Young Stars & Planets Near the Sun
Proceedings IAU Symposium No. 314, 2015
J. H. Kastner, B. Stelzer, & S. A. Metchev, eds.

doi:10.1017/S1743921315006237

The Chemistry of Nearby Disks

Karin I. Öberg

Harvard-Smithsonian Center for Astrophysics, 60 Garden St, MS 16, Cambridge, MA 02138
email: `koberg@cfa.harvard.edu`

Abstract. The gas and dust rich disks around young stars are the formation sites of planets. Observations of molecular trace species have great potential as probes of the disk structures and volatile compositions that together regulate planet formation. The disk around young star TW Hya has become a template for disk molecular studies due to a combination of proximity, a simple face-on geometry and richness in volatiles. It is unclear, however, how typical the chemistry of the TW disk is. In this proceeding, we review lessons learnt from exploring the TW Hya disk chemistry, focusing on the CO snowline, and on deuterium fractionation chemistry. We compare these results with new ALMA observations toward more distant, younger disks. We find that while all disks have some chemical structures in common, there are also substantial differences between the disks, which may be due to different initial conditions, structural or chemical evolutionary stages, or a combination of all three.

Keywords. astrochemistry, protoplanetary disks, ISM: molecules, radio lines: ISM

1. Introduction

Gas and dust-rich disks seem ubiquitous around young stars. The planet formation potential of these disks depends fundamentally on the disk dust and gas mass. Measuring disk masses is difficult, however. We are practically blind to the main constituent, cold H_2 gas. Observations of dust continuum emission is a popular proxy, assuming a constant gas-to-dust conversion ratio. Disk demographic studies relying on such measurements suggest that the material needed to assemble a planetary system similar to our Solar System is frequently present around young stars (Andrews *et al.* 2013). Even around the smallest stars, there is more than sufficient mass in grains to form several Earth-like planets. This finding is in good agreement with exo-planet statistics, including the inferred high frequency of rocky planets around M dwarfs (Dressing & Charbonneau 2015). Assuming a constant gas-to-dust ratio may be a poor approximation, however, due to a combination of dust growth into boulders that are hidden from view, decoupled dust and gas dynamics, and efficient gas photoevaporation from the disk atmosphere. CO line observations have been used as a more 'direct' tracer of the disk gas mass (Williams & Bast 2014), but suffer from their own set of constraints, including a poorly constrained chemistry and therefore CO-to-H_2 conversion factor under many disk conditions (Favre *et al.* 2013). Constraining this chemistry and therefore the utility of CO as a disk gas tracer should clearly be a priority for upcoming disk studies (Bergin *et al.* 2013). This statement can be generalized to other molecular tracers or important disk characteristics, such as temperature, density, and ionization profiles.

Understanding the chemical compositions of disks is also an end in itself. The compositions of planets depend fundamentally on the composition of the disk dust grains and disk volatiles they form from, and on how this composition varies with distance from the central star. Of especial importance for planet formation is the separation of volatiles into their gas and ice phases, which is set by the balance of adsorption ("freeze-out" of the gas phase onto solids), and desorption (back to the gas phase). We call the midplane

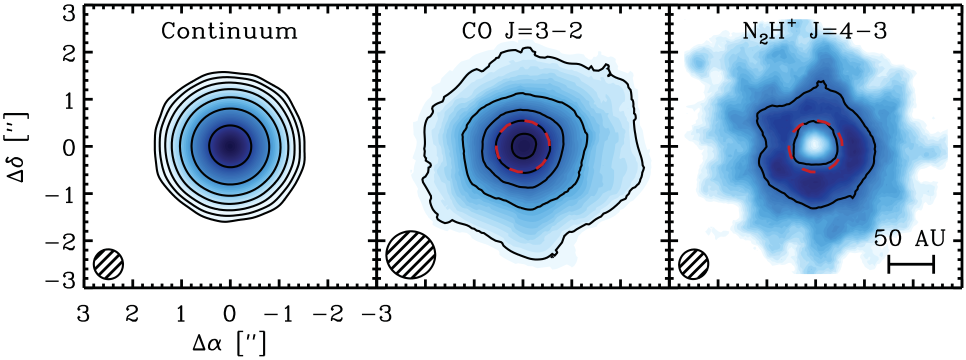

Figure 1. The dust continuum, CO and N_2H^+ emission toward TW Hya. The red dashed circle marks the inferred CO snowline location. (reprinted with permission from Qi *et al.* 2013b).

