

The Two Hot Corinos of the SVS13-A Protostellar Binary System: Counterposed Siblings

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Abstract

We present ALMA high-angular-resolution (~50 au) observations of the Class I binary system SVS13-A. We report images of SVS13-A in numerous interstellar complex organic molecules: CH₃OH, ¹³CH₃OH, CH₃CHO, CH₃OCH₃, and NH₂CHO. Two hot corinos at different velocities are imaged in VLA4A ($V_{sys} = +7.7 \text{ km s}^{-1}$) and VLA4B ($V_{sys} = +8.5 \text{ km s}^{-1}$). From a non-LTE analysis of methanol lines, we derive a gas density of $3 \times 10^8 \text{ cm}^{-3}$ and gas temperatures of 140 and 170 K for VLA4A and VLA4B, respectively. For the other species, the column densities are derived from an LTE analysis. Formamide, which is the only N-bearing species detected in our observations, is more prominent around VLA4A, while dimethyl ether, methanol, and acetaldehyde are associated with both VLA4A and VLA4B. We derive in the two hot corinos abundance ratios of ~1 for CH₃OH, ¹³CH₃OH, and CH₃OCH₃; ~2 for CH₃CHO; and ~4 for NH₂CHO. The present data set supports chemical segregation between the different species inside the binary system. The emerging picture is that of an onion-like structure of the two SVS13-A hot corinos, caused by the different binding energies of the species, also supported by ad hoc quantum chemistry calculations. In addition, the comparison between molecular and dust maps suggests that the interstellar complex organic molecules emission originates from slow shocks produced by accretion streamers impacting the VLA4A and VLA4B disks and enriching the gas-phase component.

Unified Astronomy Thesaurus concepts: Astrochemistry (75)

1. Introduction

The birth of planets inside protostellar disks has been traced back in time, as a result of recent ALMA high-angularresolution observations showing substructures in the dust distribution of young (<1 Myr) disks, which may be caused by the interaction of the disk material with forming planets (Sheehan & Eisner 2017; Segura-Cox et al. 2020; Sheehan et al. 2020). Protostellar Class 0/I disks are thus the ideal environment to investigate the initial conditions and the chemical content, which will be at least partially inherited by forming planets (e.g., Öberg & Bergin 2021). From a chemical point of view, close binaries are unique laboratories as they are expected to originate from the same parent core, i.e., the same initial gas composition and similar gas conditions, in terms of temperature, density, and UV illumination. Observed differences in the chemistry of the two binary components are then expected to be the result of a chemical evolution inside the system (e.g., Manigand et al. 2020). SVS13-A is a perfect case study because it is a very well-studied Class I protostellar system in NGC 1333, hosting a rich chemistry including emission from several interstellar complex organic molecules (hereafter iCOMs; López-Sepulcre et al. 2015; Codella et al. 2016; Bianchi et al. 2017; De Simone et al. 2017; Bianchi et al. 2019; Belloche et al. 2020; Diaz-Rodriguez et al. 2021; Yang et al. 2021). The two components of the binary system (VLA4A and VLA4B) have a separation of ~ 0.13 (~ 90 au at the source distance of 299 pc), and they have been imaged in

Original content from this work may be used under the terms of the Creative Commons Attribution 4.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. the continuum using ALMA (Tobin et al. 2016, 2018; Diaz-Rodriguez et al. 2021). Recently, the presence of two hot corinos in both VLA4A and VLA4B has been reported by Diaz-Rodriguez et al. (2021). The detection of ethylene glycol only toward VLA4A suggests the possibility of different chemistry at work in the two binaries, calling for mapping different iCOMs using different excitation transitions. In this Letter, we present ALMA high-angular-resolution observations, imaging the SVS13-A binary system using a large number of lines (17) due to both O-bearing and N-bearing iCOMs, namely methanol (CH₃OH and ¹³CH₃OH), acetalde-hyde (CH₃CHO), dimethyl ether (CH₃OCH₃), and formamide (NH₂CHO), down to planet-formation scales.

2. Observations

The system SVS13-A was observed with ALMA (2018.1.01461.S) in Band 6. Data were acquired on 2019 September 8 using the C43-6 configuration, with baselines between 43 m and 5.9 km. The observations were centered at $\alpha_{J2000} = 03^{h}29^{m}3^{s}8$, $\delta_{J2000} = +31^{\circ}16'03''$. 8. The quasar J0510 +1800 was used as bandpass and flux calibrator, while J0336 +3218 was the phase calibrator. The absolute flux calibration uncertainty is 20%. Data were calibrated using the standard ALMA calibration pipeline within CASA (McMullin et al. 2007). Phase self-calibration has been performed using the IRAM-GILDAS⁵ package, after the determination of line-free continuum channels, and the solutions applied to both the continuum and spectral cubes. The observed spectral windows, as well as the synthesized beam and the rms noise of the

⁵ http://www.iram.fr/IRAMFR/GILDAS

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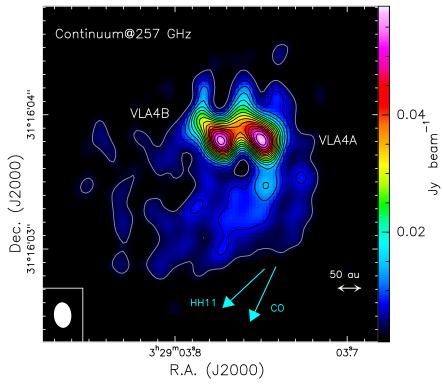


Figure 1. Dust continuum emission at 257 GHz as observed by ALMA (color scale and contours). First contours (gray) and steps (black) are 8σ , corresponding to 3.35 mJy beam⁻¹. The beam size is $0''_{...19} \times 0''_{...19} \times 0''_{...111}$ (PA = +5°). The binary system is composed of VLA4A (right) and VLA4B (left). Coordinates are $\alpha_{J2000} = 03^{h}$ 29^m 3.575, $\delta_{J2000} = +31^{\circ}16'03''_{...1911}$ for VLA4A and VLA4B, respectively. The blue arrows indicate the directions toward HH 11 (133°) as well as the main axis of the H₂/CO jet (155°) as inferred by Lefèvre et al. (2017).

continuum-subtracted line cubes, using spectral channels of $122 \text{ kHz} (0.15 \text{ km s}^{-1})$, are reported in Table B1.

3. Results

3.1. Continuum Emission

Figure 1 shows the SVS13-A map of the dust continuum emission at 1.3 mm. The two emission peaks correspond to the two components of the SVS13-A system previously observed with ALMA as well as at centimeter wavelengths (Carrasco-González et al. 2008; Tobin et al. 2018; Diaz-Rodriguez et al. 2021): VLA4A and VLA4B. In addition, the map shows arclike structures in agreement with that observed by Tobin et al. (2016, 2018) and Diaz-Rodriguez et al. (2021): a bright arc (up to 32σ) extending from the southern edge of the continuum associated with VLA4A toward the southeast and two fainter arcs (up to 16σ) parallel to the first one and extending on the east (i.e., from the southern edge of the continuum associated with VLA4B) and on the west side of VLA4A. In addition, the present image shows further three elongated structures extending from the northern edge of the continuum associated with VLA4A and B toward the north, with a slightly negative PA. As the ALMA beam is roughly elongated along the N-S direction (PA = $+5^{\circ}$), we checked for the presence of possible artifacts caused by the cleaning process by repeating the cleaning using different tapering. With a larger circular beam, all the elongated arc-like structures, including the three structures toward the north, are less evident but still present. The presence of accretion streamers, suggested for VLA4B (Diaz-Rodriguez et al. 2021), is then confirmed by the present ALMA data set also toward VLA4A, and it has an impact on

the following discussion on the origin of iCOM emission (Section 5.1).

