Constraining Spatial Densities of Early Ice Formation in Small Dense Molecular Cores from Extinction Maps

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Abstract

Tracing dust in small dense molecular cores is a powerful tool to study the conditions required for ices to form during the prestellar phase. To study these environments, five molecular cores were observed: three with ongoing low-mass star formation (B59, B335, and L483), and two starless collapsing cores (L63 and L694-2). Deep images were taken in the infrared $JHK$ bands with the United Kingdom Infrared Telescope WFCAM (Wide Field Camera) instrument and IRAC channels 1 and 2 on the Spitzer Space Telescope. These five photometric bands were used to calculate extinction along the line of sight toward background stars. After smoothing the data, we produced high spatial resolution extinction maps ($\sim$13″–29″). The maps were then projected into the third dimension using the AVIATOR algorithm implementing the inverse Abel transform. The volume densities of the total hydrogen were measured along lines of sight where ices (H$_2$O, CO, and CH$_3$OH) have previously been detected. We find that lines of sight with pure CH$_3$OH or a mixture of CH$_3$OH with CO have maximum volume densities above $1.0 \times 10^6$ cm$^{-3}$. These densities are only reached within a small fraction of each of the cores ($\sim$0.3%–2.1%). CH$_3$OH presence may indicate the onset of complex organic molecule formation within dense cores, and thus we can constrain the region where this onset can begin. The maximum volume densities toward star-forming cores in our sample ($\sim$(1.2–1.7) $\times 10^6$ cm$^{-3}$) are higher than those toward starless cores ($\sim$(3.5–9.5) $\times 10^5$ cm$^{-3}$).

Unified Astronomy Thesaurus concepts: Interstellar dust extinction (837); Interstellar extinction (841); Infrared astronomy (786); Infrared photometry (792); Molecular clouds (1072); Bok globules (171); Young stellar objects (1834); Ice formation (2092)

1. Introduction

Dust grains and the ices that form on them play an important role in the early stages of stellar and planetary formation within dense molecular cores. The dense environments shield the innermost core from interstellar radiation. The extremely cold temperatures within the core allow gases to condense onto the surface of dust grains, adding layers and complexity to the icy surfaces they have gathered together.

At relatively low densities H$_2$O is the first to freeze out, forming a monolayer of ice at an extinction $A_V = 1.6$ (Hollenbach et al. 2009). As the density within the core increases, H$_2$O is mixed with other ices such as CH$_4$, NH$_3$, and CO$_2$, and models show that at the highest densities ($n \geq 10^5$ cm$^{-3}$) CO can completely freeze out (Allamandola et al. 1999). At this point more complex ices can form such as H$_2$CO and CH$_3$OH on short timescales of $\sim 10^4$ yr (Cuppen et al. 2009). Models indicate that these molecules are vital for the onset of complex organic molecules (Fedoseev et al. 2017), and they appear to be abundant in cores even before stars form (Chu et al. 2020; Scibelli & Shirley 2020).

Ices have been observed along lines of sight through molecular cores toward background stars and young stellar objects (YSOs). Absorption features for H$_2$O (3.0 μm), CO (4.67 μm), and CO$_2$ (4.27 μm) have been well characterized (e.g., Whittet et al. 1983, 1985, 1998; Chiar et al. 1995; Goto et al. 2018). Additionally, CH$_3$OH (3.53 μm from the C–H stretching mode) has been detected along several lines of sight through molecular cores (e.g., Boogert et al. 2011; Chiar et al. 2011; Chu et al. 2020). These wavelengths are difficult to observe from the ground owing to high sky background noise and telluric features. Thus, only a limited sample of background stars and YSOs have probed the environments for ice formation. Extinction thresholds have been determined for the formation of different ices within small isolated cores and large molecular clouds. There are significant variations to this threshold between clouds, for example, the extinction, $A_V$, at which H$_2$O ice forms in Ophiuchus is $\sim$10–15 mag (Tanaka et al. 1990), while the Pipe Nebula has a threshold $A_V = 5.2 \pm 6.1$ mag (Goto et al. 2018). Even smaller thresholds were found for the Taurus Molecular Cloud (TMC) and Lupus ($A_V = 3.2 \pm 0.1$ mag and $2.1 \pm 0.6$ mag, respectively; Whittet et al. 2001; Boogert et al. 2013). For CO ice the formation threshold is typically higher, with $A_V = 6.0 \pm 4.1$ for the TMC (Chiar et al. 1995) and $A_V = 4.96 \pm 1.07$ from isolated cores (Chu et al. 2020).

Extinction thresholds can provide insight on the dust column density through the line of sight where ices can form. However, mapping the extinction across the full core can provide spatial and structural context to understand what promotes or inhibits different ice growth. Extinction maps have long been a tool to trace the dust in star-forming regions. Observations in the near-infrared (NIR) have utilized the fact that at longer wavelengths stars become less obscured by dust. Lada et al. (1994) recognized this relationship of the infrared color excess with the extinction and used it to map dust in a method called NICE (near-infrared color excess). In this method the difference between the observed and intrinsic color of a background star can produce an extinction measurement. The following equation from Lada et al. (1994) is an example of a simplified way to calculate the extinction using photometry in the $H$ and $K$ bands assuming a normal reddening law from...
Rieke & Lebofsky (1985):
\[(H - K)_{obs} = (H - K)_{int} + 0.063 \times A_V.\] (1)

The “obs” represents the color that is observed, while the “int” is the intrinsic color of the stars. The \(H-K\) colors are beneficial to use because the intrinsic colors of stars have a small scatter (e.g. Koornneef 1983). Typically a nearby field of stars with low extinction levels is measured to obtain an average intrinsic color to use in the above equation. After measuring the extinction along the line of sight toward background stars, the discrete measurements are smoothed into an extinction map. This method has some limitations because using only one color can cause significant noise in the final \(A_v\) estimate. Thus, this method was later expanded into NICER, where multiple wavelength bands could be used to determine the extinction with significantly smaller errors in \(A_v\) (Lombardi & Alves 2001). Additional improvements to this general technique have carefully removed some bias and inhomogeneities in the distribution of background stars that cause discrepancies on the small-scale structure (NICEST; Lombardi 2009). New computational methods have also been employed for these techniques, such as PNICER, which uses a machine-learning algorithm (Meingast et al. 2017), and XNICER, which uses a full Bayesian inference of the extinction for each observed object (Lombardi 2018).

