

MILLIMETER WAVE SPECTRUM AND ASTRONOMICAL SEARCH OF VINYL FORMATE

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Abstract

Previous detections of methyl and ethyl formate make other small substituted formates potential candidates for observation in the interstellar medium. Among them, vinyl formate is one of the simplest unsaturated carboxylic ester. The aim of this work is to provide direct experimental frequencies of the ground vibrational state of vinyl formate in a large spectral range for astrophysical use. The room-temperature rotational spectrum of vinyl formate has been measured from 80 to 360 GHz and analyzed in terms of Watson's semirigid rotor Hamiltonian. 2600 transitions within $J = 3 - 88$ and $K_a = 0 - 28$ were assigned for the most stable conformer of vinyl formate and a new set of spectroscopic constants was accurately determined. Spectral features of vinyl formate were then searched for in Orion KL, Sgr B2(N), B1-b, and TMC-1 molecular clouds. Upper limits to the column density of vinyl formate are provided.

Keywords: catalogs — ISM: molecules — molecular data — techniques: spectroscopic

1. INTRODUCTION

Methyl formate (CH_3OCOH) is one of the most abundant complex organic molecules in the interstellar medium (ISM). Ever since its first detection in Sgr B2 (Brown et al. 1975; Churchwell & Winnewisser 1975), large number of lines originating from the ground and torsionally excited vibrational states (Demyk et al. 2008; Kobayashi et al. 2007; Lovas 2016) as well as mono-deuterated, ^{13}C and ^{18}O isotopic species (Haykal et al. 2014; Coudert et al. 2013; Tercero et al. 2012; Margulès et al. 2010; Carvajal et al. 2009) were found in different molecular clouds. The choice of new candidates to be searched for is usually justified by analogy with already detected molecules and based on a plausible chemistry occurring in the ISM. Thus, substituted formates could be present and, rather recently, the presence of the ethyl derivative ($\text{CH}_3\text{CH}_2\text{OCOH}$) has been evidenced in Sgr B2(N) (Belloche et al. 2009, 2013) and Orion KL (Tercero et al. 2013). Several species containing the vinyl functional group have been observed in the interstellar medium: vinyl cyanide ($\text{CH}_2=\text{CHCN}$, Gardner & Winnewisser 1975; Schilke et al. 1997; Nummelin & Bergman 1999; López et al. 2014), vinyl alcohol ($\text{CH}_2=\text{CHOH}$, Turner & Apponi 2001), propenal ($\text{CH}_2=\text{CHCHO}$, Hollis et al. 2004; Requena-Torres et al. 2008), and propylene ($\text{CH}_2=\text{CHCH}_3$, Marcelino et al. 2007), leading to consider vinyl formate ($\text{CH}_2=\text{CHOCHO}$) as a good candidate. It could be formed starting from the vinyl alcohol and carbon monoxide or from formic acid and acety-

lene, all these possible precursors being already detected in the ISM.

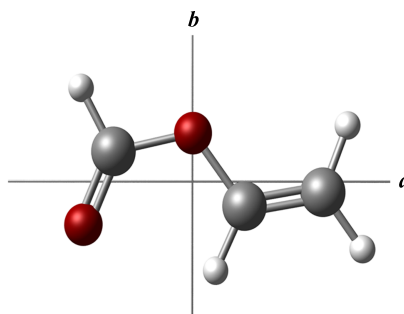


Figure 1. The most stable *cis-trans* conformer of vinyl formate defined by two dihedral angles $\phi_1(\text{O}=\text{C}-\text{O}-\text{C}) = 0^\circ$ and $\phi_2(\text{C}-\text{O}-\text{C}=\text{C}) = 180^\circ$.