The continuum emission associated with VLA4A and VLA4B has a disk-like structure. We modeled the continuum emission in the uv plane assuming two elliptical inclined disks centered on the continuum peak positions. The best fitting is second disk with axes $0.325 (0.242) \times 0.205 (0.153)$ and PA 33°.8 (0°.1) centered toward VLA4B. The integrated fluxes are 183.15 (0.87) mJy and 126.06 (0.55) mJy for VLA4A and VLA4B, respectively. The sizes are $\sim 180 \times 70$ au (VLA4A) and 90×70 au (VLA4B). From the axis ratio, we can infer an inclination of 67° and 51° (with respect to the plane of the sky) for the VLA4A and VLA4B disks, respectively. We calculate the disk masses assuming isothermal and optically thin dust emission. If we assume a dust temperature of 140 K, as derived from line analysis, a dust-to-gas ratio of 1/100, and a dust mass opacity coefficient k_{ν} of $1.0 \text{ cm}^2 \text{ g}^{-1}$ (Ossenkopf & Henning 1994), we obtain 0.029 M_{\odot} for VLA4A and 0.020 M_{\odot} for VLA4B. The value obtained for VLA4B is consistent with that reported by Diaz-Rodriguez et al. (2021), while the one for VLA4A is higher by a factor of 3. If we assume a lower dust temperature of 30 K, we obtain 0.159 M_{\odot} for VLA4A and 0.110 M_{\odot} for VLA4B, in good agreement with that found by Tobin et al. (2018).

3.2. Emission from iCOMs

We detected a total of 17 emission lines from 4 iCOMs (Table 1). More specifically, we detected four lines of CH₃OH and five lines of 13 CH₃OH, covering upper-level energies (E_{up})

Transition	ν^{a} (GHz)	E_{up}^{a}	$S\mu^{2a}$	I_{int^b} (K km s ⁻¹)		
	(GHZ)	(K)	(D ²)	VLA4A	VLA4B	VLA4A/VLA4E
				VLA4A	VLA4D	VLA4A/VLA4E
CH ₃ OH 25 _{3,22} –25 _{2,23} A	241.588758	804	102	251 (53)	112 (26)	2.2 (0.7)
CH ₃ OH 5 _{2,3} -4 _{2,2} E	241.904147	61	14	454 (95)	353 (74)	1.3 (0.4)
CH ₃ OH 5 _{-2,4} -4 _{-2,3} E	241.904643	57	13			
CH ₃ OH 16 _{3,14} –16 _{2,15} A	255.241888	365	59	410 (86)	267 (56)	1.5 (0.5)
¹³ CH ₃ OH 4 _{3,2} -4 _{2,3} A	255.203728	73	3	138 (31)	102 (23)	1.4 (0.4)
¹³ CH ₃ OH 3 _{3,0} –3 _{2,1} A	255.210605	64	2	110 (25)	76 (18)	
¹³ CH ₃ OH 7 _{3,5} -7 _{2,6} A	255.214891	113	6	195 (42)	148 (32)	
¹³ CH ₃ OH 3 _{3,1} –3 _{2,2} A ^c	255.220865	64	2	<118	$<\!\!80$	
¹³ CH ₃ OH 14 _{3,12} –14 _{2,13} A	256.826572	288	13	147 (32)	91 (21)	1.6 (0.5)
CH ₃ CHO 13 _{1.13} –12 _{1.12} E	242.106020	84	163	161 (35)	66 (16)	2.4 (0.8)
CH ₃ CHO 13 _{1,13} -12 _{1,12} A	242.118136	84	163	155 (35)	48 (13)	3.2 (1.1)
CH ₃ OCH ₃ 5 _{3 2} -4 _{2 3} AE	241.523808	26	28	>51 ^d	>41 ^d	
CH ₃ OCH ₃ 5 _{3,2} -4 _{2,3} EA	241.528318		15			
CH ₃ OCH ₃ 5 _{3,2} -4 _{2,3} EE	241.528719		69			
CH ₃ OCH ₃ 5 _{3,2} -4 _{2,3} AA	241.531026		46			
CH ₃ OCH ₃ 21 _{3,18} –20 _{4,17} AA	241.635773	226	61	<58 ^e	<60 ^e	
CH ₃ OCH ₃ 21 _{3,18} -20 _{4,17} EE	241.637303		97			
CH ₃ OCH ₃ 21 _{3,18} -20 _{4,17} AE	241.638831		37			
CH ₃ OCH ₃ 21 _{3,18} -20 _{4,17} EA	241.638834		24			
CH ₃ OCH ₃ 13 _{1,13} –12 _{0,12} EA	241.946249	81	34	131 (29)	136 (30)	1.0 (0.3)
CH ₃ OCH ₃ 13 _{1,13} -12 _{0,12} AE	241.946249		69			
CH ₃ OCH ₃ 13 _{1,13} –12 _{0,12} EE	241.946542		274			
CH ₃ OCH ₃ 13 _{1,13} -12 _{0,12} AA	241.946835		103			
CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} AE	256.135096	208	104	106 (25)	117 (27)	0.9 (0.3)
CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} EA	256.135164		69			
CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} EE	256.137180		278			
CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} AA	256.139230		174			
NH ₂ CHO 12 _{1,12} -11 _{1,11}	243.521044	79	156	267 (59)	40 (11)	7 (2)
NH ₂ CHO 12 _{4,9} -11 _{4,8}	255.058533	127	139	160 (37)	42 (12)	4 (1)
NH ₂ CHO 12 _{4.8} -11 _{4.7}	255.078912	127	139	>93 ^f	>39 ^f	

 Table 1

 Properties of the Lines Detected toward SVS13-A

Notes.

^a Frequencies and spectroscopic parameters have been provided by (Kukolich & Nelson 1971; Xu & Lovas 1997; Xu et al. 2008; Endres et al. 2009, and references therein) for CH_3OH , $^{13}CH_3OH$, CH_3OCH_3 , and NH_2CHO , respectively, and retrieved from the Cologne Database for Molecular Spectroscopy, http://www.astro.uni-koeln.de/cdms/ (Müller et al. 2005). They were provided by Kleiner et al. (1996) and retrieved from the Jet Propulsion Laboratory molecular database, https://spec.jpl.nasa.gov/ (Pickett et al. 1998) for CH₃CHO.

^b Errors on the integrated intensity include 20% of calibration.

^c Contaminated by the NH₂CHO 123,10–11_{3,9} line at 255.225651 GHz.

^d The line profile is truncated as the line is close to the edge of the spectral window.

^e Tentatively detected (line peak below 3σ detection limit).

^f The NH₂CHO 12_{3,10}-11_{3,9} line at 255.225651 GHz is also detected but not considered for the analysis as strongly contaminated by ¹³CH₃OH (see c).

from 57 K to 804 K. We also detected two CH₃CHO lines (84 K), four lines of CH₃OCH₃ (26–226 K), and three lines of NH₂CHO (79–127 K). In Figure 2, we show the emission of one representative line for each species, integrated on three velocity intervals, namely the CH₃OH $25_{3,22}$ – $25_{2,23}$ A at 241.589 GHz; the ¹³CH₃OH 14_{3,12}–14_{2,13} A line at 256.827 GHz; the CH₃CHO 13_{1,13}–12_{1,12} E line at 242.106 GHz; the 13_{1,13}–12_{0,12} EA, AE, EE, and AA transitions at 241.946 GHz; and the NH₂CHO 12_{4,9}–11_{4,8} transition at 255.059 GHz. The lines are representative of each species, independently of their upper-level energy. All the maps are reported in Figures C1–C5. Figure 2 also shows the iCOM spectra extracted in the positions corresponding to the continuum peak position of the two sources VLA4A and VLA4B. From the ¹³CH₃OH spectra, we reveal different systemic velocities for VLA4A (+7.7 km s⁻¹) and VLA4B

(+8.5 km s⁻¹). The spatial distribution of iCOMs is different for the different species. For CH₃OH and ¹³CH₃OH, in the interval between +4.0 and +7.5 km s⁻¹, the line emission traces VLA4A, with an elongation toward the north. In the velocity intervals 7.5–8.7 km s⁻¹, corresponding to the systemic velocity reported for SVS13-A, and 8.8–12.0 km s⁻¹, the line emission is associated with both protostars, peaking in between. A beam deconvolved size of 0.".6 × 0.".4 is derived from a simple 2D Gaussian fit in the image plane of the ¹³CH₃OH moment 0 emission. For CH₃OCH₃, the spatial distribution is similar but the emission between +8.8 and +11 km s⁻¹ peaks closer to VLA4B. Acetaldehyde emission between 8.8 and 11 km s⁻¹ peaks closer to VLA4A. Finally, formamide, which is the only N-bearing species detected in our observations, is peaking toward VLA4A.

