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Millimeter-wave Observations of Gaseous Species in Disks

Geoffrey A. Blake

Division of Geological & Planetary Sciences, California Institute of Technology,
Mail Stop 150–21, Pasadena, CA 91125, USA
email: gab@gps.caltech.edu

Abstract. The role of high spectral and spatial resolution spectroscopy in understanding the evolution of the gaseous component of circumstellar accretion disks is described. Millimeter-wave emission lines from trace constituents such as CO, CN, HCO^+, and HCN can be used to probe the kinematic and physico-chemical properties in the near-surface regions of disks beyond 50–100 AU, but, thanks to extensive depletion in the midplane, they are not a reliable proxy for the disk mass. For the special case of nearly edge-on circumstellar disks, the resulting ices can be directly observed through mid-infrared spectroscopy, using ground based facilities or spacecraft (*cf.* Najita, this volume). Emerging and planned millimeter-wave → THz arrays will possess sufficient sensitivity and resolution to probe much closer to the central star and to search for prebiotic compounds such as those detected in comets, meteorites and interplanetary dust particles.

Keywords. astrochemistry — solar system: formation — stars: planetary systems: formation — stars: planetary systems: protoplanetary disks

1. Introduction

As the means by which matter and angular momentum are exchanged between molecular clouds and young stars and as the birth sites of planets, circumstellar disks provide the pivotal observational link between star formation and (exo)-planetary science. Though disks must be established very early in the star formation process, this overview is concerned primarily with those systems in which the vast majority of accretion has been completed. As the accretion process wanes, reprocessing of the central stellar radiation becomes the dominant source of energy release, and in these so-called passive circumstellar disks an examination of the re-radiated longer-wavelength photons can be used to learn a great deal about the physical properties of the disk.

The basic geometry is outlined in Figure 1. Material near the star and especially at the disk surface radiates strongly in the infrared, while the more distant and interior portions of the disk can best be probed at longer millimeter wavelengths where the bulk of the dust is optically thin. Near- and mid-infrared imaging can efficiently search for the presence or absence of such excess emission, and has been used to infer the presence of disks around hundreds of young stars. Infrared surveys also yield time scale estimates of order a few million years for the disappearance of small dust grains in the inner regions of circumstellar disks (Skrutskie *et al.* 1990; Robberto *et al.* 1999) – a span similar to that measured for the creation of differentiated planetesimals in the early solar nebula from the absolute ages of chondritic meteorites (Amelin *et al.* 2002). The time scale and associated mechanism(s) by which individual optically thick disks dissipate to become the optically thin, or debris, disks are not yet quantitatively known, but are exceedingly important to nebular chemistry and to the formation of planetary systems. The more tenuous debris disks themselves are estimated to survive for several tens, perhaps hundreds, of millions of