Most recently, a new technique has been utilized to take 2D maps and project them into the third dimension using a mathematical technique called an inverse Abel transform. The Abel transform has been used, for example, by taking a 3D object with optically thin emission and integrating the emission along the line of sight to produce a 2D image. The inverse Abel transform does the opposite, where a 2D plane is projected into 3D using an axially symmetric distribution (Abel 1826). This technique has been used in several applications (Hasenberger & Alves 2020, and references therein). In Hasenberger & Alves (2020) they develop the algorithm AVIATOR to reconstruct 2D maps into 3D with the assumption that the distribution along the line of sight is similar to the distribution in the plane of projection. Typically densities of molecular cores are derived from dust continuum emission maps in the submillimeter (e.g., Kirk et al. 2005; Ysard et al. 2012). However, they usually rely on an average temperature along the line of sight and do not consider temperature gradients within the cores. Because these cores have stratified density structures that may have internal or external radiation fields, this can introduce errors on the density profile. Radiative transfer methods can also be used to model the volume density as shown in Nielbock et al. (2012) and Steinacker et al. (2016) to incorporate temperature gradients but are model dependent. The inverse Abel transformation removes some uncertainties in these methods by not needing temperature information or model-dependent parameters (Hasenberger & Alves 2020). Having 3D information is essential for observationally constraining the local densities of dust where ice forms.

In this work we present extinction maps and their 3D reconstructions for five cores at different evolutionary stages. All but one of these cores were previously studied for ongoing ice formation where column densities toward individual background stars were measured for H\(_2\)O, CO, and CH\(_3\)OH ices (Chu et al. 2020). This provides an excellent sample to compare the spatial densities of dust and gas required for the different ices to form. We will first describe the molecular cores being investigated in Section 2. Observations of the cores and data reduction methods are in Section 3. In Section 4 we present the extinction maps of each core (Section 4.1) and transform them into 3D maps (Section 4.2) where spatial densities along lines of sight toward background stars with ice detections are shown. We discuss these results in Section 5.

2. Target Selection

We have selected five molecular cores for extinction mapping and analyzing the local densities where ices form. These are all small (~0.2–1 pc), dense, mostly isolated cores. They represent different stages of evolution where two are collapsing (L63 and L694-2), two have Class 0 YSOs embedded in the core (B335 and L483), and one is quiescent with several later-stage (Class II) YSOs (B59). All of the cores were chosen because they have a high density of background stars with a position against the Galactic bulge. This allows for measurements of many lines of sight through the cores so that the extinction maps will have very fine sampling with high spatial resolutions on the sky. Because the cores are also nearby (<250 pc), there are very few foreground stars contaminating the data. The Galactic bulge contains mostly more evolved late K and M stars that have a small spread in color, reducing the uncertainty in the intrinsic color measurements used in Equation (1) (Zoccali et al. 2003). As previously mentioned, four of the five cores were studied in Chu et al. (2020), where several lines of sight displayed the presence of H\(_2\)O, CO, and CH\(_3\)OH ice. The 3D maps of the cores will allow us to probe the spatial density of hydrogen required for this ice formation. The cores are relatively simple in shape and structure, which is not necessarily the most representative of other star-forming regions, but these properties will help simplify the 3D reconstruction. Each of the cores are summarized in Table 1, and below we highlight some of the features seen in the infrared and the ices that have been detected.

2.1. L63

L63 is one of the densest regions in the northern Ophiuchus (Oph N) complex and is classified as being starless in a quasi-equilibrium collapsing stage (e.g. Nozawa et al. 1991; Ward-Thompson et al. 1994, 1999; Kirk et al. 2005; Seo et al. 2013). The distance to Oph N has been estimated from Hipparcos parallaxes to be 145 ± 2 pc (de Geus et al. 1989), but extinction-based distance modulus estimates have a range of distances between 80 and 200 pc, where some individual clouds are farther away than others (Straizys 1984; de Geus et al. 1989; Wilking et al. 2008). In Hatchell et al. (2012) an average distance of 130 pc is used, and we adopt the same for the distance to L63. The density of background stars for L63 is lower than others in our sample, and there were not any background stars that were bright enough to be included in the study by Chu et al. (2020) for the detection of ices.

2.2. B59

B59 is the densest and only known part of the Pipe Nebula where star formation has begun (Onishi et al. 1999; Forbrich et al. 2009). Using astrometric data from Gaia, the distance is measured with high precision at 163 ± 5 pc (Dzib et al. 2018). It is the largest core in our sample, with the densest regions covering ~0.8 × 0.8 pc and a total mass of ~30 \(M_\odot\) (Duarte-Cabral et al. 2012). Brooke et al. (2007) developed an extinction map for B59 with Two Micron All Sky Survey

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(2MASS) JHK data with a spatial resolution of \( \sim 100'' \). They found a peak extinction of \( A_V \sim 45 \). Within \( \sim 0.1 \) pc of the highest-density peak 13 low-mass YSOs were identified (Brooke et al. 2007). Most are classified as later Class II sources, but two are Class 0/I or I. In Chu et al. (2020) spectra of five of the Class II YSOs were observed, where \( H_2O \) ice was detected along the line of sight to all five, and four displayed frozen CO, of which two had a mixture of CO with polar ice, presumably \( CH_3OH \). They determine that the ices are most likely present in the foreground cloud and not part of the YSO’s disk or envelope.

