EVIDENCE FOR MULTIPLE PATHWAYS TO DEUTERIUM ENHANCEMENTS IN PROTOPLANETARY DISKS

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ABSTRACT

The distributions of deuterated molecules in protoplanetary disks are expected to depend on the molecular formation pathways. We use observations of spatially resolved DCN emission from the disk around TW Hya, acquired during ALMA science verification with a ∼3″ synthesized beam, together with comparable DCO⁺ observations from the Submillimeter Array, to investigate differences in the radial distributions of these species and hence differences in their formation chemistry. In contrast to DCO⁺, which shows an increasing column density with radius, DCN is better fit by a model that is centrally peaked. We infer that DCN forms at a smaller radii and thus at higher temperatures than DCO⁺. This is consistent with chemical network model predictions of DCO⁺ formation from H₂D⁺ at T < 30 K and DCN formation from additional pathways involving CHD⁺ at higher temperatures. We estimate a DCN/HCN abundance ratio of ~0.017, similar to the DCO⁺/HCO⁺ abundance ratio. Deuterium fractionation appears to be efficient at a range of temperatures in this protoplanetary disk. These results suggest caution in interpreting the range of deuterium fractions observed in solar system bodies, as multiple formation pathways should be taken into account.

Key words: astrochemistry – circumstellar matter – ISM: molecules – molecular processes – stars: pre-main sequence

Online-only material: color figures

1. INTRODUCTION

Deuterium fractionation in interstellar cloud cores, protostars, and solar system bodies is frequently used to infer important aspects of their physical and chemical histories (Brown et al. 1988; Herbst & van Dishoeck 2009; Mumma & Charnley 2011). The deuterium enhancement in Earth’s sea water, with respect to the cosmic abundance, has been used as an argument for volatile delivery to the young Earth from cold, comet-like planetesimals, even though most present-day comets have about a factor of two higher D/H ratio compared to Earth’s sea water (Mumma & Charnley 2011). Recent observations of Earth-like deuterium fractionation in a Jupiter family comet (Hartogh et al. 2011) have lent further support to this scenario. Deuterated molecules, notably DCO⁺ and DCN, are also detected in a handful of protoplanetary disks, the sites of ongoing planet formation, with abundances that imply deuterium enhancements by orders of magnitude (van Dishoeck et al. 2003; Guilloteau et al. 2006; Qi et al. 2008; Oberg et al. 2010, 2011). Understanding how and under what conditions these deuterated molecules form in disks is key to using deuterium fractionation to probe physical conditions, and to explaining the deuterium fractionation pattern in the solar system. The formation chemistry of DCN is of particular interest since the DCN/HCN ratio can be measured in both comets (e.g., Meier et al. 1998) and disks, enabling direct comparison.

Deuterium levels in molecules are enhanced above the cosmic deuterium abundance of ∼2 × 10⁻⁵ because of differences in zero-point energy between deuterated species and the non-deuterated equivalents. The reverse reactions are efficiently inhibited at low temperatures, resulting in deuterium fractionation. However, the “low-temperature” regime is different for different reactants. Deuterated species that form from reactions with H₂D⁺, in particular DCO⁺, are expected to be abundant only at temperatures below 30 K (Willacy 2007) because of the modest activation energy of 230 K for converting H₂D⁺ back to H₂ (Gerlich et al. 2002). The activation energy barrier for the conversion between CHD⁺ and CH⁺ is higher, 390 K (Asvany et al. 2004), and CHD⁺ can therefore drive a warmer deuterium chemistry. Theoretically, DCN may form through reactions with the CHD⁺ reaction product CHD, as well as with H₂D⁺, DCO⁺, D, and through grain surface reactions followed by thermal or non-thermal desorption (Aikawa & Herbst 2001; Willacy 2007). Observations of warm DCN in the Orion bar provide observational evidence for that the CHD⁺ reaction pathway is important under some interstellar conditions (Parise et al. 2009). The formation pathways of DCN that are efficient in disks have yet to be constrained by observation.