radius where freeze-out overtakes desorption for a major volatile a 'snowline'. Because of an exponential dependence of desorption rates on temperature these transitions are expected to be sharp and may thus be properly referred to as 'lines' when only considering the midplane regions. Snowlines can enhance the planet formation efficiency through a combination of increased grain surface density, rapid particle growth due to cold-head effects, pressure traps and increased grain stickiness (Ciesla & Cuzzi 2006, Johansen *et al.* 2007, Chiang & Youdin 2010, Gunlach *et al.* 2011, Ros & Johansen 2013). Snowline locations will also regulate the compositions of forming planets (Öberg *et al.* 2011) and planetesimals. In this proceeding we will only consider the CO snowline, simply because it occurs at a low temperature, i.e. far from the central star, and can thus be resolved by ALMA (§2).

A third aspect of planet formation is how Earth (and by extension, Earth-like planets and exoplanets) obtained its water. The Earth's oceans may have outgassed from the mantle, or may have been delivered by icy bodies bombarding the young Earth, or a combination of both. One approach to resolve this question is to compare the terrestrial water isotopic composition (level of deuterium enrichment) with other Solar System and interstellar water reservoirs. Using deuterium fractionation as a probe of the thermal history of terrestrial water (and other volatiles) presupposes a good understanding of the distribution and chemistry of deuterated molecules in the Solar Nebula. This chemistry is not well constrained in disks, however, and in §3 we discuss what observations of different deuterated species in the TW Hya disk and in younger disks can teach us about deuterium fractionation during planet formation.

2. Disk Snowlines

The locations of major snowlines depend on the volatile composition (e.g. whether most nitrogen is in N_2 or NH_3), a balance between freeze-out and thermal and non-thermal desorption rates at different disk locations (set by a combination of density, temperature and radiation fields), and disk dynamics (Öberg *et al.* 2011). Exact snowline locations are therefore difficult to predict from theory, and observational constraints are key to constrain planet formation models. The CO snowline is expected at the disk radius where the temperature drops below ∼20 K. Around T Tauri and Herbig Ae disks this threshold is crossed at ∼20–150 AU.

Extractions of CO snowline locations using CO observations is challenging because of the presence of large amounts of CO in the disk atmosphere (Qi *et al.* 2011). An alternative approach is to exploit chemical effects regulated by CO freeze-out to constrain the location of the CO snow line. Three proposed CO snow line tracers are N_2H^+, H_2CO, and DCO^+ (Qi *et al.* 2013, Mathews *et al.* 2013). N_2H^+ is expected to be a robust tracer of CO freeze-out because the presence of gas phase CO slows down N_2H^+ formation and speeds up N_2H^+ destruction. The predicted anti-correlation between gas-phase CO and N_2H^+ is observed in pre-stellar and protostellar environments (e.g. Caselli *et al.* 1999, Bergin *et al.* 2002, Jørgensen *et al.* 2004). Qi *et al.* (2013b) imaged N_2H^+ emission with the Atacama Large sub-Millimeter Array (ALMA) toward the disk around T Tauri star TW Hya and found a large ring with an inner edge at 30 AU, tracing the CO snowline (Fig. 1). The determined CO snowline location corresponds to a CO freeze-out temperature of 17 K, using a detailed disk density and temperature structure. This is a few degrees lower than expected, which may reflect a combination of model uncertainties and excess CO depletion due to chemical conversion of CO into other species in this old disk.

With ALMA similar measurements using N_2H^+ are possible toward samples of disks. So far only one such additional measurement exists. N_2H^+ observations with ALMA toward HD 163296 reveal a similar ring-like structure as previously observed toward TW Hya, but the inferred CO snowline location is substantially (10s of AU) closer to the star than expected from the inferred CO freeze-out temperature in the TW Hya disk. The HD 163296 CO snowline measurement corresponds to a CO freeze-out temperature of $\sim$25 K, 8 K higher than in the TW Hya disk (C. Qi, private communication). Such a high freeze-out temperature may be explained by dynamics (moving the snowline inwards due to drift of solids) or a water-rich ice morphology. CO is known to bind stronger to water ice compared to other CO molecules and even small amounts of water forming or freezing out with the CO ice could increase the CO freeze-out temperature by several degrees (Collings *et al.* 2004).

