A Survey of CH$_3$CN and HC$_3$N in Protoplanetary Disks

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Abstract

The organic content of protoplanetary disks sets the initial compositions of planets and comets, thereby influencing subsequent chemistry that is possible in nascent planetary systems. We present observations of the complex nitrile-bearing species CH$_3$CN and HC$_3$N toward the disks around the T Tauri stars AS 209, IM Lup, LkCa 15, and V4046 Sgr as well as the Herbig Ae stars MWC 480 and HD 163296. HC$_3$N is detected toward all disks except IM Lup, and CH$_3$CN is detected toward V4046 Sgr, MWC 480, and HD 163296. Rotational temperatures derived for disks with multiple detected lines range from 29 to 73 K, indicating emission from the temperate molecular layer of the disk. V4046 Sgr and MWC 480 radial abundance profiles are constrained using a parametric model; the gas-phase CH$_3$CN and HC$_3$N abundances with respect to HCN are a few to tens of percent in the inner 100 au of the disk, signifying a rich nitrile chemistry at planet- and comet-forming disk radii. We find consistent relative abundances of CH$_3$CN, HC$_3$N, and HCN between our disk sample, protostellar envelopes, and solar system comets; this is suggestive of a robust nitrile chemistry with similar outcomes under a wide range of physical conditions.

Key words: astrochemistry – ISM: molecules – protoplanetary disks

Supporting material: figure set

1. Introduction

Planets form by accreting gas and dust within the protoplanetary disk; the material present in the disk therefore sets the initial composition of planets. Observations of solar system comets suggest that the solar nebula was rich in volatile organic molecules around the time the comets were formed, usually with abundances of a few percent with respect to water ice (e.g., Mumma & Charnley 2011). Understanding how this early inventory of organic molecules developed into the vast complexity of biochemistry is key to the study of the origins of life. Recent successes in prebiotic syntheses of RNA and protein precursors suggest that nitrile-bearing molecules, characterized by the C≡N functionality, played a crucial role in prebiotic chemistry (Powner et al. 2009; Ritson & Sutherland 2012; Sutherland 2016). From cometary studies, HCN, CH$_3$CN, and HC$_3$N indeed appear to have been common in the young solar system (Mumma & Charnley 2011; Cordiner et al. 2014; Le Roy et al. 2015). To evaluate whether the nitrile chemistry of the solar nebula is typical, and in turn any implications for the chemical habitability of other planetary systems, observations of planet-forming disks are essential.

The simple nitrile species CN and HCN were first detected toward protoplanetary disks two decades ago (Dutrey et al. 1997; Kastner et al. 1997) and have since been observed toward many additional disks (see Dutrey et al. 2014). Until the advent of ALMA, observational challenges limited our ability to detect and characterize more complex nitrile species in disks. The first disk detections of HC$_3$N were made by Chapillon et al. (2012) with the IRAM 30 m telescope toward GO Tau, LkCa 15, and MWC 480. CH$_3$CN was first detected in a disk by Öberg et al. (2015) toward MWC 480 using ALMA. The molecular emission was spatially resolved, allowing radial abundance profiles of CH$_3$CN and HC$_3$N to be derived. At comet-forming disk radii the abundances were found to be similar to those measured in solar system comets, suggesting that the solar system is not unique in its nitrile chemistry.

In addition to their relevance to prebiotic chemistry, CH$_3$CN and HC$_3$N are, along with CH$_3$OH (Walsh et al. 2016), the only large organic molecules detected in protoplanetary disks to date. Because of this, these molecules are key to furthering our understanding of the growth of organic complexity in disks. Their abundances and distributions can be used to benchmark astrochemical models of disks, and in turn to help predict the chemistry of complex molecules that cannot currently be directly observed. This is of particular importance for gaining insights into the ice compositions in disks, which can be constrained only through chemical models.

To date, the number of disks with well-characterized nitrile abundances is small, and it is unclear (i) whether other disks commonly host similar nitrile abundances as the solar nebula, and (ii) how robust the nitrile chemistry is across different circumstellar environments. A larger sample of observations is required to obtain constraints on the nitrile chemistry in disks.

Here, we present observations of the complex nitrile molecules HC$_3$N and CH$_3$CN toward a diverse sample of six protoplanetary disks: our targets span over an order of magnitude in luminosity and disk age and represent both transition disks and full disks. In Section 2, we describe the observations and data reduction. The observational results are presented in Section 3. In Section 4, a parametric model is used to obtain abundance profiles of CH$_3$CN and HC$_3$N toward the bright sources MWC 480 and V4046 Sgr. Finally, in Section 5, we comment on implications for the nitrile chemistry in other circumstellar systems based on our findings.

2. Methods

2.1. Observations

During ALMA Cycle 2, the HC$_3$N 27–26 transition as well as the CH$_3$CN 14–13 $K$ ladder were observed for the disks AS
Table 1
Disk and Star Properties of Observed Sources

| Source      | Distance (pc) | Spectral Type | Age (Myr) | $M_s$ (M$_\odot$) | $L_*$ ($L_\odot$) | $M_\ast$ (10$^{-9}$ M$_\odot$ yr$^{-1}$) | Disk Inc. (deg) | Disk PA (deg) | $M_{disk}$ (M$_\odot$) | V$_{LSR}$ (km s$^{-1}$) |
|-------------|---------------|---------------|-----------|------------------|------------------|------------------------------------------|----------------|--------------|------------------------|--------------------------|
| AS 209      | 143           | K5            | 1.6       | 0.9              | 1.5              | 51                                       | 38             | 86           | 0.015                  | 4.6                      |
| IM Lup      | 161           | M0            | 1         | 1.0              | 0.93             | 0.01                                    | 50             | 144.5        | 0.17                   | 4.4                      |
| LkCa 15     | 140           | K3            | 3–5       | 0.97             | 0.74             | 1.3                                      | 52             | 60           | 0.05–0.1               | 6.3                      |
| V4046 Sgr   | 72            | K5, K7        | 24        | 1.75             | 0.49, 0.33       | 0.5                                      | 33.5           | 76           | 0.028                  | 2.9                      |
| MWC 480     | 142           | A4            | 7         | 1.65             | 11.5             | 126                                      | 37             | 148          | 0.11                   | 5.1                      |
| HD 163296   | 122           | A1            | 4         | 2.25             | 30               | 69                                       | 48.5           | 132          | 0.17                   | 5.8                      |

Note. Table adapted from Huang et al. (2017), where a full list of references can be found.

209, HD 163296, IM Lup, LkCa 15, MWC 480, and V4046 Sgr (project code 2013.1.00226). Disk and stellar properties for each source are listed in Table 1. The MWC 480 data were previously presented in Öberg et al. (2015); these lines were reanalyzed in this work to ensure that all sources were treated consistently. During Cycles 3 and 4, as part of a line survey in disks (project code 2013.1.01070.S), the HC$_3$N 31–30 and 32–31 transitions and the CH$_3$CN 15–14 and 16–15 K-ladders were observed toward MWC 480 and LkCa 15.

A detailed description of the Cycle 2 observations can be found in Huang et al. (2017). Briefly, from 2014 to 2015 Band 6 observations were taken at two spectral settings, 1.1 mm and 1.4 mm, containing 14 and 13 narrow spectral windows, respectively. Baselines spanned 18–650 m, and the total on-source time was ~20 minutes per source. Amplitude and phase calibration, as well as frequency bandpass calibration, were performed using observations of a quasar. Flux calibration was performed using observations of either Titan or a quasar. A portion of the CH$_3$CN 14–13 ladder (14$_{0}$–13$_{0}$, 14$_{1}$–13$_{1}$, and 14$_{2}$–13$_{2}$) is contained in a spectral window of 59 MHz with a channel width of 61 kHz (0.071 km s$^{-1}$) in the 1.1 mm spectral setting. The HC$_3$N 27–26 transition is contained in a spectral window of 117 MHz, also with a channel width of 61 kHz (0.075 km s$^{-1}$) in the 1.1 mm spectral setting.