TW Hydrae is the most well-studied protoplanetary disk because of its proximity (51 pc) and near face-on viewing geometry that allows for direct investigation of the radial distribution of molecular emission. Millimeter emission from CO, HCO⁺ 3–2, DCO⁺ 3–2, HCN 3–2, and DCN 3–2 lines have been spatially resolved using the Submillimeter Array (SMA). Analysis of DCO⁺ emission showed that the DCO⁺ column density increases with radial distance from the star, out to ∼90 AU, consistent with the low-temperature formation pathway from H₂D⁺ (Qi et al. 2008). The DCN emission was too weak for detailed modeling, but newly released Atacama Large Millimeter/submillimeter Array (ALMA) science verification data on DCN 3–2 toward TW Hydrae have higher signal-to-noise ratio and allow for significant constraints. In this paper, we use these new data to compare the DCN and DCO⁺ distributions, and to test whether these data suggest different pathways to deuterium enhancements in these species as predicted by some models of disk chemistry.
2. SPATIALLY RESOLVED OBSERVATIONS OF DCN AND DCO$^+$ TOWARD TW HYA

TW Hya was observed on 2011 April 20 and 23 in ALMA band 6 as a part of ALMA science verification. The calibrated visibilities and CLEANed reference images were released and made available to the public in 2011 August. These observations include the DCN $J = 3–2$ line at 217.238 GHz, which was acquired with a channel spacing of 0.16 km s$^{-1}$ (resampled to 0.2 km s$^{-1}$) and synthesized beam size $2.8 \times 2.3''$, with an rms of 12 mJy beam$^{-1}$ in the line-free channels. These data are comparable in resolution to the previous observations of Qi et al. (2008), with a noise level 14 times better for the ALMA data compared to the SMA observations.

Figure 1 displays the integrated DCN 3–2 emission toward TW Hya. The DCN emission is peaked on the TW Hya stellar position and spatially compact, barely resolved with the ALMA beam. For comparison, Figure 1 shows the integrated DCO$^+$ 3–2 emission, which does not peak at the stellar position and appears more extended. Using the DCO$^+$ velocity channel maps, especially the peanut-shaped central one that provides strict constraints on the DCO$^+$ radial distribution, Qi et al. (2008) demonstrated that the DCO$^+$ column density increases with distance from the central star out to 90 AU. Since the excitation characteristics of the DCN and DCO$^+ J = 3–2$ lines are similar, the differences in the Figure 1 images suggest different abundance distributions. In particular, DCN appears to be more abundant in the inner (warmer) disk regions compared to DCO$^+$.

3. THE DCN RADIAL PROFILE

To constrain the radial distribution of the DCN column density, we use the same methods as Qi et al. (2008) to model observations of DCO$^+$, HCO$^+$, and HCN emission from TW Hya. First, we adopt a physical structure of the TW Hya disk with density and temperature distributions from Qi et al. (2004, 2006). Second, we assume that DCN exists in a disk layer with vertical boundaries given by the best-fit values for HCN in Qi et al. (2008); the boundaries of DCN are not very well determined from the present data and chemical models predict a similar vertical distribution of DCN and HCN (Willacy 2007). Third, we model the DCN column density in this layer as a power law, $N_{10} \times (r/10^4)^{\alpha}$, where $N_{10}$ is the column density at 10 AU, $r$ is the distance from the star in AU, and $\alpha$ is the power-law index.

Based on the DCN data, the model is cut off at 100 AU, which is in agreement with previous models of DCO$^+$ and HCN. For HCN and DCO$^+$, Qi et al. (2008) found $\alpha \sim -1$ and $\alpha \sim 2$, respectively. We therefore tested models of DCN column density with three different values of power-law index, $\alpha = -1, 0, 2$, to investigate if the DCN distribution can be modeled similarly to DCO$^+$, or if it can be better described by a flat or decreasing function of radius. A more detailed characterization of the shape of the DCN radial profile requires higher spatial resolution than currently available.

For each power-law model, we optimize $N_{10}$ by minimizing the $\chi^2$ value, the weighted differences between the observed and modeled complex visibilities. The techniques are described in detail in Qi et al. (2008), and the best-fit models are shown in Figures 2 and 3. Unlike the DCO$^+$, the DCN $J = 3–2$ line is complicated by hyperfine structure. The central DCN line quartet at 217.23863 GHz is separated by 0.23 MHz (0.32 km s$^{-1}$) from a singlet at 217.23840 GHz, with 22% of the intensity of the quartet. This is close enough in frequency and strong enough in relative intensity to affect the shape and strength of emission in the channel maps. We use the Monte Carlo radiative transfer code RATRAN (Hogerheijde & van der Tak 2000), taking into account the DCN hyperfine structure, to produce model visibilities that are sampled at the appropriate spatial frequencies for comparison with the ALMA data. The relative population of the hyperfine levels are assumed to be in LTE, and the relative optical depth of the hyperfine transitions including line overlap is accounted for accurately.