While vinyl acetate, one of the simplest unsaturated carboxylic ester after vinyl formate, has been recently searched for in Orion KL (Kolesníková et al. 2015), no such trials have been conducted for vinyl formate. Detection of new complex molecules, such as vinyl formate, by millimeter and submillimeter wave astronomy is usually hampered with several difficulties: low fractional abundances with respect to H_2 , large partition functions, presence of multiple conformations, but also, to a large extent, a lack of reference laboratory spectra. Prior to this work, vinyl formate has been studied in the gas phase by a conventional Stark-modulation spectroscopy (Rao & Curl 1964; Voss et al. 1978), electron diffraction and

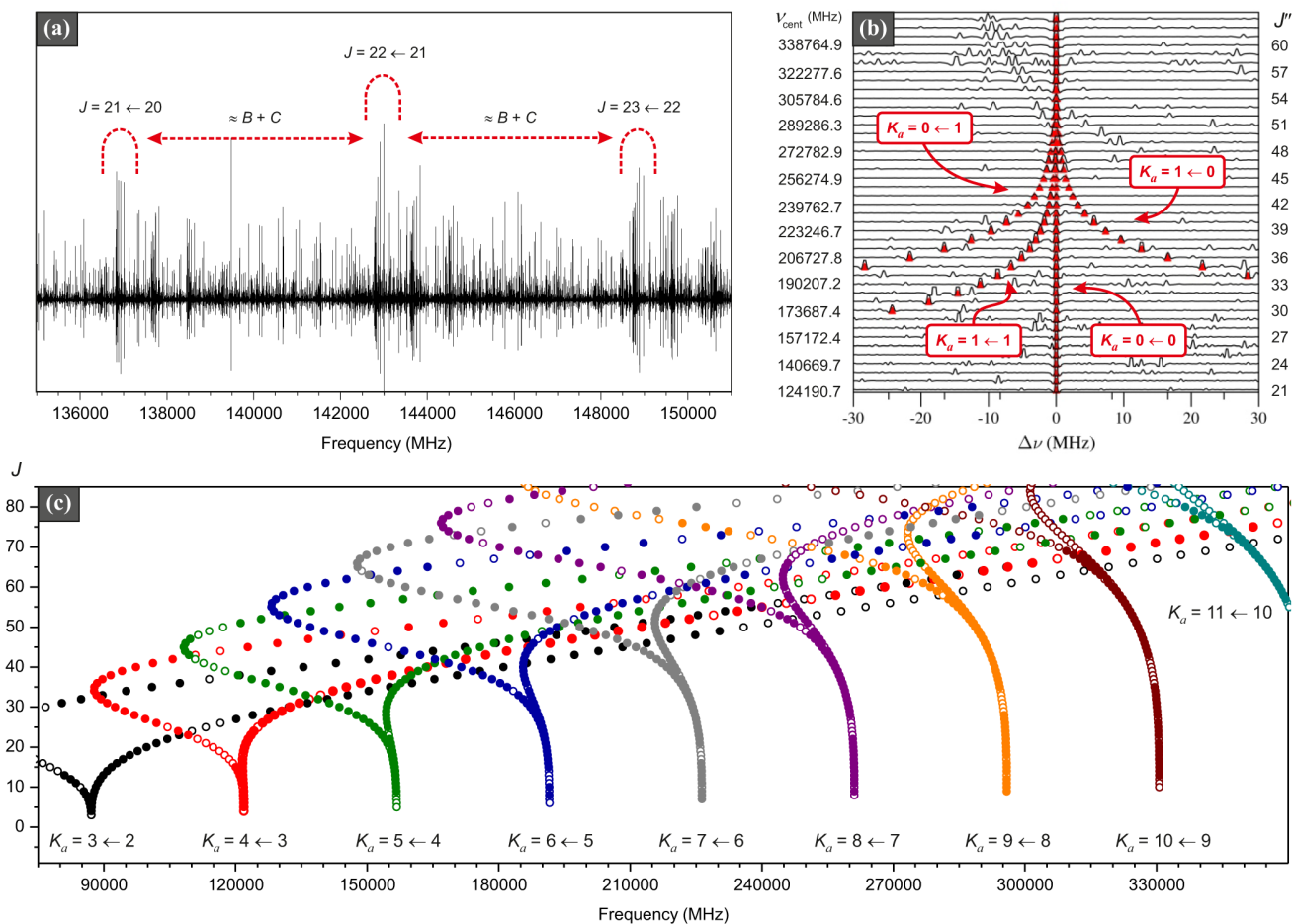


Figure 2. (a): A 16 GHz section of the room-temperature rotational spectrum of vinyl formate. Groups of the ground state a -type R -branch transitions and their approximate separations are indicated. (b): Loomis-Wood-type plot illustrating a convergence of the a -type and b -type R -branch transitions with lowest values of the K_a quantum numbers. Four different line sequences corresponding to $K_a = 0 \leftarrow 0$, $1 \leftarrow 1$, $1 \leftarrow 0$, and $0 \leftarrow 1$ can be found up to $J'' \approx 45$. At $J'' > 50$, only one strong line can be observed. Rotational transitions are lined up to the central frequencies ν_{cent} of the $K_a = 0 \leftarrow 0$ transitions and J'' quantum numbers indicated on the left and right side of the diagram, respectively. A frequency distance from the central stripe is given by $\Delta\nu$ quantity. (c): Fortrat diagram of the b -type Q -branch series of transitions analyzed in this work. The filled circles represent the experimentally measured data while the opened circles come from predictions from the final fit. All Q -branches with $K_a > 0$ are divided into two sub-branches. The lower-frequency sub-branch, which conspicuously doubles back on itself in frequency, corresponds to transitions fulfilling the $K_a + K_c = J$ condition. On the other hand, the higher-frequency sub-branch belongs to $K_a + K_c = J + 1$ transitions.