The Cycle 3/4 observations are described in full in R. Loomis (2018, in preparation). This work made use of data taken in two Band 7 correlator setups at 0.9 and 1.1 mm, each containing four spectral windows of 1920 channels with channel widths of 975 kHz (~0.99–1.06 km s$^{-1}$ for the lines of interest). Baselines spanned 15–650 m, and the total on-source integration time was ~20 minutes per source. Phase calibration, bandpass calibration, and flux calibration were all performed using quasar observations.

2.2. Data Reduction

Initial data calibration was performed by ALMA/NAASC staff. Two rounds of phase self-calibration were performed using the continuum emission from individual spectral windows, except for HD 163296, which was self-calibrated using averaged spectral windows due to weak continuum emission. Following continuum subtraction, the data cubes were imaged in CASA using the CLEAN task with a $\sigma$ noise threshold. Briggs weighting was used with a robust parameter of 2.0 for all lines except those in the source V4046 Sgr; here, a value of 1.0 was adopted to improve the angular resolution, which was possible due to higher signal-to-noise ratios. To obtain channel maps, the data were regridded to 0.5 km s$^{-1}$ and 1.1 km s$^{-1}$ spectral resolution for the Cycle 2 and Cycle 3/4 observations, respectively. CLEAN masks were drawn by hand for lines with obvious emission (V4046 Sgr HC$_3$N 27–26 and CH$_3$CN 14$_{0}$–13$_{0}$ and 14$_{1}$–13$_{1}$). For all other lines, the 5$\sigma$ continuum contour was used as the CLEAN mask.

A Keplerian mask was applied to the cleaned data cube to obtain moment zero maps, line spectra, and integrated flux densities for each transition. The use of Keplerian masks as CLEAN templates and for spectral extraction is well established (e.g., Rosenfeld et al. 2013a; Loomis et al. 2015; Öberg et al. 2015); details on the use of Keplerian masking for moment zero map generation will be presented in J. Pegues (2018, in preparation). Briefly, to construct appropriate masks, the Keplerian velocity of each image pixel was calculated based on its deprojected radius from the star, assuming disk and stellar parameters taken from the literature (Table 1). In each velocity channel, only pixels corresponding to the appropriate Keplerian velocity were included, and all other pixels were masked. The mask outer radii were chosen to encompass all HC$_3$N and CH$_3$CN emission. The masks were verified to fit the actual disk profile using H$^{13}$CN emission (Guzmán et al. 2017), which has a more obvious Keplerian structure than HC$_3$N or CH$_3$CN. An example channel map with its Keplerian mask overlaid is shown in Figure 1 for the HC$_3$N 27–26 transition in V4046 Sgr; for all other lines and sources, similar figures can be found in the online Journal.

Since the moment zero maps are produced by summing only emission within the Keplerian mask, each moment zero pixel represents the sum of a different number of channels. The rms is therefore nonuniform across the moment zero map. We approximate the moment zero rms by bootstrapping: the same Keplerian mask used to obtain the moment zero map is applied to 1000 off-source positions. The rms per pixel is determined from the standard deviation of each mask pixel across all off-source moment zero maps. The median rms value is taken to be the representative moment zero rms, and is quoted in Table 2 and used to draw contours in Figures 2 and 4. The uncertainty in the integrated flux density was estimated from the standard deviation of the integrated fluxes within 1000 off-source Keplerian masks.

In V4046 Sgr, the CH$_3$CN 14$_{1}$–13$_{1}$ line is blended with the 14$_{1}$–13$_{1}$ line (spectrum shown in Figure 2). Likewise, in MWC 480 the CH$_3$CN 15$_{0}$–14$_{0}$ and 15$_{1}$–14$_{1}$ lines are blended. To treat blended lines, two Keplerian masks (one centered on each line) were calculated and used to extract the emission from both lines, and the resulting moment zero map sums the total emission. To estimate the integrated flux density from each individual transition, we assume that emission is symmetric around the rest velocity of the source. The integrated flux for
transitions. Based on these criteria, HC3N is detected toward the same status of detection versus nondetection for all criterion of an SNR detected or not detected in a disk. A molecule is considered therefore use these lines to classify whether molecules are of six disks.

The CH3CN 140 procedure, an additional error of 30% the integrated the total blended feature minus the integrated higher-energy transition was taken to be the integrated lower-energy transition was therefore assumed to be twice the integrated flux of the lowest-velocity horn (i.e., velocities lower than the source velocity). The integrated flux of the higher-energy transition was taken to be the integrated flux of the total blended feature minus the integrated flux of the low-energy transition. To account for the added uncertainties in this procedure, an additional error of 30% the integrated flux was added in quadrature with the bootstrapped integrated flux uncertainty for blended lines.

3. Observational Results

Based on our observations, we now present the molecular line detections and nondetections in our sample. For molecules with multiple detections toward a source, we use the rotational diagram method to derive rotational temperatures and column densities. Finally, we calculate disk-averaged abundance ratios of CH3CN/HCN and HC3N/HCN for all disks by assuming a range of emission temperatures.

3.1. Molecule Detections

A summary of the line observations is presented in Table 2. The CH3CN 140–130 and HC3N 27–26 transitions were targeted toward all six disks and, compared to the other observed CH3CN and HC3N transitions, are the brightest across the sample. We therefore use these lines to classify whether molecules are detected or not detected in a disk. A molecule is considered detected if emission >3 × rms is present within the Keplerian mask in at least three channels. We also tested a detection criterion of an SNR >3 for the integrated flux density and find the same status of detection versus nondetection for all transitions. Based on these criteria, HC3N is detected toward all disks except IM Lup. CH3CN is firmly detected toward three of six disks (HD 163296, MWC 480, and V4046 Sgr). In AS 209 and LkCa 15, CH3CN is not seen at significant levels in individual channel maps but shows suggestive features at around a 3σ level in the moment zero maps, as well as positive integrated intensities in the radial profiles. Higher-sensitivity follow-up observations are required to confirm if these are indeed detections. For subsequent analysis, these lines are treated as nondetections (3σ upper limits).

Figure 1 shows the disk continuum maps as well as the CH3CN 140–130 and HC3N 27–26 line maps and spectra for each disk. In all cases, the molecular emission is more compact than the continuum emission. Comparing the nitrile emission across the sample, V4046 Sgr is by far the strongest emitter, with strong detections of both CH3CN and HC3N. Next strongest are HD 163296 and MWC 480, which both host strong HC3N and moderate CH3CN emission. AS 209 and LkCa 15 both exhibit moderate HC3N and tentative CH3CN emission, and neither molecule is detected in IM Lup.

Figure 2 shows the deprojected radial profiles for each transition. The uncertainties are estimated by dividing the median moment zero rms by the square root of the number of independent measurements (i.e., the number of pixels at each radius divided by the beam size in pixels, to account for beam convolution). For both CH3CN and HC3N, almost all detections exhibit centrally peaked emission. The exception is CH3CN and HC3N in AS 209, which peak at larger radii, indicative of a ringed structure; this can also be seen in the moment zero map (Figure 2). Although it does not have a large central dust cavity, AS 209 also exhibits a ring-like structure in the molecules H13CN, HC15N, DCN, H13CO+, and DCO+ (Guzmán et al. 2017; Huang et al. 2017), possibly due to dust opacity effects. Additionally, we note that when imaged with a smaller robust factor, HC3N and possibly CH3CN in V4046 Sgr show evidence of a central depression. Higher-resolution observations are required to confirm the morphology of these molecules at small scales.