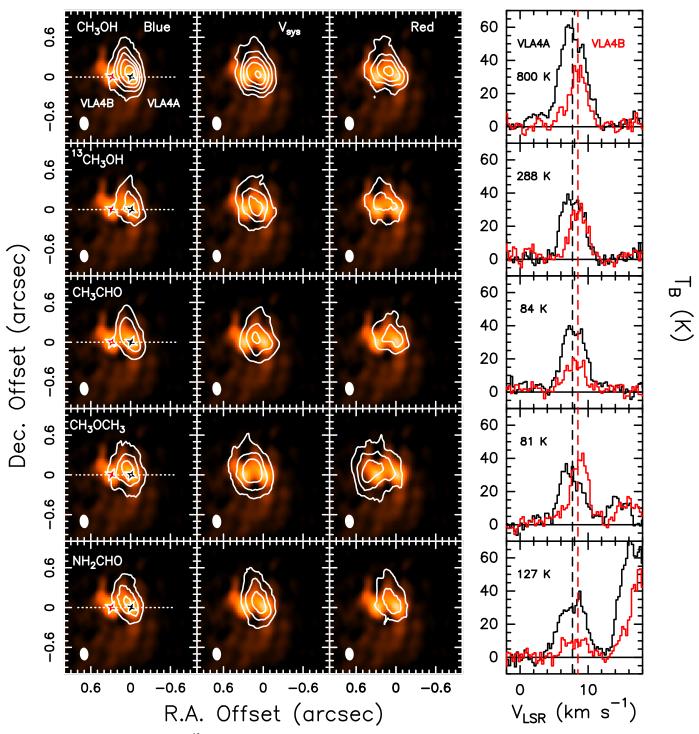


Figure 2. Integrated emission from CH₃OH, ¹³CH₃OH, CH₃CHO, NH₂CHO, and CH₃OCH₃, in white contours, superposed to the dust emission in color scale. The emission is integrated in the following velocity intervals: $4-7.5 \text{ km s}^{-1}$ in the left panels ($V_{sys} -$), 7.5–8.7 km s⁻¹ in the middle panels (V_{sys}), and 8.8–12.0 km s⁻¹ in the right panels ($V_{sys} +$). The first contours and steps are 5σ , corresponding to 35 mJy beam⁻¹, 19 mJy beam⁻¹ and 29 mJy beam⁻¹, for CH₃OH; 34 mJy beam⁻¹, 21 mJy beam⁻¹ and 28 mJy beam⁻¹ for ¹³CH₃OH; 29 mJy beam⁻¹, 19 mJy beam⁻¹ for CH₃CHO; 30 mJy beam⁻¹, 18 mJy beam⁻¹ and 29 mJy beam⁻¹ for CH₃OCH₃; and 33 mJy beam⁻¹, 24 mJy beam⁻¹, and 27 mJy beam⁻¹ for NH₂CHO, respectively. The synthesized beams are reported in white in the lower-left corner of each panel. The dashed line indicates the axes connecting VLA4A and VLA4B along which the line intensity profiles shown in Figure 3 are extracted. On the right, we report the spectra in brightness temperature units, extracted at the continuum peak position of VLA4A (black star) and VLA4B (red star). From ¹³CH₃OH spectra, we derived a systemic velocity of $+7.7 \text{ km s}^{-1}$ for VLA4A (black vertical dashed line) and $+8.5 \text{ km s}^{-1}$ for VLA4B (red vertical dashed line). Spectra are smoothed at 0.3 km s⁻¹ resolution. On the left is reported the upper-level energy of each transition in K.

In Table 1 we report the integrated line intensities extracted from the continuum peak positions of VLA4A and VLA4B, respectively, and their intensity ratios. The intensity ratios are close to the value of 1 for CH₃OCH₃, confirming that dimethyl ether is present in both protostars. For methanol and acetaldehyde, intensity ratios vary from 1.3 to 3.2, while formamide abundances are higher in VLA4A by factors of 4–7. The intensity ratios suggest chemical differentiation inside the system. To further

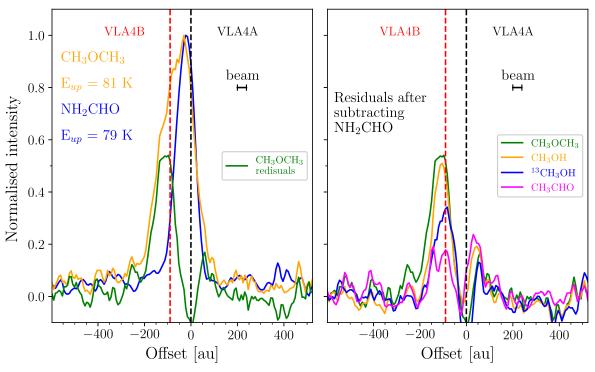


Figure 3. Left panel: normalized intensity profile of the NH₂CHO line at 243.521 GHz (blue) and the CH₃OCH₃ line at 241.946 GHz (orange) extracted along the line connecting VLA4A with VLA4B. The green line shows the residuals obtained subtracting the formamide emission from the CH₃OCH₃ profile. The two vertical dashed lines show the position of VLA4A (black) and VLA4B (red). The offset in pixel is given with respect to the position of VLA4A. The pixel size corresponds to 25 mas. Right panel: residual line profiles of CH₃OCH₃ (green), CH₃OH (orange), ¹³CH₃OH (blue), and CH₃CHO (magenta), after subtracting the formamide emission profile. The analyzed lines are the CH₃OCH₃ line at 241.964 GHz, the CH₃OH line at 241.904 GHz, the ¹³CH₃OH line at 255.204 GHz, the two detected CH₃CHO lines at 242.106 GHz and 242.118 GHz, whose intensity is added, and the NH₂CHO line at 243.521 GHz.

investigate the species spatial distribution, we compare emission lines with similar E_{up} (between 57 and 81 K) in order to minimize excitation conditions effects. Figure 3 shows the normalized integrated line profiles of CH₃OCH₃ and NH₂CHO, extracted along the horizontal axes connecting the two protostars (Figure 2). The x-axis reports the offset in astronomical units with respect to the position of VLA4A. Two vertical dashed lines indicate the positions of the two protostars. The green line is the residual emission obtained subtracting the NH₂CHO spectra from the CH₃OCH₃ emission. If we assume that NH₂CHO mainly traces VLA4A, the green profile is the additional emission from VLA4B. Figure 3 also shows the residual profiles of CH₃OCH₃, CH₃OH, ¹³CH₃OH, and CH₃CHO after subtracting the NH₂CHO emission. The figure highlights the emission of different species at the position of VLA4B. Finally, Figure A1 shows the intensity-weighted peak velocity (moment 1) maps of the brightest ¹³CH₃OH, CH₃OCHO, and NH₂CHO lines. All of the lines show velocity gradients roughly orthogonal to the outflow direction. Methanol shows the broadest velocity interval while formamide shows the tightest.

