A Subarcsecond ALMA Molecular Line Imaging Survey of the Circumbinary, Protoplanetary Disk Orbiting V4046 Sgr

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Abstract

We present a suite of Atacama Large Millimeter Array (ALMA) interferometric molecular line and continuum images that elucidate, on linear size scales of ~30–40 au, the chemical structure of the nearby, evolved, protoplanetary disk orbiting the close binary system V4046 Sgr. The observations were undertaken in the 1.1–1.4 mm wavelength range (ALMA Bands 6 and 7) with antenna configurations involving maximum baselines of several hundred meters, yielding subarcsecond-resolution images in more than a dozen molecular species and isotopologues. Isotopologues of CO and HCN display centrally peaked morphologies of integrated emission-line intensity, whereas the line emission from complex nitrile group molecules (HC3N, CH3CN), deuterated molecules (DCN, DCO+), hydrocarbons (as traced by C2H), and potential CO ice line tracers (N2H+, and H2CO) appears as a sequence of sharp and diffuse rings. The dimensions and morphologies of HC3N and CH3CN emission are suggestive of photodesorption of organic ices from the surfaces of dust grains, while the sequence of increasing radius of peak intensity represented by DCN (smallest), DCO+, N2H+, and H2CO (largest) is qualitatively consistent with the expected decline of midplane gas temperature with increasing disk radius. Empirical modeling indicates that the sharp-edged C2H emission ring lies at relatively deep disk layers, leaving open the question of the origin of C2H abundance enhancements in evolved disks. This study of the “molecular anatomy” of V4046 Sgr should serve as motivation for additional subarcsecond ALMA molecular line imaging surveys of nearby, evolved protoplanetary disks aimed at addressing major uncertainties in protoplanetary disk physical and chemical structure and molecular production pathways.

Key words: circumstellar matter – protoplanetary disks – stars: individual (V4046 Sgr) – stars: pre-main sequence

1. Introduction

Contemporary models describing viscously heated, irradiated protoplanetary disks orbiting solar-mass pre-main sequence (T Tauri) stars typically invoke a combination of gas-phase, gas-grain, and grain surface processes, some of which are driven by the intense dissociation and ionizing radiation from the central stars (e.g., Cleeves et al. 2013; Walsh et al. 2015). The physical and chemical disk structures that emerge from this complex admixture at late disk evolutionary stages give rise to the formation of molecular disk “ice lines” and “dead zones” and hence ultimately determine the orbits, masses, and compositions of any resulting planets (Öberg & Bergin 2016; Cridland et al. 2017). At late disk evolutionary stages these processes are accompanied by planet–disk (dynamical) interactions and radiation-driven disk photoevaporation, generating steep gradients in density, molecular abundance, and dust grain size that manifest themselves in the form of disk holes, rings, and gaps (e.g., Gorti et al. 2015; Dong & Fung 2017).

The handful of examples of nearby (D \( \lesssim \) 100 pc), evolved (age \( \sim 5–20 \) Myr) pre-main-sequence stars of roughly solar mass that are orbited by and actively accreting from primordial circumstellar disks offer unparalleled opportunities to investigate these and other late-stage planet formation processes (Kastner 2016). Two of these star–disk systems, TW Hya and V4046 Sgr—which lie at \( D = 60.09 \pm 0.14 \) pc and 72.47 \( \pm 0.34 \) pc, respectively (Gaia Collaboration et al. 2018)—have been among the most popular subjects for early millimeter-wave interferometric imaging studies of disks carried out with the Atacama Large Millimeter Array (ALMA). These initial ALMA studies are yielding new insight into the late physical and chemical evolution of protoplanetary disks (e.g., Qi et al. 2013b; Andrews et al. 2016; Bergin et al. 2016; Nomura et al. 2016; Guzmán et al. 2017; Hily-Blant et al. 2017; Huang et al. 2017, 2018).

Although TW Hya is thus far (and by far) the more heavily scrutinized of these two nearby, evolved disks, V4046 Sgr is in certain respects even more interesting. A member of the ~23 Myr old \( \beta \) Pic Moving Group (Mamajek 2016), V4046 Sgr is even older than TW Hya (age \( \sim 8 \) Myr; Ducourant et al. 2014); furthermore, V4046 Sgr is a close (\( P \sim 2.4 \) day) binary system consisting of nearly equal-mass, \( \sim 0.9 \) \( M_\odot \) components (Donati et al. 2011; Rosenfeld et al. 2012, and references therein). Despite its advanced system age, V4046 Sgr is orbited...
by a chemically rich circumbinary disk (Kastner et al. 2008, 2014; Rapson et al. 2015c) whose radial extent (~350 au; Rodriguez et al. 2010) and estimated gas mass (~0.09 \( M_\odot \); Rosenfeld et al. 2013) are even larger than those of the TW Hya molecular disk (~200 au and ~0.05 \( M_\odot \), respectively; Andrews et al. 2012; Bergin et al. 2013). Thus, the V4046 Sgr system presents a prime target for the purposes of understanding the process of circumbinary planet formation around near-solar-mass stars in tight orbits.

Our single-dish molecular line surveys have established that the TW Hya and V4046 Sgr disks display remarkably similar molecular spectra, with particularly strong emission from HCO\(^+\), HCN, CN, and C\(_2\)H, in addition to CO (Kastner et al. 1997, 2008, 2014). However, the two disks have sharply contrasting submillimeter continuum emission morphologies: the submillimeter surface brightness of TW Hya is centrally peaked, with a sharp outer edge at ~60 au and a set of superimposed gaps (Andrews et al. 2016), whereas V4046 Sgr appears as a compact ring that peaks at a radius of ~30 au (Rosenfeld et al. 2013). The inner radius of this ringlike submillimeter continuum emission structure is far too large to be the result of dynamical interactions between the disk and central binary, and is instead the hallmark of a “transition disk”—i.e., a disk that has developed an inner cavity that is devoid of large dust grains as a consequence of its relatively advanced evolutionary state (e.g., Andrews et al. 2011, and references therein).