### 2.3. L483

L483 is a small isolated core with an embedded low-mass (0.1–0.2 \( M_\odot \); Oya et al. 2017) protostar, IRAS 18148–0440 (Parker 1988). Though the protostar is deeply embedded at \( A_V \sim 70 \), it appears to be the source of a variable nebula that is only visible in the infrared (Connelley et al. 2009). The variability is most likely due to opaque clouds within \( \sim 1 \) au that cast shadows and change the illumination of the nebula. In Fuller & Wootten (2000) they model the central region within 3000 au of the source to have infalling material from the surrounding core. L483 is typically associated with the Aquila Rift region at a distance of 200 pc (Dame & Thaddeus 1985), but Very Long Baseline Array and Gaia-DR2 astrometry shows that the distance to Aquila is upward of 436 ± 9 pc (Ortiz-León et al. 2018); however, the parallaxes and extinction of stars near L483 still indicate a closer distance of 200–250 pc (Jacobsen et al. 2019), and thus we adopt the average distance of 225 pc. Signatures of \( H_2O \), \( CO_2 \), CO, and \( CH_3OH \) ice have been measured through lines of sight into this core to background stars outside of the influence of the protostellar envelope (Boogert et al. 2011; Chu et al. 2020).

### 2.4. B335

B335 is a Bok globule with a Class 0 YSO deeply embedded in the core (Frerking & Langer 1982; Keene et al. 1983; Chandler et al. 1990; Hodapp 1998). The protostar appears to be less evolved than the protostar in L483 with a lower mass (0.02–0.06 \( M_\odot \); Imai et al. 2019) and very low levels of rotation (Jacobsen et al. 2019). In the infrared there are emission features where a bipolar outflow from the protostar has broken through the globule on both sides. At 8 \( \mu m \) a shadow extends \( \sim 3000–7500 \) au with \( A_V > 100 \), and core shine can be seen at shorter wavelengths (Stutz et al. 2008). The distance is 150 ± 50 pc, but with higher uncertainty than some of the other cores in our sample (Stutz et al. 2008).

### 2.5. L694-2

The isolated core L694-2 is collapsing with a strong infall with speeds faster than those within L63 and increasing toward the center (Lee et al. 2004; Seo et al. 2013). However, the core appears to be starless (Harvey et al. 2002, 2003; Evans et al. 2003; Suresh et al. 2016). There is a compact centrally condensed core (Lee et al. 2001) with a mass of \( \sim 1 M_\odot \), and within the next 10\(^4\) yr a point mass is expected to form (Williams et al. 2006). The distance to L694-2 was originally assumed to be similar to the distance of B335 since it is nearby (Tomita et al. 1979), but Kawamura et al. (2001) revised this distance based on star counts to be 230 ± 30 pc, which is adopted here. In Chu et al. (2020) ice features were detected toward background stars including \( H_2O \) and CO. For one line of sight just outside the densest part of the core \( CH_3OH \) ice was detected.

### 3. Observations and Data Reduction

#### 3.1. UKIRT Photometry

Observations of each core were taken in the \( J \) (1.25 \( \mu m \)), \( H \) (1.64 \( \mu m \)), and \( K \) (2.20 \( \mu m \)) band filters (Hewett et al. 2006) with the 3.8 m United Kingdom Infrared Telescope (UKIRT) using the Wide Field Camera (WFCAM) instrument (Casali et al. 2007). WFCAM has four 2048 \( \times \) 2048 pixel detectors, each with 0\('4\) resolution for a total area of coverage of 0.19 deg\(^2\) per detector. Integration times were typically longer for the \( J \) band than the \( H \) and \( K \) bands and ranged from 1.0 to 5.6 hr (total integration times for each band are presented in Figure 1). Observations were made during the 2014A and 2016A semesters.

Images were processed with the Cambridge Astronomical Survey Unit as described in Irwin et al. (2004) and retrieved from the WFCAM Science Archive (Hambly et al. 2008). All of the cores fit onto one detector except for B59, where we...
Figure 1. On the left $JHK$ color-composite images of each core are shown with the size scale labeled using the reported distances to the cores in the text. The following are the total exposure times used for each cloud: $B59—J = 1.0$ hr, $H = 1.2$ hr, $K = 1.4$ hr; $L483—J = 5.6$ hr, $H = 2.8$ hr, $K = 2.8$ hr; $B335—J = 4.0$ hr, $H = 2.8$ hr, $K = 3.2$ hr; $L694-2—J = 3.2$ hr, $H = 2.0$ hr, $K = 2.0$ hr; $L63—J = 4.0$ hr, $H = 3.2$ hr, $K = 3.6$ hr. On some of the images circles show lines of sight that have ice measurements from Chu et al. (2020), where blue has H$_2$O ice; green has H$_2$O and CO ice; red has H$_2$O, CO, and CO$_{2}$ ice; and yellow has H$_2$O, CO, CO$_{2}$, and CH$_3$OH ice (CO$_{2}$ is CO mixed with polar ice). Black squares identify other YSOs where lines of sight were not measured. The magenta box in the $JHK$ color images is also shown in color images with $K$, channel 1, and channel 2 from Spitzer to display background stars detected in the highest-density region. The right panels are the corresponding grayscale extinction maps where the color bar is in $A_V$. The black centers of some cores show where the extinction level saturates. Overlaid contours have step sizes $A_V = 4$ represented by different colors. The size of the smoothing resolution is shown in the upper left corner.
Figure 1. (Continued.)
treated each chip individually for analysis before combining as a mosaic image. Using stacked images, we obtained the positions of stars using IRAF’s daofind with an FWHM of 5 pixels and a 4σ detection threshold. Then, using this source list, we extracted the stellar photometry in each band for individual frames using point-spread function (PSF) fitting with the IRAF routine daophot. A sample of 18 stars for each core was used to produce a model PSF that was used to obtain the photometry for all stars. Aperture photometry was not possible because of the crowded star fields. To calibrate the photometry, we used the source catalogs that are also products of the standard reduction pipeline (Hodgkin et al. 2009) that are calibrated to 2MASS (Skrutskie et al. 2006). We matched these catalogs from each individual frame to find the average photometry for each star. Then, using this master list, any stars in the 12–18 mag range with errors ≤0.07 mag were matched to targets we detected, and a calibration was done for each frame. The final photometry was an average between the individual frames. The limiting magnitudes vary slightly between the different cores depending on the total integration times and are complete to the 90% level corresponding to ~21.0 mag in J band and ~20.0 mag in H and K bands. Stars were saturated below ~10 mag.