3.3. Column Densities and Abundances

In order to characterize the two hot corinos, we analyzed their methanol emission on the dust peaks (Table 1) via the non-LTE LVG (large velocity gradient) code grelvg, developed by Ceccarelli et al. (2003). We used the collisional coefficients with para-H₂, computed by Rabli & Flower (2010) between 10 and 200 K for the first 256 levels and provided by the BASECOL database (Dubernet et al. 2013). We assumed the A/E CH₃OH ratio equal to 1 (Flower et al. 2006) and ${}^{12}C/{}^{13}C = 60$ (e.g.,

Milam et al. 2005). To compute the line escape probability as a function of the line optical depth, we adopted a semi-infinite slab geometry and a line width equal to 4 km s^{-1} , as measured. We ran a large grid of models (~10,000) to cover the χ^2 surface in the parameters space: the total (A- plus E-) methanol column density N(CH₃OH) from 1×10^{13} to 2×10^{18} cm⁻², the H₂ density n_{H2} from 1×10^5 to $\times 10^{10}$ cm⁻³ and the temperature T from 40 to 200 K. We fitted the measured ¹³CH₃OH-A line intensities by comparing them with those predicted by the model, leaving $N(^{13}CH_3OH)$, n_{H2} , and T as free parameters. We obtained a good fit ($\chi^2 = 1.1$) with the following parameters: $N(^{13}\text{CH}_3\text{OH}) = (1.0 \pm 0.2) \times 10^{17} \text{ cm}^{-2}$, $T = (140 \pm 40)$ K, and $n_{\text{H2}} = 3 \times 10^8 \text{ cm}^{-3}$ with a lower limit of $2 \times 10^7 \text{ cm}^{-3}$, indicating that the lines are LTE populated.⁶ Line optical depths are estimated using the non-LTE predictions. The predicted opacity of the ¹³CH₃OH-A line is between 0.1 to 0.4. Because the ¹²CH₃OH-E lines are predicted to be very optically thick $(\tau \sim 60)$, we derive the column density of the main isotopologue from the ¹³CH₃OH one, assuming the same temperature of 140 K, and we obtain $N(CH_3OH) = (6 \pm 1) \times$ 10^{18} cm⁻². We repeated the same analysis also for VLA4B and obtained the following parameters (reduced $\chi^2 = 0.95$): $N(CH_3OH) = (5 \pm 1) \times 10^{18} \text{ cm}^{-2}$, $T = (170 \pm 50)$ K, and $n_{\text{H2}} = 3 \times 10^8 \text{ cm}^{-3}$ with a lower limit of $2 \times 10^7 \text{ cm}^{-3}$, again indicating that the lines are LTE parameter. indicating that the lines are LTE populated. Please note that the line with $E_{up} = 800$ K cannot be modeled by the non-LTE code because of the lack of collisional coefficients. Assuming that the line upper level is LTE populated, the predicted intensity is

⁶ Note that the obtained values are in good agreement with those derived by the non-LTE analysis of 18 ¹³CH₃OH lines detected by the IRAM 30 m ASAI survey (Bianchi et al. 2017).

 Table 2

 Results of the Non-LTE LVG and LTE Rotational Diagram Analysis of the iCOM Emission Observed toward VLA4A and VLA4B

		VLA4A			VLA4B		VLA4A/VLA4B ^a
Species	T _{rot} (K)	$\frac{N_{ m tot}}{(m cm^{-2})}$	X _{CH3OH} ^b	T _{rot} (K)	$\frac{N_{\rm tot}}{({\rm cm}^{-2})}$	X _{CH3OH} ^c	,
			Non-I	LTE Analysis			
CH ₃ OH ^c ¹³ CH ₃ OH	140 ^d 140(40)	$\begin{array}{c} 6(1)\times 10^{18} \\ 1.0(0.2)\times 10^{17} \end{array}$		170 ^d 170(50)	$5(1) imes 10^{18}$ $8(2) imes 10^{16}$		1.2 (0.3) 1.3 (0.4)
			Rotational	Diagram Analy	vsis		
CH ₃ CHO CH ₃ OCH ₃ NH ₂ CHO	140^{d} 140^{d} 140^{d}	$\begin{array}{l} 2.4(0.4)\times10^{16}\\ 7.5(1.2)\times10^{16}\\ 5.9(0.9)\times10^{15}\end{array}$	$\begin{array}{l} 4.0 \ (1.0) \times 10^{-3} \\ 1.3 \ (0.3) \times 10^{-2} \\ 4.0 \ (0.9) \times 10^{-3} \end{array}$	170 ^d 170 ^d 170 ^d	$\begin{array}{c} 1.1(0.2)\times10^{16}\\ 1.0(0.2)\times10^{17}\\ 1.4(0.3)\times10^{15} \end{array}$	$\begin{array}{l} 2.2 \; (0.6) \times 10^{-3} \\ 2.0 \; (0.6) \times 10^{-3} \\ 2.8 \; (0.8) \times 10^{-4} \end{array}$	2.2 (0.5) 0.8 (0.2) 4 (1)

Notes.

^a Column density ratios.

^b Abundance ratio with respect to CH₃OH.

^c Derived from ¹³CH₃OH assuming ${}^{12}C/{}^{13}C = 60$.

^d Assumed, as derived by the methanol non-LTE analysis.

about a factor of 2 lower than the observed one.⁷ Yet, it is very likely this high-lying line is subthermally populated so that the predicted intensity even has to be considered an upper limit. It has already been found by other authors that high-lying (with $E_{up} \ge 500$ K) methanol lines are most likely due to radiatively populated methanol rather than collisionally populated, as discussed in Leurini et al. (2007).

Because the methanol non-LTE analysis showed that both the VLA4A and VLA4B hot corinos have large densities, we carried out an LTE rotational diagram analysis for the other iCOMs, assuming a rotational temperature of 140 and 170 K for VLA4A and VLA4B, respectively, as derived from the methanol analysis. The results of the analysis are reported in Table 2. Synthetic LTE spectra generated using Weeds (Maret et al. 2011) are reported in Figures E1–E4. The column density ratios between VLA4A and VLA4B are consistent with the line intensity ratios reported in Table 1. In Table 2 we also report the column density ratios of the other iCOMs with respect to methanol, which is in agreement with the ASAI analysis (Bianchi et al. 2019).

4. Discussion and Conclusions

4.1. Accretion Streamers and Hot Corinos

The three continuum arc structures observed toward the south and the three fingers toward the north could be either accretion streamers or alternatively, outflow cavity walls. The brightest arclike structure in the south has been reported on similar spatial scales by Tobin et al. (2018) in the 1.3 mm continuum emission and in blueshifted C¹⁸O(2–1) emission. Tobin et al. (2018) stressed that this one-armed spiral pattern is similar to that observed in L1448 IRAS3B (Tobin et al. 2016) and associated with a disk inclined by ~45° surrounding the triple system. The SVS13-A disks are closer to edge on (i = 67° and 50°) than L1448 IRAS3B. Although the contribution of cavities opened by the precessing jets/outflows cannot be excluded, recent studies have shown that accretion streamers feeding disks are common phenomena from Class 0 to Class II objects (Yen et al. 2019; Pineda et al. 2020; Garufi et al. 2022), where planet formation is possibly already ongoing. Their presence may strongly affect the disk chemical composition because they can produce slow shocks when impacting the disk. The chemistry occurring in the shocked gas could synthesize new molecules that would eventually accrete into the disk and, consequently, enrich it. Further observations of typical shock tracers such as SO and SO₂ (e.g., Garufi et al. 2022) are needed to confirm the presence of accretion streamers in VLA4A and VLA4B.

On the other hand, iCOM emission is compact, confirming the presence of two hot corinos, one in VLA4A and a second one in VLA4B. The molecular emission sizes (0."3–0."5) are consistent with thermal sublimation of the icy mantles, namely the classical definition of a hot corino (Ceccarelli 2004). The velocity gradient roughly perpendicular to the outflow direction (see Figure A1) suggests the presence of rotating gas, either from two protostellar disks or from the inner portion of the infalling envelope.

Thanks to the superb angular resolution (0."13 in the east–west direction), the blueshifted line emission appears to be elongated in the north direction up to \sim 150 au, being spatially coincident with the northern accretion streamers (Figure C1–C5). The iCOM emission could be associated with material accreting from the streamer and inducing a slow shock in the protostellar disk, similarly to what was found in, e.g., L1527 (Sakai et al. 2014; Oya et al. 2015; Sakai et al. 2017). Moreover, we cannot exclude the possibility that the system has a higher multiplicity, including multiple unresolved cores. Observations of different molecular tracers at extremely high angular resolution (tens of astronomical units), as well as an accurate physical model of the system, are necessary to conclude the origin of iCOM emission.

Finally, the data suggest chemical segregation between formamide, tracing mainly VLA4A and the rest of the observed iCOMs, in the inner 100 au of the system. In Appendix D we discuss the possibility that the observed chemical segregation is due to opacity effects. While dust and line opacity effects cannot completely be excluded, our data suggest a real chemical differentiation of the two hot corinos instead of temperature gradients or excitation effects.