infrared spectroscopy (Pyckhout et al. 1986). All of those studies indicate that the *cis-trans* structure, presented in Fig. 1, is the most stable conformer of gaseous vinyl formate at room temperature, in agreement with *ab initio* calculations (Pyckhout et al. 1986; Aroney et al. 1976). Although the previous microwave data (10 – 20 GHz, $J \leq 8$ and $K_a \leq 2$) provided first rotational constants of this conformer, they cannot be used to accurately predict its frequencies in the millimeter wave domain. Large frequency uncertainties resulting from the extrapolation outside the experimentally known data region prevent to analyze confidently an astronomical survey of interstellar molecular clouds. The absence of accurate laboratory millimeter wave data thus stimulated new spectroscopic measurements up to 360 GHz. The precise set of the spectroscopic constants is provided and has been used to search for this species in the interstellar medium.

2. EXPERIMENTAL DETAILS

2.1. Chemical synthesis

Vinyl formate is a colorless liquid compound with boiling point of 46°C (Rostovskii & Barinova 1963) and was synthesized as follows. Gaseous acetylene (C_2H_2) was bubbled for 2 hours into 100 g of 100% formic acid ($HCOOH$) and 4% mercury phosphate ($Hg_3(PO_4)_2$) giving vinyl formate ($CH_2CHOCHO$) and 1,1-ethanediol diformate ($CH_3CHOC(O)H_2$). The temperature was maintained at 50 – 55°C during the reaction. The crude mixture was then fitted on a vacuum line (0.1 mbar) and the low boiling compounds were distilled. A first trap at $-65^\circ C$ selective condensed high boiling compounds while vinyl formate was selectively trapped in a second trap cooled at $-120^\circ C$. A second purification by distillation in vacuum was performed to

obtain a pure compound. Yield: 45%.

