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# Photochemical origin of SiC<sub>2</sub> in the circumstellar envelope of carbon-rich AGB stars revealed by ALMA

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The fact that whether SiC<sub>2</sub> is a parent species, formed in the photosphere or as a by-product of high-temperature dust formation, or a daughter species, formed in chemistry driven by the photodestruction of the parent species in the outer envelope, has been debated for a long time. In this study, we analyze the Atacama Large Millimeter Array (ALMA) observations of four SiC<sub>2</sub> transitions in the circumstellar envelopes (CSEs) of three C-rich asymptotic giant branch (AGB) stars (AI Vol, II Lup, and RAFGL 4211) and find that SiC<sub>2</sub> exhibits an annular, shell-like distribution in these targets, suggesting that SiC<sub>2</sub> can be a daughter species in the CSEs of carbon-rich AGB stars. The results may provide important references for future chemical models.

## KEYWORDS

asymptotic giant branch stars, mass loss, circumstellar envelope, C-rich, SiC<sub>2</sub>, AI Vol, II Lup, RAFGL 4211

## 1 Introduction

Late evolutionary stars with masses between 0.8 and 8 M<sub>⊙</sub> (Höfner and Olofsson, 2018) experience dramatic mass losses. The stellar wind continues to eject material outward, eventually forming a circumstellar envelope (CSE), often referred to as the molecular space factory. According to different C/O ratios, asymptotic giant branch (AGB) stars are divided

into three classes: O-rich AGB stars (oxygen-rich,  $C/O < 1$ ), S-type AGB stars ( $C/O \approx 1$ ), and C-rich AGB stars (carbon-rich,  $C/O > 1$ ). Over 105 molecular species have been detected in the circumstellar envelope of the evolved stars (Decin, 2021). These species, distributed in different areas of CSEs, can help us trace shell properties, such as local temperature and gas composition, and help us understand the chemical synthesis within the objects. A large number of carbon-bearing species are observed in abundance surrounding the carbon stars, for instance, CO, CS,  $HC_3N$ , and  $C_2H$ , some of which come from the inner layers of CSEs, while some are formed in the outer regions (Decin et al., 2008; Li et al., 2016).

Silacyclopopynylidene ( $SiC_2$ ) was first detected and confirmed in IRC +10216 by Thaddeus et al. (1984), who derived a fairly large column density,  $1.5 \times 10^{14} \text{ cm}^{-2}$ . Glassgold et al. (1986) suggested that  $SiC_2$  was formed by the reaction of  $Si^+$  with  $C_2H_2$  or  $C_2H$ , followed by dissociative recombination with electrons. Glassgold et al. (1991) suggested alternative pathways, initiated by reactions of  $SiS$  with  $C_2H_2^+$  or  $C_2H_3^+$ . All these routes need the presence of UV photons to form cations and radicals and, thus, treat  $SiC_2$  as a daughter species.

The spatial distribution of  $SiC_2$  in IRC +10216 was discussed by Takano et al. (1992) and Guelin et al. (1993), who showed a spherical shell-like structure indicative of a daughter species. Lucas et al. (1995) and Gensheimer et al. (1995) used the Plateau de Bure and the Berkeley-Illinois-Maryland Array (BIMA), respectively, to map  $SiC_2$  emissions, showing that it had a shell structure. The first confirmation that  $SiC_2$  was present close to the star came from Cernicharo et al. (2010), who used the Herschel Space Observatory to detect some 55 transitions from energy levels 500–900 K above the ground state, implying that  $SiC_2$  was present in the dust-forming zone. Subsequently, Fonfría et al. (2014), using the CARMA interferometer, and Prieto et al. (2015), using the Atacama Large Millimeter Array (ALMA), detected emissions from both the central region and the outer shell.

In a work devoted to single-dish observations of 25 C-rich AGB stars (Massalkhi et al., 2018),  $SiC_2$  and  $SiC$  were detected in about half of the sources. They found that the abundance of  $SiC_2$  decreased with the increasing envelope density, indicating that  $SiC_2$  is a parent species in these CSEs. De Beck and Olofsson (2020) detected  $SiC_2$  in the S-type AGB star W Aql, and showed that the emission occurs in a ring of a radius of  $1-2''$ .

Most evidence shows that  $SiC_2$  is formed in LTE conditions close to the star, although IRC +10216 has an increase in the abundance of  $SiC_2$  at approximately  $10''$ , indicating an additional formation in the outer regions of CSEs. To date, no millimeter-wave interferometric array observation of  $SiC_2$  has been published in CSEs of C-rich AGB stars other than IRC +10216. In this work, we provide evidence that  $SiC_2$  seems to be a daughter molecule through high-resolution observations of three C-rich AGB stars. We describe the observations in Section 2. The results are discussed in Section 3. The conclusion is presented in Section 4. The spatial distribution and the fractional abundance of  $SiC_2$  in AI Vol together with  $5_{0,5} - 4_{0,4}$  transitions in RAFGL 4211 are discussed in the main paper, while the rest of the results are presented in the Supplementary Material.

## 2 Observations

Observations were made using the ALMA 12-m array. The spectral line observations in three bands of AI Vol, RAFGL 4211, and II Lup covering four Windows with a bandwidth of 2 GHz were performed on 16 August 2015 (2013.1.00070.S, PI: Nyman, Lars-Åke). The data were extracted from the ALMA Archive<sup>1</sup>. For AI Vol, the configuration used for the observation is a 12-m main array, with baselines 21–783 m. The image cube per spw averages every  $2 \times 488$  kHz channel. The rms requirement is 3 mJy per 1 arcsec beam, per 0.9 MHz ( $\sim 2.7 \text{ km s}^{-1}$ ). The synthesized rms is 1.3 mJy/beam, and the synthesized beam is  $1.4'' \times 0.9''$ . The parameters of the observed transitions are shown in Table 1. The frequency resolution during the observation is 1,128.9984 kHz, corresponding to the velocity resolution of 2.526–3.122  $\text{km s}^{-1}$ . The wide frequency range covers four lines of  $SiC_2$  ( $4_{0,4} - 3_{0,3}$ ,  $4_{2,3} - 3_{2,2}$ ,  $4_{2,2} - 3_{2,1}$ , and  $5_{0,5} - 4_{0,4}$ ).

AI Vol, RAFGL 4211, and II Lup are all carbon-rich AGB stars with mass losses. A survey conducted by Smith et al. (2015) at the 3-mm band revealed that the three carbon-rich stars possess abundant molecules but the sensitive detection of molecular spatial distributions relies on more advanced telescopes, such as ALMA. In this study, we present the physical parameters taken from the literature and the synthesized beam for the observed sources, which are listed in Table 2.

