

The millimeter wave spectrum of *s-cis*- and *s-trans*-acrylic acid in its ground vibrational state

E. R. Alonso^a, L. Kolesníková^a, I. Peña^a, S. T. Shipman^b, B. Tercero^c, J. Cernicharo^c,
and J. L. Alonso^{a,*}

^a *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopia y Bioespectroscopia, Parque Científico UVA, Unidad Asociada CSIC, Universidad de Valladolid, 47011 Valladolid, Spain*

^b *Division of Natural Sciences, New College of Florida, Sarasota, FL 34243, USA*

^c *Instituto de Ciencia de Materiales de Madrid, CSIC, C/ Sor Juana Inés de la Cruz 3, 28049 Cantoblanco, Spain.*

Abstract

The millimeter wave spectrum of acrylic acid ($\text{CH}_2=\text{CH}-\text{COOH}$), the simplest unsaturated carboxylic acid, was measured and analyzed from 130 to 360 GHz. Additional measurements from 18 to 26.5 GHz were also made using a waveguide CP-FTMW spectrometer. More than 4000 rotational lines were assigned to *s-cis*- and *s-trans*-acrylic acid in their ground vibrational states. New laboratory data of acrylic acid were then used to search for its spectral features in Orion KL, Sgr B2, and W51 molecular clouds. An upper limit to the column density of acrylic acid in Orion KL is provided.

Keywords: Acrylic acid, Millimeter wave spectrum, Rotational spectrum, Interstellar medium

*Corresponding author: Phone: +34 983186348; Fax: +34 983186349
E-mail address: jlonso@qf.uva.es

1. Introduction

Active regions of high-mass star formations, such as the Orion KL and Sgr B2 molecular clouds, show incredibly rich chemistry as a result of the interaction of the newly formed stars with their environment and are the prime targets of several current astrochemical investigations. The search for complex organic molecules (COMs) undoubtedly belongs among them. In the context of astrochemistry, COMs are defined as organic molecules with six or more atoms [1] and are considered crucial molecules due to their connection with organic and biochemical processes occurring on the Earth. One of the most important techniques for studying these molecular clouds and searching for COMs is mm/submm astronomy, which probes the rotational spectra of gas phase molecules and, in addition to the characterization of the species, provides valuable information about the physical conditions of the gas. Although a large variety of simpler molecules as well as COMs have been found in these sources [2, 3], thousands of spectral features are still observed in the line surveys captured by numerous observational facilities working on the ground (e.g. IRAM, ALMA, GBT, NRAO, BIMA, CARMA, CSO, SEST) or in space (Herschel/HIFI). The new generation of telescopes, especially such as the ALMA project, is bringing scientifically very important data, since the sensitivity and angular resolution are substantially improved in comparison with other currently used single-dish telescopes, and these capabilities open more possibilities towards detections of interstellar molecules in smaller abundances than before. The frequency coverage of the ALMA interferometer from 84 to 720 GHz thus motivates laboratory spectroscopists to record and analyze the rotational spectra in the millimeter and sub-millimeter wave region and to gather an atlas of line positions and intensities for potentially detectable molecules. Acrylic acid (prop-2-enoic acid, $\text{CH}_2=\text{CH}-\text{COOH}$) is the simplest unsaturated carboxylic acid and seems to be a logical molecule to search for since it shares the carboxyl ($-\text{COOH}$) and vinyl ($-\text{CH}=\text{CH}_2$) functional groups with other already detected

interstellar and circumstellar molecules: formic acid (H-COOH) [4-8], acetic acid (CH₃-COOH) [6, 9-12], vinyl alcohol (CH₂=CH-OH) [13], vinyl cyanide (CH₂=CH-CN) [7, 14-17], propenal (CH₂=CH-CHO) [18, 19], and propylene (CH₂=CH-CH₃) [20]. Tentative detection of another complex vinyl containing species, vinyl acetate, has been discussed recently [21].