2.2. Rotational spectra measurements

The room-temperature rotational spectra were recorded at the pressure of approximately 20 μ bar using the Valladolid millimeter wave absorption spectrometer (Daly et al. 2014). A sequential multiplication of the basic synthesizer frequency (≤ 20 GHz) by a set of active and passive multipliers (6 \times , 9 \times , 12 \times , and 18 \times multiplication factors, VDI, Inc.) allowed to cover the frequency region from 80 to 360 GHz. The synthesizer output was frequency modulated at the modulation frequency $f = 10.2$ kHz and modulation depth between 30 and 40 kHz. The signal was detected by solid-state zero-bias detectors (VDI, Inc.) and further processed by lock-in amplifier using $2f$ detection. The second derivative shape of the lines was fit to the Gaussian profile function. The uncertainty of the line center frequency is estimated to be better than 50 kHz.

3. ANALYSIS OF THE SPECTRA

The molecular structure of *cis-trans* conformer of vinyl formate is shown in Fig 1. It is a planar near-prolate asymmetric rotor ($\kappa = -0.95$) of C_s symmetry with electric dipole moment oriented in the ab inertial plane. Two nonzero dipole moment components were determined by Rao & Curl (1964) to $|\mu_a| = 1.1$ (1) D and $|\mu_b| = 1.0$ (1) D. **A portion of the room-temperature millimeter wave spectrum is illustrated in Fig. 2(a). Groups of a -type R -branch transitions dominate the millimeter wave spectrum and can be easily identified due to their typical $(B + C)$ periodicity (see Fig. 2(a)). These groups are interspersed by b -type R -branch transitions which do not cluster into any characteristic pattern. However, as J increases, the rotational energy levels with lowest- K_a quantum numbers become near-degenerate and pairs of b -type transitions involving these energy levels form quartets of similar intensity with corresponding pairs of a -type transitions before they coalesce into one quadruply degenerate line. A good visibility of this progressive line blending with the use of graphical Loomis-Wood-type plot (AABS package, Kisiel et al. (2005)) is shown in Fig. 2(b).** Finally, bands of b -type Q -branch transitions form another easily recognizable feature of the millimeter wave spectrum of vinyl formate. Typical contour and properties of the Q -branch series can be displayed in the Fortrat diagram, demonstrated in Fig. 2(c), which plots the individual transition frequencies versus J quantum number.

At the initial stage of the line assignment, predictions based on the spectroscopic constants from (Rao & Curl 1964) were used. Intense R -branch transitions involving $K_a = 0, 1$ energy levels were searched for at first. Subsequently, higher K_a R -branch transitions together with several Q -branch and some P -branch transitions were assigned. Finally, 2600 transition lines were measured and the ranges of J and K_a quantum numbers were extended up to 88 and 28, respec-

Table 1. Ground state spectroscopic constants of vinyl formate (S -reduction, I' -representation).

Constant	Unit	Value ^a
A	MHz	20391.47934 (25)
B	MHz	3184.151243 (37)
C	MHz	2757.735370 (37)
D_J	kHz	0.717093 (18)
D_{JK}	kHz	-8.82527 (25)
D_K	kHz	118.0508 (36)
d_1	kHz	-0.1379641 (20)
d_2	kHz	-0.00877161 (90)
H_J	Hz	0.0003413 (28)
H_{JK}	Hz	-0.008785 (93)
H_{KJ}	Hz	0.05985 (66)
H_K	Hz	-2.099 (16)
h_1	mHz	0.00513 (30)
h_2	mHz	0.02057 (20)
h_3	mHz	0.003154 (53)
L_{JJK}	mHz	0.0001869 (97)
L_{JK}	mHz	-0.005498 (81)
L_{KKJ}	mHz	0.08838 (74)
σ_{fit}^b	kHz	24

^aThe numbers in parentheses are 1σ uncertainties in units of the last decimal digit. ^bRoot mean square deviation of the fit.

tively. The fits and predictions were made in terms of Watson's S -reduced Hamiltonian in I' -representation (Watson 1977) with Picketts SPFIT/SPCAT program suite (Pickett 1991). The present data allowed determination of the rotational constants and full set of quartic and sextic centrifugal distortion constants. Three octic constants were necessary to fit the $K_a \geq 18$ transitions within the experimental uncertainty. The spectroscopic constants are collected in Table 1 and the measured transitions are reported in Table 2.