In V4046 Sgr, MWC 480, and LkCa 15, multiple transitions from the same molecule were observed. Figure 4 shows the moment zero maps for these additional transitions. The CH3CN 141–131 and 142–132 lines were covered within the same spectral window as the 140–130 transition, and in V4046 Sgr these higher-K lines were strong enough to be detected. Additionally, for MWC 480 and LkCa 15 the CH3CN 150–140 and 160–150, and HC3N 31–30 and 32–31 lines were observed in a separate program (R. Loomis, 2018 in preparation). In MWC 480, CH3CN 150–140, and HC3N 31–30 and 32–31 were detected. These additional lines were not detected in LkCa 15.
Table 2

| Transition      | Frequency (GHz) | Source  | Beam (") | Beam PA (") | Channel rms$^c$ (mJy beam$^{-1}$) | Mom. Zero rms$^b$ (mJy beam$^{-1}$ km s$^{-1}$) | Int. Flux Density$^d$ (mJy km s$^{-1}$) |
|-----------------|-----------------|---------|-----------|-------------|----------------------------------|---------------------------------------------|----------------------------------------|
| CH$_3$CN 14$_n$-13$_0$ | 257.5274        | AS 209  | 0.51 × 0.45 | −66.2       | 3.1                              | 4.3                                         | <39                                     |
|                 |                 | IM Lup  | 0.47 × 0.43 | 83.4        | 3.0                              | 4.1                                         | <33                                     |
|                 |                 | LkCa 15 | 0.67 × 0.51 | −15.5       | 2.8                              | 4.7                                         | <28                                     |
|                 |                 | V4046 Sgr | 0.59 × 0.48 | 84.9        | 2.9                              | 7.9                                         | 299 ± 94$^d$                           |
|                 |                 | MWC 480 | 0.76 × 0.49 | −8.6        | 2.8                              | 4.8                                         | 42 ± 11                                 |
|                 |                 | HD 163296 | 0.60 × 0.46 | −87.1       | 2.3                              | 4.2                                         | 53 ± 11                                 |
| CH$_3$CN 14$_{-1}$-13$_{-1}$ | 257.5224        | V4046 Sgr | 0.59 × 0.48 | 84.9        | 2.9                              | 7.9                                         | 259 ± 82$^d$                           |
| CH$_3$CN 15$_{-1}$-14$_{-1}$ | 257.5076        | V4046 Sgr | 0.59 × 0.48 | 84.9        | 3.0                              | 4.7                                         | 113 ± 17                               |
| CH$_3$CN 15$_{-1}$-14$_{-0}$ | 275.9156        | LkCa 15 | 1.17 × 1.04 | −43.6       | 2.8                              | 8.7                                         | <30                                     |
|                 |                 | MWC 480 | 1.30 × 1.07 | −7.3        | 2.7                              | 10.0                                        | 44 ± 23$^d$                            |
| CH$_3$CN 15$_{-1}$-15$_{-0}$ | 275.9103        | MWC 480 | 1.30 × 1.07 | −7.3        | 2.7                              | 10.0                                        | 42 ± 19$^d$                            |
| CH$_3$CN 16$_{-1}$-15$_{-0}$ | 294.3024        | LkCa 15 | 1.35 × 0.85 | −56.5       | 5.3                              | 16.0                                        | <54                                     |
|                 |                 | MWC 480 | 1.41 × 0.86 | −45.6       | 4.8                              | 16.0                                        | <67                                     |
| HC$_3$N 27-26   | 245.6063        | AS 209  | 0.54 × 0.46 | −64.0       | 3.4                              | 5.4                                         | 103 ± 15                               |
|                 |                 | IM Lup  | 0.51 × 0.45 | 69.5        | 3.1                              | 4.2                                         | <29                                     |
|                 |                 | LkCa 15 | 0.71 × 0.53 | −14.5       | 2.9                              | 4.8                                         | 44 ± 9                                  |
|                 |                 | V4046 Sgr | 0.60 × 0.50 | 86.7        | 3.4                              | 6.0                                         | 352 ± 20                                |
|                 |                 | MWC 480 | 0.81 × 0.51 | −8.5        | 3.1                              | 5.3                                         | 136 ± 11                                |
|                 |                 | HD 163296 | 0.62 × 0.48 | −86.1       | 2.7                              | 4.6                                         | 201 ± 13                                |
| HC$_3$N 31-30   | 281.9768        | LkCa 15 | 1.40 × 0.86 | −56.4       | 4.6                              | 12.9                                        | <44                                     |
|                 |                 | MWC 480 | 1.45 × 0.90 | −44.7       | 4.1                              | 11.4                                        | 92 ± 15                                 |
| HC$_3$N 32-31   | 291.0684        | LkCa 15 | 1.40 × 0.86 | −56.4       | 5.0                              | 15.2                                        | <48                                     |
|                 |                 | MWC 480 | 1.38 × 0.90 | −43.7       | 5.0                              | 14.2                                        | 59 ± 20                                 |

Notes.

$^a$ For 0.5 km s$^{-1}$ channel widths.

$^b$ Median rms; see Section 2.2.

$^c$ 3σ upper limits are reported for nondetections.

$^d$ Uncertainty includes an additional 30% of the integrated flux due to line blending.

3.2. Population Diagrams

For molecules with multiple detections, rotational diagrams can be used to determine the disk-averaged column densities and rotational temperatures of emission (Figure 5). In most cases, only detected lines were used in fitting rotational diagrams; the exception is for HC$_3$N in LkCa 15, as only a single line is detected. In this case, the 3σ upper limits on the nondetected transitions were used to obtain an upper limit for the rotational temperature.

Assuming LTE and optically thin emission, the disk-integrated flux density $S_{\nu}$ for each transition is taken to be the minimum angular extent of emission. $S_{\nu}$ is then used to determine the disk-averaged column densities and rotational temperatures.

$$N_a = \frac{4\pi S_{\nu} \Delta V}{A_{\text{rot}} \Omega h c}$$

where $S_{\nu}$ is the flux density, $\Delta V$ is the line width, $A_{\text{rot}}$ is the Einstein coefficient, and $\Omega$ is the solid angle of the source. For a disk-averaged column density, $\Omega$ is the same for each transition of a molecule. To estimate $\Omega$ for each molecule, we use the deprojected radial profile of the brightest line (Figure 3) to identify the maximum angular extent of emission. $\Omega$ is taken to be the solid angle subtended by a circle with this radius. In turn, the total column density $N_T$ and rotational temperature $T_{\text{rot}}$ can be determined from the upper level populations given by the Boltzmann distribution:

$$N_u = \frac{N_T}{Q(T_{\text{rot}})} e^{-E_u/T_{\text{rot}}}$$

Here, $g_u$ is the upper state degeneracy, $Q$ is the molecular partition function, and $E_u$ is the energy of the upper state (K). To calculate the partition functions for CH$_3$CN and HC$_3$N, we use the symmetric top and linear polyatomic approximations respectively (Gordy & Cook 1984; Magun & Shirley 2015):

$$Q(T, \text{CH}_3\text{CN}) = 1.78 \times 10^6 \left(\frac{T}{A B^2}\right)^{1/2}$$

$$Q(T, \text{HC}_3\text{N}) = \frac{kT}{h B_0} e^{h B_0/3kT},$$

where $A, B$, and $B_0$ are the rotational constants for CH$_3$CN and HC$_3$N.