The imaging process of the calibrated data was manually performed using CASA 4.3.1<sup>2</sup> software. The “clean” task was employed, and to achieve a balance between the spatial resolution and noise gain in the resulting image, the Briggs weighting function was applied along with adjustments to the “robust” parameter of 0.5. The rms was calculated near the center of the field, excluding all emissions within the region. The rms values for all channel maps were obtained using the task “imstat” in CASA software. Each pixel on the image plane corresponded to a size of 0.2 arcseconds. Then, we used Python software to map and analyze ALMA product data. To calculate the molecular column density, we employed shell fitting using GILDAS software<sup>3</sup>, along with Splatalogue<sup>4</sup> and CDMS databases<sup>5</sup> (Müller et al., 2005).

## 3 Result

### 3.1 Spatial distribution of $SiC_2$

We found four transitions of  $SiC_2$  from each source, except for the  $4_{2,2} - 3_{2,1}$  transition, which was not observed in II Lup. Based on  $S_{\mu}^2$  from Table 3, the  $4_{2,2} - 3_{2,1}$  transition of  $SiC_2$  in the 3-mm wavelength range ranked third in terms of signal intensity. However, we did not detect any signal. Our data were obtained from the ALMA Archive, and from the data information, we found that the other

1 <https://almascience.nao.ac.jp/aq>

2 <https://casa.nrao.edu/>

3 <http://www.iram.fr/IRAMFR/GILDAS>

4 <https://splatalogue.online//advanced.php>

5 <http://www.astro.uni-koeln.de/cdms/catalog>

TABLE 1 Spectral line parameters of different transitions in SiC<sub>2</sub> obtained via shell fitting using GILDAS.

Transition	AI Vol				RAFGL 4211				II Lup				
	Frequency (GHz)	rms (mK)	$\int T_{\text{Rdb}} \text{ (K km s}^{-1}\text{)}$	$T_{\text{peak}} \text{ (K)}$	S/N	rms (mK)	$\int T_{\text{Rdb}} \text{ (K km s}^{-1}\text{)}$	$T_{\text{peak}} \text{ (K)}$	S/N	rms (mK)	$\int T_{\text{Rdb}} \text{ (K km s}^{-1}\text{)}$	$T_{\text{peak}} \text{ (K)}$	S/N
$J_{K_a, K_c} = 4_{0,4} - 3_{0,3}$	93.06363900	6.70	1.26 ( $\pm 0.21$ )	0.14	20.45	16.40	1.48 ( $\pm 0.52$ )	0.14	8.60	21.49	9.51 ( $\pm 0.75$ )	0.54	25.11
$J_{K_a, K_c} = 4_{2,3} - 3_{2,2}$	94.24539300	2.73	0.29 ( $\pm 0.09$ )	0.03	10.99	10.70	0.53 ( $\pm 0.34$ )	0.06	5.51	25.13	6.82 ( $\pm 0.88$ )	0.37	14.82
$J_{K_a, K_c} = 4_{2,2} - 3_{2,1}$	95.57938100	2.55	0.32 ( $\pm 0.08$ )	0.04	13.73	16.30	0.91 ( $\pm 0.52$ )	0.10	6.13	47.30	-	-	-
$J_{K_a, K_c} = 5_{0,5} - 4_{0,4}$	115.38238880	6.64	0.48 ( $\pm 0.21$ )	0.04	5.27	40.60	4.45 ( $\pm 1.30$ )	0.33	8.08	72.80	17.20 ( $\pm 2.55$ )	0.80	11.03

Note: the uncertainties are indicated in parentheses. S/N is calculated by  $T_{\text{peak}}/\text{rms}$ .

three transitions of SiC<sub>2</sub> and the data from two additional sources had map sizes of 800 × 800 or 640 × 640 pixels. In contrast, the data without signal detection only covered a map size of 300 × 300 pixels. We speculate that there may have been some unknown special circumstances during the observations that led to the absence of a signal.

AI Vol does not have the strongest spectral line signal, but the signal-to-noise ratio of the spatial brightness distribution is higher than that of the other two stars. Cernicharo et al. (2015) have reported the observations and model results of a C-rich AGB star, IRC +10216. They suggest that a companion star may explain the spiral structure of its CSE. Lykou et al. (2018) reported spiral structures of several parent molecules in II Lup, suggesting that a companion star is the main forming mechanism of mass loss. The results show that the spectral line signal of AI Vol is stronger than RAFGL 4211 (in Figure 6; Supplementary Figure SA9). In order to get reliable results, we concentrate on analyzing the distribution around the center star of AI Vol (in Section 3.1.1). The rotational diagram method was used to calculate fractional abundance, and its detailed analysis is presented in Section 3.2.

### 3.1.1 AI Vol

Figures 1, 2 show the SiC<sub>2</sub> ( $4_{0,4} - 3_{0,3}$  and  $4_{2,2} - 3_{2,1}$ ) radial velocity channel map toward the C-rich AGB star AI Vol (the other transitions are shown in Supplementary Figures SA1, A2). Around the local standard of the rest velocity  $V_{\text{LSR}}$  of AI Vol ( $-39 \text{ km s}^{-1}$ ), SiC<sub>2</sub> shows a ring distribution around the center star with a diameter of  $\sim 4\text{--}6''$  ( $\sim 2,840.95\text{--}4,258.08 \text{ au}$ ), and the signal strength reaches 20.4 and  $13.7\sigma$  for  $4_{0,4} - 3_{0,3}$  and  $4_{2,2} - 3_{2,1}$  transitions. Based on the images presented by Decin et al. (2015), it is evident that the parent molecules, such as SiO, exhibit a concentrated distribution within a compact structure surrounding the central star. In contrast, our observation reveals a characteristic pattern specific to the daughter molecules, distributed in hollow rings around the star (Agúndez et al., 2015; 2017). The brightness distributions of Figures 1, 2 under different velocity components are all generated from the transitions ( $4_{0,4} - 3_{0,3}$  and  $4_{2,2} - 3_{2,1}$ ) without the spatial extension caused by the fine structure.

The brightness distribution of the  $4_{0,4} - 3_{0,3}$  transition of SiC<sub>2</sub> and the 2–1 transition of SiO around  $V_{\text{LSR}}$  channels (from 32.3 to 46.5  $\text{km s}^{-1}$ ) are shown in Figure 3. We can see that the maximum emission of SiC<sub>2</sub> occurs at the radius of  $\sim 3''$ , with a hole in the distance from the star  $\sim 2''$ . The studies conducted by Takano et al. (1992) and Agúndez et al. (2015) showcased the spatial distribution of the daughter species centered around  $V_{\text{LSR}}$ . SiO is present as the parent species in three types of AGB stars (Cherchneff, 2006; Ramstedt et al., 2009). SiC<sub>2</sub> and SiO, shown in Figure 3, represent the spatial distribution characteristics of the daughter species and parent species, respectively, exhibiting distinct hollow and compact structures.