4. SEARCHING FOR VINYL FORMATE IN SPACE

The new spectroscopic results presented in this work allow us to carry out a rigorous search for vinyl formate in space. High-mass star-forming regions are the best candidates for this search: on the one hand, both methyl and ethyl formate (CH_3OCOH and $\text{CH}_3\text{CH}_2\text{OCOH}$) have been detected in Orion KL (Tercero et al. 2013) and Sgr B2 (Belloche et al. 2009, 2013), being the former species one of the most abundant molecules in these regions. On the other hand, vinyl cyanide (CH_2CHCN) is other of the most abundant species in those sources (López et al. 2014; Belloche et al. 2013) and also is related to its extremely abundant methyl and ethyl counterparts. Therefore, we mainly focused on the available astronomical data of Orion KL and Sgr B2.

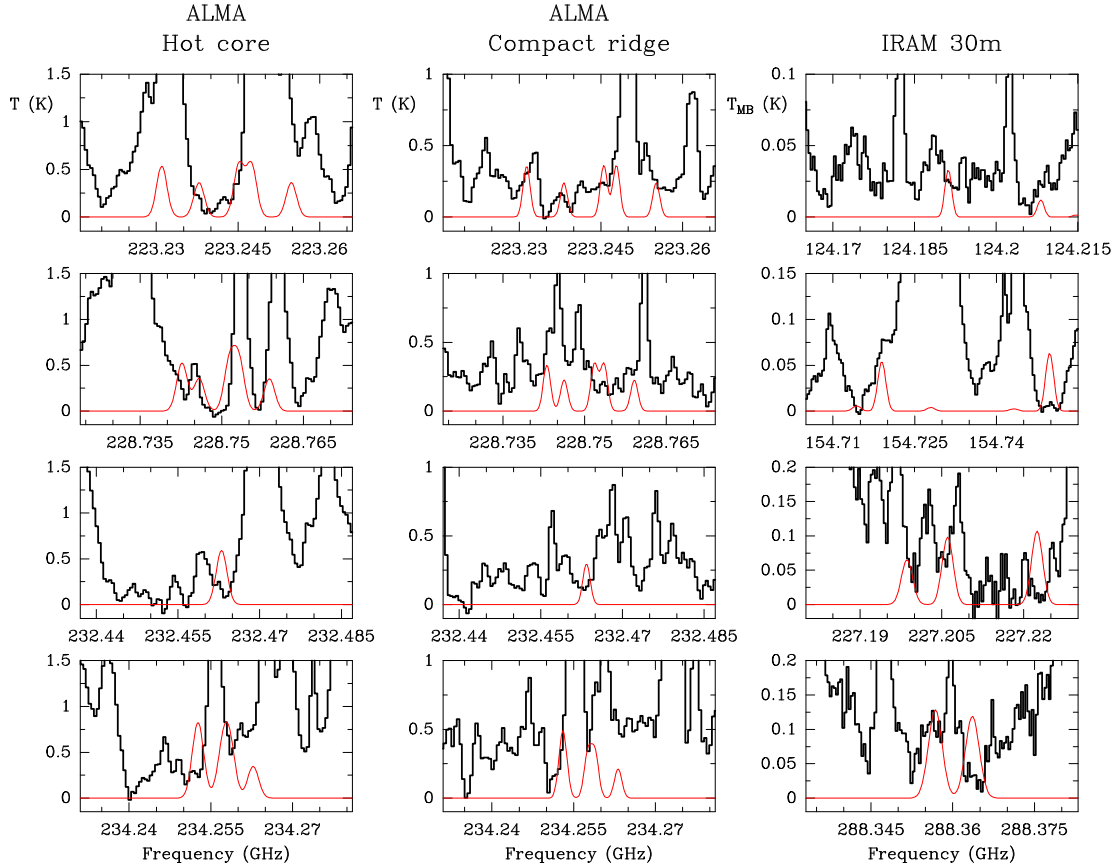


Figure 3. ALMA SV data of two different positions and IRAM 30m data at selected frequencies together with the synthetic spectra of vinyl formate obtained using the column densities shown in Table 3. A v_{LSR} of $+9.0 \text{ km s}^{-1}$ is assumed.