As in the case of TW Hya (Rapson et al. 2015b), scattered-light, near-IR observations of V4046 Sgr with the Gemini Planet Imager revealed a dust ring system within the giant planet formation region of the disk (Rapson et al. 2015a). The outer (radius 30–45 au) faint scattering halo imaged in the near-IR overlaps the ring detected in submillimeter continuum imaging of the disk, while the inner (radius 12–18 au) bright ring seen in scattered light lies fully interior to the submillimeter emission “hole,” demonstrating that the apparent (submillimeter) cavity within ~30 au is actually rich in small grains that have “filtered” through to smaller radii. When considered in the context of theoretical predictions of the effects of planets on disk structure (e.g., Rice et al. 2003; Paardekooper & Mellema 2006; Zhu et al. 2012), the combination of a disk “gap” near 20 au, an inner disk hole, and evidence for grain size segregation is indicative of recent or ongoing giant-planet-building activity (Rapson et al. 2015a).

Initial ALMA disk studies have included V4046 Sgr among small samples of objects that were the subjects of molecular line imaging surveys focused on disk deuterium chemistry (Huang et al. 2017), nitrogen isotopic ratios (Guzmán et al. 2017), and molecular ice lines (C. Qi et al. 2018, in preparation). In addition, we recently carried out an ALMA line imaging study of V4046 Sgr that was aimed at investigating the origin of the large CN and C\(_2\)H abundances that are evidently characteristic of evolved molecular disks (see, e.g., Kastner et al. 2014, 2015; Punzi et al. 2015; Bergin et al. 2016). All of these ALMA line surveys of V4046 Sgr have been undertaken in the 1.1–1.4 mm wavelength range (ALMA Bands 6 and 7) with antenna configurations involving maximum baselines of several hundred meters, yielding subarcsecond-resolution images in more than a dozen molecular species and isotopologues. Here, we bring together the results of these observations of the disk orbiting V4046 Sgr. Collectively, these ALMA images serve to elucidate, on linear size scales of ~30–40 au, the chemical structure of an evolved, circumbinary, protoplanetary disk.

### 2. Observations

The library of ALMA images of V4046 Sgr presented here was compiled from data obtained during the course of ALMA programs 2013.1.00226.S (Cycle 2; PI: K. Öberg), 2015.1.00671.S (Cycle 3; PI: J. Kastner), and 2015.1.00678.S (Cycle 3; PI: C. Qi). Table 1 lists the species and transitions...
Data obtained for program 2015.1.00671.S during a shorter (~360 s) integration on 2016 July 31 in a second spectral setup optimized for the CO $J = 2 \rightarrow 1$ and CN $N = 2 \rightarrow 1$ transitions (in the 226–231 GHz frequency range) could not be properly calibrated and are hence unusable.

### Table 2

| Program          | $\nu$ (GHz) | Beam (PA)$^a$ | Flux$^b$ (mJy) |
|------------------|-------------|---------------|----------------|
| 2013.1.00226.S   | 235         | 0°70 × 0°43 (+84°) | 338 ± 34      |
| 2013.1.00266.S   | 251         | 0°52 × 0°43 (+82°) | 353 ± 35      |
| 2015.1.00671.S   | 264         | 0°69 × 0°49 (−77°) | 327 ± 33      |
| 2015.1.00678.S   | 284         | 0°38 × 0°29 (−73°) | 472 ± 47      |

Notes.

$^a$ Major and minor axes and position angle of the synthesized beam.

$^b$ Integrated fluxes above the 3σ level in continuum images; listed errors assume (10%) systematic calibration uncertainties dominate over pixel-to-pixel rms uncertainties.

### 3. Results

#### 3.1. Images

The resulting clean beam sizes and integrated fluxes (within apertures encompassing the source flux above ~3σ levels) are listed in Tables 1 and 2 for the line and continuum imaging, respectively. The formal uncertainties on the line fluxes listed in Table 1 were estimated by propagating the rms per-channel errors, accounting for the radial extent of the emission in the moment 0 image as well as the line widths (see, e.g., Kastner et al. 2010); the minimum uncertainties are ~10%, after accounting for typical systematic ALMA calibration errors. Our integrated continuum and 12CO and 13CO line flux measurements are consistent with those obtained in previous SMA imaging of V4046 Sgr within the respective uncertainties (Rodriguez et al. 2010; Öberg et al. 2011), with the possible exception of the 264 GHz continuum measurement (which is ~20% lower than previously measured by Öberg et al. 2011).

3. The resulting ALMA 235 GHz and 264 GHz continuum images and moment 0 line images for the molecular species and transitions listed in Table 1, as well as a moment 1 $^{12}$CO(2–1) image, are presented in Figure 1 in 12″ × 12″ fields of view and in Figures 2 and 3 in 6″ × 6″ fields of view. The moment 0 images displayed in these figures have been integrated over channel ranges that span the detectable emission; for all images apart from H2CO and N2H$,^+$, the component channel maps were clipped at the 1σ level in order to isolate the signal.

The continuum, $^{12}$CO, and $^{13}$CO images reproduce, at higher spatial resolution and signal-to-noise, the basic features seen in the best previous 1.3 mm continuum and CO imaging of V4046 Sgr, which were obtained with the SMA and presented in Rosenfeld et al. (2013). Specifically, the millimeter-wave continuum emission appears as a partially filled ring, peaking at ~0″3 (~22 au) from the star, with a sharp intensity cutoff at its outer radius of ~0″8 (~60 au), whereas the CO is strongly centrally peaked and the $^{12}$CO emission outer radius (~4″, i.e., ~300 au) is far larger than that of the continuum. As was the case for the previous SMA imaging (Rodriguez et al. 2010; Rosenfeld et al. 2013), the large-scale Keplerian rotation of the disk is readily apparent in the moment 1 image of $^{12}$CO(2–1).

The molecular emission-line images in Figures 2 and 3 are grouped according to their morphological properties (see also Huang et al. 2017), wherein Figure 2 displays images with intensity (moment 0) and intensity-weighted mean radial velocity (moment 1) images discussed in Section 3.
centrally peaked morphologies and Figure 3 displays images with ringlike morphologies that range from distinct to somewhat diffuse. Correspondingly, in Figures 4 and 5, respectively, we display radial profiles extracted from the centrally peaked and ringlike molecular emission-line images (see Section 3.2).