⁷ Note that we used the same beta escape probability β as a function of the line opacity τ used in the non-LTE LVG code, namely $\beta = \frac{1 - \exp[-3\tau]}{3\tau}$ (de Jong et al. 1980), where τ is estimated to be 0.3.

4.2. A Real Chemical Segregation?

A different spatial distribution between O-bearing and N-bearing molecules has been observed in Orion KL (Blake et al. 1987; Peng et al. 2013, and references therein) and in other high-mass star-forming regions on scales of thousands of astronomical units (Allen et al. 2017; Csengeri et al. 2019). Investigating whether a similar segregation is present also in the inner 100 au around low-mass protostars is more complicated as only a few system have been observed with enough angular resolution. An intriguing chemical segregation between formamide and acetaldehyde has been observed in the jet-induced shock L1157-B1, at a distance of >0.1 pc from the protostar (Codella et al. 2017). In this case, the dichotomy is reproduced well by chemical models that assume that the formamide formation is dominated by gas-phase reactions (chemistry effect). A chemical differentiation has also been observed in the prototypical Class 0 binary system IRAS 16293-2422 (Manigand et al. 2020). The abundance of CH₃OCH₃ relative to methanol is similar in the two components of the IRAS 16293-2422 system, while it differs by a factor of 2 for CH₃CHO and 4 for NH₂CHO, similarly to what was found in VLA4A and VLA4B. In IRAS 16293-2422, the observed differences are interpreted as a result of the onion-like structure of the hot corino (physical effect). In particular, the NH₂CHO rotational temperature is slightly higher ($T \sim 140-300$ K) than what was derived for other iCOMs ($T \sim 100$ K) (Jørgensen et al. 2016, 2018; Manigand et al. 2020), suggesting that N-bearing species trace hotter gas, closer to the protostar. On the other hand, recent ALMA observations of other two Class 0 protostars, Perseus B1-c and Serpens S68N, do not show a significant difference in the excitations conditions of N-bearing and O-bearing species (van Gelder et al. 2020; Nazari et al. 2021), leaving the question open. Further observations in different N-bearing and O-bearing complex species are required to clarify the origin of the chemical segregation observed in SVS13-A and inferred in IRAS 16293-2422 A and B but not in other low-mass protostars. The spatial distribution of iCOM emission in SVS13-A supports the idea that formamide is formed in a compact region closer to the protostar and thus, contrarily to other iCOMs, can be more easily obscured by the dust. The fact that the dust emission of VLA4B is optically thicker than that of VLA4A supports this scenario. Note also that the binding energy, recently computed by Ferrero et al. (2020), of formamide (average \sim 8400 K) is larger than the one of methanol (average \sim 6200 K), in agreement with the possible onion-like structure of the two SVS13-A hot corinos. Interestingly, Diaz-Rodriguez et al. (2021) report the detection of ethylene glycol only toward VLA4A, suggesting that the observed chemical segregation in SVS13-A is not exclusive of formamide. Because no binding energy of ethylene glycol is available in the literature, we carried out new ab initio quantum chemistry calculations to evaluate its binding energy over an 18 water molecule cluster (see Appendix F). In order to compare ethylene glycol with formamide, we also recalculated the binding energy of the latter. We found that the binding energy of ethylene glycol has an average value of \sim 7100 K, while that of formamide is equal to \sim 4700 K. We emphasize that the difference with respect to Ferrero et al. (2020) is due to a different water cluster used. The

important point here is the relative binding energy of ethylene glycol with respect to formamide, which is not expected to change with the water cluster used. This means that if the calculation by Ferrero et al. (2020) was performed for ethylene glycol, the binding energy would be even higher than that of formamide (~8400 K). This justifies the similar spatial distribution of formamide and ethylene glycol, different from that of methanol. Overall, the new calculated binding energies support the hypothesis that the observed chemical differentiation is caused by the onion-like structure of the two SVS13-A hot corinos instead of spatial segregation between O-bearing and N-bearing species. Further observations at high angular resolution (tens of astronomical units) with ALMA and at centimeter wavelengths with JVLA (and, in the future, with ngVLA and SKA) are needed to further investigate the chemical stratification inside the two hot corinos VLA4A and VLA4B and to quantify the dust opacity effects.

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Software: astropy (Astropy Collaboration et al. 2013, 2018), matplotlib (Hunter 2007), GAUSSIAN16 (Frisch et al. 2016), CASA (McMullin et al. 2007).

Appendix A Moment 1 Maps

Figure A1 reports the intensity-weighted velocity peak (moment 1) maps of the following lines: 13 CH₃OH at 256.8265 GHz, CH₃CHO at 242.1060 GHz, and NH₂CHO at 255.058 GHz. The two stars indicate the VLA4A and VLA4B positions. The systemic velocities of the two protostars are indicated as horizontal lines in the wedge.

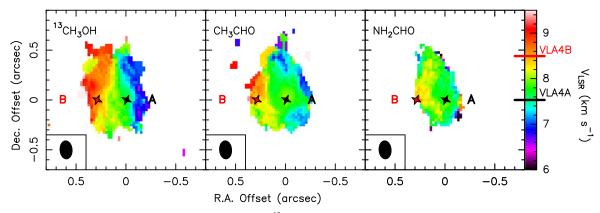


Figure A1. Moment 1 (intensity-weighted velocity peak) map of the lines ¹³CH₃OH at 256.8265 GHz, CH₃CHO at 242.1060 GHz, and NH₂CHO at 255.058 GHz (see Table 1). The two stars indicate the VLA4A and VLA4B positions. The systemic velocities of the two protostars are indicated as horizontal lines in the wedge.

Appendix B ALMA Observations

Table B1 reports the parameters of the observed ALMA setup.

Table B1 Observations				
Frequencies (GHz)	Synthesized beam (")	rms (mJy/beam kms ⁻¹)	Detected Transitions	
241.528–241.647	0."21 × 0."14	4.8	CH ₃ OH 25 _{3,22} -25 _{2,23} A CH ₃ OCH ₃ 5 _{3,2} -4 _{2,3} EA, AE, EE, AA CH ₃ OCH ₃ 21 _{3,18} -20 _{4,17} EA, AE, EE, AA	
241.900–242.020	0."21 × 0."14	4.9	CH ₃ OH 5 _{2,3} -4 _{2,2} E CH ₃ OH 5 _{-2,4} -4 _{-2,3} E CH ₃ OCH ₃ 13 _{1,13} -12 _{0,12} EA, AE, EE, AA	
242.076-242.135	$0.''20 \times 0.''13$	4.8	CH ₃ CHO 13 _{1,13} –12 _{1,12} E, A	
243.491–243.550	0.22×0.14	6.2	NH ₂ CHO 12 _{1,12} -11 _{1,11}	
255.020-255.080	$0!'20 \times 0!'13$	5.3	NH ₂ CHO 12 _{4,9} –11 _{4,8} NH ₂ CHO 12 _{4,8} –11 _{4,7}	
255.196–255.255	0."20 × 0."13	5.3	CH ₃ OH 16 _{3,14} –16 _{2,15} A ¹³ CH ₃ OH 4 _{3,2} –4 _{2,3} A ¹³ CH ₃ OH 3 _{3,0} –3 _{2,1} A ¹³ CH ₃ OH 7 _{3,5} –7 _{2,6} A ¹³ CH ₃ OH 3 _{3,1} –3 _{2,2} A	
256.107–256.167	$0.''19 \times 0.''13$	5.1	CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} AE, EA, EE, AA	
256.797–256.856	0″19 × 0″13	5.6	¹³ CH ₃ OH 14 _{3,12} –14 _{2,13} A CH ₃ OCH ₃ 19 _{5,14} –19 _{4,15} AE, EA, EE, AA	

Table	B1
Observa	tions

Appendix C Channel Maps of the Present ALMA Data Set

In this section, we report the images of all the 17 transitions of the 4 iCOMs (CH₃OH, ¹³CH₃OH, CH₃CHO, NH₂CHO, and CH₃OCH₃) observed in SVS13-A.