In summary: there are two measurements of CO snowline locations and the results are two substantially different CO freeze-out temperatures. The causes for these differences are unclear, though there are several candidates, including disk dynamics and ice chemistry. This result entails that we cannot currently use theory to predict the CO freeze-out temperature or the location of the CO snowline in a disk, including the Solar Nebula. There is a clear need for a survey of CO snowline locations toward disks to 1. constrain how CO freeze-out depends on disk structure and evolution, and 2. establish the 'typical' CO freeze-out temperature during planet formation.

3. Deuterium Fractionation

Deuterium fractionation is commonly used to infer (thermal) properties about volatile formation locations. Molecules become enriched in deuterium due to small differences in zero-point energies between deuterated and non-deuterated molecules, which results in preferential formation of deuterated molecules at low temperatures. Based on this understanding, the high D/H ratio in terrestrial H_2O has been used to infer delivery of water from asteroids and comets, which both assembled in the colder, outer Solar System (Hartogh *et al.* 2011). The generally high D/H ratio in Solar System water has further been used to infer a cold pre-Solar origin of most Solar System H_2O (Cleeves *et al.* 2014).

So far only two deuterated molecules have been detected in disks, DCO^+ and DCN (van Dishoeck *et al.* 2003, Qi *et al.* 2008). Figure 2 shows Submillimeter Array (SMA) observations of DCO^+ in the TW Hya disk. The DCO^+ emission presents a low SNR ring. When compared with HCO^+ toward TW Hya, this ring implies an increasing level of deuterium fractionation with disk radius. This is in agreement with theoretical

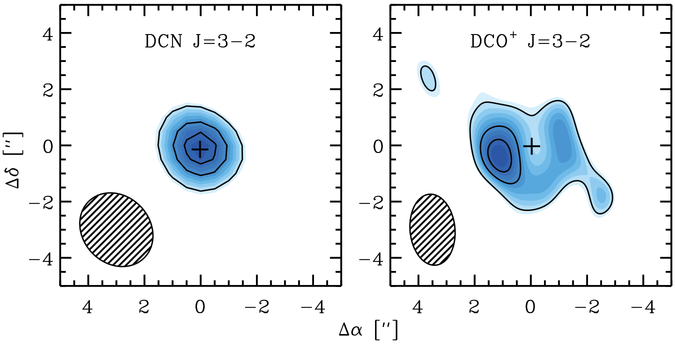

Figure 2. Integrated images of the TW Hya disk in (*left:*) DCN J=3-2 emission (ALMA science verification) and (*right:*) DCO$^+$ J=3-2 emission (SMA data from Qi *et al.* (2008)). The contour levels are at 50%, 75% and 90% of the peak value. The cross marks the peak of the continuum emission, which locates the position of the central star. Reprinted with permission from Öberg *et al.* (2012).

expectations, since the temperature in the disk midplane decreases with increasing disk radius. By contrast, DCN emission presents a centrally peaked feature toward the TW Hya disk (Fig. 2). This suggests that deuterium fractionation in HCN occurs at higher temperatures compared to HCO$^+$. There are clearly multiple pathways to deuterium fractionation in disks, which operate in different temperature regimes (Öberg *et al.* 2012). This already complicates the use of deuterium fractionation as a thermal history probe.

The picture is complicated further by recent observations of DCO$^+$ and DCN toward a small sample of disks with ALMA. Figure 3 shows the different DCO$^+$ and DCN 3–2 emission morphologies toward three disks around T Tauri stars AS 209, V 4046 Sgr and IM Lup. These disks were observed during 2014 and 2015 with the Atacama Large Millimeter/Submillimeter Array (ALMA; project code 2013.1.00226) with ~30 antennas, spanning baselines of 15–650 m. The total on source integration time was ~20 minutes. The visibility data were calibrated by ALMA staff. Each individual SPW was further phase and amplitude self-calibrated in CASA 4.2.2. In each SPW, the continuum was subtracted using line-free channels. The fully calibrated visibilities were Fourier inverted and CLEANed.