The best-fit CH$_3$CN and HC$_3$N column densities and rotational temperatures are listed in Table 3. The rotational temperature of CH$_3$CN in V4046 Sgr is 29 ± 2 K and in MWC 480 is 73 ± 23 K. By comparison, the rotational temperature of CH$_3$CN was recently measured in the disk around the solar analog TW Hya to be 29 K; follow-up chemical modeling predicted abundant gas-phase CH$_3$CN between temperatures of 25–50 K, corresponding to the warm molecular layer of the disk (Loomis et al. 2018b). The measured rotational temperature in V4046 Sgr is consistent with these TW Hya results, while CH$_3$CN in MWC 480 is warmer. MWC 480 is a Herbig Ae star and hosts a stronger radiation field than the Taurus stars TW Hya and V4046 Sgr, which may explain the warmer emission. However, we emphasize that given the line blending of CH$_3$CN (see Section 2.2) the rotational temperature is rather poorly constrained.

Moreover, at densities below $\sim 10^7$ cm$^{-3}$, the CH$_3$CN and HC$_3$N transitions targeted in this survey will...
Figure 2. First column: dust continuum maps (1.1 mm), with contour lines corresponding to 5, 10, 30, 100, 200, 400, and 800 σ emission. Second and third columns: CH$_3$CN 140–130 and HC$_3$N 27–26 moment zero maps, integrated within the Keplerian masks shown in Figure 1 in the online journal. Emission below the minimum rms value is not shown. Contours correspond to 3, 6, and 10 × the median moment zero rms (Section 2.2). For all moment zero maps, the synthesized beam is shown in the lower left corner, and the continuum centroid is marked with a +. Fourth column: disk-integrated spectra extracted with Keplerian masks for CH$_3$CN 140–130 (blue lines) and HC$_3$N 27–26 (orange lines). For V4046 Sgr, the CH$_3$CN line is blended with the 141–131 transition.
be subthermally excited. Modeling in Loomis et al. (2018b) suggests that CH$_3$CN emission can arise from regions with densities down to $10^6$ cm$^{-3}$; therefore, the rotational temperatures listed in Table 3 may underestimate the kinetic temperature of the emission region.

We note that in V4046 Sgr, the derived CH$_3$CN rotational temperature also corresponds to the kinetic gas temperature: for symmetric top molecules, the populations of different $K$ levels with the same $J$ value are a direct result of collisions (e.g., Loren & Mundy 1984). This is not the case for MWC 480 since the multiple lines detected consist of different $J$ levels within the same $K$ ladder.

HC$_3$N in MWC 480 has a measured rotational temperature of 49 $\pm$ 6 K, consistent within the uncertainties with the warm CH$_3$CN temperature found in the same source. Additional observations are needed to determine whether there is a real difference in the emission temperature (and therefore emission location) of CH$_3$CN and HC$_3$N within a disk. In LkCa 15, only one HC$_3$N line was firmly detected, resulting in a rotational temperature upper limit of 103 K.

### 3.3. Disk-averaged Abundance Ratios

Disk-averaged abundance ratios of HC$_3$N and CH$_3$CN with respect to HCN are calculated using the integrated fluxes listed in Table 2 and adopted rotational temperatures. H$^{13}$CN integrated fluxes are taken from Guzmán et al. (2017); we assume a standard $^{12}$C/$^{13}$C ratio of 70 (with an uncertainty of 15%) to convert to HCN column densities. HC$_3$N/HCN and CH$_3$CN/HCN abundance ratios are calculated for rotational temperatures of 30, 50, and 70 K corresponding to the range of observed rotational temperatures. In this treatment, we assume that HC$_3$N and CH$_3$CN are cospatial with HCN. If all molecules are emitting from the molecular layer between the midplane and the disk atmosphere, this is a reasonable approximation vertically; however, differences in the radial extent of emission for each molecule may introduce some error into the abundance ratios. IM Lup is excluded from this analysis since only upper limits are available for all species.

The derived abundance ratios are listed in Table 4. For all rotational temperatures, HC$_3$N is more abundant than CH$_3$CN. The CH$_3$CN abundance is on the order of a few percent with respect to HCN for all choices of rotational temperature. For a given rotational temperature, the CH$_3$CN/HCN ratios are consistent within the uncertainties with a single value across the entire disk sample. The derived HC$_3$N/HCN abundance ratios are a few percent for a 70 K rotational temperature but significantly higher ($\sim$50% for AS 209, LkCa 15, and V4046 Sgr, and over 100% for MWC 480 and HD 163296) for a 30 K rotational temperature. In MWC 480, the only source with a well-constrained HC$_3$N rotational diagram, the derived temperature is close to 50 K; therefore, for at least the Herbig Ae stars, the 50 K abundances ($\sim$20%) are likely the most reliable.

### 4. Abundance Profile Modeling

The strong emission of both CH$_3$CN and HC$_3$N in MWC 480 and V046 Sgr enables a more detailed modeling of the radial abundance profiles within each disk.

#### 4.1. V4046 Sgr Model

The physical model for V4046 Sgr is adapted from the parametric model of the V4046 Sgr disk described in Rosenfeld et al. (2013b) and is further developed in Guzmán et al. (2017). For fitting CH$_3$CN and HC$_3$N emission, we use the same physical disk model as that described in Guzmán et al. (2017).
Molecular abundance profiles are assumed to follow a power law, following, e.g., Qi et al. (2008, 2013):

\[ X(r) = X_{100} \left( \frac{r}{R_{100}} \right)^\alpha, \]  

where \( X \) is the abundance with respect to the total hydrogen density, \( X_{100} \) is the abundance at the characteristic radius of \( R_{100} = 100 \text{ au} \), and \( \alpha \) is the power-law index. An outer radius cutoff \( R_{\text{out}} \) of 100 au was adopted based on the extent of emission in the deprojected radial profile (Figure 3). In the disk atmosphere, photodissociation is assumed to destroy most molecules, and the molecular abundances are attenuated by a factor of \( 10^8 \) above \( z/r = 0.5 \). To account for depletion in the disk midplane, molecule abundances are attenuated by a factor of \( 10^3 \) at temperatures below 25 K. This temperature does not correspond to a purely thermal freeze-out boundary for nitriles, but was chosen empirically based on the boundary where gas-phase CH$_3$CN disappears in the chemical model presented in Loomis et al. (2018b), and is also consistent with the \( \sim 30 \text{ K} \) rotational temperature found for CH$_3$CN in this disk. This depletion boundary is similar to the expected CO freeze-out temperature, and likely arises due to either a coincidence with the photodesorption boundary of the nitrile molecules, or an increase in gas-phase nitrile chemistry driven by CO sublimation.

CH$_3$CN and HC$_3$N were fit independently for the free parameters \( X_{100} \) and \( \alpha \). While we use the same physical disk model as in Guzmán et al. (2017), the boundary conditions for the molecular abundance profiles are slightly different here; since we ultimately wish to normalize CH$_3$CN and HC$_3$N with respect to H$^{13}$CN, we also refit the H$^{15}$CN observations to ensure consistency.