3.2. Spitzer Photometry

Our five cores were observed with Spitzer IRAC’s channels 1 and 2 (3.6 and 4.5 μm, respectively; Fazio et al. 2004) during the warm mission (cycles 11 and 12, program ID 11028). Observations had 100 s exposures with total integration times of 1 hr per core, producing a 1σ limiting flux of 0.36 μJy in channel 2. This was significantly deeper than previous observations of the same fields found in the Spitzer Heritage Archive, with integrations of only ~100 s producing 1σ limiting fluxes of 2.16 μJy (Program ID 139, PI Evans, N. for B59, L63, L483, and L694-2; Program ID 94, PI Lawrence, C. for B335; Program ID 20119, PI Lada, C. for B59). Observations for our program were made in the high dynamic range (HDR) mode, and channel 2 observations were taken immediately after channel 1 in order to remove any possible uncertainty due to variability in the stars. The dither pattern used a 36-point dither.
Images were processed by the Spitzer Science Center pipeline S19.2.0. The photometry was measured using mosaics created with MOPEX following the guidelines and best inputs explained in the IRAC Instrument Handbook v2.1. We performed point-response function (PRF) photometry with the APEX procedure because PSF fitting with IRAC has proven to be problematic in channels 1 and 2.

4. Results

4.1. Extinction Mapping

Employing the NICER method from Lombardi & Alves (2001), we derive extinction maps for the five cores using multiple photometric bands. Equation (1) shows a simple method to determine the extinction using only the $H$–$K$ color, but NICER can implement multiple color measurements to reduce errors in the final extinction measurement. First, we use the $JHK$ data and Spitzer IRAC channels 1 and 2 (ch1 and ch2) to take the covariance matrix of the $J$–$H$, $H$–$K$, $K$–ch1, and ch1–ch2 intrinsic colors. The reddening vectors ($A_V/A_J$) for the different color combinations are taken from Rieke & Lebofsky (1985) for $JHK$ colors and from Indebetouw et al. (2005) for IRAC channels. In Indebetouw et al. (2005) the extinction law is derived using $A_K$ as a reference rather than $A_V$ and can vary between different environments. The variation is characterized by the reddening parameter $R_V = A_V/E_{B-V}$, where $E_{B-V}$ is the color excess. For $R_V = 3.1$, $A_V/A_K \sim 8.8$, but for regions where $R_V = 5$, $A_V/A_K \sim 7.5$ (Cardelli et al. 1989). We adopt $R_V = 3.1$ for all of the coefficients used in the NICER equations since we have used the color combinations from Rieke & Lebofsky (1985) for $JHK$, which is appropriate for the $R_V = 3.1$ environment. Knowing the reddening vectors and intrinsic colors then allows us to calculate the $A_V$ along the line of sight toward each background star. Following are the NICER equations used similar to that found in Equation (1):

\begin{align*}
(J - H)^{obs} &= (J - H)^{int} + 0.11 \times A_V \tag{2} \\
(H - K)^{obs} &= (H - K)^{int} + 0.063 \times A_V \tag{3} \\
(K - [3.6])^{obs} &= (K - [3.6])^{int} + 0.048 \times A_V \tag{4} \\
([3.6] - [4.5])^{obs} &= ([3.6] - [4.5])^{int} + 0.015 \times A_V \tag{5}
\end{align*}

We do not use the NICEST routine (Lombardi 2009) since our cores are relatively simple in structure and nearby to where contamination by foreground stars is not significant. Even with some foreground stars, the density of background stars is high, and the foreground stars would appear as outliers and have a small impact on the final extinction map.

4.1.1. Intrinsic Colors

In previous studies (e.g., Lada et al. 1994; Lombardi & Alves 2001; Lombardi et al. 2006; Lada et al. 2009) average intrinsic colors of background stars are obtained by using a nearby control field with negligible extinction levels. This also accounts for any reddening due to intervening dust in the interstellar medium (ISM). However, in our study we did not obtain nearby control fields for each core since it would have nearly doubled our observing time. Thus, we demonstrate a two-step approach to simulate a control field.

Using galactic simulations of stars from the TRILEGAL model4 (Girardi et al. 2005), we can estimate the intrinsic colors of background stars in the direction of each molecular core individually. This model uses four major components to simulate stars in a particular region of the sky: (1) a library of stellar evolutionary tracks, (2) a library of synthetic spectra, (3) the instrumental setup for a given telescope, and (4) a description of Galaxy components such as the Galactic thin and thick disk, halo, and bulge. The input requires the equatorial or galactic inputs for the region of the sky of interest and a total field area dimension. We chose the coordinates that are close to the center of each core with an area of 0.1 deg$^2$. Then, a photometric system is selected with a chosen magnitude limit where we set the limiting magnitude to 20 mag in $H$ band. Other parameters such as the initial mass function, binary fraction, and galactic components were kept at the default, and the dust extinction was set to zero. The output produces a list of stars with expected stellar parameters for the particular region of the sky, including temperature, mass, and the expected magnitude in the 2MASS $JHK$ and Spitzer IRAC channel 1–4 filters. The distribution from the simulations allows us to identify the expected intrinsic color for the four color combinations mentioned above ($J$–$H$, $H$–$K$, $K$–ch1, and ch1–ch2).

To ensure that the simulation produced accurate colors, we tested a field of stars used in Lada et al. (1994): IC 5146 (R.A.: 328.4577; decl.: 47.2566 (J2000)). They determine the average $H$–$K$ color to be 0.13, but in our simulation, with a field of view of 0.5 deg$^2$ and a limiting magnitude of 14 in $K$ band (corresponding to the approximate limiting magnitude in our work), we find an intrinsic $H$–$K$ color of 0.063. This is because the theoretical values do not account for any interstellar dust in the foreground or behind the molecular core, along the line of sight. Using the Galactic Dust Reddening and Extinction website,5 the data from the Infrared Astronomy Satellite (IRAS) mission and the DIRBE experiment (Diffuse InfraRed Background Experiment) on board the COBE satellite produce the visual extinction for a given location (Schlegel et al. 1998). Newer estimates of dust reddening were also measured by Schlafly & Finkbeiner (2011) using the Sloan Digital Sky Survey. Toward a low-extinction region near IC 5146 (R.A.: 328.4–329.0; decl.: 47.5–47.7) the $A_V$ is $\sim$0.72–0.87 (depending on which reddening data are used). Using the average $A_V = 0.80$ and the reddening law used in Rieke & Lebofsky (1985; to remain consistent with the NICER calculations), the ISM reddening of $H$–$K$ is $\sim$0.05, and thus the sum of the intrinsic color and ISM reddening in $H$–$K$ is $\sim$0.113, which is in agreement with Lada et al. (1994).