Similarly to the TW Hya disk, the DCO$^+$ emission maps always present a hole or depressions toward the warm disk center. In contrast to the previous TW Hya observations, the DCN emission maps also present central depressions toward all three disks. This may simply be an effect of the increased spatial resolution employed for these observations, however. A second similarity between TW Hya and the disk sample is that the DCN emission appears to be more compact than the DCO$^+$ emission, suggesting that cold deuterium fractionation chemistry is generally more important for DCO$^+$ production compared to DCN. These structural similarities between TW Hya and the younger disk sample in Fig. 3 are accompanied by several important differences, however.

Figure 3 shows the relative sizes of the DCO$^+$ and DCN central emission depressions vary between different disks. Toward AS 209, the radius of the central DCO$^+$ hole is smaller than the DCN hole radius. The opposite is true for the relative hole sizes of DCO$^+$ and DCN in the transition disk around V4046 Sgr, which also presents the largest DCO$^+$ hole in the sample. IM Lup presents the most surprising morphology, a set of concentric rings in DCO$^+$ emission (Öberg *et al.* 2015, submitted to ApJ). DCN is barely detected in this source. Together with TW Hya, this small disk sample reveals that there is no simple relationship between disk radius and the deuterium pathways that results in deuterium

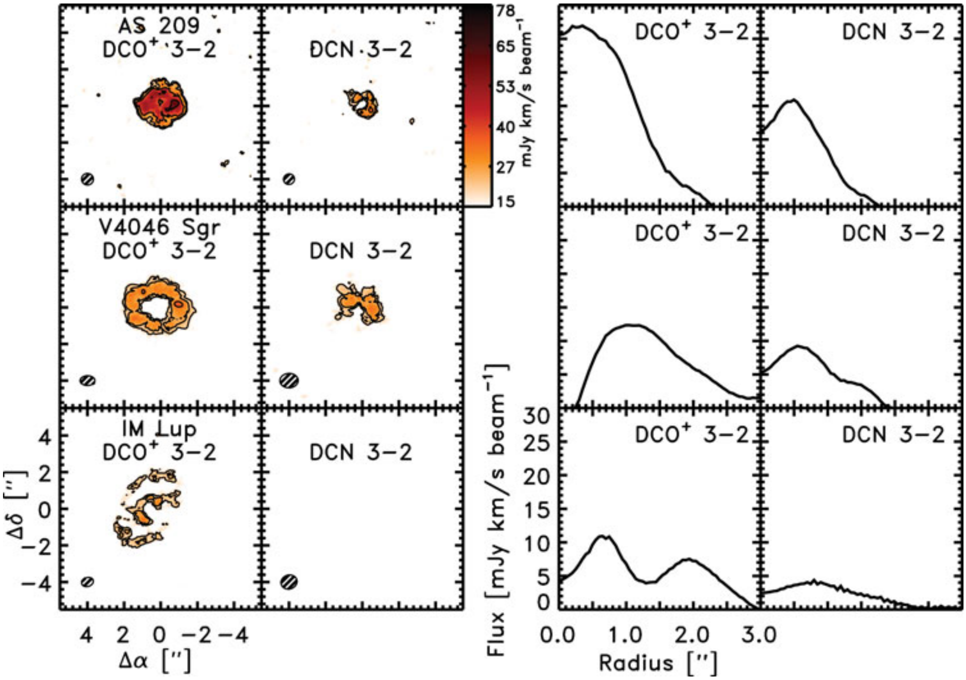

Figure 3. DCO^+ and DCN emission toward three protoplanetary disks. The left panels show the integrated emission maps of DCO^+ and DCN with the color scale marking the flux density in mJy km/s beam^{-1} (the beam is shown in the bottom left of each panel). The right panels show the corresponding deprojected and azimuthally averaged radial profiles.

enrichments of either HCO^+ or HCN. In particular DCN does not always extend further in toward the central star compared to DCO^+. In summary: even when only considering two molecules, the deuterium enrichment pattern observed toward TW Hya does not appear to be universal in protoplanetary disks.