4.1. Orion KL

Combining the IRAM 30m survey (Tercero et al. 2010, 2015) and the ALMA Science Verification (SV) data of this source we could analyze a wide frequency band (80–306 GHz) and focus on different positions characterized each one of them by a typical chemistry: the compact ridge where the emission peak of methyl and ethyl formate is located (see Tercero et al. 2015; Favre et al. 2011a) and a position in the middle of the hot core clumpy structure (see e.g. Favre et al. 2011b) that corresponds with the emission peak of ethylene glycol ($\text{HOCH}_2\text{CH}_2\text{OH}$; Brouillet et al. 2015) and methyl isocyanate (CH_3NCO ; Cernicharo et al. 2016). Vinyl formate was implemented in the MADEX code (Cernicharo 2012) to obtain a synthetic spectrum of this species according to the typical physical parameters of the source (see Table 3 and, e.g., Cernicharo et al. 2016; Tercero et al. 2015). As Fig. 3 shows, we did not detect vinyl formate above the confusion limit of these data. Hence, we can only estimate upper limits to its column density, which are shown in Table 3. In Fig. 3 the model is shown by the red curve over imposed on the IRAM 30m and ALMA SV data at selected frequencies and positions. Above the limit established by these models, we see that most of the vinyl formate lines are missing.

We found that in the compact ridge of Orion KL vinyl formate is 240 and 2 times less abundant than methyl formate and ethyl formate, respectively (see Tercero et al. 2015, for the derived column densities of methyl and ethyl formate).

4.2. Sgr B2

We continued the search for vinyl formate in space checking public data of Sgr B2. As in the Orion case, we did not find this species above the detection limit of the data, either in the PRIMOS survey at low frequencies from 7 to 50 GHz (Neill et al. 2012) or in the IRAM 30m data at 3 mm (80–115 GHz) of Sgr B2(N) provided by Belloche et al. (2013). According to the physical parameters derived for methyl formate in the source by Belloche et al. (2013), we provide upper limits to the vinyl formate column density in these cloud components (see Table 3, Sgr B2(N), warm gas) and a $N(\text{CH}_3\text{OCOH})/N(\text{CH}_2\text{CHOCOH})$ ratio ~ 10 . In addition, we also derived upper limits to its column density for the cold gas of the region adopting the physical parameters derived by (Brünken et al. 2010) for HOCN (see Table 3, Sgr B2(N), cold gas).

4.3. Dark clouds

Table 2. List of the assigned transitions for the ground state rotational spectrum of vinyl formate.^a

J'	K'_a	K'_c	J''	K''_a	K''_c	$\nu_{\text{obs}}^{\text{b,c}}$ (MHz)	$\nu_{\text{obs}} - \nu_{\text{calc}}^{\text{d}}$ (MHz)
14	0	14	13	0	13	80380.074 (50)	0.008
15	0	15	14	0	14	85861.916 (50)	0.011
30	6	25	29	6	24	179245.443 (50)	-0.008
31	6	26	30	6	25	185284.508 (50)	0.010
56	10	46	55	10	45	334748.164 (50)	-0.021
57	10	47	56	10	46	340796.726 (50)	-0.012
23	4	19	23	3	20	109175.845 (50)	-0.007
24	4	20	24	3	21	106882.004 (50)	-0.001
37	9	28	37	8	29	293853.995 (50)	0.010
38	9	29	38	8	30	293617.252 (50)	-0.007
36	2	34	35	3	33	201778.534 (50)	-0.010
37	2	35	36	3	34	209007.174 (50)	0.004
56	5	51	55	6	50	260889.572 (50)	-0.007
57	5	52	56	6	51	273516.082 (50)	0.027