Acrylic acid exists in two stable planar forms, *s-cis* and *s-trans* (IUPAC nomenclature), defined by the arrangement of two double bonds about the single C-C bond (see Fig. 1). The *s-cis* structure has been established to be the more stable one by only $58 \pm 20 \text{ cm}^{-1}$ [22]. Rotational spectra of both isomeric forms were measured for the first time by Bolton et. al. [22] from 18 to 40 GHz by a conventional Stark-modulated spectrometer. Later on, Calabrese et. al. [23] used the supersonic-jet Fourier transform microwave and Stark-modulated free-jet techniques to record the spectra in the frequency ranges 6 – 18.5 and 52 – 74.4 GHz. Very recently, during the course of this study, another work in several narrow frequency windows was performed: 95.7 – 104, 108.7 – 109.2, 289.4 – 294, and 391.3 – 397.3 GHz [24]. Authors assigned almost 600 new lines and improved the determination of spectroscopic constants for both isomers. Predicted transitions of acrylic acid at frequencies above 480 GHz were then searched for towards the star forming region DR21(OH) using the Herschel Science Archive data with negative results.

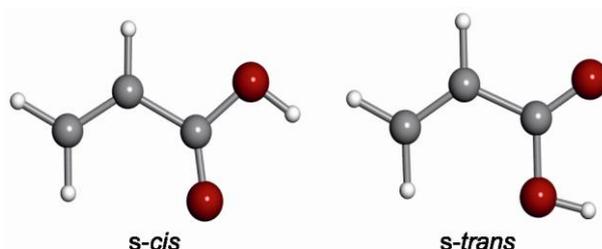


Fig. 1: Two planar isomeric forms of acrylic acid.

The aim of this work was similar to those of Calabrese et. al. [24], i.e. extension of the measurements of the acrylic acid rotational spectrum to higher frequencies that may facilitate its detection in the interstellar medium. The continuous broadband spectrum measured from 130 to 360 GHz allowed to assign more than 4000 lines and to derive the spectroscopic constants for both *s-cis* and *s-trans* isomers up to the sixth order. In comparison with previous work, direct laboratory data obtained in this study were used to search for the acrylic acid in several more sensitive surveys. Orion KL, Sgr B2, and W51 molecular clouds, which are known for their rich organic chemistry, were chosen and results are discussed in section 4.

2. Experimental details

A commercial sample of acrylic acid (b.p. 139 °C) was used without any further purification. Rotational spectra measurements were carried out on two different spectrometers. A waveguide chirped-pulse Fourier transform microwave spectrometer at New College of Florida was used to record the spectrum in the 18–26.5 GHz region at a temperature of –15 °C and a pressure of 3 mTorr. Details about the spectrometer can be found elsewhere [25]. In each spectrum, 100 million free induction decays of 4 μ s duration were averaged and Fourier transformed using a Kaiser–Bessel window function. The frequency accuracy was set to 50 kHz.

Rotational spectra from 130 to 360 GHz were taken at room temperature and a pressure of approximately 15 mTorr by the millimeter wave spectrometer at the University of Valladolid. Information concerning the synthesizer, cascade frequency multipliers as well as detectors can be found in Daly et. al. [26]. All spectra were recorded in 1 GHz scans using the frequency modulation technique with $2f$ lock-in detection, where $f = 10.2$ kHz is the modulation frequency, and modulation depth of 30 kHz. Frequency accuracy of isolated well-developed lines was estimated to be better than 50 kHz.