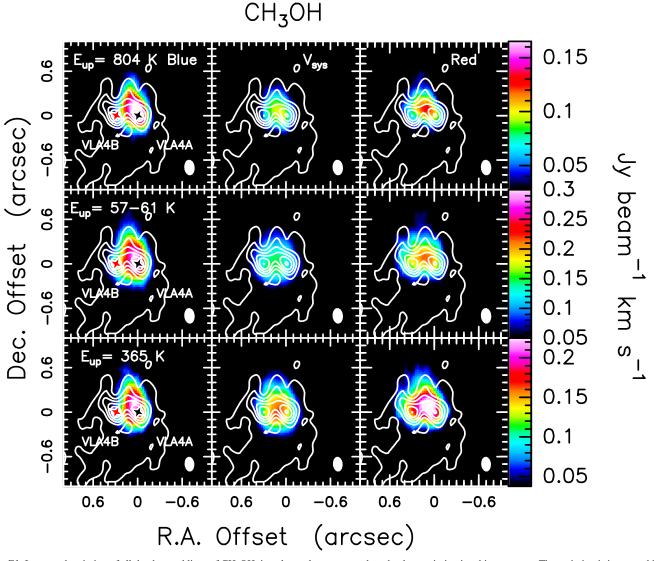


Figure C1. Integrated emission of all the detected lines of CH₃OH, in color scale, superposed on the dust emission in white contours. The emission is integrated in the following velocity intervals: $4-7.5 \text{ km s}^{-1}$ in the left panels (blue), $7.5-8.7 \text{ km s}^{-1}$ in the middle panels (V_{sys}), and $8.8-12.0 \text{ km s}^{-1}$ in the right panels (red). The first contours are 10σ , corresponding to 4 mJy beam⁻¹, and steps are 25σ , corresponding to 10.46 mJy beam⁻¹. The synthesized beams are reported in white in the lower-right corner of each panel. On the left is reported the upper-level energy of each transition in Kelvin.

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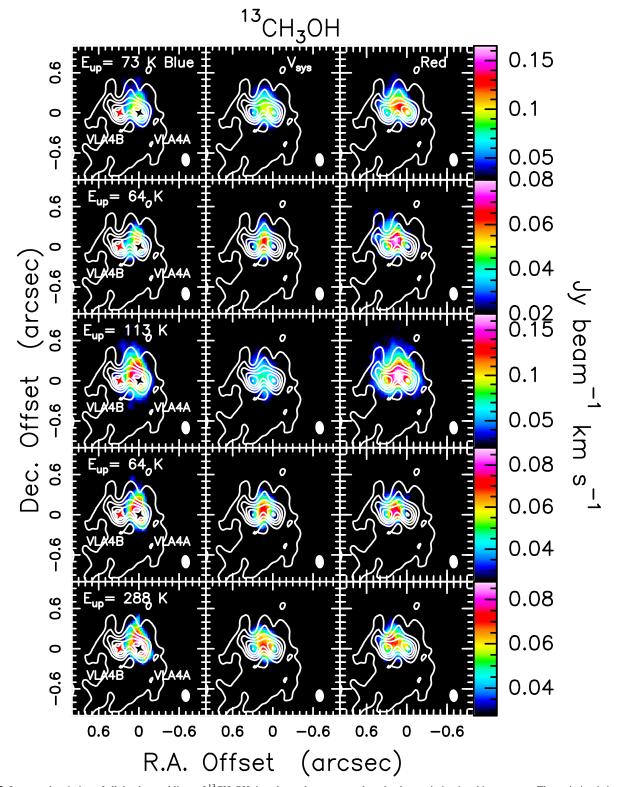


Figure C2. Integrated emission of all the detected lines of ¹³CH₃OH, in color scale, superposed on the dust emission in white contours. The emission is integrated in the following velocity intervals: $4-7.5 \text{ km s}^{-1}$ in the left panels (blue), $7.5-8.7 \text{ km s}^{-1}$ in the middle panels (V_{sys}), and $8.8-12.0 \text{ km s}^{-1}$ in the right panels (red). The first contours are 10σ , corresponding to 4 mJy beam⁻¹, and steps are 25σ , corresponding to 10.46 mJy beam⁻¹. The synthesized beams are reported in white in the lower-right corner of each panel. On the left is reported the upper-level energy of each transition in Kelvin.

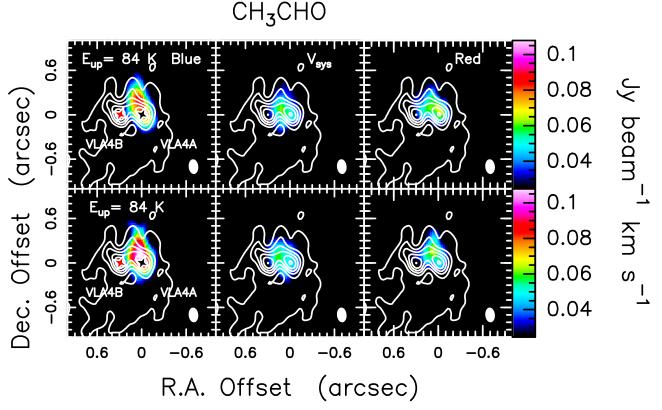


Figure C3. Integrated emission of all the detected lines of CH₃CHO, in color scale, superposed on the dust emission in white contours. The emission is integrated in the following velocity intervals: $4-7.5 \text{ km s}^{-1}$ in the left panels (blue), $7.5-8.7 \text{ km s}^{-1}$ in the middle panels (V_{sys}), and $8.8-12.0 \text{ km s}^{-1}$ in the right panels (red). The first contours are 10σ , corresponding to 4 mJy beam⁻¹, and steps are 25σ , corresponding to 10.46 mJy beam⁻¹. The synthesized beams are reported in white in the lower-right corner of each panel. On the left is reported the upper-level energy of each transition in Kelvin.

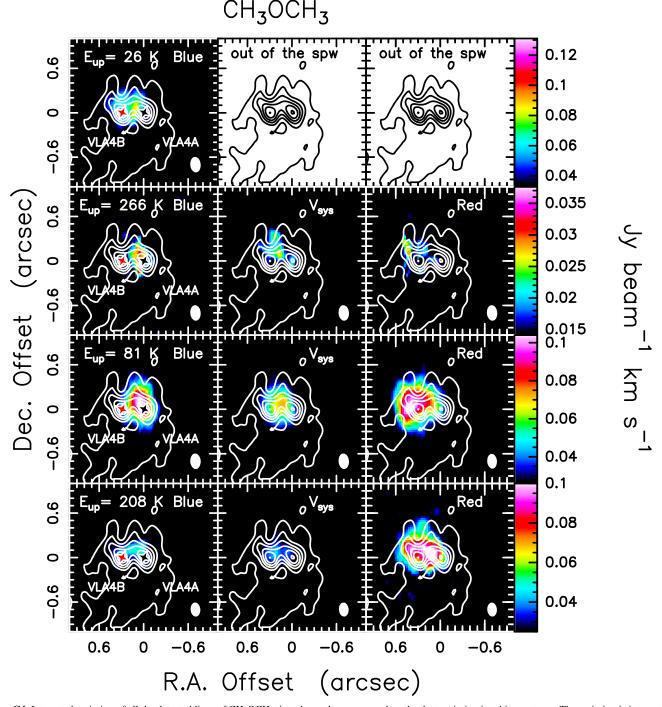


Figure C4. Integrated emission of all the detected lines of CH_3OCH_3 , in color scale, superposed on the dust emission in white contours. The emission is integrated in the following velocity intervals: 4–7.5 km s⁻¹ in the left panels (blue), 7.5–8.7 km s⁻¹ in the middle panels (V_{sys}), and 8.8–12.0 km s⁻¹ in the right panels (red). The first contours are 10σ , corresponding to 4 mJy beam⁻¹, and steps are 25σ , corresponding to 10.46 mJy beam⁻¹. The synthesized beams are reported in white in the lower-right corner of each panel. On the left is reported the upper-level energy of each transition in Kelvin. The panels showing only the continuum contours refer to line emission partially outside the observed spectral window (spw). Please note that each line is composed of four blended transitions very close in frequency (AE, EA, EE, AE). This structure, due to the rotation in the CH₃OCH₃ molecule of two functional groups CH₃-, leads to some contamination in the channel maps. However, we would like to stress that this velocity blending does not affect the line spatial distribution.