**Centrally peaked morphologies (Figures 2 and 4).** The images of C and O isotopologues of CO and C and N isotopologues of HCN all display centrally peaked morphologies. The line emission from the rare CO and HCN isotopologues is far more compact than that of the most abundant isotopologues ($^{12}$C$^{16}$O and H$^{12}$C$^{14}$N), as expected in light of the smaller optical depths and resulting lower fluxes in the lines of the rare isotopologues.

**Distinct ringlike morphologies (Figures 3 and 5).** The HC$_3$N, CH$_3$CN, DCO$^+$, and C$_2$H line images display ringlike emission morphologies wherein the emission rings have clearly defined central holes, relatively sharp outer edges, or both. The emission from the cyanide group molecules, HC$_3$N and CH$_3$CN, arises from compact regions whose outer radii are similar to those of the 1.1–1.4 mm continuum emission ring (see Section 3.2). Due to their low signal-to-noise ratios and small angular sizes, we find that the depths of the inner holes within the HC$_3$N and CH$_3$CN emitting regions are sensitive to the adopted visibility weighting during the image reconstruction (cleaning) process, while the degree of azimuthal asymmetry is sensitive to channel noise clipping in constructing the moment 0 images. However, the overall ringlike morphologies of HC$_3$N and CH$_3$CN—ewith the CH$_3$CN ring possibly more asymmetric and filled in than HC$_3$N—appear to be a robust result of these observations.

**Diffuse ringlike morphologies (Figures 3 and 5).** The DCN, H$_2$CO$^+$, N$_2$H$^+$, and H$_2$CO line images all display diffuse emission morphologies and appear as rings to a greater or lesser degree. The DCN(4–3) image presented here, which has a higher signal-to-noise ratio than the DCN(3–2) image presented in Huang et al. (2017), confirms the ringlike DCN emission morphology hinted at in that survey. Evidently, the diffuse DCN ring is more compact than the sharper C$_2$H or DCO$^+$ rings, while the H$_2$CO$^+$ ring dimensions appear to
more closely resemble those of DCN than those of DCO$^+$. The radius of peak integrated line intensity within the bright $N_2H^+$ ring is comparable to the radius of peak integrated $C_2H$ line intensity, but with its filled in central hole and outer halo, the $N_2H^+$ ring is much larger and more diffuse in appearance. The outer radius of the H$_2$CO emitting region appears to be similar to that of CO, but (unlike CO) the H$_2$CO has a central hole. As in the case of DCO$^+$ and C$_2$H, the inner holes of the $N_2H^+$ and H$_2$CO line emission rings, though poorly defined, appear to be similar to the outer radii of the continuum rings.

3.2. Radial Profiles of Integrated Molecular Line Intensity

In Figures 4 and 5 we display radial profiles extracted from unclipped versions of the moment 0 molecular emission-line images of V4046 Sgr, as well as the radial profile of the 264 GHz continuum image. These profiles were extracted after deprojecting the images assuming a disk inclination $i = 33.5^\circ$ and position angle of $67^\circ$ (Rosenfeld et al. 2013). The error bars indicate statistical uncertainties, which we estimated as $\sigma_r = \sigma_{\nu\nu} \sqrt{\Delta V/\delta \nu} (1/\sqrt{N})$, where $\sigma_{\nu\nu}$ is the rms flux density deviation in a channel map (as determined from an emission-free region of the map), $\Delta V$ is the line width, $\delta \nu$ is the channel width (such that $\Delta V/\delta \nu$ is the number of velocity channels over which the line emission was integrated), and $N$ is the number of pixels included within the radial bin.

Figure 4 provides a comparison of the radial profiles of integrated emission from isotopologues of CO and HCN, which have centrally peaked image morphologies (Figure 2). Some caution must be applied in comparing these profiles in detail, since the beam widths of the CO isotopologue images are $\sim 40\%$ larger than those of the HCN isotopologues (Table 1). The radial profiles of both $^{12}$CO and H$^{12}$CN show inflection points (slope changes) at $\sim 1.5$ ($\sim 100$ au) that are suggestive of bright cores surrounded by larger halo structures. Such features can be produced by subtraction of optically thick continuum emission from optically thick line emission (Weaver et al. 2018), but that is unlikely to be the case here, given that the inflection points lie well beyond the outer edge of the continuum ring ($\sim 0.7\arcsec$). The $^{12}$CO falls off steeply with radius within the inner continuum ring, whereas the H$^{12}$CN profile is shallow within this same region. The radial profiles demonstrate that detectable emission extends to $\sim 2.5\arcsec$ ($\sim 180$ au) and $\sim 4\arcsec$ ($\sim 300$ au) for H$^{12}$CN and $^{12}$CO, respectively, with $^{12}$CO.
intensity displaying a sharp outer edge that is best seen in the comparison of radial intensity profiles of CO isotopologue emission presented in Section 4.1.

In the left and right panels of Figure 5, we compare the radial profiles of integrated emission from molecular lines exhibiting sharply ringlike and more diffuse ringlike morphologies, respectively (Figure 3). Such a direct comparison of these radial profiles is enabled by the similar beam sizes of the data collected for all of these transitions (i.e., their beam widths differ by <15%; Table 1). A sequence is apparent in the radial position of peak intensity and (hence) central hole size within these rings of molecular line emission. The smallest rings are those of the cyanide group molecules (CH$_3$CN and HC$_3$N), which peak near $\sim$0"25 ($\sim$18 au), just inside the peak continuum emission (see Figure 6). The largest rings are the sharp-edged C$_2$H and diffuse N$_2$H$^+$, both of which peak at $\sim$1"2 ($\sim$90 au), and H$_2$CO, which displays a broad peak at $\sim$1"6 ($\sim$115 au). The emission rings of the deuterated species DCN and DCO$^+$, which peak at $\sim$0"6 ($\sim$45 au) and $\sim$0"8 ($\sim$60 au), respectively, are intermediate in size. While we do not display the radial profile of H$^{13}$CO$^+$ due to its relatively poor signal-to-noise ratio (S/N), this faint ring appears to more closely trace DCN than DCO$^+$ (Figure 3; see also Figure 2 in Huang et al. 2017).
The upper left panels of Figure 5 illustrate the close correspondence of the radial profiles of emission from the cyanide group molecules (HC$_3$N and CH$_3$CN) to each other and to that of the 264 GHz continuum emission profile, which peaks at $\sim 0^\circ3$ ($\sim 22$ au) and has an outer radius (at 10% of peak) of $\sim 0^\circ8$ ($\sim 60$ au). The peak intensities of HC$_3$N and CH$_3$CN emission appear to lie just inside that of the continuum, and the lack of a central hole is apparent in the case of CH$_3$CN. The radial distributions of HC$_3$N and CH$_3$CN line emission both display sharp outer radial cutoffs, falling to $\sim 10\%$ of peak intensity at $\sim 0^\circ7$ ($\sim 50$ au).