Figure 3 shows a comparison between the observed DCN $J = 3–2$ line channel maps and the best-fit models for power-law indices $\alpha = -1, 0, 2$. The model with $\alpha = -1$ clearly provides the best fit to the data, as models with $\alpha = 0$ and $\alpha = 2$ underestimate the emission in the line wings, show offsets from the observed peaks, and appear more elongated in the central channel than the data. Note that the peanut-shaped feature in the systemic velocity channel map of DCN Model 3 is not as obvious as for DCO$^+$ (Qi et al. 2008) because of the blending of DCN hyperfine components. The better fit of the model with a negative power index is reflected in the $\chi^2$ values of the models, which increase from 2296194 for Model 1, to
2298334 for Model 2, and to 2300603 for Model 3. (Note that we have not excluded the possibility that DCN is even more centrally peaked than assumed in Model 1.)

Using Model 1 and the HCN profile reported by Qi et al. (2008), we calculate the DCN/HCN abundance ratio to be \(\sim 0.017\) in the TW Hya disk. This result does not depend strongly on the model power-law indices; varying the power-law indices by \(\pm 2\) changes the ratio by less than 30%. This ratio is similar to the previously measured DCO\(^+\)/HCO\(^+\) abundance ratio of 0.035 in the TW Hya disk (van Dishoeck et al. 2003).

4. DISCUSSION

The observations demonstrate that DCN is centrally peaked on the size scales observed, ruling out common radial distributions for DCN and DCO\(^+\). The presence of DCN closer to the star, in regions that are warmer due to stellar irradiation, together with the comparable estimates for the DCN/HCN and DCO\(^+\)/HCO\(^+\) abundance ratios, suggests a mechanism for efficient deuterium enhancement in disk material at higher temperatures than implied by reactions solely with H\(_2\)D\(^+\) at \(T < 30\) K. This agrees with standard model predictions in that DCN can form from gas-phase reactions involving CH\(_2\)D\(^+\) at \(T > 30\) K. However, there are several alternative chemical mechanisms that have the potential to affect the relative distributions of DCO\(^+\) and DCN, including photochemistry, additional gas-phase reactions that result in HCN deuterium fractionation, grain surface formation of DCN followed by desorption, and molecule-specific destruction such as depletion onto interstellar grains. Since the origins of DCO\(^+\) are reasonably well understood, we will focus on the mechanisms that affect the DCN distribution.

Before doing so, we note that it is possible for dynamical processes to transport cold chemistry products to warmer disk regions. If the destruction rates are slow compared to formation, then high deuterium fractionation at \(T > 30\) K does not a priori imply warm deuterium chemistry. In the context of the DCN and DCO\(^+\) distributions observed in the TW Hya disk, both DCN and DCO\(^+\) could form cold, and then DCO\(^+\) could be destroyed during gas diffusion inward, while most DCN survives. Such a scenario seems unlikely in light of recent models of disk chemistry with diffusion that show HCN chemistry is faster than that for HCO\(^+\) (Semenov & Wiebe 2011). An HCN deuterium fractionation mechanism that differs from DCO\(^+\) chemistry is thus required to explain the observed DCN distribution.

Photochemistry can produce deuterium fractionation and Thi et al. (2010) show that high HDO/H\(_2\)O ratios in disk gas can be achieved through photochemistry at \(T > 100\) K, where the HDO formation rate depends on the O+HD reaction. DCN can similarly form through CN+HD. This reaction has a barrier of \(\sim 3000\) K (Johnston & Bersohn 1989), however, and formation of DCN from CN+HD seems unlikely to contribute significantly to the TW Hya DCN distribution on \(>50\) AU size scales in the absence of significant vibrational or electronic excitation of the CN. This is consistent with the HDO model results, where the same mechanism seems to be exclusive to the atmosphere of the inner disk where UV fluxes are very high. Since ultraviolet induced photochemistry should operate mainly in the disk atmosphere, resolved observations of multiple DCN transitions that can constrain the DCN excitation and vertical abundance distribution could be used to address the viability of this mechanism.

Freeze-out onto grain surfaces has the potential to regulate the DCN distribution relative to DCO\(^+\) because of the different binding energies of DCN and CO. Gas absorption onto grains is predicted to produce molecule-specific “snowlines” beyond which abundances drop dramatically. This mechanism clearly works in a centrally peaked abundance distribution, though warm deuterium chemistry would still be required to produce DCN in the first place. It seems unlikely, however, that freeze-out could regulate the HCN and DCN distributions on the observed size scales. HCN has a comparable adsorption energy to H\(_2\)O (Aikawa et al. 1996), which, for the TW Hya disk, results in a snowline at a radius \(<10\) AU (Qi et al. 2008). This does not exclude the possibility that the DCN distribution is directly regulated by depletion onto grain surfaces at smaller radii. In fact, in the inner hot region of several disks, where HCN is detected at infrared wavelengths, the abundances are much higher than observed in outer disks at millimeter wavelengths, suggestive of an abundance drop at a few AU due to ice formation beyond this radius (Salyk et al. 2011).