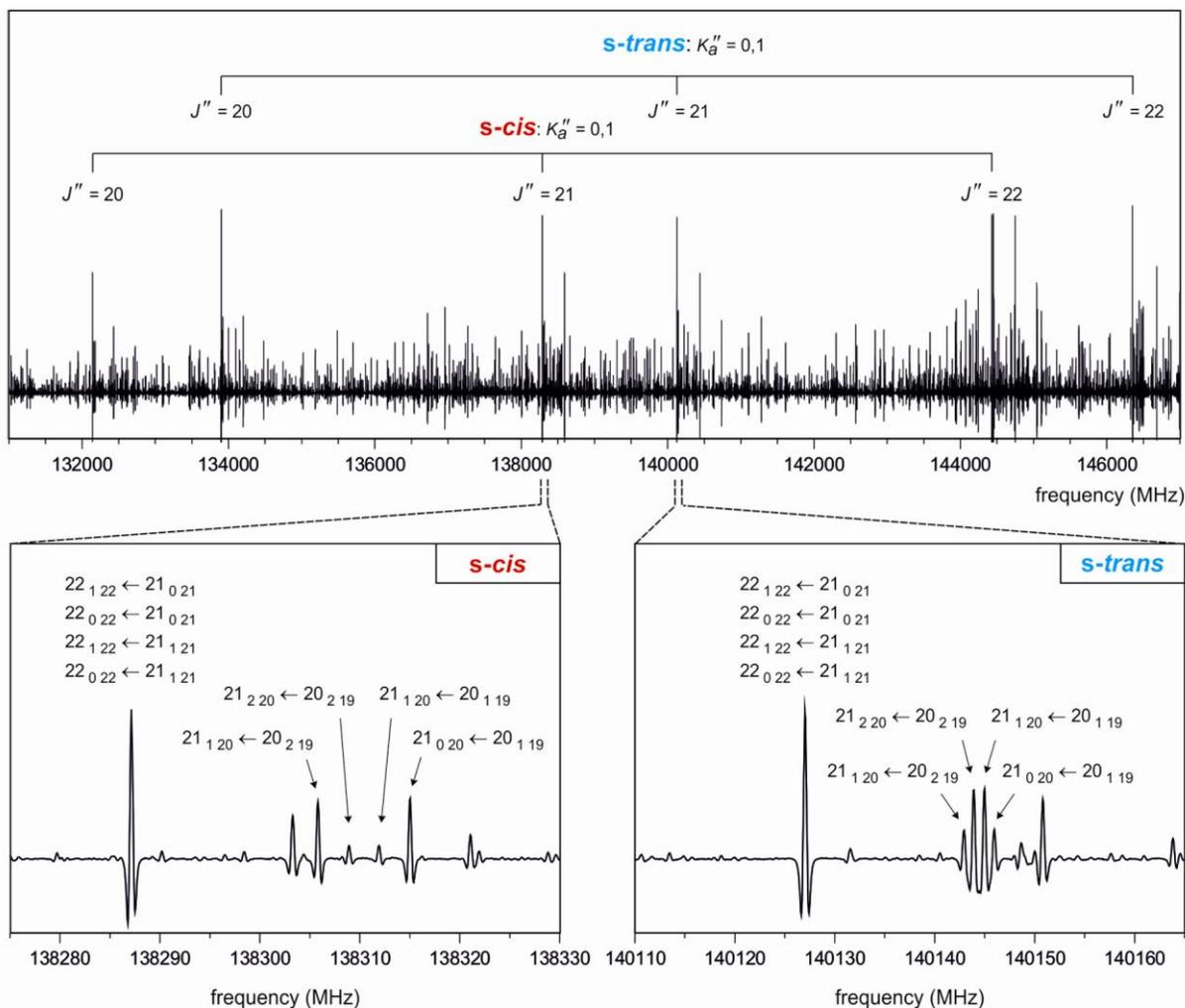


Fig. 2: Upper panel: section of the acrylic acid rotational spectrum with assignment of the strongest spectral features for the *s-cis* and *s-trans* isomers. Lower panels: quartets of *a*-type and *b*-type *R*-branch rotational transitions between nearly degenerate pairs of levels with lowest values of K_a quantum number.