**Table 3**

| Source   | Molecule | \( N_T \left(10^{12} \text{ cm}^{-2}\right) \) | \( T_{\text{rot}} \) (K) |
|----------|----------|---------------------------------|-----------------|
| MWC 480  | CH$_3$CN | \(1.8 \pm 0.4\)                  | \(73 \pm 23\)   |
| V4046 Sgr| CH$_3$CN | \(6.2 \pm 1.8\)                  | \(29 \pm 2\)    |
| MWC 480  | HC$_3$N  | \(5.8 \pm 2.8\)                  | \(49 \pm 6\)    |
| LkCa 15  | HC$_3$N  | \(>0.8\)                         | \(<103\)        |

**Figure 4.** Moment zero maps for molecules with multiple observed transitions, integrated within the Keplerian masks shown in Figure 1 in the online journal. Emission below the minimum rms value is not shown. Contours correspond to 3, 6, and 10\times\text{rms} levels. For all moment zero maps, the synthesized beam is shown in the lower left corner, and the continuum centroid is marked with a +.

**Figure 5.** Rotational diagrams for multiple line detections. Full circles show detections and open circles show 3\sigma upper limits for nondetected lines. For LkCa 15, the rotational diagram is fit using upper limit constraints since only one line is detected.
The fitting was performed by generating synthetic observations of the brightest line emission, holding the gas density and temperature profiles constant and adopting the disk inclination, position angle, stellar mass, and systemic velocity listed in Table 1. The synthetic images had a spectral resolution of 0.5 km s\(^{-1}\) and spanned -2.0 to 14.5 km s\(^{-1}\) for CH\(_3\)CN (including both the 140\,-\,130 and 141\,-\,131 transitions) and -3.0 to 9.0 km s\(^{-1}\) for HC3N. The radiative transfer code RADMC-3D (Dullemond 2012) was used to calculate level populations for each synthetic image assuming LTE conditions. The vis sample Python package\(^4\) (Loomis et al. 2018a) was then used to sample the synthetic image at the \(u\,\nu\) points of the observations. The likelihood function was calculated from the weighted difference between observations and the model in the \(u\,\nu\) plane. The affine-invariant MCMC package emcee (Foreman-Mackey et al. 2013) was used to sample posterior distributions of both parameters \(X_{100}\) and \(\alpha\). A flat prior was used for each parameter when generating new samples: \(10^{-20} < X_{100} < 10^{-8}\) and \(-3 < \alpha < 2\). The resulting best-fit values are listed in Table 5. Figure 6 shows channel maps of the observations along with the best-fit model and residuals for CH\(_3\)CN and HC3N (H\(^{13}\)CN and CH\(_3\)CN 141\,-\,132 can be found in the Appendix); the observations are well reproduced by the model.

To ensure that the choice of depletion boundary does not significantly impact our results, the models were also run with an adopted depletion boundary of 19 and 30 K. For CH\(_3\)CN the best-fit \(X_{100}\) at 19 and 30 K are within 25% of the 25 K value, and the best-fit \(\alpha\) are within 15%. For HC3N there was less than 3% change for both \(X_{100}\) and \(\alpha\). The results are therefore not highly sensitive to the choice of depletion boundary. To further confirm the derived abundances, we use the best-fit \(X_{100}\) and \(\alpha\) values from the CH\(_3\)CN 140\,-\,130 line to create a synthetic image of the 142\,-\,132 transition. The higher-frequency transition is well reproduced by the lower-frequency best-fit values (shown in the Appendix), indicating that the adopted model is appropriate.

Since V4046 Sgr is a transition disk with a large inner gap, we also test whether a model with a large cavity produces a better fit to the observations. The fiducial model uses a cavity radius of 3 au based on the CO line emission and SED of V4046 Sgr (Rosenfeld et al. 2013b). An adopted 29 au radius, corresponding to the millimeter dust radius hole, produces a worse fit to the data for both molecules.

### Table 4

| Source   | CH\(_3\)CN/HCN (%) | HC\(_3\)N/HCN (%) |
|----------|---------------------|-------------------|
|          | 30 K                | 50 K                  | 70 K                  | 30 K        | 50 K                  | 70 K                  |
| AS 209   | <4.7                | <2.5                | <2.0                 | 69.7 ± 17.7 | 10.8 ± 2.8 | 4.9 ± 1.2 |
| LkCa 15  | <4.3                | <2.3                | <1.8                 | 43.4 ± 13.2 | 6.7 ± 2.0 | 3.0 ± 0.9 |
| V4046 Sgr| 5.1 ± 1.8           | 2.7 ± 0.9           | 2.2 ± 0.8            | 37.9 ± 6.2  | 5.9 ± 1.0  | 2.7 ± 0.4 |
| HD 163296| 5.6 ± 1.6           | 2.9 ± 0.9           | 2.4 ± 0.7            | 134.1 ± 28.0| 20.9 ± 4.4| 9.4 ± 2.0 |
| MWC 480  | 5.9 ± 1.9           | 3.1 ± 1.0           | 2.5 ± 0.8            | 121.9 ± 24.0| 19.0 ± 3.7| 8.5 ± 1.7 |

Note. For disks with measured rotational temperatures, the closest corresponding abundance is marked in bold.

### Table 5

| Source   | V4046 Sgr | MWC 480 |
|----------|-----------|---------|
|          | \(X_{100}\) | \(\alpha\) |
|          |           |         |
| CH\(_3\)CN | 8.1 ± 0.4 \times 10^{-12} | 0.6 ± 0.1 |
| HC\(_3\)N  | 2.8 ± 0.2 \times 10^{-11} | 1.3 ± 0.1 |
| H\(^{13}\)CN| 1.2 ± 0.1 \times 10^{-12} | -0.5 ± 0.1 |
|          |           |         |
|          | 7.97 ± 1.6 \times 10^{-13} | -0.1 ± 0.3 |
|          | 1.2 ± 0.1 \times 10^{-11} | 0.8 ± 0.1 |
|          | 1.2 ± 0.2 \times 10^{-13} | -1.1 ± 0.1 |

\(^4\) https://pypi.python.org/pypi/vis_sample

4.2. MWC 480 Model

In Öberg et al. (2015), the CH\(_3\)CN 140\,-\,130 and HC\(_3\)N 27\,-\,26 profiles in MWC 480 were fit by obtaining the minimum \(\chi^2\) value from a grid of calculated abundance models. Here, we adopt the same parametric physical model for the disk density and temperature described in that paper but use the MCMC fitting procedure described in the previous section to constrain \(X_{100}\) and \(\alpha\). This allows us to better explore the parameter space and therefore to obtain more robust constraints on the fit parameters and their uncertainties. Also in contrast to Öberg et al. (2015), we use RADMC-3D instead of the non-LTE LIME code for radiative transfer calculations to ensure consistency with the V4046 Sgr results.