3.3. Line Profiles

In Figure 7, we display line profiles extracted from the interferometric data cubes for molecular species observed by ALMA subsequent to the observations presented in Huang et al. (2017) and Guzmán et al. (2017) or whose profiles were not presented in those papers. The extraction regions were ellipses whose major and minor axes approximately correspond to the $\sim 3\sigma$ noise levels in the individual velocity channel images. Whereas the $^{12}$CO and $^{13}$CO line profiles display the classical double-peaked profiles characteristic of Keplerian rotation (as was already apparent in single-dish observations; Kastner et al. 2008), the profile of C$^{18}$O—which is presented here for the V4046 Sgr disk for the first time—appears more rounded, with stronger wings relative to the line core. This difference reflects the smaller detectable extent of the C$^{18}$O emission, which effectively suppresses the emission at the low radial velocities characteristic of the outer disk relative to the higher-velocity emission characteristic of the central disk. Similar arguments appear to pertain to the line profiles of isotopologues of HCN, wherein the line profile of the most abundant isotopologue appears double-peaked and those of the rare isotopologues are more rounded. The line profiles of N$_3$H$^+$ and H$_2$CO lack high-velocity wings, as expected given their...
large, diffuse, ringlike morphologies. The triple-peaked C2H and CH3CN line profiles result from the superposition of double-peaked emission lines in neighboring hyperfine transitions (compare with C2H and CH3CN line profiles displayed in Kastner et al. 2014; Öberg et al. 2015, respectively).

4. Discussion

4.1. Radial Dependencies of CO Isotopologue Emission Ratios

Given their similar beam areas (which differ by <5%) and comparable sensitivities, the images in $J = 2 \rightarrow 1$ emission from $^{12}$CO, $^{13}$CO, and C$^{18}$O (Figure 2) afford the opportunity to investigate the ratios of CO isotopologue emission-line intensity as functions of radial position across the V4046 Sgr disk. These ratios in turn can be used to assess the optical depths of $^{12}$CO, $^{13}$CO, and C$^{18}$O emission. Specifically, given an assumed (constant) isotopologue abundance ratio $X_{12,18}$ within the disk, the ratio of line emission intensities in two isotopologues at radial position $r$ can be related to optical depth in the first (more abundant) isotopologue, $\tau_1$, via

$$R_{12}(r) = \frac{1 - \exp(-\tau_1(r))}{1 - \exp(-\tau_1(r)/X_{12,18})}$$

(e.g., Kastner et al. 2014; Schwarz et al. 2016 carried out such an analysis of $\tau(r)$ for the TW Hya disk). Caution must be applied in interpreting estimates for $\tau_1(r)$ as deduced from $R_{12}(r)$, given that emission from the different isotopologues likely arises from different vertical disk layers (e.g., Zhang et al. 2017). Furthermore, the optical depth can vary significantly both spatially (within the synthesized beam), as well as across the line profile over which the intensity is integrated. Hence, we restrict the present discussion to a qualitative analysis of the radial regimes over which the various isotopologue emission lines appear to be optically thick or thin.

Comparisons of the radial profiles in the various isotopologues, as well as the radial profiles of the intensity ratios of CO isotopologue emission, are presented in Figure 8. The integrated intensity of $^{12}$CO emission shows a precipitous drop at $\sim 4''$ (∼300 au), indicative of either the steep outer edge of the gas disk or a sharp decline in CO abundance; the latter would presumably be due to UV photodissociation. The maximum radii of detectable $^{13}$CO and C$^{18}$O emission are $\sim 3''$ (∼220 au) and $\sim 1''$ (∼75 au), respectively. These radii set the respective limits within which we can measure the $^{12}$CO:$^{13}$CO and $^{13}$CO:C$^{18}$O (and $^{12}$CO:C$^{18}$O) emission-line ratios. We find the ratio of $^{12}$CO:$^{13}$CO line emission intensities to be essentially independent of $r$ given the uncertainties, with a value $R_{12,13} \sim 2.5$, while the $^{12}$CO:C$^{18}$O line ratio increases from $R_{12,18} \sim 5$ to $R_{12,18} \sim 18$ over the radial range $r \lesssim 25$ au to $r \sim 75$ au. The ratio of $^{13}$CO:C$^{18}$O line emission intensities $R_{13,18}$ increases from $R_{13,18} \sim 2$ to $R_{13,18} \sim 7$ over this same radial range.

For the values of $X_{12,13}$ and $X_{12,18}$ typically assumed in the astrophysical literature—i.e., $X_{12,13}$ from $\sim 40$ to $\sim 70$, and $X_{12,18} \sim 480$ (Kastner et al. 2014; Zhang et al. 2017, and references therein)—these small values of $R_{12,13}$ and $R_{12,18}$ imply, not surprisingly, that the $^{13}$CO(2–1) emission is very optically thick (i.e., $\tau_{12} \gg 1$) across the disk surface. Meanwhile, the observation that $R_{13,18} < 7$ (i.e., $R_{13,18} < X_{13,18}$ assuming $X_{12,13} = 70$) within $\sim 75$ au indicates that $\tau_{13} > 1$, at least in the inner disk; the small, near-constant value of $R_{12,13}$ furthermore implies that $^{13}$CO(2–1) is optically thick throughout the disk. Assuming that the ratio of $^{13}$CO to C$^{18}$O optical depths is identical to their abundance ratio, the foregoing results for $\tau_{13}$ for V4046 Sgr also imply that C$^{18}$O is optically thin throughout much of the disk. These results for $\tau_{13}$ and $\tau_{18}$ are similar to those inferred for TW Hya by Schwarz et al. (2016). We note, however, that Zhang et al. (2017) find that C$^{18}$O(3–2) is optically thick in the innermost regions ($r \lesssim 20$ au) of the TW Hya disk.