Edward of the cores in our sample we calculate the sum of the intrinsic and ISM colors in this way to determine the overall extinction. Errors on the intrinsic colors come from the standard deviation of the intrinsic colors from the TRILEGAL simulation. Table 2 reports these values. The errors for $E(B-V)$ are provided by the Galactic Dust Reddening and Extinction website, and we propagate the errors from both reddening estimates to determine the error on the ISM extinction (Table 2).

The ISM extinction can introduce systematic errors to the overall extinction measurement depending on the extinction law adopted. Since we use the relation in Rieke & Lebofsky (1985) for the NICER technique, we use the ISM $A_V$ where $R_V = 3.1$ throughout this work to remain consistent, but dense cores may have a higher reddening vector such as $R_V = 5.5$

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4 http://stev.oapd.inaf.it/cgi-bin/trilegal

5 https://irsa.ipac.caltech.edu/applications/DUST/
Weingartner & Draine 2001). We explore how this could affect the overall extinction, and in Table 2 we show the average $A_V$ for the ISM used for each core with both $R_V = 3.1$ and $R_V = 5.5$. The difference between the two extinction laws introduces a discrepancy in $A_V$ by $\sim 1$ mag (or $\sim 2$ mag for L483). In low-extinction regions this could have a large effect, but in higher-extinction regions a difference in the ISM of $\sim 1$–2 mag becomes small. However, if the extinction in the ISM may increase by a factor of $\sim 1.8$ depending on whether the $R_V$ chosen is 3.1 or 5.5, this suggests that the $A_V$ in the core could potentially be underestimated by a similar factor when using $R_V = 3.1$. Until we have a better understanding of the extinction law in dense cores, we are limited to this additional systematic error for the $A_V$ in the core.

### 4.1.2. Map Smoothing

Once the extinction toward each line of sight through the core is calculated, extinction maps are constructed. L483, B335, and B59 harbor YSOs, but the YSOs were excluded in producing the extinction maps. The YSOs in L483 and B335 are highly extincted and thus were not even detected in the Spitzer data. For B59 we also removed 13 YSOs in our sample that were identified by Forbrich et al. (2009) and Brooke et al. (2007). These YSOs include the five identified in Section 4.2.1; the remaining seven are identified in Figure 1. The extinction maps are then created using a weighted mean smoothing with a Gaussian smoothing kernel. The weighted mean assumes that the resolution to be a good balance in order to not lose actual structure within the core. The grayscale smoothed extinction maps are shown in Figure 1 beside color-composite images of the cores. Contours are shown representing levels with $\Delta A_V = 4$. The smoothing resolutions are listed in Table 2 for each core and displayed on the extinction maps.

In order to demonstrate where the extinction measurement is unreliable as a result of undersampling, regions in the center of each core are shown in black, where the third-nearest neighbor is less than twice that of the smoothing resolution. This means that the extinction value for the given pixel is interpolated from three or fewer nearby stars. For L63, there were no regions that were undersampled by this criterion. Additionally, the errors on the $A_V$ value for each pixel were determined as the interpolated value of the variance divided by the effective number of stars that contribute to the measurement of that pixel. The variance is converted to a $1\sigma$ value, and we divide the $1\sigma$ values by the $A_V$ for each pixel to determine the error fraction. We then determine the median error fraction for each core in the range $4 \leq A_V < 32$ and $A_V > 32$ to represent the significance of the errors and how the errors may be impacted at higher levels of extinction. We do not consider low-extinction regions ($A_V < 4$) since, as discussed previously, the errors on the intrinsic colors and extinction law can be rather significant and dominate. In Table 3 we convert this error fraction to a percent and find that for extinction values $4 \leq A_V < 32$ the errors are on the 2.5%–8.2% level. For higher-extinction regions the errors are slightly worse except for L63 and B59, where the high-extinction regions are still decently sampled.

### 4.2. Three-dimensional Reconstruction of Molecular Cores

Each of the five extinction maps were prepared for the AVIATOR algorithm to reconstruct a 3D volume density distribution from the 2D maps (Hasenberger & Alves 2020). This algorithm calculates the volume density assuming that a distribution perpendicular to the plane of projection is similar to that in the plane of projection, without requiring symmetry in the plane of projection. Because of computational time restrictions, the maps were first binned to have a resolution of $2.5''$ pixel$^{-1}$ (B335), $4''$ pixel$^{-1}$ (L483), $5''$ pixel$^{-1}$ (L694-2),

| Core   | $J-H$  | $H-K$  | $K-C1$  | $C1-C2$  | $\sigma_{A_V}$ | $\sigma_{A_V}$ |
|--------|--------|--------|--------|--------|---------------|---------------|
| L63    | 0.616 ± 0.120 | 0.166 ± 0.068 | 0.162 ± 0.096 | 0.024 ± 0.038 | 0.98 ± 0.10 | 1.77 ± 0.18 |
| B59    | 0.440 ± 0.107 | 0.109 ± 0.022 | 0.067 ± 0.013 | −0.015 ± 0.025 | 0.99 ± 0.09 | 1.75 ± 0.16 |
| L483   | 0.804 ± 0.122 | 0.299 ± 0.071 | 0.258 ± 0.109 | 0.050 ± 0.040 | 2.69 ± 0.25 | 4.75 ± 0.45 |
| B335   | 0.530 ± 0.146 | 0.130 ± 0.064 | 0.092 ± 0.084 | −0.001 ± 0.040 | 0.73 ± 0.14 | 1.31 ± 0.12 |
| L694-2 | 0.613 ± 0.146 | 0.174 ± 0.063 | 0.136 ± 0.081 | 0.010 ± 0.039 | 1.10 ± 0.15 | 2.03 ± 0.26 |