The northeast part of the shell emission has relatively stronger spectral signals. The SiC<sub>2</sub> ( $4_{0,4} - 3_{0,3}$ ) transition for AI Vol is stronger than the other transitions, and the hollow shell structure can be seen more clearly. SiC<sub>2</sub> at different velocity components showed an elongated cavity extending from the inner region to a location with a southern radius of  $\sim 2''$ . This structure may be

**TABLE 2** Source and observational parameters.

Name	IRAS	Mass loss rate ( $M_{\odot}\text{yr}^{-1}$ )	Distance (pc)	$V_{\text{LSR}}$ ( $\text{km s}^{-1}$ )	$V_{\text{exp}}$ ( $\text{km s}^{-1}$ )	$\theta_{\text{beam}}$ ( $''$ )
AI Vol	IRAS 07454-7112	4.9(-6) <sup>(2)</sup>	710 <sup>(2)</sup>	-39.0 <sup>(2)</sup>	12.0 <sup>(2)</sup>	1.51 × 0.99 <sup>(1)</sup>
RAFGL 4211	IRAS 15082-4808	1.0(-5) <sup>(3)</sup>	850 <sup>(4)</sup>	-3.0 <sup>(5)</sup>	19.5 <sup>(3)</sup>	1.00 × 1.00 <sup>(1)</sup>
II Lup	IRAS 15194-5115	1.7(-5) <sup>(2)</sup>	500 <sup>(2)</sup>	-15.5 <sup>(2)</sup>	21.5 <sup>(2)</sup>	0.75 × 0.45 <sup>(1)</sup>

Note:  $a(b) = a \times 10^b$ . Mass loss, distance, local standard of rest ( $V_{\text{LSR}}$ ), and expansion ( $V_{\text{exp}}$ ) velocities from the literature and synthesized beam,  $\theta_{\text{beam}}$ . References: <sup>(1)</sup>this work; <sup>(2)</sup>Danilovich et al. (2018); <sup>(3)</sup>Woods et al. (2003); <sup>(4)</sup>Groenewegen et al. (2002); <sup>(5)</sup>Smith et al. (2015).

**TABLE 3** Upper energy,  $E_u$ , and  $S\mu^2$  of molecular SiC<sub>2</sub> in the observed transitions extracted from the “Splatologue” database.

Transition	$E_u$ (K)	$S\mu^2$ (Debye <sup>2</sup> )
$J_{Ka, Kc} = 4_{0,4} - 3_{0,3}$	11.23	22.82
$J_{Ka, Kc} = 4_{2,3} - 3_{2,2}$	19.12	17.18
$J_{Ka, Kc} = 4_{2,2} - 3_{2,1}$	19.22	17.18
$J_{Ka, Kc} = 5_{0,5} - 4_{0,4}$	16.77	28.46

caused by a companion star, but AI Vol has no spiral structure typical of a companion star (Cernicharo et al., 2015). The gas expands at a lower velocity near the star, and lower-excited state transitions farther from the star are more spatially distributed than higher-excited state transitions of the same source. This is seen in Figure 4, where the zeroth-order moment map of the ( $5_{0,5} - 4_{0,4}$ ) transition has a smaller extent than the ( $4_{0,4} - 3_{0,3}$ ) transition.

The difference between Figures 3, 4 lies in their representation of data. In Figure 3, we present channel maps which provide images of vertical slices through the expanding envelope, while Figure 4 shows the line intensity integrated over all velocities. From Figure 3, we can see the clear feature of SiC<sub>2</sub> as a daughter molecule. Figure 4 offers a broader perspective by showcasing the distribution of all signals. Moreover, it reveals that the gas intensity spatial distribution of AI Vol for different transitions varies in size. Compared to transitions with low rotational quantum numbers, transitions with high rotational quantum numbers are distributed closer to the star.

The inner region of AGB stars is at  $\leq 20R_{\odot}$  ( $3.89 \times 10^{14}$  cm), and the intermediate area of the CSE of AI Vol is at  $\leq 70R_{\odot}$  ( $1.36 \times 10^{15}$  cm) (Decin et al., 2008). So the radius of SiC<sub>2</sub> molecules in AI Vol coincides with the region of the daughter species in the model (Li et al., 2016).

### 3.1.2 RAFGL 4211 and II Lup

Figure 5; Supplementary Figures SA3–A5 show the channel maps of the four transitions of SiC<sub>2</sub> for RAFGL 4211. The synthesized beam of observation is  $1.00 \times 1.00''$ , with position angles (PA) 0°. Signal strengths range from 5 $\sigma$  to 8 $\sigma$ . The brightness distribution radius is  $\sim 5''$  at approximately  $V_{\text{LSR}} = -3.0$  km s<sup>-1</sup> velocity (distance from the star center to peak intensity). A hollow shell structure exists within the radius  $\sim 3''$  of the star. The SiC<sub>2</sub> spatial distribution range of RAFGL 4211 is found to be  $\sim 6.36 \times 10^{16}$ – $8.90 \times 10^{16}$  cm. In addition to focusing on the

brightest component, we see some clump distributions in the outer regions.

Supplementary Figures SA6–A8 show the channel map of the three transitions of II Lup. The emissions  $4_{2,2} - 3_{2,1}$  have no notable signals and linewidths (the third panel at the bottom of Supplementary Figure SA9). The synthesized beam of observation is  $0.75 \times 0.45''$ . The signal strengths range from 6 $\sigma$  to 11 $\sigma$ . Supplementary Figure SA8 shows that  $5_{0,5} - 4_{0,4}$  emission has the form of a ring around the central position. The brightness distribution radius of the II Lup near  $V_{\text{LSR}} = 15.5$  km s<sup>-1</sup> velocity is  $\sim 10''$ . The SiC<sub>2</sub> spatial distribution range of II Lup is found to be  $\sim 3.74 \times 10^{16}$ – $7.48 \times 10^{16}$  cm. As with RAFGL 4211, some clumps can be seen at  $\sim 16''$ . These clumps may be a part of a spiral structure caused by a companion star.