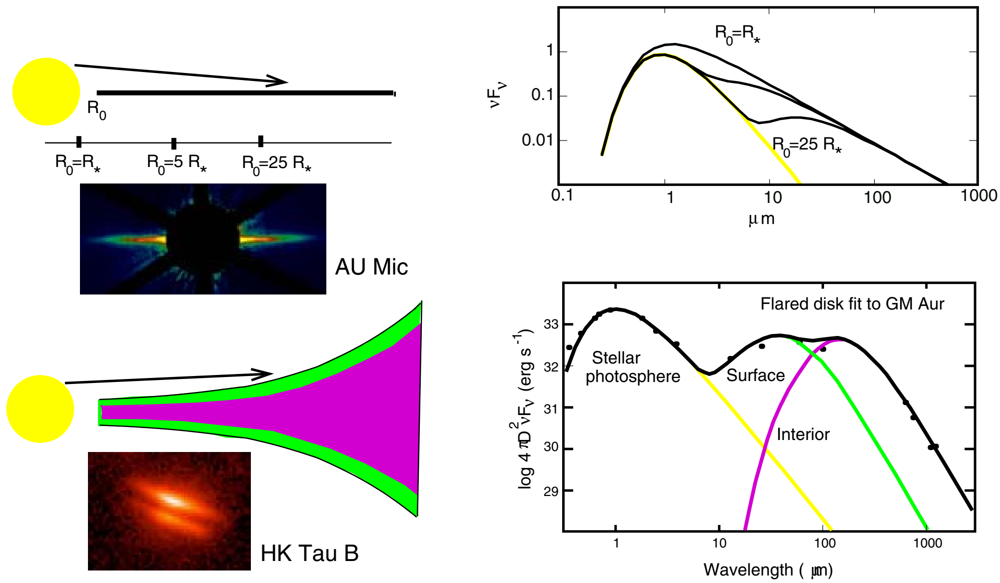

Figure 1. Schematic disk structure cross sections for passive flat *vs.* flaring (hydrostatic equilibrium) disks, and the spectral energy distributions (SEDs) that result. Conceptual models of the latter predict that the infrared portion of the SED is dominated by optically thin radiation from the disk surface layers exposed to the stellar radiation field, while the millimeter-wave emission is dominated by the cooler disk interior (Chiang & Goldreich 1997). Adapted from van Zadelhoff (2002), with inset images of AU Mic and HK Tau C from the Keck telescope (Liu 2004) and HST (Stapelfeldt *et al.* 1998), respectively. The top right panel illustrates the changes in the SED for successively larger inner holes in the dust distribution.

years in at least 15% of young main sequence stars, as judged from mid- and far-infrared continuum excesses of nearby stars (Rieke *et al.* 2005).

The spatio-temporal properties of disks as inferred from SEDs, namely masses of 0.001–0.1 $M_\odot$ and sizes of 10's to 100's of AU, are similar to those inferred for the Minimum Mass Solar Nebula (MMSN; Hayashi 1981); and have been verified for a *handful* of objects by detailed imaging, with millimeter-wave CO studies providing among the earliest and most conclusive evidence for the expected ∼Keplerian velocity fields (see Koerner *et al.* 1993; Dutrey *et al.* 1994). Direct optical/IR imaging and, especially, interferometry (Monnier & Millan-Gabet 2002) has begun to probe closer to the central stars, but cannot directly constrain critical disk properties such as the surface mass density or accretion flows, while at present millimeter-wave studies can only probe the outer regions of disks. Similarly, disk dissipation studies based on infrared excesses tell us little about the gas content of such objects. The discovery of extrasolar 'hot Jupiters' some 0.05 AU from their parent stars (Marcy, Cochran & Mayor 2000) has highlighted the important role of star-disk-protoplanet interactions and time scales, and demands new tools that can investigate the critical planet-forming zone of disks. As described by Najita (this volume), mid-infrared spectroscopy provides one current route to studies of gas in the inner disk. Below I briefly outline future possibilities with the millimeter-wave arrays presently under construction or expansion.

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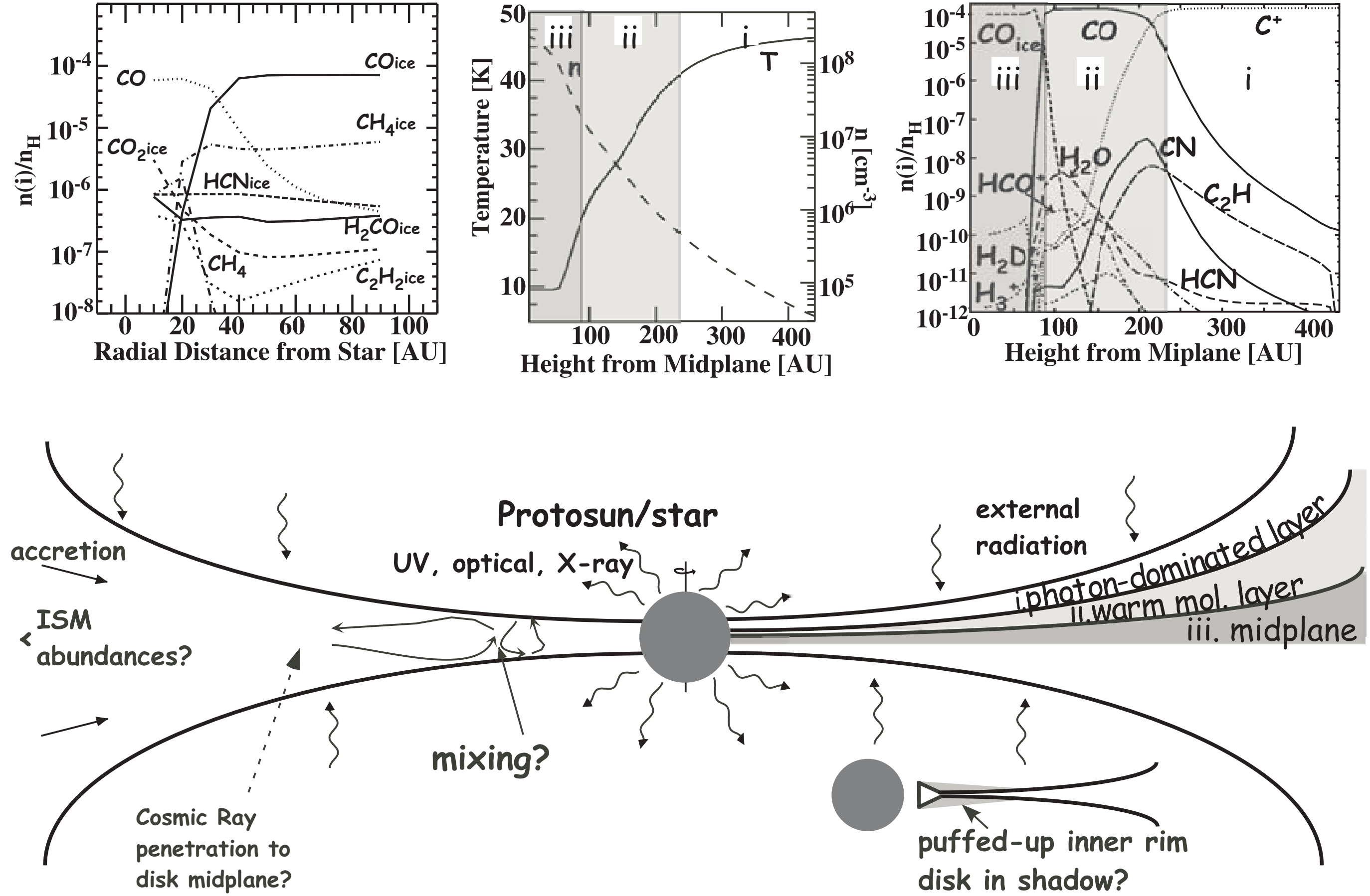