Beyond this snowline, ice formation products may be returned to the gas phase through photodesorption (e.g., Öberg et al. 2009). Both laboratory experiments and observations of grain
surface products show that deuterium fractionation can be very efficient in interstellar ices (Nagaoka et al. 2005; Parise et al. 2006). Theoretically, the DCN/HCN ratio in ices can reach values of 2 × 10^{-2}, similar to the ratios predicted from pure gas-phase chemistry (Aikawa & Herbst 1999; Willacy 2007). Recent determinations of low abundances of cold H2O gas toward TW Hya and DM Tau (Bergin et al. 2010; Hogerheijde et al. 2011) suggest, though, that H2O ice evaporation is not efficient outside of a few AU radius. Because of the low abundances of HCN and DCN relative to H2O, these species are likely to act as minor impurities when formed in the ice, and desorb only where H2O ice desorbs. Thus, while we cannot rule out ice photodesorption as a contributor to the observed DCN distribution, it is unlikely to be the dominant process.

Having dismissed dynamics, photochemistry, and mechanisms requiring grains as plausible routes to significant deuterium fractionation in the outer disk, this leaves additional gas-phase formation routes of DCN as the main alternative to the reactions involving CH2D+. In the gas phase, DCN can form from HNC+D+ (e.g., Willacy 2007). The deuterium fractionation in HCN then depends on the gas-phase D/H ratio. The D/H ratio is predicted to be <10^{-3} at large disk radii (250 AU in a generic disk model), while it reaches and possibly exceeds 10^{-2} in the inner disk midplane (17–50 AU; Willacy 2007; Willacy & Woods 2009). Thus, reactions between D and HCN provide a plausible pathway to deuterium fractionation in HCN in some regions of the disk, and detailed modeling is needed to provide predictions on the vertical and radial abundance profiles resulting from this formation mechanism.

In summary, several reaction and destruction mechanisms may contribute to the DCN abundance pattern observed in the TW Hya disk. However, warm CH2D+ -driven deuterium chemistry in the inner disk and cold H2D+ -driven deuterium chemistry in the outer disk are likely to dominate over the alternatives at the disk radii probed by the observations, and these pathways form a consistent picture on their own. A warm CH2D+ -driven deuterium chemistry was also the favored explanation for the observations of DCN in the Orion bar (Parise et al. 2009). To determine definitively which formation pathway(s) dominate in disks will require interferometric observations with higher spatial resolution, observations of related molecules and isotopologs, and more detailed models of DCN radial distributions for the different chemical scenarios. For example, if photodesorption is important, then DCN should spatially correlate with other grain surface products, and a powerful photochemistry may enhance the 15N/14N ratio in HCN, analogous to what is observed in Titan’s atmosphere (Liang et al. 2007). Whichever DCN formation pathway dominates, the substantial deuterium enrichment in warmer regions of the TW Hya disk challenges the conventional wisdom that the high deuterium fractions in comets are necessary evidence for a cold (T < 30 K) chemical history (Mumma & Charnley 2011). Most comet deuterium fractions are measured from the D/H ratio in cometary water. In Oort cloud comets this ratio is ~3 × 10^{-4}, enhanced by an order of magnitude compared to the cosmic D/H ratio. Higher D/H ratios of 0.0023–0.025 have been observed for DCN/HCN in Hale-Bopp, consistent with models of gas-phase deuterium followed by freeze-out (Meier et al. 1998; Blake et al. 1999). In light of the TW Hya results, even this high ratio does not imply a cold, T < 30 K origin of the comet material, but may instead reflect the existence of a lukewarm pathway to deuterium enhancements in the Solar Nebula. The radial distributions of DCN and DCO+ in disk material around TW Hya and other T Tauri stars should be revisited by ALMA at higher resolution to investigate whether the observed deuterium chemistry trends persist at smaller scales. Until then, care should be exercised in interpreting the D/H ratios in cometary material.

In general, resolved distributions of molecular emission in disks have the potential to put stronger and more direct constraints on key aspects of chemical evolution than (global) abundance ratios. In the case of DCN, the DCN/HCN abundance ratio of ~10^{-2} is consistent with a range of chemical models that assume different formation pathways. However, the observation of different radial distributions of DCN and DCO+ immediately suggests the presence of different formation pathways for these species and rule out that DCN is mainly formed through reactions with H2D+.

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