### 3.1.3 Summary of morphology

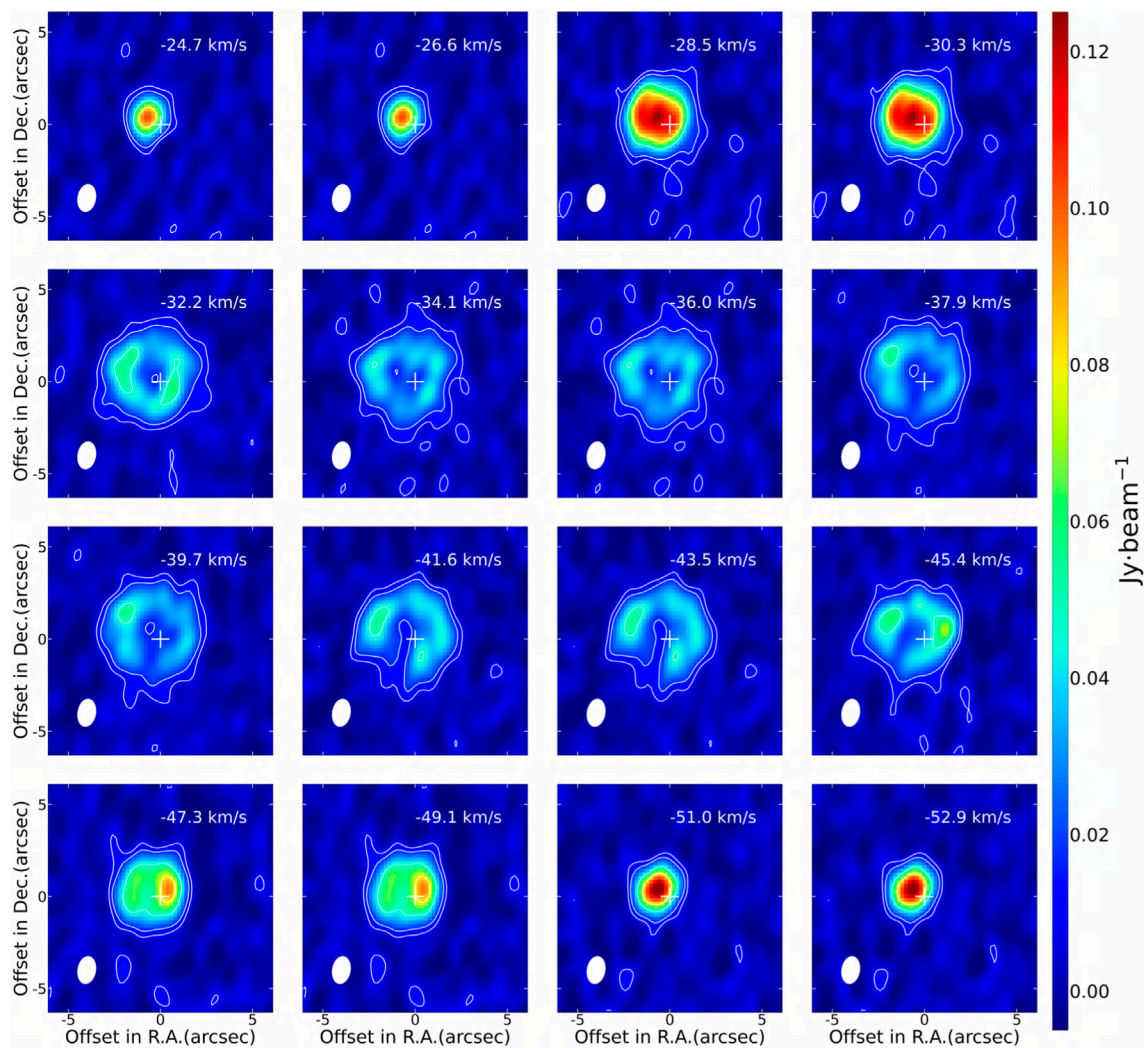
The SiC<sub>2</sub> channel map (Figures 2, 5) of AI Vol and RAFGL 4211 shows distinct daughter species characteristics. The SiC<sub>2</sub> radius greater than the  $20R_{\odot}$  distribution in the three C-rich AGB stars is consistent with the distribution of daughter species in O-rich AGB stars (Li et al., 2014). The distribution in hollow rings of the three sources indicates that SiC<sub>2</sub> is formed in the star’s outer layer through chemical reactions. This is the same as the ring distribution of SiC<sub>2</sub> in IRC +10216 (Takano et al., 1992). Gensheimer et al. (1995) reported that the inner and outer radii of SiC<sub>2</sub> of IRC +10216 are mainly distributed in the range of  $\sim 2 \times 10^{16}$ – $6 \times 10^{16}$  cm. In the analyzed observations of three sources, the SiC<sub>2</sub> spatial distribution range is approximately  $2.12 \times 10^{16}$ – $8.90 \times 10^{16}$  cm. Altogether, combining the ring brightness distribution of SiC<sub>2</sub> obtained in this work, we confirm that SiC<sub>2</sub> is the daughter molecule in the CSEs of C-rich AGB stars.

## 3.2 Abundance

We use the rotational diagram method to estimate the abundance of SiC<sub>2</sub>, and the spectral line profiles of the four transitions are shown in Figure 6. Using the parameters in Table 1, the molecular excitation temperature and column density are calculated under the assumption of LTE, and the equation is as follows (Zhang et al., 2009; Wang et al., 2014, e.g.):

$$\ln\left(\frac{3kW}{8\pi^3\nu S\mu^2}\right) = \ln\left(\frac{N}{Q}\right) - \frac{E_u}{kT_{\text{ex}}}. \quad (1)$$

Here,  $N$  represents the total column density of the molecule,  $Q$  represents the partition function,  $E_u$  represents the upper-level



**FIGURE 1**

Channel maps of  $\text{SiC}_2$  ( $4_{0,4} - 3_{0,3}$ ) toward AI Vol. The shape of the synthesized beam is shown in the lower left corner of each panel with a size of  $1.51 \times 0.99''$ , with PA  $9.82^\circ$ . The systemic velocity is displayed in the top right corner of each panel. The white cross represents the position of the star on the map. The white contour maps display the flux levels of the  $\text{SiC}_2$  transition at 5, 10, 30, and 50 times the rms noise,  $1\sigma = 1.6 \text{ mJy}\cdot\text{beam}^{-1}$ . The selected range of the color bar can show the spatial distribution of molecules better. The brightness distribution of the elongated cavity is similar to that in IRC +10216 (Lucas et al., 1995).

energy,  $T_{\text{ex}}$  represents the excitation temperature,  $k$  represents the Boltzmann constant,  $\nu$  (Hz) represents the rest frequency,  $W$  ( $\int T_{\text{R}} d\nu$ ) represents the spectral line integral intensity, and  $S\mu^2$  represents the product of the line strength and the square of the electric dipole moment. The values of  $S\mu^2$  and  $E_u/k$  are taken from the Splatalogue database<sup>6</sup>. As the upper energy levels are close in temperature, the errors in the derived quantities are rather large.