If both $^{12}$CO(2–1) and $^{13}$CO(2–1) are optically thick, their line ratio is diagnostic of the characteristic temperatures of the regions from which the bulk of the emission in each line originates. Hence, Figure 8 indicates that the optically thicker $^{12}$CO(2–1) emission arises from a warmer and hence higher-lying disk layer than $^{13}$CO(2–1), as expected given the vertical
temperature inversion that is a feature of models of irradiated disks (e.g., Zhang et al. 2017). Higher spatial resolution ALMA imaging of CO isotopologue emission from the V4046 Sgr disk, as well as observations of $^{12}$C$^{18}$O emission analogous to those carried out for TW Hya (Zhang et al. 2017), would test the foregoing qualitative inferences concerning the radial dependencies of the optical depths of CO isotopologue emission and would provide important additional constraints on disk vertical structure, molecular mass, and $^{12}$C/$^{13}$C abundance ratio.

4.2. The Potential Connection between Complex Nitriles and Dust

V4046 Sgr stands out among disks surveyed thus far by ALMA for its unusually bright emission from both HC$_3$N and CH$_3$CN (Bergner et al. 2018). As in the case of MWC 480, the first disk detected in both of these complex nitrile (cyanide-bearing) species (Oberg et al. 2015), there appears to be a spatial correspondence between the HC$_3$N and CH$_3$CN line emission and the continuum emission from large (millimeter-sized) dust grains in the V4046 Sgr disk. However, the subarcsecond ALMA imaging of V4046 Sgr presented here makes apparent the ringlike morphologies of HC$_3$N and, possibly, CH$_3$CN (Figure 3). These morphologies closely correspond to those of the continuum emission as well as scattered light from small grains just interior to the continuum ring (Rapson et al. 2015a)—and they contrast with the centrally peaked emission from the rare HCN isotopologues (Figure 6)—suggesting a connection between the presence of dust rings and the production of gas-phase HC$_3$N and CH$_3$CN. Various pure gas-phase production routes for HC$_3$N and CH$_3$CN and potential grain surface chemistry production of CH$_3$CN are discussed by Bergner et al. (2018) in the context of their survey of complex nitriles in V4046 Sgr and several other disks. Here, we point out one possible interpretation of the apparent morphological correspondence between emission from these species and that of emission from (and scattering off) dust grains within the V4046 Sgr disk.

Specifically, based on the results of simulations (Walsh et al. 2014; Cleeves et al. 2016) and laboratory experiments (Mendoza et al. 2013), it is possible that the ringlike HC$_3$N and CH$_3$CN emitting regions are generated by stellar irradiation of ice-coated grains. In such a scenario, HC$_3$N, CH$_3$CN, and other more complex organics either form in the disk, or were inherited from the prestellar core that spawned V4046 Sgr. In either case, a significant mass of organics likely subsequently accretes (freezes out) onto grains in the present-day disk and/or at earlier phases of the protostellar (Class 0/I) disk. The intense stellar UV and X-irradiation from V4046 Sgr (e.g., Argiroffi et al. 2012) impinging on the well-defined rings of dust grains within the disk then results in efficient desorption of the organic ice coatings, generating detectable column densities of HC$_3$N and CH$_3$CN (Walsh et al. 2014). Interestingly, HC$_3$NH$^+$ is one of the dominant products of X-irradiation of pyrimidine ice-coated grains in laboratory experiments (Mendoza et al. 2013). This suggests that the abundances of HC$_3$N might be enhanced in UV- and X-irradiated regions that are sufficiently rich in pyrimidine and (perhaps) other organic ices, such that both the abundance of HC$_3$NH$^+$ and the molecular gas ionization fraction are elevated. On the other hand, it is not clear whether either HC$_3$N or CH$_3$CN would then survive long in the gas-phase, given the large photodissociation rates within such a hostile radiation environment.

Similar arguments pertain to the production of gas-phase H$_2$CO via UV and X-ray photodesorption of hydrogenated grain (CO) ice mantles (Walsh et al. 2014; Oberg et al. 2017). Indeed, the Walsh et al. (2014) modeling predicts that the column density of gas-phase H$_2$CO thus generated should peak at, and remain elevated out to, much larger disk radii than the column densities of HC$_3$N and CH$_3$CN. Qualitatively, these model predictions also seem to be borne out by the ALMA imaging presented here (Figure 5; see also Section 4.3). We note, however, that the Walsh et al. (2014) model assumes a smoothly varying disk dust component, which does not describe evolved protoplanetary disks like the one orbiting V4046 Sgr, with its relatively narrow, compact ring of large grains and interior small-grain dust ring/gap system. The HC$_3$N and CH$_3$CN images presented here hence serve as motivation for future simulations aimed at ascertaining whether and how the processes of photodesorption and photodissociation of organics in a protoplanetary disk depend on the extent...
of dust grain coagulation and transport within the disk. Given that thermal excitation of the $\sim260$ GHz transitions observed here requires gas kinetic temperatures of $\sim100$ K, sensitive observations of lower-lying transitions of HC$_3$N and CH$_3$CN in V4046 Sgr would also help test the hypothesis that photodesorption is responsible for production of these molecules. As noted by Bergner et al. (2018), the extant data are not sensitive to emission from these molecules within cooler disk regions at larger radii.