### Notes.

a Intrinsic colors from TRILEGAL simulations including the intervening interstellar dust extinction. Errors shown are the standard deviation of the intrinsic colors.

b Spitzer IRAC channels 1 and 2.
c The interstellar dust extinction from the Galactic Dust Reddening and Extinction website using the extinction law from Rieke & Lebofsky (1985) with reddening $R_V = 3.1$.
d The interstellar dust extinction from the Galactic Dust Reddening and Extinction website using the extinction law from Weingartner & Draine (2001) with reddening $R_V = 5.5$.
e Smoothing resolution used for extinction maps.

| Core   | Median $A_V$ Errors |
|--------|----------------------|
| 4 ≤ $A_V < 32$ | $A_V > 32$ |
| L63    | 5.7% | 4.6% |
| B59    | 2.5% | 0.8% |
| L483   | 6.1% | 8.8% |
| B335   | 8.2% | 10.4% |
| L694-2 | 5.0% | 5.9% |

Notes.

a The median errors calculated as $\sigma_{AV}/A_V$ and converted to a percentage for all pixels with $4 \leq A_V < 32$.
b The median errors calculated as $\sigma_{AV}/A_V$ and converted to a percentage for all pixels with $A_V > 32$. 

Table 2: Extinction Mapping Parameters

Table 3: Median $A_V$ Errors
These pixel sizes do not necessarily represent the resolutions in the 3D maps. Threshold levels of the extinction are required for the reconstruction, and we chose a threshold with a step size of 0.02, meaning that each threshold level is at least 2% higher than the previous level. The algorithm then produces a 3D data cube (map) of extinction where the sum along the lines of sight reproduces the original 2D map, with errors typically on the 2%–5% level and increasing to errors of $A_V = 2$ in the highest-extincted regions highlighted as undersampled regions in Figure 1. The undersampled regions were used in creating the 3D maps, as they retain information related to the ice chemistry in the densest parts of the core (see Section 4.2.1 for further discussion). For each core we find the point with the maximum extinction within the core. Because the dimension of each voxel (3D pixel) is the same, the size of a single pixel in the $x$- and $y$-direction (assuming that the distances to the cores are accurate in Table 1) is the same as along the $z$-direction. This allows us to calculate the distance for every voxel in the core from the point with the maximum extinction. Using this distance, a volume density of hydrogen ($n[cm^{-3}]$) can also be determined where the relation $N_H/A_V = 1.79 \times 10^{21} \text{ cm}^{-2} \text{ mag}^{-1}$ represents the total hydrogen column (H and H$_2$; Predehl & Schmitt 1995). This relationship is discussed further in Section 4.2.2. Figure 2 shows the volume density ($n[cm^{-3}]$) for each voxel as a function of distance from the maximum density in parsecs. The voxel with the maximum density in each core comes from more undersampled regions in the core, but since the undersampled regions are due to high extinction representing the center of the core, we can still use it to draw conclusions about the core structures and make comparisons between the cores. Errors on the maximum volume density are calculated as the standard deviation of the density values for the surrounding voxels out to the distance of the

Figure 2. The voxel volume density of each point within the core as a function of distance from the densest point in the core derived from the AVIATOR algorithm (black points). The colored points show the specific lines of sight toward YSOs and background stars. The colored data are only showing the lines of sight through the pixel corresponding to the center of the star’s R.A. and decl. The colors are the same as in Figure 1, representing the different ices detected.
smoothing resolution for each core (Table 4). In some cases this produces errors that are unreasonably small, as the voxels are not completely independent values, which is required when taking the standard deviation. These uncertainties also do not account for errors arising from the AVIATOR reconstruction, the variation in the $N_H/A_V$ relationship, and the uncertainties in distances to the cores, which are all discussed separately and in some cases are much larger than those found from the standard deviation. Below are descriptions of the features observed in these figures and some analysis with comparisons to features seen in the extinction maps.

$L_63$.—The highest-density region appears to be a very small region within the core, and there is a steep drop-off to lower-density regions. There is a second peak in the density at a little farther distance ($\sim0.05$ pc) from the highest-density region, which is another dense region that can be seen in the extinction map. In the 2D map we see a peak in the southeast portion of the cloud and two other dense regions north and west of the highest-density region. These dense regions are possibly artifacts from the smoothing kernel used because the structures are smaller than the smoothing resolution. The maximum density reached is $(9.0 \pm 1.7) \times 10^5$ cm$^{-3}$.

$L_694.2$.—There is a high peak in the density reaching $(6.5 \pm 1.3) \times 10^5$ cm$^{-3}$ that drops off somewhat rapidly to lower-density regions. There are many points in the core that reach a density $\sim1.5 \times 10^5$ cm$^{-3}$ that extends nearly 0.2 pc away from the densest region. Similar to $L_{483}$, this is most likely due to the elongated feature of infalling material in the southeast direction in the core (Figure 1).

$B59$.—This core has a very broad region of high density extending to distances beyond 0.1 pc. The peak density is the highest of any of the cores and is not shown in the figure at $(1.7 \pm 0.5) \times 10^6$ cm$^{-3}$. There are several high-density peaks ($>2 \times 10^5$ cm$^{-3}$) at much farther distances. The extinction map also shows a very irregular shape with spots of higher extinction. This core is actively forming several stars, and it is evident that there are multiple areas with higher densities for this star formation to occur.

$L_{483}$.—Similar to $B59$, the relationship is somewhat broad at the highest density levels. It then has several parts of the core that reach a density between $\sim3 \times 10^5$ cm$^{-3}$ and $\sim6 \times 10^5$ cm$^{-3}$, and this represents the more extended feature in the northwest direction from the core (Figure 1). This core has one of the highest spatial densities out of the five cores at $(1.5 \pm 0.5) \times 10^6$ cm$^{-3}$. However, it also has one of the highest uncertainties in distance estimates, and the standard deviation is high, making this maximum density more unreliable.