3. Analysis of the spectra

Previous Stark measurements provided the dipole moment components of $|\mu_a^{s-cis}| = 0.56(10)$ D, $|\mu_b^{s-cis}| = 1.35(5)$ D, $|\mu_a^{s-trans}| = 1.70(4)$ D, and $|\mu_b^{s-trans}| = 1.10(5)$ D [22] indicating that both *a*-type and *b*-type transitions are relevant for both isomers. Predictions based on previous work of Calabrese et. al. [23] significantly facilitated the assignments at lower frequencies as well as their extension into the millimeter wave range. A section of the rotational spectrum at the millimeter wavelengths is shown in Fig. 2. *a*-type and *b*-type *R*-

branch transitions between near degenerate pairs of levels for low values of K_a quantum number form the most intense lines of the acrylic acid rotational spectrum (see Fig. 2, upper panel). For $K_a = 0$ and 1, these transitions are overlapped and one absorption line, repeating with a period of $\approx 2C$, thus corresponds to a pair of a -type and a pair of b -type transitions. In such cases, four transitions were assigned to one experimental frequency and were fitted to their intensity weighted averages. With increasing K_a , these transitions form quartets (see Fig. 2, lower panels) which become degenerate as J increases. For the *s-cis* isomer, a total of 2381 distinct frequency lines were newly assigned in this work to 3107 a -type and b -type Q - and R -branch transitions and several b -type P -branch transitions ($2 \leq J \leq 74$, $0 \leq K_a \leq 24$). These data were collected into a single data set with 24 lines from Bolton et. al. [22] and 76 lines from Calabrese et. al. [23] and were least-squares fitted using the Watson's semi-rigid Hamiltonian in S -reduction and F' -representation [27]. For the *s-trans* isomer, 1697 distinct frequency lines were assigned to 2323 a -type and b -type Q - and R -branch transitions and a few b -type P -branch transitions ($2 \leq J \leq 76$, $0 \leq K_a \leq 24$). These transition lines were combined with 28 lines from Bolton et. al. [22] and 73 lines from Calabrese et. al. [23] and were analyzed in the same way as the *s-cis* isomer data. The resulting spectroscopic constants for both isomers of acrylic acid are listed in Table 1 and the complete lists of the rotational transitions included in the fits are given in Tables S1 and S2 of the electronic supplementary material. The present data sets improve the determination of quartic centrifugal distortion constants and allowed for the derivation of a complete set of sextic ones leading to stronger predictive power of many additional lines for both *s-cis* and *s-trans* isomer at higher frequencies if necessary.

Table 1: Spectroscopic constants of *s-cis* and *s-trans* acrylic acid (*S*-reduction, *I'*-representation)^a.

Constant	Unit	<i>s-cis</i>	<i>s-trans</i>
<i>A</i>	MHz	11078.87327 (19)	10716.20452 (45)
<i>B</i>	MHz	4251.971260 (81)	4388.30110 (13)
<i>C</i>	MHz	3073.397662 (83)	3114.31077 (10)
<i>D_J</i>	kHz	0.662086 (58)	0.683756 (71)
<i>D_{JK}</i>	kHz	5.20116 (16)	5.42718 (82)
<i>D_K</i>	kHz	4.70200 (73)	3.9778 (44)
<i>d₁</i>	kHz	−0.2248528 (98)	−0.244260 (28)
<i>d₂</i>	kHz	−0.0731989 (40)	−0.084519 (12)
<i>H_J</i>	mHz	0.107 (12)	−0.102 (18)
<i>H_{JK}</i>	mHz	−4.723 (33)	−6.89 (37)
<i>H_{KJ}</i>	mHz	−2.95 (19)	−11.0 (32)
<i>H_K</i>	mHz	32.53 (89)	184 (14)
<i>h₁</i>	mHz	0.0535 (17)	−0.0126 (69)
<i>h₂</i>	mHz	0.0511 (11)	−0.0147 (56)
<i>h₃</i>	mHz	0.04074 (20)	0.0390 (12)
<i>N_{lines}</i> ^b		2381	1697
σ_{fit} ^c	kHz	38	49

^a The numbers in parentheses are 1σ uncertainties in the units of the last decimal digit.

^b Number of the distinct frequency lines in the fit.

^c Root mean square deviation of the fit.