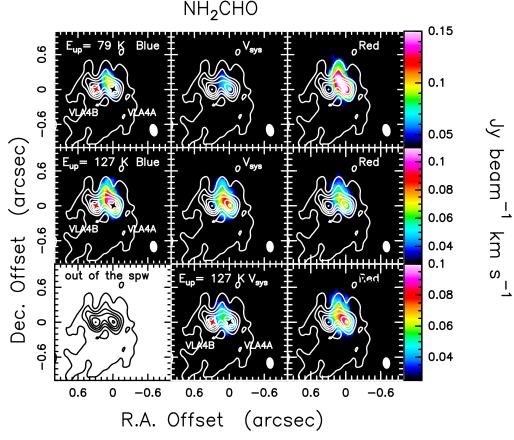


Figure C5. Integrated emission of all the detected lines of NH₂CHO, in color scale, superposed on the dust emission in white contours. The emission is integrated in the following velocity intervals: $4-7.5 \text{ km s}^{-1}$ in the left panels (Blue), $7.5-8.7 \text{ km s}^{-1}$ in the middle panels (V_{sys}), and $8.8-12.0 \text{ km s}^{-1}$ in the right panels (Red). The first contours are 10σ , corresponding to 4 mJy beam⁻¹, and steps are 25σ , corresponding to 10.46 mJy beam⁻¹. The synthesized beams are reported in white in the lower-right corner of each panel. On the left is reported the upper-level energy of each transition in Kelvin. The panel showing only the continuum contours refers to line emission partially outside the observed spectral window (spw).

Appendix D Dust and Line Opacity Effects

Previous studies of the binary system IRAS 4A have shown that dust could dramatically obscure molecular emission at (sub)millimeter wavelengths (De Simone et al. 2020). In particular, while iCOM emission is observed only toward one of the two protostars of the binary system at (sub)millimeter wavelengths (López-Sepulcre et al. 2017), a similar emission is instead observed at radio wavelengths, which are less affected by dust opacity (De Simone et al. 2020). In the case of the binary system SVS13-A, dust opacity effects may also play a role. In particular, at 1.2 mm, the flux density of VLA4A is higher by a factor of 1.4 with respect to that of VLA4B, while VLA4B is brighter at shorter wavelengths (Diaz-Rodriguez et al. 2021). Moreover, the spectral index is different toward the two sources (2.2–2.4 in VLA4B and 3.0–3.1 in VLA4A). This suggests (a) possible grain growth toward VLA4B,

implying a large fraction of large dust grains that enhance the flux at 9 mm wavelengths or, alternatively, (b) optically thick dust at 1.3mm toward VLA4B. In this second hypothesis, dust opacity could prevent us from detecting molecular emission toward VLA4B, similarly to the case of IRAS 4A. In any case, as all the observed transitions are at similar frequencies, dust opacity is expected to affect the emission from iCOMs in the same way if they originate from the same region. Another explanation for a different spatial distribution of molecular species could be line opacity. Optically thick lines could trace an external shell of the protostellar envelope, more extended than the one traced by optically thin lines. The simultaneous observations of lines covering a broad range of upper-level energies (26-804 K) allow us to verify that molecular lines from the same species show a similar spatial distribution, regardless of the upper-level energy of the transition (see Figures C1–C5). We conclude that the observed iCOM spatial distribution is not driven by excitation effects.

Appendix E Comparison with LTE Modeling

We report here the synthetic LTE spectra generated with Weeds using the gas parameter derived from the LVG and rotational diagram analysis (see Section 3.3).

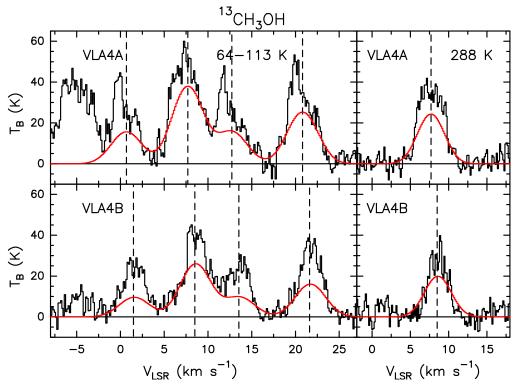


Figure E1. Synthetic LTE spectra generated with Weeds using the gas parameter in Table 2.

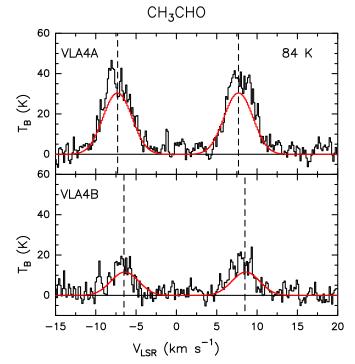


Figure E2. Synthetic LTE spectra generated with Weeds using the gas parameter in Table 2.

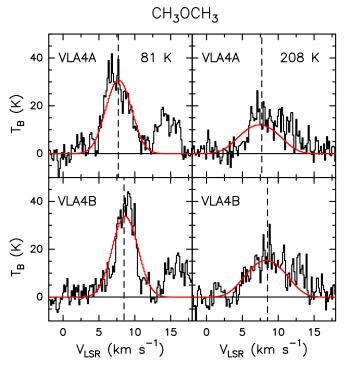


Figure E3. Synthetic LTE spectra generated with Weeds using the gas parameter in Table 2.

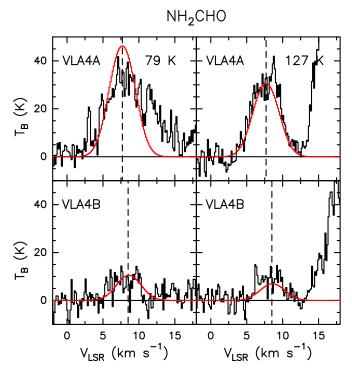


Figure E4. Synthetic LTE spectra generated with Weeds using the gas parameter in Table 2.

Appendix F Quantum Chemical Computations

We have carried out quantum chemical calculations with the GAUSSIAN16 (Frisch et al. 2016) in order to calculate the binding energies of ethylene glycol and formamide on an amorphous water-ice surface made of 18 water molecules. We employed the hybrid-DFT functional BHandHLYP (Lee et al. 1988; Becke 1993), corrected for dispersion with Grimme's G3(BJ) a posteriori correction (Grimme et al. 2010, 2011). Geometry optimization and frequency calculations were carried out with the 6-311+G(d,p) basis set (Hehre et al. 1972; Hariharan & Pople 1973; Krishnan et al. 1980). Density functional theory (DFT) energies were further refined at the 6-311++G(2df,2pd). This functional has been shown to

provide high-quality binding energies for organic fragments (e.g., Enrique-Romero et al. 2019, 2021, 2022).

Several binding geometries were found for each molecule. For each one of them, we provide a binding energy value calculated following $E_{\text{bind}} = -(E_{\text{complex}} - E_{\text{admol}} - E_{\text{surf}})$, where E_{complex} , E_{admol} , and E_{surf} correspond to the zero-point-corrected energies of the complex (surface + molecule), the molecule (isolated), and the surface (isolated), respectively. Both the geometries and their binding energy values are shown Figure F1.

As can be seen, ethylene glycol has a higher binding energy, ranging from \sim 50–70 kJ mol⁻¹ (6300–8400 K), than formamide (\sim 25–55 kJ mol⁻¹, 2970–6600K) as a consequence of its flexibility and size, which allow ethylene glycol to establish two to four H bonds, while formamide can only make two to three at most, on our water surface model.