In order to determine the relative abundance of  $\text{SiC}_2$  to  $\text{H}_2$ , it is necessary to evaluate the average  $\text{H}_2$  column density within the radius occupied by  $\text{SiC}_2$ . This can be achieved by employing the

following equation (Gong et al., 2015):

$$N_{\text{H}_2} = \frac{\dot{M}R/V_{\text{exp}}}{\pi R^2 m_{\text{H}_2}} = \frac{\dot{M}}{\pi R V_{\text{exp}} \mu m_{\text{H}}} \quad (2)$$

For AI Vol,  $\dot{M} = 4.9 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$  (Danilovich et al., 2018).  $R$  is the radius of the peak of the highest brightness point in Figure 4, which is  $3''$ ;  $V_{\text{exp}}$  represents the expansion velocity of  $12 \text{ km s}^{-1}$  (Nyman and Olofsson, 1995);  $m_{\text{H}}$  represents the mass of hydrogen; and  $\mu$  represents the mean molecular weight of 2.8, as described in Gong et al. (2015). The derived column density of  $\text{H}_2$  is  $5.52 \times 10^{20} \text{ cm}^{-2}$ . In the rotational analysis using Eq. 1, we carried out error propagation and obtained the error of excitation temperature ( $\delta T_{\text{ex}}$ ) and column density ( $\delta N$ ), with the integral intensity of  $1\sigma$

<sup>6</sup> <https://splatalogue.online//advanced.php>

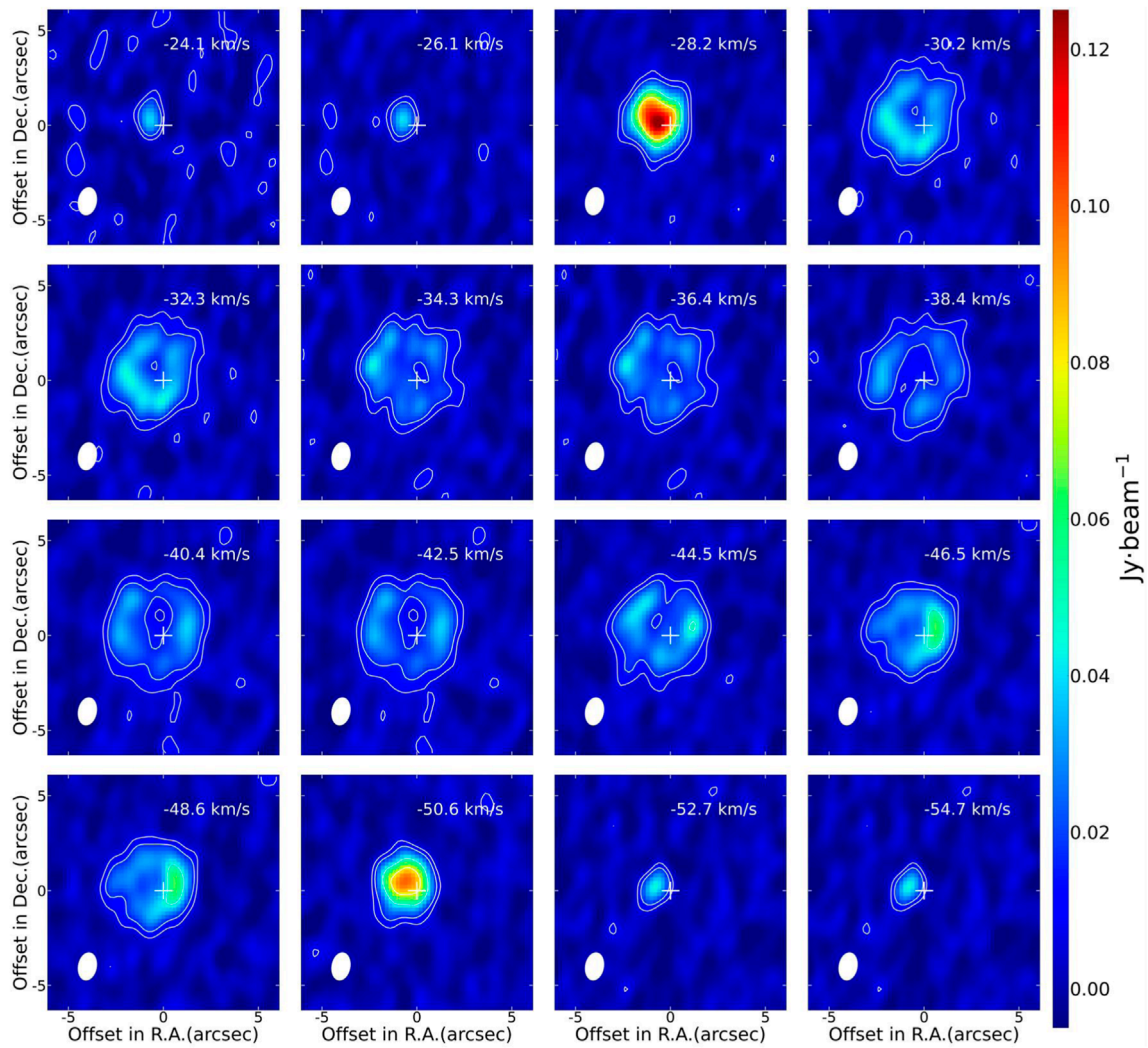


FIGURE 2

Channel maps of  $\text{SiC}_2$  ( $4_{2,2} - 3_{2,1}$ ) toward AI Vol. The shape of the synthesized beam is shown in the lower left corner of each panel with a size of  $1.48 \times 0.98''$ , with PA  $10.44^\circ$ . The velocity ( $\text{km s}^{-1}$ ) is displayed in the top right corner of each panel. The white cross represents the center of the star in the map. The white contours display the flux levels of the  $\text{SiC}_2$  transition at 5, 10, 30, and 50 times the rms noise,  $1\sigma = 1.5 \text{ mJy beam}^{-1}$ .