To retrieve molecular abundances, we use the same power-law prescription (Equation (5)) as in Section 4.1. Again the abundances are attenuated above a \(z/r\) of 0.5 to account for photodestruction. We adopt a depletion boundary of \(z/r < 0.05\), which roughly corresponds to the cutoff in the V4046 Sgr model. As in the V4046 Sgr model, this does not correspond to the nitrile freeze-out boundary but likely corresponds to where photodesorption of nitriles and/or CO-driven gas-phase chemistry become efficient. A higher cutoff of \(z/r < 0.2\) was also tested, corresponding to the lower boundary of CH\(_3\)CN emission in the model of Loomis et al. (2018b). An outer radius \(R_{\text{out}}\) of 180 au was chosen, corresponding to the extent of emission in the MWC 480 radial profiles (Figure 3). The MCMC fitting procedure is otherwise the same as described above. CH\(_3\)CN, HC\(_3\)N, and H\(^{13}\)CN were each fit with spectral resolutions of 0.5 km s\(^{-1}\) and velocity ranges of 1–9.5 km s\(^{-1}\), 0–14.5 km s\(^{-1}\), and 0–14.5 km s\(^{-1}\), respectively. The resulting model channel maps and residuals are shown in the Appendix. The best-fit values of \(X_{100}\) and \(\alpha\) are listed in Table 5. For both V4046 Sgr and MWC 480, CH\(_3\)CN and HC\(_3\)N appear to have increasing or flat abundance profiles, while H\(^{13}\)CN shows a decreasing abundance profile.
Such as for V4046 Sgr, we can use the constraints from additional lines to confirm the validity of the best-fit model. For both depletion boundaries of $z/r < 0.05$ and $z/r < 0.2$, we created synthetic images of the upper-level CH$_3$CN and HC$_3$N lines based on the best-fit $X_{100}$ and $\alpha$ values from the lower-level lines. Rotational diagram calculations were performed for CH$_3$CN and HC$_3$N using the modeled fluxes. We obtain very similar rotational temperatures for $z/r < 0.05$ and $z/r < 0.2$ models: 20 and 23 K for CH$_3$CN, and 44 and 45 K for HC$_3$N, respectively. The HC$_3$N model temperatures are very close to the observed values, while the CH$_3$CN temperatures are low. Because the modeled CH$_3$CN rotational temperature is not substantially improved by increasing the $z/r$ cutoff, a more complex parametric model is likely required to fully describe the disk physical and/or abundance structure. For instance, modeling of H$_2$CO emission in TW Hya required both a hot inner component and a cool extended component to match observations ("Oberg et al. 2017); the possible presence of a warm inner component in MWC 480 would not be captured by the single power-law profile used in our models, resulting in a potential underprediction of the observed rotational temperature. We emphasize, however, that the observed rotational temperature of CH$_3$CN in MWC 480 is not well constrained due to a small lever arm in upper energy levels as well as line blending uncertainties, and may in reality be closer to the modeled rotational temperature. Of the two depletion boundaries, the $z/r < 0.05$ cutoff produced better fits to the higher-$J$ lines as determined by the reduced $\chi^2$, and therefore all future discussion pertains to the $z/r < 0.05$ model results. Channel maps for these models are shown in the Appendix.

4.3. CH$_3$CN and HC$_3$N Column Densities and Abundances

The best-fit CH$_3$CN and HC$_3$N abundance profiles derived for V4046 Sgr and MWC 480 are shown in Figure 7, along with the derived radial column density profiles. For comparison, we also show the column densities of HC$_3$N and CH$_3$CN predicted by a disk chemistry model for a generic T Tauri star and disk (Walsh et al. 2014). CH$_3$CN column densities from the disk chemistry model are within an order of magnitude to those derived in this work for V4046 Sgr and MWC 480, while HC$_3$N column densities are underestimated by over an order of magnitude in the model. However, neither V4046 Sgr nor MWC 480 is well-described by the disk physical structure adopted by Walsh et al. (2014), and further tuning of models is required to make conclusive comparisons. Comparing the relative shapes of the radial column density profiles, the extremely centrally peaked profile in the model is not reproduced in the profiles derived in this work. However, we note that due to the high upper-state energies of the lines fitted (92 K for CH$_3$CN and 165 K for HC$_3$N), our observations are not sensitive to cool material and therefore may not reflect the true spatial distributions of the molecules.

To illustrate this, we use the modeled best-fit abundance profiles to determine the fraction of emitting molecules (i.e., molecules in the upper energy state of the observed transition) in temperature bins from 10 to 200 K, following Bergin et al. (2013). The number density of a species in the upper energy state $n_u$ is related to the total number density $n_T$ by the Boltzmann distribution (Equation (2)). $n_u$ is integrated over the disk to find the number of upper-state molecules in target temperature bins. The fraction of upper-state molecules in each temperature bin relative to the total number of upper-state molecules, $f_u(T)$, is shown in Figure 8 as a cumulative distribution function.

For both CH$_3$CN and HC$_3$N in V4046 Sgr and MWC 480, roughly half of the emitting molecules are in gas warmer than 50 K, with virtually no contribution from 30 K gas. This indicates that our observations are mostly probing warm
emission. Since most gas in disks exists at <50 K temperatures, there may be a substantial amount of material that our observations are not sensitive to. As further discussed in Section 5, follow-up observations of lower-J transitions of HC3N and CH3CN will be helpful in addressing this issue.

Because the retrieved abundance profiles may depend on the physical disk structure assumed in the model, we also present the CH3CN and HC3N abundance profiles normalized with respect to HCN. This should be less sensitive to the details of the physical model structure assuming that all three molecules are emitting cospatially; this is already implicit in our model since we used the same freeze-out and photodissociation boundary conditions to retrieve molecular abundances within a given source. H13CN is converted to HCN using the standard isotopic ratio of 70 with an uncertainty of 15%.

The resulting CH3CN and HC3N abundance profiles with respect to HCN in V4046 Sgr and MWC 480 are shown in Figure 9. The derived gas-phase abundances with respect to HCN in the inner 100 au of the disks are on the order of a few percent for CH3CN and a few tens of percent for HC3N. These model-derived inner disk abundances are consistent with the range of disk-averaged abundances calculated assuming 30–70 K rotational temperatures (Table 4).

5. Discussion

In a sample of six protoplanetary disks, we have detected the complex nitrile molecules HC3N and CH3CN in five and three disks respectively. These molecules therefore appear common in other nascent planetary systems. The disks in our sample host a range of physical conditions, which can be used to evaluate the nitrile chemistry in disks. We begin by surveying the possible origins of complex nitriles in disks, followed by an evaluation of our source sample.

5.1. Nitrile Formation in Disks

5.1.1. Chemical Pathways

HC3N is proposed to form efficiently in the gas phase, via either CN + C2H2 or HCN + C2H (Fukuzawa & Osamura 1997), and has no known efficient grain-surface formation pathways. In contrast, CH3CN can form via both gas-phase and grain-surface processes. In current astrochemistry codes, the dominant gas phase CH3CN formation channel is \(C^+ + C^+ \rightarrow C_3N\) followed by dissociative recombination. On grain surfaces, CH3N is converted to HCN using the standard isotopic ratio of 70 with an uncertainty of 15%.

The resulting CH3CN and HC3N abundance profiles with respect to HCN in V4046 Sgr and MWC 480 are shown in Figure 9. The derived gas-phase abundances with respect to HCN in the inner 100 au of the disks are on the order of a few percent for CH3CN and a few tens of percent for HC3N. These model-derived inner disk abundances are consistent with the range of disk-averaged abundances calculated assuming 30–70 K rotational temperatures (Table 4).
there may be important contributions from as yet unexplored chemistry that leads to CH$_3$CN formation.

5.1.2. Nitrile Abundance Correlations

To explore the relationship among different nitrile-bearing species in our disk sample, Figure 10 shows the distance-normalized fluxes of the CH$_3$CN 14–13 and HC$_3$N 27–26 transitions each plotted against the H$^{13}$CN 3–2 transition. The HC$_3$N emission strength has no clear relation to H$^{13}$CN. However, interpreting this lack of correlation is complicated by the high upper energy of the HC$_3$N 27–26 line: with an excitation temperature of 165 K, this transition is not sensitive to cool HC$_3$N molecules, which may be abundant in some disks. Indeed, the enhanced HC$_3$N emission around the Herbig Ae stars compared with the T Tauri stars is consistent with a thermal effect (Figure 10), as there will be more hot molecular material around more luminous stars. Observations of lower-J HC$_3$N transitions are needed to determine whether the HC$_3$N chemistry is related to the other nitrile chemistry in disks.