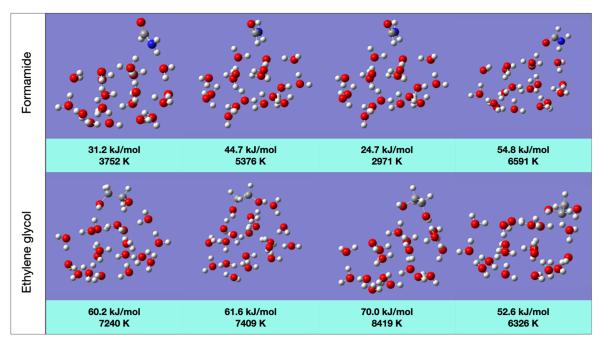


Figure F1. Optimized binding geometries and energies. The energetics include zero-point-energy corrections.

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References

- Allen, V., van der Tak, F. F. S., Sánchez-Monge, Á, Cesaroni, R., & Beltrán, M. T. 2017, A&A, 603, A133
- Astropy Collaboration, Robitaille, T. P., Tollerud, E. J., et al. 2013, A&A, 558, A33
- Astropy Collaboration, Price-Whelan, A. M., Sipőcz, B. M., et al. 2018, AJ, 156, 123
- Becke, A. D. 1993, JChPh, 98, 1372
- Belloche, A., Maury, A. J., Maret, S., et al. 2020, A&A, 635, A198
- Bianchi, E., Codella, C., Ceccarelli, C., et al. 2017, MNRAS, 467, 3011
- Bianchi, E., Codella, C., Ceccarelli, C., et al. 2019, MNRAS, 483, 1850
- Blake, G. A., Sutton, E. C., Masson, C. R., & Phillips, T. G. 1987, ApJ, 315, 621
- Carrasco-González, C., Anglada, G., Rodríguez, L. F., Torrelles, J. M., & Osorio, M. 2008, AJ, 136, 2238
- Ceccarelli, C. 2004, in ASP Conf. Ser. 323, The Hot Corinos of Solar Type Protostars, ed. D. Johnstone et al. (San Francisco, CA: ASP), 195
- Ceccarelli, C., Maret, S., Tielens, A. G. G. M., Castets, A., & Caux, E. 2003, A&A, 410, 587
- Codella, C., Ceccarelli, C., Cabrit, S., et al. 2016, A&A, 586, L3
- Codella, C., Ceccarelli, C., Caselli, P., et al. 2017, A&A, 605, L3
- Csengeri, T., Belloche, A., Bontemps, S., et al. 2019, A&A, 632, A57
- de Jong, T., Boland, W., & Dalgarno, A. 1980, A&A, 91, 68
- De Simone, M., Codella, C., Testi, L., et al. 2017, A&A, 599, A121
- De Simone, M., Ceccarelli, C., Codella, C., et al. 2020, ApJL, 896, L3
- Diaz-Rodriguez, A. K., Anglada, G., Blázquez-Calero, G., et al. 2021, arXiv:2111.11787
- Dubernet, M.-L., Alexander, M. H., Ba, Y. A., et al. 2013, A&A, 553, A50
- Endres, C. P., Drouin, B. J., Pearson, J. C., et al. 2009, A&A, 504, 635
- Enrique-Romero, J., Ceccarelli, C., Rimola, A., et al. 2021, A&A, 655, A9
- Enrique-Romero, J., Rimola, A., Ceccarelli, C., et al. 2019, ESC, 3, 2158
- Enrique-Romero, J., Rimola, A., Ceccarelli, C., et al. 2022, ApJS, 259, 39
- Ferrero, S., Zamirri, L., Ceccarelli, C., et al. 2020, ApJ, 904, 11
- Flower, D. R., Pineau Des Forêts, G., & Walmsley, C. M. 2006, A&A, 449, 621
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., et al. 2016, Gaussian 16 Revision C.01, https://gaussian.com/citation/
- Garufi, A., Podio, L., Codella, C., et al. 2022, A&A, 645, A145

- Grimme, S., Antony, J., Ehrlich, S., & Krieg, H. 2010, JChPh, 132, 154104
- Grimme, S., Ehrlich, S., & Goerigk, L. 2011, JCoCh, 32, 1456
- Hariharan, P. C., & Pople, J. A. 1973, Theoret. Chim. Acta, 28, 213
- Hehre, W. J., Ditchfield, R., & Pople, J. A. 1972, JChPh, 56, 2257
- Hunter, J. D. 2007, CSE, 9, 90
- Jørgensen, J. K., van der Wiel, M. H. D., Coutens, A., et al. 2016, A&A, 595, A117
- Jørgensen, J. K., Müller, H. S. P., Calcutt, H., et al. 2018, A&A, 620, A170
- Kleiner, I., Lovas, F. J., & Godefroid, M. 1996, JPCRD, 25, 1113
- Krishnan, R., Binkley, J. S., Seeger, R., & Pople, J. A. 1980, JChPh, 72, 650
- Kukolich, S. G., & Nelson, A. C. 1971, CPL, 11, 383
- Lee, C., Yang, W., & Parr, R. G. 1988, PhRvB, 37, 785
- Lefèvre, C., Cabrit, S., Maury, A. J., et al. 2017, A&A, 604, L1
- Leurini, S., Schilke, P., Wyrowski, F., & Menten, K. M. 2007, A&A, 466, 215
- López-Sepulcre, A., Jaber, A. A., Mendoza, E., et al. 2015, MNRAS, 449, 2438
- López-Sepulcre, A., Sakai, N., Neri, R., et al. 2017, A&A, 606, A121
- Manigand, S., Jørgensen, J. K., Calcutt, H., et al. 2020, A&A, 635, A48
- Maret, S., Hily-Blant, P., Pety, J., Bardeau, S., & Reynier, E. 2011, A&A, 526, A47
- McMullin, J. P., Waters, B., Schiebel, D., Young, W., & Golap, K. 2007, in ASP Conf. Ser. 376, CASA Architecture and Applications, ed. R. A. Shaw, F. Hill, & D. J. Bell (San Francisco, CA: ASP), 127
- Milam, S. N., Savage, C., Brewster, M. A., Ziurys, L. M., & Wyckoff, S. 2005, ApJ, 634, 1126
- Müller, H. S. P., Schlöder, F., Stutzki, J., & Winnewisser, G. 2005, JMoSt, 742, 215
- Nazari, P., van Gelder, M. L., van Dishoeck, E. F., et al. 2021, A&A, 650, A150
- Öberg, K. I., & Bergin, E. A. 2021, PhR, 893, 1
- Ossenkopf, V., & Henning, T. 1994, A&A, 291, 943
- Oya, Y., Sakai, N., Lefloch, B., et al. 2015, ApJ, 812, 59
- Peng, T. C., Despois, D., Brouillet, N., et al. 2013, A&A, 554, A78
- Pickett, H. M., Poynter, R. L., Cohen, E. A., et al. 1998, JQSRT, 60, 883
- Pineda, J. E., Segura-Cox, D., Caselli, P., et al. 2020, NatAs, 4, 1158
- Rabli, D., & Flower, D. R. 2010, MNRAS, 406, 95
- Sakai, N., Sakai, T., Hirota, T., et al. 2014, Natur, 507, 78
- Sakai, N., Oya, Y., Higuchi, A. E., et al. 2017, MNRAS, 467, L76
- Segura-Cox, D. M., Schmiedeke, A., Pineda, J. E., et al. 2020, Natur, 586, 228
- Sheehan, P. D., & Eisner, J. A. 2017, ApJ, 851, 45
- Sheehan, P. D., Tobin, J. J., Federman, S., Megeath, S. T., & Looney, L. W. 2020, ApJ, 902, 141
- Tobin, J. J., Looney, L. W., Li, Z.-Y., et al. 2016, ApJ, 818, 73
- Tobin, J. J., Looney, L. W., Li, Z.-Y., et al. 2018, ApJ, 867, 43
- van Gelder, M. L., Tabone, B., Tychoniec, Ł., et al. 2020, A&A, 639, A87
- Xu, L.-H., & Lovas, F. J. 1997, JPCRD, 26, 17
- Xu, L.-H., Fisher, J., Lees, R. M., et al. 2008, JMoSp, 251, 305
- Yang, Y.-L., Sakai, N., Zhang, Y., et al. 2021, ApJ, 910, 20
- Yen, H.-W., Gu, P.-G., Hirano, N., et al. 2019, ApJ, 880, 69