error. The formulas for  $\delta T_{\text{ex}}$  and  $\delta N$  are as follows:

$$\delta T_{\text{ex}} = \frac{1}{m_R^2} \delta m_R \quad (3)$$

and

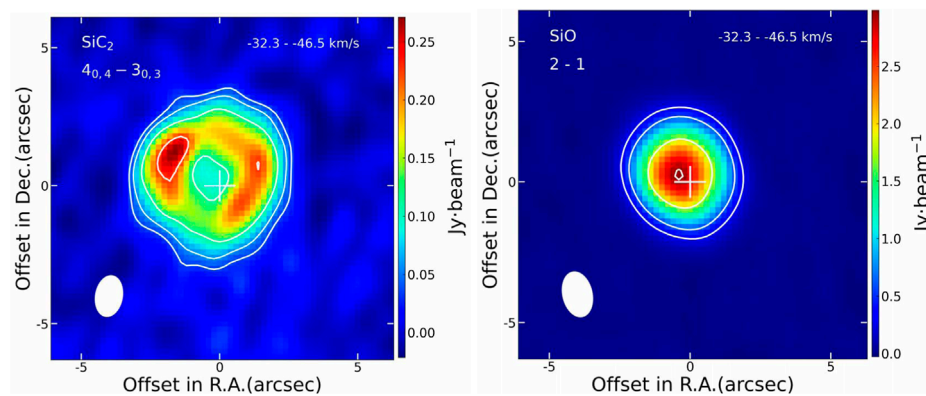
$$\delta N = \sqrt{\delta_{N,Q}^2 + \delta_{N,C_R}^2}. \quad (4)$$

The slope is represented by  $m_R$ , and the intercept is represented by  $C_R$ .  $\delta N$  is the uncertainty contribution from the rotation partition function and the intercept of the rotational diagram.

In practical calculations, first, the excited temperature and column density of  $\text{SiC}_2$  are fitted by using the rotation diagram method that is described in Eq. 1 and plotted in Figure 7; second, the fractional abundance of  $\text{SiC}_2$  is calculated by  $f = N/N_{\text{H}_2}$ . In AI Vol,

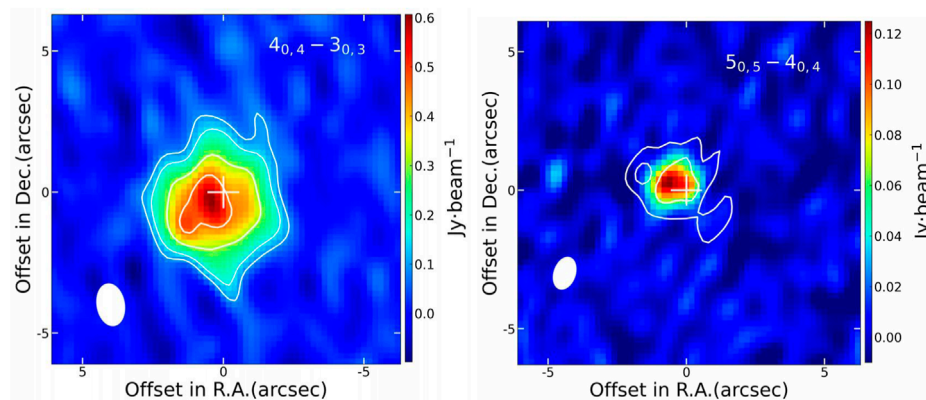
we obtained  $f(\text{SiC}_2) = 1.55 \times 10^{-8}$ , which is an order of magnitude lower than  $\text{SiC}_2$  abundance in IRC +10216, which is approximately  $10^{-7}$  (Cernicharo et al., 2010; Agúndez et al., 2012; Fonfría et al., 2014; Vellilla-Prieto et al., 2018). Table 4 presents fractional abundances, column densities, and excitation temperatures of  $\text{SiC}_2$  for all three stars. We found that the fractional abundance of  $\text{SiC}_2$  increases with the increasing wind density in the three observed C-rich AGB stars.

In the previous astrochemical models of C-rich CSEs of AGB stars,  $\text{SiC}_2$  is always treated as a parent species with an initial abundance of  $\sim 10^{-5}$  (Li et al., 2014; Massalkhi et al., 2018; Van de Sande and Millar, 2022). However, this study clearly shows that this molecule is a daughter species, and therefore, the chemistry of  $\text{SiC}_2$  in chemical models needs to be reinvestigated.



**FIGURE 3**

Brightness distribution of  $\text{SiC}_2$  (left panel) and  $\text{SiO}$  (right panel) transitions at the source velocity ( $-32.3$ – $-46.5$   $\text{km s}^{-1}$ ) in AI Vol. The color bar shows the brightness distribution of different regions. The white cross represents the center of the star in the map. The beam size of the observation in  $\text{SiC}_2$  is  $1.51 \times 0.99''$ , with PA  $9.82^\circ$ . The beam size of the observation in  $\text{SiO}$  is  $1.64 \times 1.06''$ , with PA  $-12.99^\circ$ . The white contours display the flux levels of  $\text{SiC}_2$  at 3, 5, 10, and 20 times the rms noise, with  $1\sigma = 11.3$   $\text{mJy-beam}^{-1}$ . For  $\text{SiO}$  (2–1), the flux levels are at 5, 10, 30, and 50 times the rms noise, where  $1\sigma = 58.9$   $\text{mJy-beam}^{-1}$ .



**FIGURE 4**

Zeroth moment map of the  $\text{SiC}_2$  ( $4_{0,4} - 3_{0,3}$  and  $5_{0,5} - 4_{0,4}$ ) line at 93.063639 and 115.382375 GHz toward AI Vol. The beam size of observation is  $1.51 \times 0.99''$ , with PA  $9.82^\circ$ . The molecular transitions are displayed in the top right corner of each panel. In the right panel, the beam size of observation is  $1.20 \times 0.79''$ , with PA  $18.86^\circ$ . In the left panel, the white contours display the flux levels at 3, 5, 10, and 15 times the rms noise, with  $1\sigma = 30.5$   $\text{mJy-beam}^{-1}$ . In the right panel, the flux levels are shown at 3 and  $5\sigma$  ( $1\sigma = 0.1$   $\text{mJy-beam}^{-1}$ ).

### 3.3 $\text{SiC}_2$ chemistry

Previous studies on silicon chemistry in CSEs of AGB stars mainly arise from these models constructed for the carbon-rich AGB star IRC +10216. The detailed discussion on the chemistry of the triangular molecule  $\text{SiC}_2$  in the inner CSE can be found in Willacy and Cherchneff (1998) and in the outer CSE in Takano et al. (1992), Gensheimer et al. (1995), and MacKay and Charnley (1999), where  $\text{SiC}_2$  is found to be mainly formed via ion-neutral reactions and are broken down into  $\text{SiC}$  due to photodissociation induced by the photons from the interstellar medium. Cernicharo et al. (2010) introduced three key reactions to the formation of  $\text{SiC}_2$  (i.e., Si reacts with  $\text{C}_2\text{H}_2$ , Si reacts with  $\text{C}_2\text{H}$ , and  $\text{Si}^+$  reacts

with  $\text{C}_2\text{H}$ ), and then, it can successfully explain the enhanced abundance of  $\text{SiC}_2$  from observations. The chemistry of these cyclic molecules is complex. The study of  $c\text{-SiC}_3$  by Yang et al. (2019) suggested that the carbon-silicon molecules in the CSE may not only come from complex ion-molecule reactions or the photodissociation of high-molecular weight carbon-silicon molecules but also from bimolecular neutral-neutral reactions, leading to the formation of naked carbon-silicon molecules via photochemical dehydrogenation. Since  $\text{SiC}_2$  is likely the gas-phase precursor in forming  $\text{SiC}$  dust in carbon stars (Massalkhi et al., 2018), the interaction between gas and dust, in addition to the non-spherical and clumpy structures of the envelopes of the stars, will need to be considered in future chemical models.