From the available data, CH$_3$CN emission appears to correlate with H$^{13}$CN, although more detections are required to establish if this relationship is real. We note that CH$_3$CN exhibits no such correlation with C$^{18}$O emission strength; the tentative correlation with H$^{13}$CN is therefore not simply a trend with the amount of gas in the disk. If additional data points confirm this correlation, it may be evidence for an active gas-phase contribution to CH$_3$CN formation, as this is currently the only chemical pathway with a direct link between HCN and CH$_3$CN. Other potential gas-phase and grain-surface channels to CH$_3$CN formation, which could explain a correlation with HCN but are not currently included in models, should also be explored.

5.1.3. Nitrile Spatial Correlations

Correlations in the spatial extent of molecules within a disk can also be used to constrain their formation chemistry. Across the disk sample, the spatial distributions of CH$_3$CN and HC$_3$N (Figure 2) as well as H$^{13}$CN (see Guzmán et al. 2017, for H$^{13}$CN maps) are all compact, typically well within the bounds of the dust continuum. This spatial similarity of nitrile emission within each disk is consistent with a chemical scheme in which CH$_3$CN and HC$_3$N depend on abundant HCN (or its photo-product CN) to form. We note that this is a stronger constraint for CH$_3$CN and H$^{13}$CN than for HC$_3$N because, as discussed above, the emission from high-J transitions of HC$_3$N may not reflect the true distribution of molecules within the disk, and lower-energy transitions are required to confirm a compact distribution.

Determining whether the spatial distributions of HC$_3$N and its proposed precursor C$_2$H are related will provide important constraints on the HC$_3$N formation chemistry. Spatially resolved observations of C$_2$H toward TW Hya show a ringed structure peaking near the edge of the submillimeter continuum; DM Tau similarly demonstrates an outer ring near the dust edge and an inner ring cophasal with the continuum (Kastner et al. 2015; Bergin et al. 2016). A ringed morphology may be a feature of hydrocarbons more generally, and indeed is reproduced for the slightly larger hydrocarbon C$_2$H$_2$ (Qi et al. 2013a; Bergin et al. 2016). The apparent anti-correlation of HC$_3$N and C$_2$H suggests that the proposed HC$_3$N formation pathway of C$_2$H + HCN may not be efficient. If the ringed morphology is common to all hydrocarbons, this is also problematic for the C$_2$H$_2$ + CN pathway, although the relationship between C$_2$H and C$_2$H$_2$ distributions is unconstrained. Yet again we note that due to the high-energy HC$_3$N transitions and comparatively low angular resolution of our observations we cannot exclude the possibility of HC$_3$N rings. Higher-resolution observations of lower-J HC$_3$N transitions combined with C$_2$H observations in the same sources will be important for constraining whether the current HC$_3$N formation paradigm is viable.

5.2. Physical Drivers of Nitrile Chemistry in Disks

The physical conditions of a protoplanetary disk set what chemistry can occur, while myriad properties have been proposed as chemical drivers in disks, we focus here on those that are, to some degree, testable based on the properties of our sample, namely the radiation field, disk structure, and evolutionary stage.

5.2.1. Radiation Field

The quiescent luminosity and accretion luminosity of a host star both contribute to the overall radiation environment in a disk. The FUV emission in T Tauri stars arises dominantly from accretion luminosity, while Herbig Ae stars should have significant FUV contributions from quiescent stellar photospheric emission in addition to accretion luminosity (e.g., Kurucz 1993; Matsuyama et al. 2003). Figures 11(a)–(b) shows the distance-normalized disk-integrated fluxes of CH$_3$CN 14–13 and HC$_3$N 27–26 plotted against the quiescent luminosity and the mass accretion rate of each star. For comparison, the CH$_3$CN 14–13 flux calculated for TW Hya based on the observations of Loomis et al. (2018b) is also included, with a bolometric luminosity and mass accretion rate taken from Van Boeckel et al. (2017) and Herczeg & Hillenbrand (2008) respectively. For CH$_3$CN, we do not see any obvious trends with $L_*$ or $M_\ast$. This lack of correlation with the radiation field could indicate emission from the colder UV-shielded layers of the disk, but is also possibly due to the small number of CH$_3$CN detections. HC$_3$N appears to correlate with both the stellar luminosity and the mass accretion rate, suggesting that the UV field may play an important role in driving its chemistry. However, due to the high upper energy of the 27–26 transition, this could be due in part to the presence of hotter gas in high-UV environments rather than increased abundances of HC$_3$N; observations of lower-J HC$_3$N lines will be able to break this degeneracy.

5.2.2. Disk Age

As disks evolve, processes such as viscous accretion, dust growth/settling, and radial drift reshape the physical structure of the disk (reviewed in Williams & Cieza 2011). Astrochemical
modelers have recently begun to explore how a dynamically evolving disk impacts the chemistry, with a particular focus on the C/O ratio over time (Piso et al. 2015; Eistrup et al. 2017). Modeling by Du et al. (2015) shows that the abundance of nitrile species can be greatly enhanced as a result of gas-phase carbon and oxygen depletion: as the system ages and more CO and H2O are depleted from the gas phase, the nitrile abundances should correspondingly increase. Observationally, Kastner et al. (2014) observed enhanced CN abundances toward the evolved disks around TW Hya and V4046 Sgr.

Figure 11(c) shows the CH3CN 14ν=13ν and HC3N 27–26 integrated fluxes normalized to a distance of 140 pc and plotted against the disk age. Again, the CH3CN 14ν=13ν flux in TW Hya calculated from the observations of Loomis et al. (2018b) is included for comparison. V4046 Sgr, the oldest disk in the sample, shows anomalously high CH3CN emission. However, in all other disks, CH3CN detections and upper limits are fairly clustered, showing no obvious trend with age. Likewise, HC3N emission does not appear to be related to disk age. With the existing data, there is therefore insufficient evidence for an evolutionary trend in nitrile emission. We note that the discrepancy in CH3CN emission between V4046 Sgr and TW Hya is somewhat surprising given that the line intensities of other small molecules in the two disks are quite similar (Kastner et al. 2014).

5.2.3. Inner Dust Cavity

The disk structure determines how radiation is processed through the disk. Transitional disks, characterized by inner gaps in millimeter dust emission, may host a distinct chemistry due to increased UV radiation in the inner disk (e.g., Cleeves et al. 2011). LkCa 15 and V4046 Sgr are both transition disks and yet exhibit very different nitrile chemistries: V4046 Sgr is strongly detected in both CH3CN and HC3N, while LkCa 15 is weakly detected in HC3N and tentatively or not detected in CH3CN. There is therefore no strong global impact of an inner cavity on the disk’s nitrile chemistry; observations toward other transition disks are needed to confirm this in a larger sample.

On smaller scales, we expect that the presence of an inner gap would result in warmer gas and a higher UV field within the cavity. Suggestively, there is a slight peak in the radial profile of CH3CN in LkCa 15 out to ~50 au scales (Figure 3), consistent with the cavity radius derived by Piétu et al. (2006); however, this emission is not significant at the 3σ level and therefore no firm conclusions can be drawn.

5.3. Nitriles in Different Circumstellar Environments

We now compare the disk-averaged abundance ratios for our sample with the abundances measured in similar objects at different evolutionary stages. Low-mass protostars are the evolutionary precursors to the \(<2M_\odot\) stars in our sample, while comets formed out of the midplane of the protosolar nebula and should preserve material from the time of planet formation. We note the environments in these different types of objects span a wide range of temperatures, densities, radiation fields, and other physical conditions.

As discussed in Section 4.3, for V4046 Sgr and MWC 480 the model-derived CH3CN/HCN and HC3N/HCN abundances in the inner 100 au are consistent with the range of disk-averaged abundances calculated for 30–70 K rotational temperatures. In this section, we use the range of disk-averaged abundances as a representation of the inner 100 au of the disk in order to compare across the entire disk sample.