4. Conclusions

TW Hya has been and will continue to be an important starting point when studying disk chemistry (see, e.g., Kastner *et al.* 1997, Thi *et al.* 2004, Qi *et al.* 2013b). Its proximity, well-established disk density and temperature structure and rich molecular inventory makes it ideal to develop new chemical probes. The chemistry of the TW Hya disk may be far from typical, however. The disk around TW Hya is old compared to most other gas-rich circumstellar disks, and disk chemistry is time dependent. In this proceeding we compared the observed chemistry in the TW Hya disk with other, younger disks focusing on two key processes: the chemical imprint of CO freeze-out, and deuterium fractionation. In both cases we found several similarities between the TW Hya disk and the other targets, but also substantial differences. For example, the CO snowline locations in the TW Hya and HD 163296 disks do not seem to correspond to the same CO freeze-out temperature, and the more centrally peaked DCN emission compared to DCO^+ observed toward TW Hya is not reproduced toward all other disks. Whether these differences trace different initial conditions, present differences in disk temperature, density and radiation structures, or different chemical evolutionary stages is currently unclear. Larger surveys of disk chemistry should be able to answer some of these questions, when combining the survey results with detailed disk density, temperature and radiation structures, theory and laboratory work. Only then can we expect to establish the 'typical' chemistry present during planet formation, and further, the origins of the present-day Solar System chemical composition.

This paper makes use of the following ALMA data: ADS/JAO.ALMA#2013.1.00226.S. ALMA is a partnership of ESO (representing its member states), NSF (USA) and NINS (Japan), together with NRC (Canada) and NSC and ASIAA (Taiwan), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ. The National Radio Astronomy Observatory is a facility of the National Science Foundation operated under cooperative agreement by Associated Universities, Inc. KIÖ also acknowledges funding from the Alfred P. Sloan Foundation, and the Packard Foundation.

References

Andrews, S. M., Rosenfeld, K. A., Kraus, A. L., & Wilner, D. J. 2013, *ApJ*, 771, 129
Bergin, E. A., Alves, J., Huard, T., & Lada, C. J. 2002, *ApJL*, 570, L101
Bergin, E. A., Cleeves, L. I., Gorti, U., et al. 2013, *Nature*, 493, 644
Caselli, P., Walmsley, C. M., Tafalla, M., Dore, L., & Myers, P. C. 1999, *ApJL*, 523, L165
Chiang, E. & Youdin, A. N. 2010, *Annual Review of Earth and Planetary Sciences*, 38, 493
Ciesla, F. J. & Cuzzi, J. N. 2006, *Icarus*, 181, 178
Cleeves, L. I., Bergin, E. A., Alexander, C. M. O., *et al.* 2014, *Science*, 345, 1590
Collings, M. P., Anderson, M. A., Chen, R., *et al.* 2004, *MNRAS*, 354, 1133
Dressing, C. D. & Charbonneau, D. 2015, ArXiv e-prints
Favre, C., Cleeves, L. I., Bergin, E. A., Qi, C., & Blake, G. A. 2013, *ApJL*, 776, L38
Gundlach, B., Kilias, S., Beitz, E., & Blum, J. 2011, *Icarus*, 214, 717
Hartogh, P., Lis, D. C., Bockelée-Morvan, D., *et al.* 2011, *Nature*, 478, 218
Johansen, A., Oishi, J. S., Low, M.-M. M., *et al.* 2007, *Nature*, 448, 1022
Jørgensen, J. K. 2004, *A&A*, 424, 589
Kastner, J. H., Zuckerman, B., Weintraub, D. A., & Forveille, T. 1997, *Science*, 277, 67
Mathews, G. S., Klaassen, P. D., Juhász, A., *et al.* 2013, *A&A*, 557, A132
Öberg, K. I., Murray-Clay, R., & Bergin, E. A. 2011a, *ApJL*, 743, L16
Öberg, K. I., Qi, C., Wilner, D. J., & Hogerheijde, M. R. 2012, *ApJ*, 749, 162
Qi, C., D'Alessio, P., Öberg, K. I., *et al.* 2011, *ApJ*, 740, 84
Qi, C., Öberg, K. I., & Wilner, D. J. 2013a, *ApJ*, 765, 34
Qi, C., Öberg, K. I., Wilner, D. J., *et al.* 2013b, *Science*, 341, 630
Qi, C., Wilner, D. J., Aikawa, Y., Blake, G. A., & Hogerheijde, M. R. 2008, *ApJ*, 681, 1396
Ros, K. & Johansen, A. 2013, *A&A*, 552, A137
Thi, W., van Zadelhoff, G., & van Dishoeck, E. F. 2004, *ApJ*, 425, 955
van Dishoeck, E. F., Thi, W., & van Zadelhoff, G. 2003, *A&A*, 400, L1
Williams, J. P. & Best, W. M. J. 2014, *ApJ*, 788, 59