4.3. The Nested Molecular Rings Orbiting V4046 Sgr

Beyond the $\sim50$ au outer radius of the continuum and HC$_3$N and CH$_3$CN emission in the V4046 Sgr disk, emission from the species DCN, DCO$^+$, N$_2$H$^+$, C$_2$H, and H$_2$CO appears as a sequence of rings with an increasing radius of peak intensity (i.e., intensity peaks at $\sim45$, 60, 90, 90, and 110 au, respectively) and varying sharpness in terms of inner and outer cutoff radii (Figure 5). Among these rings, the sharp-edged morphology of C$_2$H is perhaps most striking; this emission ring is modeled and discussed in detail in Section 4.4. Here, we briefly comment on some potential implications of this molecular ring “sequence.”

The main routes proposed for formation of DCO$^+$ and DCN require the presence (destruction) of H$_2$D$^+$ and CH$_3$D$^+$, respectively (Huang et al. 2017, and references therein). Because survival of H$_2$D$^+$ requires temperatures $\lesssim$30 K, whereas survival of CH$_3$D$^+$ is energetically favorable up to $\sim$80 K, one expects DCN to peak in abundance at smaller disk radii than DCO$^+$ (Huang et al. 2017). Such a relationship is indeed observed in the case of V4046 Sgr. As formation of DCO$^+$ also depends on the presence of gas-phase CO, one further expects DCO$^+$ to be confined to a disk temperature regime and hence a (midplane) radial regime where the disk is not warm enough for destruction of H$_2$D$^+$ (which requires temperatures in excess of $\sim$30 K) but not cold enough that there is significant freeze-out of CO (temperatures below $\sim$25 K). This rather narrow range of temperatures favorable to DCO$^+$ formation may explain the ringlike appearance of DCO$^+$ in V4046 Sgr and other disks (e.g., HD 163296; Qi et al. 2015). On the other hand, Huang et al. (2017) caution against concluding that DCO$^+$ serves to trace the specific disk regime that lies just above the CO freeze-out temperature (snow line), citing the lack of a clear relationship between the radial extents of DCN and DCO$^+$ in many of the disks they surveyed.

As discussed in Qi et al. (2013a, 2013b, 2015) and Öberg et al. (2017), millimeter-wave emission lines of the species N$_2$H$^+$ and H$_2$CO (particularly the former) should provide particularly effective tracers of the CO snow line, albeit for complementary reasons: N$_2$H$^+$ is destroyed via reactions with gas-phase CO, forming HCO$^+$, while, as noted, H$_2$CO can be efficiently generated through hydrogenation of CO ice mantles on dust grains followed by photodesorption. Hence, the largest expected N$_2$H$^+$ and H$_2$CO abundance enhancements are in disk regions cold enough for CO freeze-out (although there are also warm formation pathways for H$_2$CO; Öberg et al. 2017). In general terms, this expectation appears to be borne out in V4046 Sgr, i.e., the N$_2$H$^+$ and H$_2$CO rings both reach their peak intensities beyond the peaks of the DCN and DCO$^+$ rings. However, in contrast to the TW Hya and HD 163296 disks—both of which have N$_2$H$^+$ emission rings with sharp inner cutoffs (Qi et al. 2013b, 2015)—there is no clear central hole within the N$_2$H$^+$ ring in the V4046 Sgr disk. As a result, the precise radial position of putative midplane CO freeze-out is difficult to ascertain for V4046 Sgr on the basis of its radial profile of N$_2$H$^+$ line intensity. Such an interpretation is rendered even more difficult by the possibility that the N$_2$H$^+$ column density may smoothly increase beyond the midplane CO snow line, and/or that there may be significant abundances of N$_2$H$^+$ in disk surface layers (see discussions in Nomura et al. 2016; van’t Hoff et al. 2017). Further detailed analysis of the ALMA N$_2$H$^+$ and H$_2$CO imaging results for V4046 Sgr will be presented in a forthcoming paper (C. Qi et al. 2018, in preparation).

4.4. An Empirical Model for the C$_2$H Ring

Our molecular line surveys of TW Hya, V4046 Sgr, and the disk orbiting LkCa 15 (age $\sim5$ Myr) established that the emission-line intensities of C$_2$H from these evolved disks rival or exceed those of, e.g., $^{13}$CO (Kastner et al. 2014; Punzi et al. 2015). Follow-up SMA and ALMA imaging of C$_2$H emission from TW Hya (Kastner et al. 2015; Bergin et al. 2016) revealed that the C$_2$H line emission exhibits a ringlike morphology. Our ALMA imaging has now established that the C$_2$H emission from V4046 Sgr displays the same well-defined, ringlike morphology (a result already apparent in our previous SMA C$_2$H imaging; Kastner et al. 2016), indicating that sharp-edged C$_2$H rings are a common feature of evolved disks.

Given the paucity of bright molecular line tracers of disk chemical and physical conditions, it is essential to understand the production mechanism(s) responsible for the large abundances of C$_2$H and its ringlike distribution in these and other disks (e.g., DM Tau; Bergin et al. 2016). Based on the SMA C$_2$H imaging results for TW Hya and consideration of the excitation of C$_2$H, we proposed that the C$_2$H ring traces particularly efficient UV/X-ray photodesstruction of hydrocarbons derived from small grains and grain ice mantles in the low-density ($n < 10^5$ cm$^{-3}$), large-grain-depleted surface layers of the outer (>45 au) regions of the TW Hya disk (Kastner et al. 2015). Subsequent ALMA C$_2$H imaging and accompanying modeling supports the general notion that efficient C$_2$H production in evolved disks is a signpost of grain size segregation and stellar irradiation (Bergin et al. 2016). However, Bergin et al. (2016) concluded that TW Hya’s ringlike C$_2$H emission morphology is also a result of C depletion in the inner disk, and that the emission arises from disk layers with $n > 10^6$ cm$^{-3}$. If so, then the presence of a C$_2$H ring would most likely be the result of pure gas-phase and/or gas-grain processes deep within the disk, with little or no influence from stellar irradiation (see the discussion in Kastner et al. 2015, and references therein).

