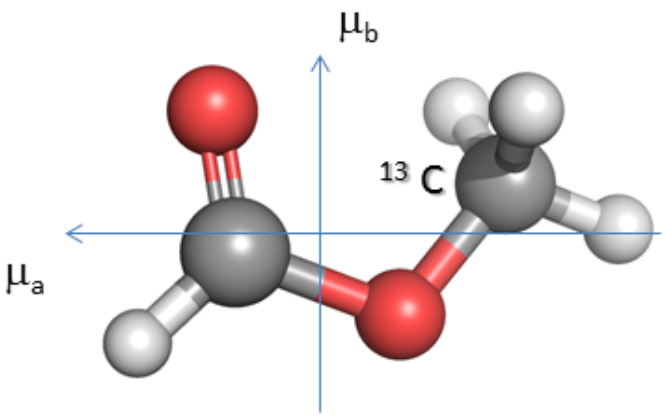
High signal to noise ratio



New accomplishments

- New spectra were recorded in Lille from 50 to 940 GHz
- Measurement and assignment of the ν_t = 0 was proceeded up to 940 GHz
- The first torsional state ν_t=1 was assigned up to 630 GHz
- A global fit of ν_t =0 and 1 is done with the BELGI program
- Determination of higher order parameters is essential for improving the reproduction of the experimental spectrum.