Figures 12(a)–(b) show the range of CH3CN/HCN and HC3N/HCN abundances measured in solar system comets (Mumma & Charnley 2011) compared to the gas-phase abundances measured in our disk sample. The disk abundances of CH3CN are within a few percent of the values measured in solar system comets for sources with detections. The upper limits for AS 209 and LkCa 15 are somewhat lower but still possibly within a few percent of cometary.

For HC3N, the disk abundances are up to an order of magnitude higher than cometary for an adopted 30 K rotational temperature; however, given the warmer (50 K) HC3N rotational temperature derived for MWC 480, we expect that the abundances calculated assuming a 30 K temperature...
overestimate the HC$_3$N/HCN ratio for the Herbig Ae disks at least. Restricting the comparison to the 50–70 K values, the HC$_3$N abundances are quite close to cometary.

Figure 12(c) shows the range of CH$_3$CN/HC$_3$N ratios measured in a sample of 16 low-mass protostellar envelopes (Bergner et al. 2017). HCN column densities toward these sources are not available; however, the CH$_3$CN/HC$_3$N ratio still provides a useful proxy for the relative efficiency of different complex nitrile chemistries. The ratios across the disk sample are mostly consistent with the values measured in protostellar envelopes, with the exception of V4046 Sgr, which is somewhat enhanced in CH$_3$CN/HC$_3$N compared to the other disks and protostars.

Based on this comparison, we see that the gas-phase nitrile abundances relative to other N-bearing molecules are consistent across various physical environments: disk molecular layers, protostellar envelopes, and the midplane of the solar nebula. We note that with these observations alone we cannot directly compare the comet- and planet-forming material in our sample with that of the protosolar nebula, as this would require extrapolations (i) from the molecular layer down to the midplane, and (ii) from gas-phase to ice abundances. Nonetheless, the consistency of nitrile abundances across a wide range of physical conditions demonstrates a robust nitrile chemistry with similar outcomes in different environments. CH$_3$CN abundance ratios (and upper limits) in particular appear to be especially regular both across the disk sample and in comparison with comets and protostars. Complex nitrile species should therefore be reliably produced in a variety of different star- and planet-forming environments.

While the abundances of N-bearing molecules appear internally consistent across a range of physical environments, there is evidence that the ratio of N- to O-bearing COMs in disks is distinct compared to other environments. In both comets and protostellar envelopes, the CH$_3$CN/CH$_3$OH ratio is typically on the order of a few percent (Mumma & Charnley 2011; Bergner et al. 2017). By contrast, in the one disk where CH$_3$OH has been detected (TW Hya), the column density ratio of CH$_3$CN/CH$_3$OH is about unity (Walsh et al. 2016; Loomis et al. 2018b), indicative of an oxygen-poor chemistry. Similarly, our observations covered a number of CH$_3$OH transitions in the 5–4 ladder, with no CH$_3$OH detections despite the strong nitrile emission. This suggests that the underabundance of gas-phase O- versus N-bearing COMs is systematic in disks. A nitrogen-rich, oxygen-poor chemistry is qualitatively consistent with an oxygen-starved environment due to, e.g., the depletion of H$_2$O and CO from the gas phase (Du et al. 2015). Such a scenario would indicate a predominantly gas-phase formation pathway for CH$_3$CN in disks. Another possible factor is if the photodesorption efficiency of intact CH$_3$CN is high compared to CH$_3$OH, which has been shown to photodesorb mainly as fragments (Bertin et al. 2016; Cruz-Diaz et al. 2016). Since photodesorption from grains is thought to be of primary importance in disks, compared to mainly thermal desorption in protostars and comets, this could also contribute to the observed discrepancy in CH$_3$CN/CH$_3$OH across circumstellar environments. Further exploration of the nitrile formation chemistry in disks using astrochemical models is needed to resolve the origin of this unique chemistry.

6. Conclusions

Based on ALMA observations of the complex nitrile species CH$_3$CN and HC$_3$N toward six protoplanetary disks, we conclude the following:

1. Complex nitrile molecules are commonly observed in protoplanetary disks, with five of six disks detected in HC$_3$N and three of six disks detected in CH$_3$CN.

2. Rotational temperatures derived for sources with multiple line detections are consistent with emission from the temperate molecular layer of the disk. V4046 Sgr exhibits cool (29 ± 2 K) CH$_3$CN emission consistent with the temperature measured in TW Hya (Loomis et al. 2018b). CH$_3$CN and HC$_3$N in MWC 480 are both characterized by warmer emission, with rotational temperatures of 73 ± 23 K and 49 ± 6 K respectively. The increased radiation field around Herbig Ae disks compared to T Tauri disks may be responsible for this difference.
3. Parametric models of the CH$_3$CN, HC$_3$N, and H$^{13}$CN abundances in MWC 480 and V4046 Sgr are used to fit the observed emission and constrain radial abundance profiles. Within 100 au, CH$_3$CN/HCN abundances are on the order of a few percent and HC$_3$N/HCN abundances on the order of tens of percent.

4. Across the disk sample, we observe a tentative correlation of CH$_3$CN with H$^{13}$CN emission; if confirmed by further detections, the formation chemistry of CH$_3$CN should be revisited to explain this relationship. We see evidence for a possible anticorrelation in the spatial distributions of HC$_3$N and its precursor C$_2$H; if confirmed in lower-J HC$_3$N transitions this would seem to rule out the current proposed HC$_3$N formation path.

5. We use the heterogeneous physical properties of our disk sample to explore whether the UV field, disk age, or presence of an inner dust cavity impact the nitrile chemistry. We observe no strong trends relating these environmental properties to the nitrile emission strength. We emphasize the need for observations of lower-energy HC$_3$N lines to help constrain any relationships with disk physical properties.

6. Disk-averaged CH$_3$CN and HC$_3$N abundances relative to other N-bearing molecules are compared to values measured in solar system comets and protostellar envelopes and found to be consistent across these different environments, although the HC$_3$N/HCN uncertainties are large due to sensitivity to the adopted rotational temperature. These molecules appear to be reliably produced under a wide variety of physical conditions, demonstrating a robust nitrogen chemistry with similar outcomes in different environments.

7. Our results are suggestive of a disk chemistry systematically rich in N-bearing relative to O-bearing COMs when compared to other circumstellar environments. The origin of this unique chemistry observed in disks compared to other stages of star and planet formation remains to be resolved.

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Software: NumPy (Van Der Walt et al. 2011), Matplotlib (Hunter 2007), Astropy (Astropy Collaboration 2013), emcee (Foreman-Mackey et al. 2013), RADMC-3D (Dullemond 2012), scikit-image (Van Der Walt et al. 2014), vis_sample (Loomis et al. 2018a).

Appendix

Abundance Models

Modeling results for H$^{13}$CN and CH$_3$CN 14$\rightarrow$13 in V4046 Sgr are shown in Figure 13. Figure 14 shows modeling results for MWC 480 CH$_3$CN 14$\rightarrow$13, HCN 27$\rightarrow$26, H$^{13}$CN 3$\rightarrow$2, CH$_3$CN 15$\rightarrow$14, and HC$_3$N 31$\rightarrow$30.
Figure 14. Observations (top), model (middle), and residuals (bottom) for CH$_3$CN 14$_0$-13$_0$, HC$_3$N 27-26, H$^{13}$CN 3-2, CH$_3$CN 15$_{10}$-14$_0$, and HC$_3$N 31-30 in MWC 480. Contour levels indicate 3, 5, 7, and 10 $\times$ rms.
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