This uncertainty in the vertical location of C$_2$H within the TW Hya disk is a consequence of the model degeneracies inherent to its near-pole-on orientation (i = 7°; Andrews et al. 2012, and references therein). Given the more intermediate inclination of the V4046 Sgr disk (i = 33°5; Rosenfeld et al. 2013), this disk potentially provides a means to distinguish between the various alternative C$_2$H production models—i.e., surface-layer, irradiation-driven production versus midplane, pure gas-phase production—to explain the presence of bright C$_2$H rings in these two disks.

To investigate the potential of the ALMA C$_2$H imaging in this regard, we have modeled the ringlike C$_2$H line emission.
following the methodology described in detail in Qi et al. (2013b) and Kastner et al. (2015). Briefly, as in Qi et al. (2013b), we adopt a physically self-consistent accretion disk model (D'Alessio et al. 2006, and references therein) that matches the spectral energy distribution (SED), with the disk geometric (i.e., scale height and surface density profile) parameters fixed to values previously determined via SED fitting for V4046 Sgr (Rosenfeld et al. 2013). Within this framework, we then investigate a limited parameter set that describes the disk layer from which the molecular emission originates. Specifically, we invoke the presence of a molecular emission layer of constant abundance that is confined to a range of vertical column densities between \(10^{21} \times (1.59 \times 10^{20}) \text{cm}^{-2}\) and \(10^{22} \times (1.59 \times 10^{21}) \text{cm}^{-2}\). The column density of the molecular layer is then allowed to vary within radial annuli ranging from an arbitrarily small inner radius \(R_0\) that is much smaller than the beam size (in this case, \(R_0 = 10\) au), through an effective inner radius \(R_{in}\) (where the column density increases to detectable values; see below), out to an outer cutoff radius \(R_{out}\). The model grid interval is 10 au in the outer disk \((r > 50\) au) to roughly 5 au in the inner disk \((r < 50\) au). The radial column density dependence is characterized by a set of radial power-law slopes \(p_n\) at breakpoints \(R_{n-1}\): for our purposes we set \(n = 2\). For a selected set of free parameters of interest—in this case, \(R_{in}, R_{out}, p_1, p_2, R_1\), for given \(Z_1, Z_2\)—radiative transfer calculations are carried out via the RATRAN code to determine the resulting sky-projected integrated line intensity distribution. Model-integrated line intensity distributions are then realized over a wide range for each parameter, and fitting to the interferometric molecular emission-line data is performed in visibility space via a grid search approach.

We carried out this model-fitting procedure for the 262.004 GHz hyperfine transition complex of C\(_2\)H emission from the V4046 Sgr disk (we did not model the 262.064 GHz transition complex, but given its similar excitation conditions, we would expect similar results). The resulting best-fit radial column density profile and vertical and radial distributions of the C\(_2\)H emitting region are illustrated in Figure 9. The parameters of the best-fit model are \(Z_1 = 0.5, Z_2 = 1.5\)—i.e., the emitting layer is confined to vertical disk column densities of between \(~5 \times 10^{21} \text{cm}^{-2}\) and \(~5 \times 10^{22} \text{cm}^{-2}\)—with inner and outer radii \(R_{in} = 30\) au and \(R_{out} = 130\) au. The uncertainties in the former (vertical) layer parameters \((Z_1, Z_2)\) are of the order of 0.5 (i.e., a factor \(~\times 3\) uncertainty in vertical disk column density), and the uncertainties in the latter (radial) emission region boundaries are of the order of \(~5\) au. We find a model surface density power-law breakpoint of \(R_1 = 100\) au, with a radial power-law slope of \(p_1 = +0.6\) between 30 au and 100 au and a (much steeper) slope of \(p_2 = +1.8\) between 100 au and 130 au. In the model, the C\(_2\)H column density \((N_{C_2H})\) behaves essentially as a step function at \(R_{in} = 30\) au, increasing from \(~10^{13} \text{cm}^{-2}\) to \(~10^{14} \text{cm}^{-2}\) over the (unresolvable) span of just a few au. \(N_{C_2H}\) then slowly increases to \(~2 \times 10^{14} \text{cm}^{-2}\) at \(R_1 = 100\) au before sharply increasing over the outer \(~30\) au in radius, to \(N_{C_2H} \sim 3.3 \times 10^{14} \text{cm}^{-2}\) at the outer cutoff radius \(R_{out} = 130\) (Figure 9, left).

In Figure 10, we compare the ALMA C\(_2\)H moment 0 image and line profile for V4046 Sgr with the corresponding image and line profile obtained from the best-fit model. In the latter Figure, the ALMA and model image data have been reconstructed with a robust value of 2.0, resulting in \(~0.08\) resolution images. It is evident that the modeling procedure has yielded a reasonable match to the ALMA C\(_2\)H image, as intended. However, we caution that, as we have not employed a rigorous parameter space study, the robustness and uniqueness of this particular model fit, as well as the precise uncertainties in the various model parameters, are difficult to assess.

The ALMA C\(_2\)H modeling results illustrated in Figure 9 (left) supercede previous extrapolations of (much larger) \(N_{C_2H}\) in the V4046 Sgr disk, based on low S/N single-dish (APEX) spectroscopy (Kastner et al. 2014). Given the kinetic temperature regime in the emitting region \((T \sim 40\) K; Figure 9, right), the model \(N_{C_2H}\) values indicate that the C\(_2\)H emission is optically thin; this inference is consistent with the fact that the measured ratio of total line intensities in the 262.004 and 262.064 GHz hyperfine complexes, \(1.37 \pm 0.1\), is in good agreement with the theoretical ratio of 1.41 (Ziurys et al. 1982).

In terms of disk scale height, the best-fit model C\(_2\)H emitting layer corresponds to the region between \(z/r \sim 0.1\) and \(z/r \sim 0.3\) over the radial range \(~30\)–\(~130\) au (Figure 9, right). This (relatively deep) vertical emitting region position contrasts with the surface-layer position we inferred for the TW Hya disk, i.e., \(z/r \sim 0.5\) (corresponding to far smaller vertical disk column

*Figure 9. Left: radial profile of C\(_2\)H column density, for the best-fit model. Right: radial and vertical distribution of the C\(_2\)H emitting layer in the best-fit model (gray shaded region), overlaid on contours of gas temperature.*
densities, in the range \( \sim (5-8) \times 10^{18} \text{ cm}^{-2} \). However, as noted, we based our inference that the C\(_2\)H lies near the TW Hya disk surface on the apparently subthermal excitation of C\(_2\)H in that disk (Kastner et al. 2015). In contrast to TW Hya, our empirical modeling of the integrated intensity image and line profile of C\(_2\)H emission from V4046 Sgr provides more direct constraints on the scale height of its emitting C\(_2\)H. Our results for V4046 Sgr hence suggest that the C\(_2\)H emitting layer may lie deeper within the TW Hya disk than we inferred previously. However, we caution that the vertical density and temperature structures of the V4046 Sgr and TW Hya disks, and protoplanetary disks more generally, are subject to large uncertainties.