4. Search for acrylic acid in space

The spectroscopic data of acrylic acid (CH_2CHCOOH) from Table 1 allow us to search for this species in space. Hot molecular clouds (HMCs) in which acetic acid (CH_3COOH) has been detected seem the best places to find this species. Acetic acid was discovered towards Sgr B2(N) by Mehringer et al. [9]. After this detection, acetic acid has been identified in other HMCs (w51e2 [10], G34.3+0.15 [11], and G19.61−0.23 [12]) and in low mass star-forming regions (IRAS 16293−2422 [6]). Moreover, the survey of acetic acid in different sources carried out by Remijan et al. [11] pointed out that this species seems to appear in regions where the emission from O- and N-containing species is co-spatial, while in sources for which

we know that there is a spatial separation between these species, acetic acid has not been detected (see Ref. [28] for further discussion). However, using the available ALMA data, we have detected acetic acid towards the South hot core of Orion KL [29]. For the search of acrylic acid, we use several public data sets (see Table 2) of Sgr B2(N), W51, and Orion KL. We did not find acrylic acid in any of these sources above the detection limit of the data. Fig. 3 shows the lack of positive detection of lines of *cis*-CH₂CHCOOH (the most stable conformer) towards Sgr B2(N) and Orion KL. Several lines corresponding to *b*-type transitions (μ_b is the largest dipole moment component) with high line strength (S_{ij}) and in a large variety of upper level energies (E_u) (see Table 3) have been selected according to the typical physical conditions of each source. For panels showing the Sgr B2(N) data, the red vertical line marks the expected rest frequency of the selected transition. For Orion KL, the panels between 214 – 244 GHz show two different positions of the ALMA SV data: the compact ridge (region rich in organic O-bearing species, blue line connecting dots) and the acetic acid peak (from Ref. [29], black histogram spectra). Using MADEX [30], LTE approximation, and assuming these physical and line parameters: source size 3'' (telescope dilution is considered), $T_K = 110$ K, $v_{\text{LSR}} = 7.5$ km s⁻¹, $v = 1.5$ km s⁻¹, we derive an upper limit to the column density of *cis*-acrylic acid in Orion KL of $(3 \pm 1) \times 10^{15}$ cm⁻² and of $(5 \pm 2) \times 10^{14}$ cm⁻² for the IRAM 30m data and the ALMA SV data, respectively. The thin red curve in Fig. 3 shows the synthetic spectrum of *cis*-acrylic acid for the adopted physical parameters.

Table 2: Data sets used to search for the acrylic acid rotational transitions.

Frequency (GHz)	Telescope	Source	Reference
7.7 – 10.7, 11.4 – 15.6, 17.6 – 26.4	GBT ^a	Sgr B2(N)	[31] ^g
30.0 – 41.7, 42.4 – 49.3			
130 – 171	NRAO ^b 12m	Sgr B2(N)	[32] ^{g, h}
218 – 264	SEST ^c	Sgr B2(N)	[33]
260 – 286	CSO ^d	Sgr B2(N)	[34]
18 – 26	GBT	W51	[35] ^g
130 – 171	NRAO 12m	W51 M	[32] ^{g, h}
80 – 115.5, 123.5 – 176, 196.7 – 307	IRAM ^e 30m	Orion KL	[17, 36]
213.71 – 246.63	ALMA ^f	Orion KL	[37]

^a Green Bank Telescope.

^b National Radio Astronomy Observatory.

^c Swedish-ESO Submillimetre Telescope.

^d Caltech Submillimeter Observatory.

^e Institut de Radioastronomie Millimétrique.

^f Atacama Large Millimeter/submillimeter Array.

^g See this reference for full observational details, data reduction procedures, and analysis.

^h These observations are a part of the “Barry E. Turner Legacy Survey”.

5. Conclusions

In the present work, new direct laboratory data allowed to search for the acrylic acid in the interstellar medium, namely in the regions of Orion KL, Sgr B2, and W51 molecular clouds, using the publically available spectral surveys captured by GBT, NRAO, SEST, CSO, IRAM, and ALMA telescopes. Although no spectral features of acrylic acid were found towards these clouds, present data can be confidently used in future to search for this molecule in another interstellar sources.