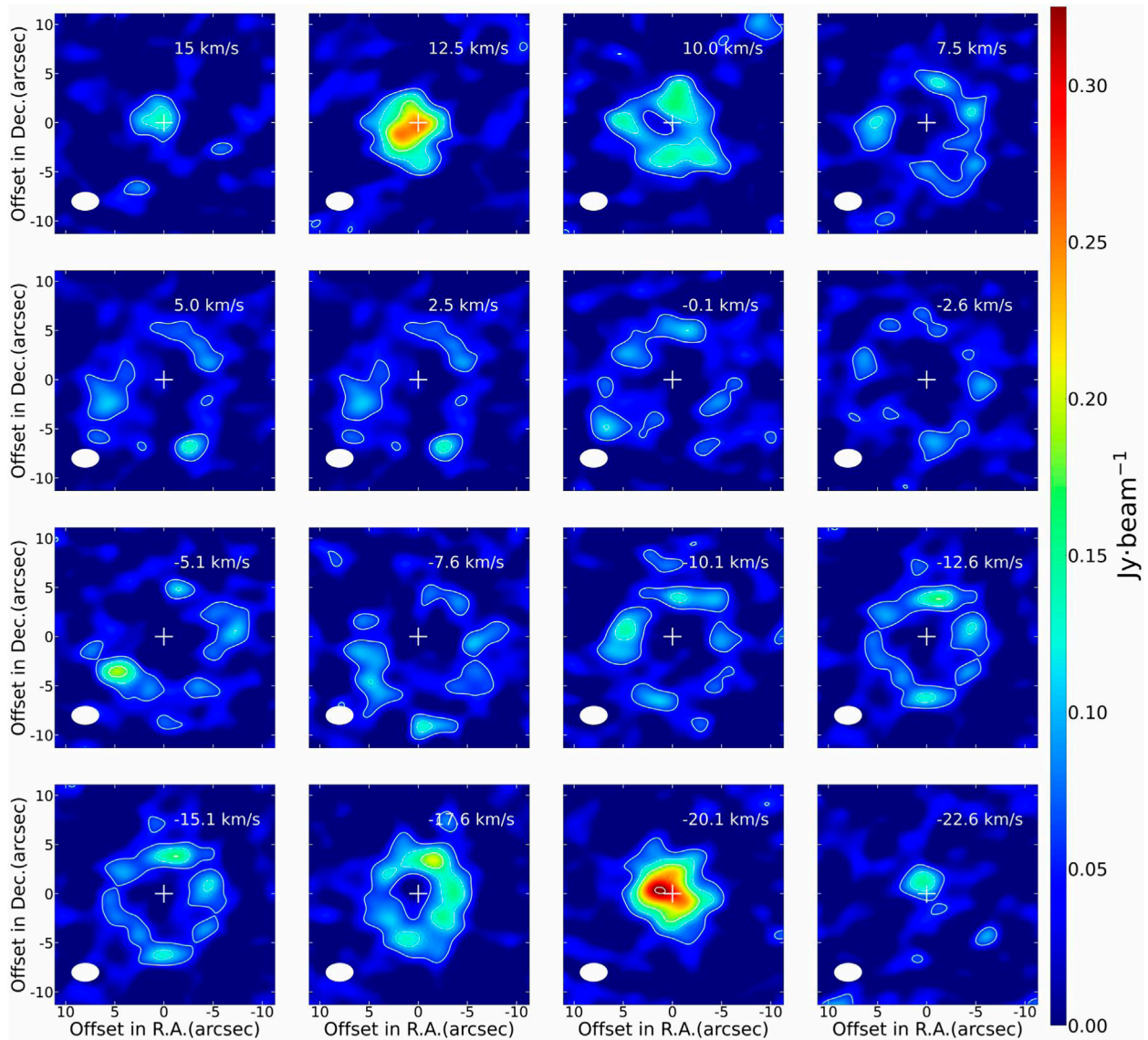


FIGURE 5

Channel maps of  $\text{SiC}_2$  ( $5_{0,5} - 4_{0,4}$ ) toward RAFGL 4211. The shape of the synthesized beam is shown in the lower left corner of each panel with a size of  $140 \times 0.93''$ , with PA  $89.13^\circ$ . The white cross represents the center of the star in the map. The white contours delineate the flux levels of  $\text{SiC}_2$ , indicating increments of 5, 10, 15, and 30 times the rms noise ( $1\sigma = 11.0 \text{ mJy-beam}^{-1}$ ).

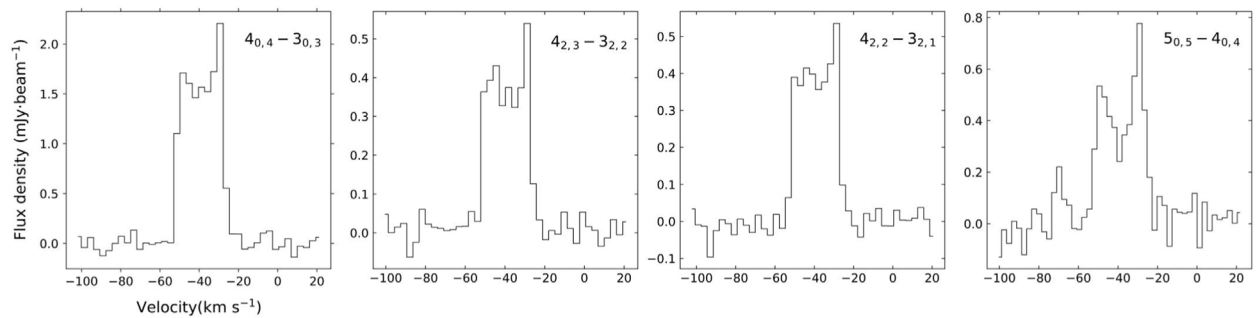


FIGURE 6

Spectral line shapes of  $\text{SiC}_2$  toward AI Vol, integrated with a  $100 \times 100$  pixel range centered on the star.