The vertical position of the emitting layer within V4046 Sgr is somewhat deeper in the disk than, but is not necessarily inconsistent with, the vertical C\(_2\)H layer position predicted by models in which production of C\(_2\)H is irradiation-driven; in particular, Walsh et al. (2010) found that the C\(_2\)H abundance should peak at \( z/r \approx 0.3 \). On the other hand, the low temperature (\( \sim 20 \text{ K} \)) and high densities (\( > 10^7 \text{ cm}^{-3} \)) of the disk layers corresponding to the region between \( z/r \approx 0.1 \) and \( z/r \approx 0.3 \) would imply that pure gas-phase production, perhaps enhanced by a large C/O ratio in the outer disk, is responsible for the large inferred C\(_2\)H column densities within the emission ring (see discussions in Kastner et al. 2015; Bergin et al. 2016). Indeed, whereas pure gas-phase, deep-disk-layer production mechanisms appear to be able to generate ringlike C\(_2\)H emission morphologies (Henning et al. 2010), surface-layer irradiation production mechanisms—such as photodesorption of hydrocarbon-coated grains or photodestruction of small grains—may require ad hoc assumptions such as inner disk shadowing (Kastner et al. 2015). Furthermore, under either (irradiation or pure gas-phase) production scenario, the “cusp” of high C\(_2\)H abundance at the outer edge of the C\(_2\)H ring that is required by our best-fit empirical model (in the form of an abrupt steepening of the power-law slope near \( R_{\text{out}} \); Figure 9, left) appears to be very difficult to explain. Observations of C\(_2\)H emission from other disks that are viewed at higher inclinations and are similarly nearby and well-resolved by ALMA (e.g., T Cha; Huélamo et al. 2015), in combination with additional theoretical efforts aimed at better understanding C\(_2\)H production, are essential if we are to pinpoint the processes that lead to large abundances of C\(_2\)H within evolved protoplanetary disks.

5. Summary

We have presented a library of ALMA molecular line and continuum images of the circumbinary disk orbiting V4046 Sgr, obtained during the course of three ALMA programs carried out in Cycles 2 and 3. All of these ALMA line surveys of V4046 Sgr have been undertaken in the 1.1–1.4 mm wavelength range (ALMA Bands 6 and 7) with ALMA antenna configurations involving maximum baselines of several hundred meters, yielding subarcsecond-resolution images in more than a dozen molecular species and isotopologues. Collectively, the resulting subarcsecond ALMA molecular line images of V4046 Sgr serve to elucidate, on linear size scales of \( \sim 30–40 \text{ au} \), the chemical structure of an evolved, circumbinary, protoplanetary disk.

The molecules CO and HCN and their isotopologues display centrally peaked velocity-integrated line intensity morphologies.

Figure 10. Top three panels: comparison of ALMA moment 0 image of C\(_2\)H 262.004 GHz emission from V4046 Sgr (top panel), with the moment 0 image obtained from the best-fit model (center panel); the residuals of the fit are shown in the bottom panel. Bottom panel: comparison of observed and model line profiles of C\(_2\)H 262.004 GHz emission, with the systemic velocity of V4046 Sgr (vertical dashed line) and the velocity offset corresponding to the hyperfine splitting of the C\(_2\)H transition indicated.
The radial profiles of the intensity ratios of CO isotopologue emission serve to constrain the opacities in the $2 \rightarrow 1$ transitions of $^{13}$CO and $^{12}$CO. We find that both lines are optically thick throughout the disk. Their near-constant ratio of $\sim 2.5$ across the disk then indicates that the $^{13}$CO emission arises from cooler, deeper disk layers than the $^{12}$CO emission, consistent with the predictions of irradiated disk models.

The integrated intensity of line emission from relatively complex nitriles (HC$_3$N, CH$_3$CN), deuterated molecules (DCN, DCO$^+$), hydrocarbons (as traced by C$_2$H), and potential CO ice line tracers (N$_2$H$^+$ and H$_2$CO) appears as a sequence of sharp and diffuse rings. The compact HC$_3$N and CH$_3$CN molecular emission regions appear as rings with dimensions similar to those of the central continuum emission and scattered-light rings within the V4046 Sgr disk. This correspondence suggests that the production of gas-phase HC$_3$N and CH$_3$CN may be over stellar high-energy, radiation-driven production of C$_2$H, nitriles, and other potentially robust tracers of disk irradiation. Either mechanism would be further enhanced by C enrichment (relative to O) in the outer disk.

There is clearly far more to be learned about the V4046 Sgr disk via ALMA observations. Higher-resolution observations of its millimeter-wave continuum and CO emission, complex nitrile emission, and HCN isotopologue emission have been carried out or are forthcoming (during Cycle 5). However, there have been no successful observations of CN to date, and none are presently scheduled, leaving open key questions as to the production of CN and its utility as a tracer of cosmic nitrogen isotope ratios (Hily-Blant et al. 2017). More generally, the molecular “anatomical” study of the V4046 Sgr disk presented here should serve to motivate additional subarcsecond ALMA molecular line imaging surveys of similarly evolved and nearby protoplanetary disks spanning a range of inclinations, as well as further detailed chemical modeling. Such efforts should address the many uncertainties in protoplanetary disk physical and chemical structure and molecular production pathways touched on by the present study, such as the abundance distributions and (hence) production and destruction mechanisms of C$_2$H, nitriles, and other potentially robust tracers of disk irradiation and gas-grain processes.

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