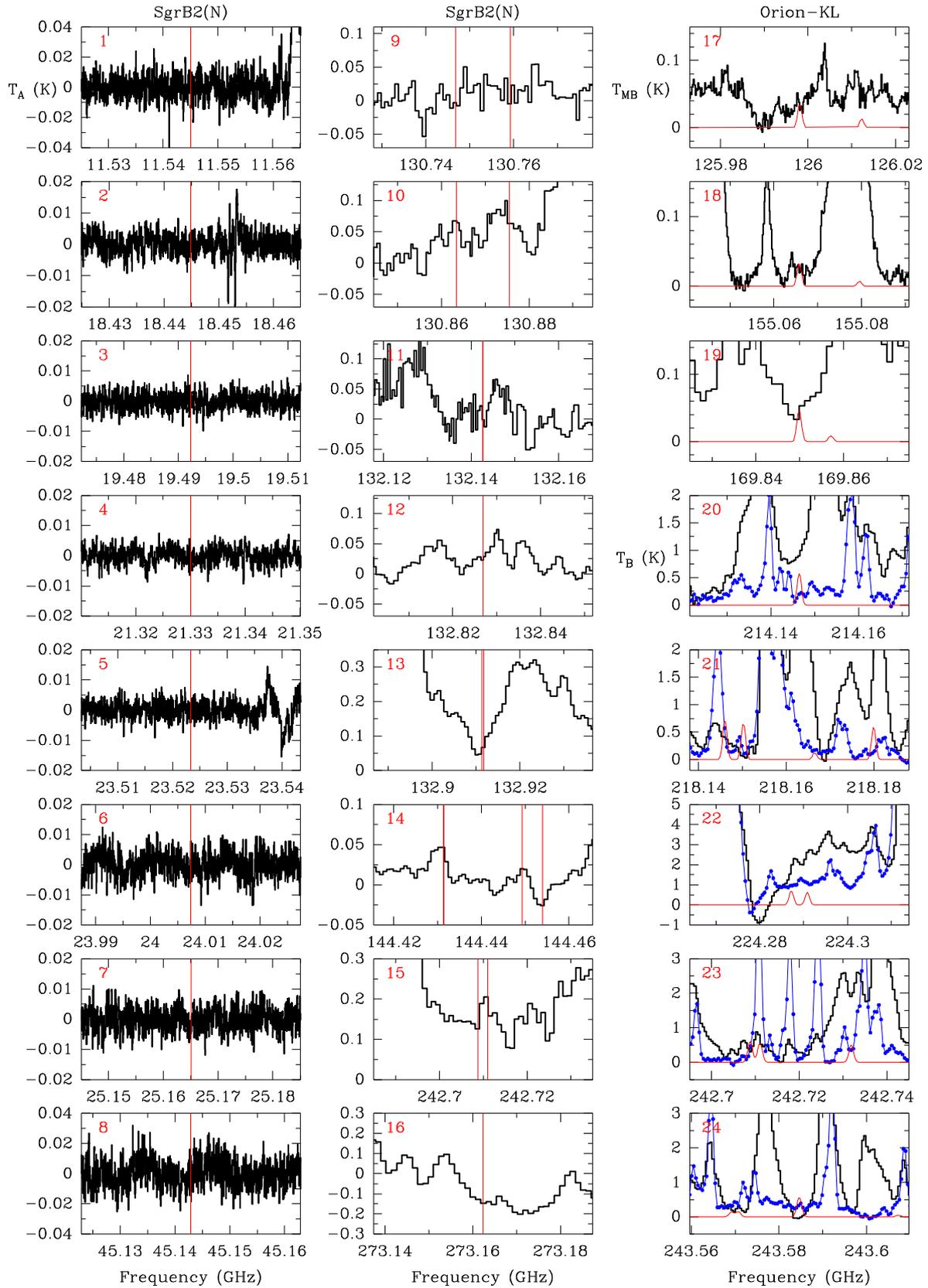


Fig. 3: Negative detection of *cis*-CH₂CHCOOH towards Sgr B2(N) ($v_{\text{LSR}} = 64 \text{ km s}^{-1}$ is assumed) and Orion KL ($v_{\text{LSR}} = 7.5 \text{ km s}^{-1}$ is assumed), see the text.