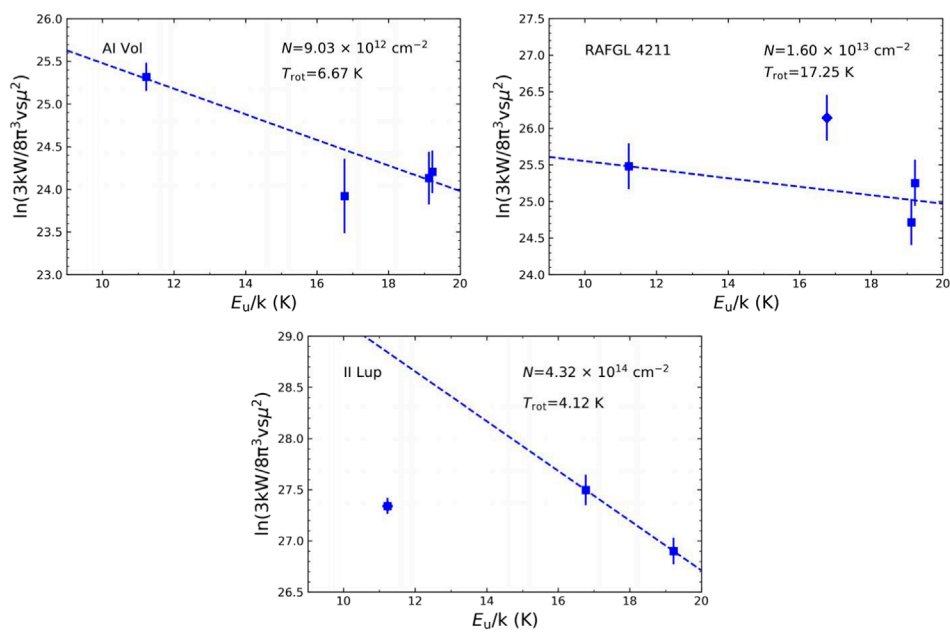


FIGURE 7

Rotational diagram for the observed SiC<sub>2</sub> lines toward AI Vol, RAFGL 4211, and II Lup. The blue dotted lines represent the results from linear least squares fitting by taking into account the weights of the errors. During fitting procedures, the data for SiC<sub>2</sub> transitions of 5<sub>0,5</sub>–4<sub>0,4</sub> (blue diamond) in RAFGL 4211 and 4<sub>0,4</sub>–3<sub>0,3</sub> (blue diamond) in II Lup were excluded. The upper right corner in each panel shows the fitted column density and excitation temperature.

**TABLE 4** Deduced excitation temperature ( $T_{\text{ex}}$ ), column density ( $N$ ), and fractional abundance ( $f$ ) of SiC<sub>2</sub> relative to H<sub>2</sub> in the target sources by the rotational diagram method, along with the previous observational results.

Source	This work			Other observations			
	$T_{\text{ex}}$ (K)	$N \times 10^{13}$ (cm <sup>-2</sup> )	$f \times 10^{-8}$	$T_{\text{ex}}$ (K)	$N \times 10^{13}$ (cm <sup>-2</sup> )	$f \times 10^{-7}$	$\dot{M} / V_{\text{exp}} \times 10^{-7}$ ( $M_{\odot} \text{yr}^{-1} \text{km}^{-1} \text{s}$ )
AI Vol	6.66 (±1.33)	0.90 (±0.49)	1.64	14.00 (±16.00) <sup>(b)</sup>	0.40 (±0.50) <sup>(b)</sup>	2.30 <sup>(a)</sup>	4.08 <sup>(c)</sup>
RAFGL 4211	17.25 (±13.07)	1.60 (±2.10)	4.62	35.00 (±51.00) <sup>(b)</sup>	4.00 (±3.00) <sup>(b)</sup>	4.90 <sup>(a)</sup>	5.13 <sup>(c)</sup>
II Lup	4.12	43.22	47.46	19.00 (±11.00) <sup>(b)</sup>	4.00 (±2.00) <sup>(b)</sup>	12.00 <sup>(a)</sup>	7.91 <sup>(a, c)</sup>

Note:  $\dot{M} / V_{\text{exp}}$  is proportional to the CSE wind density. The uncertainties are listed in parentheses, which are obtained by considering the 1 $\sigma$  signal via error propagation. The fitting of II Lup was performed using only two data points, which resulted in a lower precision and the absence of error estimation. References: <sup>(a)</sup>Woods et al. (2003); <sup>(b)</sup>Smith et al. (2015); <sup>(c)</sup>Danilovich et al. (2018).

## 4 Conclusion

To explore whether SiC<sub>2</sub> is a parent or a daughter species, we have analyzed the ALMA observations of SiC<sub>2</sub> (4<sub>0,4</sub>–3<sub>0,3</sub>, 4<sub>2,3</sub>–3<sub>2,2</sub>, 4<sub>2,2</sub>–3<sub>2,1</sub>, and 5<sub>0,5</sub>–4<sub>0,4</sub>) for the three carbon stars and compared them with SiC<sub>2</sub> results in the C-rich AGB star IRC +10216. The abundance of SiC<sub>2</sub> in the three stars is calculated by the rotational diagram method. Our analysis revealed that SiC<sub>2</sub> molecules in the CSEs of carbon stars exhibited a hollow shell structure, with a distinct brightness distribution at different velocities; therefore, we conclude that SiC<sub>2</sub> exists as a daughter molecule in the CSEs of these sources. Our results are in contrast to some previous reports which concluded that SiC<sub>2</sub> is a parent molecule in the envelopes of carbon stars. More sensitive observations may, of course, detect SiC<sub>2</sub> emissions at low levels in

the inner CSE. Our findings provide new insights into the chemical processes occurring in the CSEs of evolved stars and contribute to our understanding of the chemical evolution of ISM. A further detailed understanding of SiC<sub>2</sub> formation requires studying and comparing more C-rich AGB stars by combining the results of single-dish and high-resolution interferometric observations.

## Data availability statement

Publicly available datasets were analyzed in this study. These data can be found in the following: the datasets analyzed for this study can be found in the ALMA Science Archive: <https://almascience.nrao.edu>. This paper makes use of the following ALMA data: ADS/JAO.ALMA 2013.1.00070.S.

## Author contributions

YF prepared the project, processed the ALMA Archive data, and wrote the draft. XL initiated the project, guided the work, and revised the manuscript. TM was involved in interpreting the results, and reviewing and revising the manuscripts. RS provided continuous manuscript revisions. KW provided insights and feedback during the analysis process of the results. FX helped with the data analysis. DQ, SQ, XF, BJ, QC, G-LH, FL, and YZ provided comments and suggestions on the manuscript. JT, ZM, RM, JS, and JY were involved in analyzing the results and provided suggestions for the manuscript. All authors contributed to the article and approved the submitted version.

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## Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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## Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fspas.2023.1215642/full#supplementary-material>

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