Notes.

a Name given to identify the cloud the star samples, and whether it is a background target (B) or YSO (Y); these match the alias in Chu et al. (2018).

b Ice abundances taken from Chu et al. (2020).

c CO$_2$ represents the long-wavelength wing detected in the CO ice feature indicating a mixture with polar ice—most likely CH$_3$OH ice.

d The maximum volume density associated with a voxel, with errors as the standard deviation of the volume density for surrounding voxels within the resolution of the extinction maps.
CO, and a mixture of CO with polar ice (CO$_P$); and two have all of these ices and additionally CH$_3$OH ice. The ice column densities for each are in Table 4, and Figure 1 identifies where the ices are located in the core.

Along the lines of sight toward all 13 ice detections we calculate discrete extinction values by taking the $A_V$ for each voxel with the $x$- and $y$-coordinate corresponding to the background star or YSO and averaging the $A_V$ with its surrounding voxels in the $x$- and $y$-direction, essentially as a form of binning the data further. This is to minimize artifacts from possible oversampling of the data in the 3D maps; however, structures smaller than $\sim 0.01$ pc are not reliable. The spatial density of total hydrogen ($\text{H} + \text{H}_2$) in $n_\text{H} [\text{cm}^{-3}]$ is then calculated from these averaged voxel $A_V$ measurements along the lines of sight as explained in Section 4.2 using the $N_{\text{H}}/A_V$ relationship from Predehl & Schmitt (1995). Figures 3 and 4 show the lines of sight for each source and are separated into background stars and YSOs. Table 4 reports the maximum volume density along each line of sight, with errors calculated similarly to the maximum volume density in each core.

Table 5 shows the total $A_V$ along the lines of sight produced using NICER for each star and the $A_V$ from the beam-averaged extinction map (using the beam size corresponding to each map’s resolution). The spectra for the background stars were also modeled in Chu et al. (2020) producing the extinction, $A_K$. Using the conversion $A_V/A_K = 8.93$ (Rieke & Lebofsky 1985), this $A_V$ is also reported in Table 5. YSO spectra could not be modeled for extinction owing to a lack of suitable stellar templates for YSOs.

The two lines of sight where CH$_3$OH ice is detected have a maximum volume density of $(3.6 \pm 0.66) \times 10^5$ cm$^{-3}$ and $(1.3 \pm 0.0054) \times 10^5$ cm$^{-3}$ (L483-B2 and L694-B2, respectively). Because the mixture of CO ice with polar ice (CO$_P$) is most likely due to a mixture with CH$_3$OH (Cuppen et al. 2011; Penteado et al. 2015), we would expect that maximum densities would be similar to those with independent CH$_3$OH ice features. Indeed, the background star in B335 has a strong detection of CO$_P$ and the maximum density is similar to the lines of sight with CH$_3$OH ($(1.16 \pm 0.019) \times 10^5$ cm$^{-3}$). In Chu et al. (2020) the lack of the direct detection of CH$_3$OH ice was explained for this target as being at an extinction that is too low for CH$_3$OH to be prolific since CH$_3$OH has only been detected above $A_V > 20$. In Table 5 it appears that the total $A_V$ along the line of sight toward B335-B1 is overestimated with both the NICER measurement and beam-averaged measurement compared to the directly modeled spectrum. This could mean that the volume density is an overestimate and not dense enough to form CH$_3$OH as abundantly as toward L483-B2 and L694-B2. All of the other lines of sight toward background stars have $A_V$ measurements that agree within $3\sigma$ of the spectral models.

Along two other lines of sight toward YSOs where polar CO ice was detected, the maximum volume density reached is also high ($(2.1 \pm 0.16) \times 10^5$ and $(2.7 \pm 0.11) \times 10^5$ cm$^{-3}$) and would also indicate that there may be an abundance of CH$_3$OH ice. In Chu et al. (2020) the upper limits of CH$_3$OH were high (Table 4), and thus the ice was possibly missed owing to sensitivity limits. We cannot determine whether the volume densities are also overestimated because the YSO spectra could not be modeled, and there are some discrepancies between the NICER $A_V$ and the beam-averaged $A_V$ because the NICER $A_V$ is unreliable if there remains an envelope or disk around the YSO.

The low sensitivities of the ice measurements in Chu et al. (2020) for B59-B1 and B59-Y3 also mean that the high maximum densities could allow for the presence of ices beyond our detection limits. These sensitivity constraints in B59 also explain how there is no apparent differentiation on the location where different ices have formed in the core (Figure 2), and potentially lines of sight that sample denser parts of the core do indeed have other undetected ices. It is noteworthy that B59 has high overall maximum densities along the different lines of sight, and so another possibility is that shocks or radiation fields from the YSOs have altered the ice abundances, making them lower despite dense environments.

We can conclude that CH$_3$OH appears to only form above densities of $\sim 1.0 \times 10^5$ cm$^{-3}$. The fraction of the total core that has densities above $1.0 \times 10^5$ cm$^{-3}$ is $0.2\%$ (L63), $0.4\%$ (B59), $2.1\%$ (B335), $0.7\%$ (L483), and $0.3\%$ (L694-2) meaning that CH$_3$OH exists in a very small fraction of the cores.

The relationship of the extinction for each point along the line of sight toward the ices as a function of distance from the highest-density region is shown in Figure 2. In L483 it is clear that the CH$_3$OH ice forms much closer to the densest region at AV$_{max}$ than to B59 and L694-2. The peak density. In B335 the core is smaller and the ice features are detected at a closer distance to the core’s densest region. In B59 there is little separation in the distances where different sets of ices are found, again probably due to the sensitivity in ice detections.