	ν_t=0	ν_t=1
Number of lines	6435	2865
J_{MAX}	65	60
$K_{a_{MAX}}$	35	26

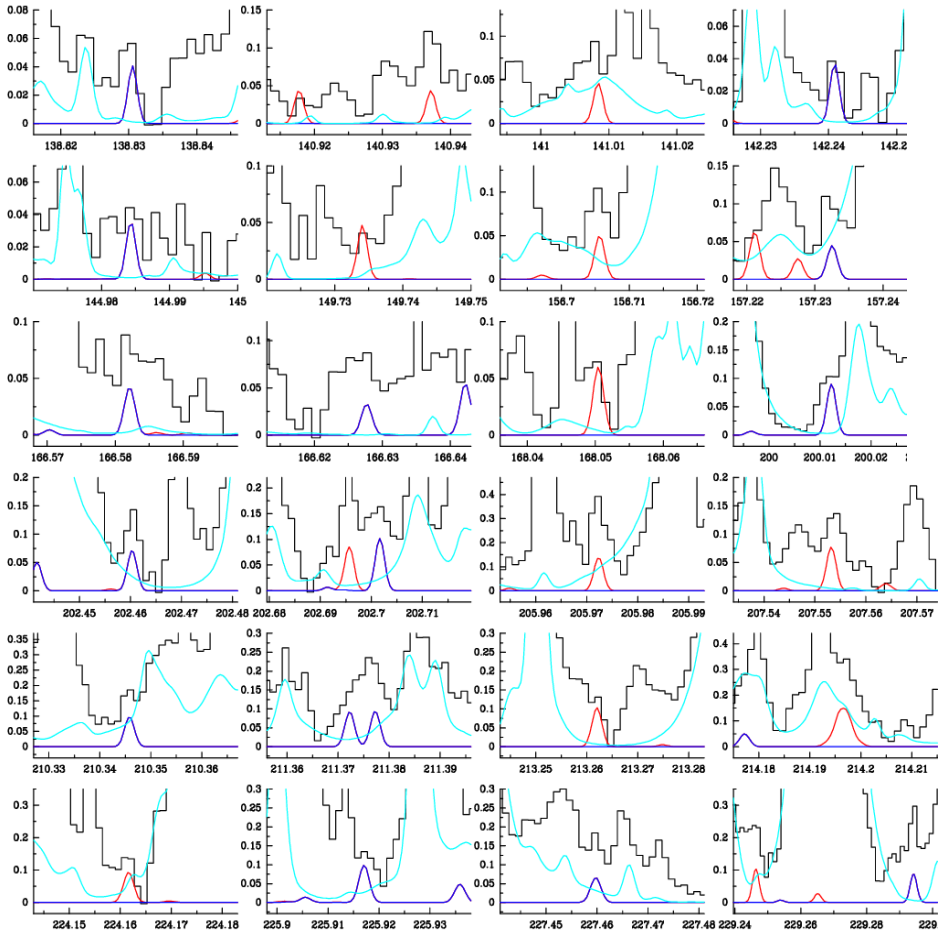


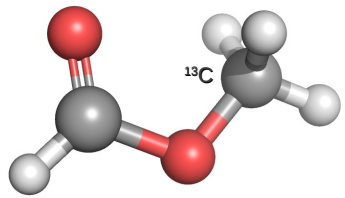
Results

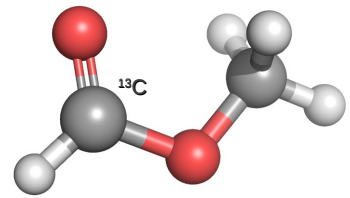
nlm	Operator	Parameter	Previous work ν_t=0	Present work ν_t=0 and 1
220	$1/2(1-\cos 3\gamma)$	V_3	407.1549(147) [a]	369.93430(395)
	P^2_γ	F	5.69168218 [b]	5.4785451(463)
211	$P_\gamma P_a$	ρ	0.0845207(106)[a]	0.084338308(343)
202	P^2_a	A_{RAM}	0.5857484(245)[a]	0.58659069(178)
	P^2_b	B_{RAM}	0.2959971(182)[a]	0.29681943(200)
	P^2_c	C_{RAM}	0.1729010(134)[a]	0.17349674(143)
		θ_{RAM}/deg	-23,7[a]	-23,8
		Nb Parms	28[a]	52
		Nb of lines	936[a]	9300
		J_{MAX}, K_{aMAX}	63,34[a]	65,35
		$freq_{MAX}$/GHz	700[a]	940
		WRMS	1.08[a]	0.78

a. Carvajal et al. *A&A*, **500**, 1109, (2009)
b. fixed to the value of the parent specie

Detection of ν_t=1 in Orion KL







- The Violet lines represent the detected lines for the $HCOO^{13}CH_3$
- The Red lines represent the detected lines for the $H^{13}COOCH_3$
- The Cyan lines represent the total model based on the previous molecular detections

Column densities

Species	Total Column density for each A and E state	Source	Reference
^{12}C	$2\ 10^{16} cm^{-2}$	Orion	Carvajal et al. *A&A*, **500**, 1109, (2009)
Both ^{13}C isotopologs	$7{,}3\ 10^{14} cm^{-2}$	Orion	Carvajal et al. *A&A*, **500**, 1109, (2009)
Both ^{18}O isotopologs	$1\ 10^{14} cm^{-2}$	Orion	Tercero et al. *A&A*, **538**, A119, (2012)
$DCOOCH_3$	$7{,}8\ 10^{14} cm^{-2}$	Orion	Margulès et al. *ApJ*, **714**, 1120, (2010)
(A/S) $HCOOCH_2D$	$5\ 10^{14} cm^{-2}$	Orion	Paper in preparation
Both ^{13}C isotopologs	$6.6\ 10^{14} cm^{-2}$	Orion	Based on the present work

Summary and perspectives

1. The Methylformate is an interstellar molecule with a methyl group capable of internal rotation at the low temperatures in the ISM
2. The latest work on the g.s. of the ^{13}C-2 isotopolog has been continued up to 940 GHz
3. The ν_t = 1 was analysed and a global fit with the BELGI program of ν_t = 0 and 1 resulted in the determination of 58 parameters providing a better ability of reproducing the experimental spectra's
4. Thanks to the present laboratory analysis, lines of the first torsional excited state were detected in IRAM 30 m line survey for Orion
5. The analysis and fitting procedures are still in progress with the aim of reaching higher quantum numbers
6. *The article dissecting the present work is in preparation*


THANK YOU FOR YOUR ATTENTION !