^aThis table is available in its entirety in machine-readable format in the electronic edition of the online journal. A portion is shown here for guidance regarding its form and content. ^bObserved frequency. Spectral lines containing two or more unresolved transitions were excluded from the fit if the difference of predicted frequencies of individual transitions is larger than 30 kHz. If their difference is less than 30 kHz, only one transition was assigned to the observed line. ^cValues in parentheses are uncertainties of the observed frequency in kHz. ^dObserved minus calculated frequency.

Finally, although we mainly expected vinyl formate in the warm gas, we explored the IRAM 30m surveys of B1-b and TMC-1 (Cernicharo et al. 2012) to derive new constraints to the chemistry of these objects. The upper limits to the CH₂CHOCO column density in these dark clouds are shown in Table 3.

4.4. Vinyl species in Orion

From the results of acrylic acid (CH₂CHCOOH, see Alonso et al. 2015), we estimated an upper limit to the column density of vinyl formate of $1.5 \times 10^{16} \text{ cm}^{-2}$ in Orion. In this work, we find a lower upper limit for the abundance of this molecule in the source. As we discussed in Alonso et al. (2015), the upper limit on the column density of vinyl derivatives such as vinyl formate or acrylic acid puts strong constraints to the production mechanisms of

vinyl species. These species in Orion are associated with cyanide groups rather than with alcohols, formates, or acetates. Interestingly, emission from vinyl and ethyl cyanide is strongly concentrated in a hot ($T_{\text{rot}} \approx 350 \text{ K}$) region of Orion KL (see Daly et al. 2013; López et al. 2014; Cernicharo et al. 2016). Neither ethyl alcohol nor methyl and ethyl formate are associated to components at this high temperature, being the warm gas ($\sim 150 \text{ K}$) the responsible for the bulk of the emission of these later species. Therefore, as well as possible different mechanisms to produce the vinyl derivatives for each functional group, small differences in the gas temperature may play an important role in the production of the vinyl species.

Although we do not detect vinyl formate in this work, the search for this species should be considered in future spectroscopic analysis of star forming regions where the gas temperatures are high and large abundances of methyl formate are found. The present data can be used with confidence in future searches for vinyl formate in space.

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Software: AABS (Kisiel et al. 2005), SPFIT/SPCAT (Pickett 1991), MADEX (Cernicharo 2012).

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Table 3. Physical parameters of the considered cloud cores.

Source	v_{LSR} (km s ⁻¹)	Δv_{FWHM} (km s ⁻¹)	d_{sou} (")	T_{rot} (K)	$N(\text{CH}_2\text{CHOCO}) \times 10^{15}$ (cm ⁻²)
Orion KL (IRAM 30m)	8	3	5	150	$\leq (4.0 \pm 1.2)$
Orion KL (ALMA SV) Hot core	8	3	3	150	$\leq (2.0 \pm 0.6)$
Orion KL (ALMA SV) Compact Ridge	7.5	2	3	100	$\leq (1.0 \pm 0.3)$
Sgr B2(N)(IRAM 30m) Warm gas	63.5	7	4	80	$\leq (50 \pm 15)$
	73.5	7	4	80	$\leq (20 \pm 6)$
Sgr B2(N)(IRAM 30m) Cold gas	64	9	60	14	$\leq (0.5 \pm 0.2)$
	75	12	60	14	$\leq (0.5 \pm 0.2)$
B1-b (IRAM 30m)	6.7	0.7	60	12	$\leq (0.005 \pm 0.002)$
TMC-1 (IRAM 30m)	6.0	0.7	60	10	$\leq (0.005 \pm 0.002)$

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