### 4.2.2. Uncertainty in Relation between $N_{\text{H}}$ and $A_V$

Several studies have calculated the $N_{\text{H}}/A_V$ ratio, where $N_{\text{H}}$ is the total number of hydrogen atoms and molecules (H and H$_2$). There are variations due to the methods used for calculating the ratio and the regions of the sky used to develop the relation. Using two X-ray binaries with two extended sources GCX and Cas A, Reina & Tarenghi (1973) were the first to derive the relation $N_{\text{H}}/A_V = 1.85 \times 10^{21}$ cm$^{-2}$ mag$^{-1}$. Later Gorenstein (1975) used independent optical extinction and column density measurements for several supernova remnants (SNRs) to obtain $N_{\text{H}}/A_V = (2.22 \pm 0.14) \times 10^{21}$ cm$^{-2}$ mag$^{-1}$, which was very close to the value later found in Güver & Özel (2009). A survey of the column densities of H I toward 100 stars in Bohlin et al. (1978) shows a smaller relation of $N_{\text{H}}/A_V = 9.4 \times 10^{20}$ cm$^{-2}$ mag$^{-1}$ and is typically used to describe the diffuse ISM. In Predehl & Schmitt (1995) X-ray point sources from ROSAT observations and four SNRs produced the ratio $N_{\text{H}}/A_V = (1.79 \pm 0.03) \times 10^{21}$ cm$^{-2}$ mag$^{-1}$, which is a very common relationship to use. Hotzel et al. (2002) later considered column densities that probed the dense cloud NGC2024 IRS2 (Lacy et al. 1994) and found that the relation was similar at $N_{\text{H}}/A_V = 1.9 \times 10^{21}$ cm$^{-2}$ mag$^{-1}$. The uncertainties were fairly large because it was based on a single source, but compared to the diffuse ISM value in Bohlin et al. (1978), it is suggested that the ratio may increase in dense cloud cores. Since all of these estimates only vary by a factor of $\sim 2$, we decided to adopt the relation in Predehl & Schmitt (1995), which is similar to the median value from these studies. The errors on this relation are also very small, and the same relation was adopted for some analysis in Chu et al. (2020), making for easier comparisons in this work.
5. Discussion

Previous work by Roy et al. (2014) and Hasenberger & Alves (2020) utilized the inverse Abel transform to construct 3D maps of the dense starless cores B68 and L1689B. They start with column density maps using data from the Herschel and Planck satellites. For B68 they find a peak volume density of \((3.8 \pm 0.3) \times 10^5\) cm\(^{-3}\) and \((3.7 \pm 0.3) \times 10^5\) cm\(^{-3}\) (Roy et al. 2014; Hasenberger & Alves 2020, respectively). This is

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Figure 3. The volume density distribution of hydrogen (H and H\(_2\)) along the line of sight toward background stars with different ices detected. The volume densities are calculated using the relationship between \(N_{\text{H}}\) and \(A_V\) explained in Section 4.2. The distances on the x-axis are calculated based on the distances to the cores in Table 1. The blue data represent lines of sight with only H\(_2\)O ice detected; green data show where H\(_2\)O and CO ice are detected; red data are for lines of sight with H\(_2\)O, CO, and a polar ice mixture with CO (CO\(_p\)); and finally black data show H\(_2\)O, CO, CO\(_p\), and CH\(_3\)OH ices. Ice detections were reported in Chu et al. (2020).
Figure 4. Similar to Figure 3, this samples lines of sight for YSOs only in B59. Colors and axes are the same as in Figure 3.
similar to the central density of $3.4^{+0.9}_{-0.5} \times 10^5$ cm$^{-3}$ found in Nielsen et al. (2012) using radiative transfer models. For L1699B the peak density values from Roy et al. (2014) and Hasenberger & Alves (2020) are $(9.5 \pm 1.0) \times 10^5$ cm$^{-3}$ and $(9.5 \pm 0.5) \times 10^5$ cm$^{-3}$, respectively. Both of these maxima are similar to those found for the starless collapsing cores L694-2 and L63. The other cores in our sample have higher maximum densities of $\sim$1(1.2–1.7) $\times 10^6$ cm$^{-3}$ and are star-forming. B59 has the highest maximum density and also has several YSOs already formed in later Class II stages. Since B68 is not yet collapsing and has the lowest maximum density, the trend of increasing maximum density as the cores evolve into star-forming cores is clear.

The trend for the local densities where different ices can form is not as straightforward. As mentioned in the introduction, H$_2$O ice can form at low extinctions typically, and above an extinction of $A_V \sim$ 5 CO freezes out. It would be expected that lower local densities would have H$_2$O and at higher densities CO and CH$_3$OH would be formed. Our results show that this is generally the case, but the lack of ice detections due to sensitivity limits complicates evidence of this trend.

In Chu et al. (2020) it is shown that only a small amount of CO is frozen out ($<$15%), but $\sim$30% of the CO ice is mixed with CH$_3$OH ice in two cores (L483 and L694-2). This implies that this mixture traces some of the densest parts of the core. Our results confirm this, showing that less than $\sim$2% of the volume of L4823 and L694-2 is dense enough for CH$_3$OH formation to occur. This small region of the core is, however, sufficient in converting CO into CH$_3$OH efficiently and allowing for complex organic molecule growth.

### 6. Summary

Five dense molecular cores were studied to constrain the total hydrogen volume densities where ice formation occurs and understand how densities vary in different protostellar environments. Using cores with a large population of background stars, NIR photometry was used to develop extinction maps with very high spatial resolutions. Implementing the new AVIATOR algorithm, these maps were projected into 3D space, allowing for measurements of the maximum density reached in each core. We find that the maximum density increases from cores that have not yet begun collapse to those that have infalling material, and finally the highest densities are in star-forming cores. The 3D maps also provided a way to determine the density required along the lines of sight where different ices form. We are particularly interested in the density at which CH$_3$OH forms, since that may indicate the initiation of more complex organic molecular growth. It is apparent that the CH$_3$OH ice forms at higher densities than other ices above $1 \times 10^6$ cm$^{-3}$. For the cores where CH$_3$OH was detected these densities are only reached in less than $\sim$2% of the total core; hence, CH$_3$OH and other complex organic molecules only trace very small dense regions.

Our method demonstrates a way to use NIR photometry to determine volume densities without the dependency on submillimeter emission data or radiative transfer models that introduce different assumptions. Extinction maps, however, also have drawbacks near the core center, due to a lack of background stars. With the upcoming James Webb Space Telescope fainter targets will be observable even in the most extincted regions, which should improve these measurements of the densest cores.

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