Table 3: Selected transitions of *cis*-CH₂CHCOOH.

Panel ^a	<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>	Frequency (MHz) ^b	<i>E_u</i> (K) ^c	<i>S_{ij}</i> ^d
1	3	1	2	3	0	3	11545.083	2.6	2.8
2	5	2	3	5	1	4	18444.902	6.9	4.32
3	3	2	1	3	1	2	19492.290	3.6	2.05
4	7	2	5	7	1	6	21330.072	11.8	5.83
5	4	0	4	3	1	3	23523.363	3.4	2.32
6	12	4	9	11	5	6	24007.389	33.5	1.15
7	6	1	5	6	0	6	25165.034	8.2	2.82
8	7	0	7	6	1	6	45142.910	9.2	5.49
9	24	2	22	24	1	23	130746.753	105	5.15
	24	3	22	24	2	23	130759.296	105	5.15
10	27	10	17	27	9	18	130863.491	170.5	15
	28	10	19	28	9	20	130875.507	180.6	15.8
11	21	0	21	20	1	20	132142.620	71.2	19.7
	21	1	21	20	0	20	132142.771	71.2	19.7
12	9	5	4	8	4	5	132826.894	24.8	4.5
13	7	6	2	6	5	1	132911.383	22.7	5.43
13	7	6	1	6	5	2	132911.805	22.7	5.43
14	23	0	23	22	1	22	144431.393	84.8	21.7
	23	1	23	22	0	22	144431.427	84.8	21.7
	22	1	21	21	2	20	144449.277	84	18
	21	2	19	20	3	18	144449.320	82.5	14.1
	22	2	21	21	1	20	144453.949	84	18
15	39	0	39	38	1	38	242708.781	235.8	37.7
	39	1	39	38	0	38	242708.781	235.8	37.7
	38	1	37	37	2	36	242711.01	235	34
	38	2	37	37	1	36	242711.01	235	34
16	14	12	3	13	11	2	273162.328	88.2	11.4
	14	12	2	13	11	3	273162.328	88.2	11.4
17	20	0	20	19	1	19	125997.968	64.9	18.7
	20	1	20	19	1	19	125998.070	64.9	19.8
	20	0	20	19	0	19	125998.179	64.9	19.8
	20	1	20	19	0	19	125998.281	64.9	18.7
18	8	7	2	7	6	1	155065.783	30.1	6.43
	8	7	1	7	6	2	155065.809	30.1	6.43
19	8	8	1	7	7	0	169849.934	35.4	7.46
	8	8	0	7	7	1	169849.934	35.4	7.46
20	10	10	1	9	9	0	214146.459	54.9	9.46
	10	10	0	9	9	1	214146.459	54.9	9.46

21	35	0	35	34	1	34	218146.019	191	33.7
	35	1	35	34	0	34	218146.019	191	33.7
	34	1	33	33	2	32	218150.228	190.2	30
	34	2	33	33	1	32	218150.228	190.2	30
	18	6	12	17	5	13	218166.531	74.2	4.63
	33	2	31	32	3	30	218179.902	188.7	26.3
22	33	3	31	32	2	30	218179.995	188.7	26.3
	36	0	36	35	1	35	224287.182	201.7	34.7
	36	1	36	35	0	35	224287.182	201.7	34.7
	35	1	34	34	2	33	224290.825	201	31
23	35	2	34	34	1	33	224290.825	201	31
	39	0	39	38	1	38	242708.781	235.8	37.7
	39	1	39	38	0	38	242708.781	235.8	37.7
	38	1	37	37	2	36	242711.010	235	34
24	38	2	37	37	1	36	242711.010	235	34
	14	10	5	13	9	4	243584.624	72.7	9.42
	14	10	4	13	9	5	243584.626	72.7	9.42

^a Number of each panel given in Fig. 3.

^b Rest frequency.

^c Upper level energy.

^d Line strength.

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