Figure 2. Chemical structure of protoplanetary disks. The disk is schematically divided into three zones: a photon-dominated layer, a warm molecular layer, and a midplane freeze-out layer. The CO freeze-out layer disappears at $r \lesssim 100$ AU as the mid-plane temperature increases. Various non-thermal inputs, cosmic ray, UV, and X-ray, drive chemical reactions. Viscous accretion and turbulence transport the disk material both vertically and radially. The *upper panel* shows the vertical distribution of molecular abundances at $r \sim 300$ AU in a typical disk model (van Zadelhoff *et al.* 2003) and a sample of the hydrogen density and *dust* temperature at the same distance (D'Alessio *et al.* 1999). In upper layers ($\gtrsim 150$ AU) the *gas* temperature will exceed the dust temperature by $\gtrsim 25$ K (Jonkheid *et al.* 2004).

2. The Basic Physical and Chemical Structure of Disks

What do disk structures such as those outlined in Figure 1 imply for chemistry? Molecular abundances are determined by both the physical conditions, such as density and temperature, and transport time scales (see Kamp *et al.*, Markwick, this volume). Recent years have seen significant progress in characterizing disk physical structure, which aids in understanding disk chemical processes. As shown below, disks that are well isolated from intense radiation fields can be quite extended with $R_{out} \sim$ few hundred AU (Simon, Dutrey, & Guilloteau 2000), much larger than expected from comparison with the MMSN. The radial distributions of midplane column density and temperature have been estimated by observing thermal emission of dust; they are fitted by a power law $\Sigma(r) \propto r^{-p}$ and $T(r) \propto r^{-q}$, with $p = 0 - 1$ and $q = 0.5 - 0.75$. At a distance of 1 AU, T(1 AU)$\sim$100–200 K, while Σ(100 AU)$\sim$0.1–10 g cm^{-2} (e.g., Beckwith *et al.* 1990).

The vertical physical structure is estimated by calculating the hydrostatic equilibrium for the density and radiation transfer for the temperature (see Kamp *et al.*, this volume). Beyond several AU the disk is mainly heated by the central star. The stellar radiation is absorbed by grains at the disk surface, which then emit thermal radiation to heat the disk interior (Calvet *et al.* 1992; Chiang & Goldreich 1997). Hence the temperature decreases towards the midplane, as shown in Figure 2. For small radii ($r <$ few AU), however, heating by mass accretion is not negligible and the midplane can be warmer than the disk surface. At $r = 1$ AU, for example, the midplane temperature can be as high as 1000 K, if the accretion rate is large (D'Alessio *et al.* 1999). The density distribution is basically Gaussian, $\exp[-(Z/H)^2]$, with some deviation due to vertical temperature variations (see Figure 2). As a whole, a gas-rich disk has a flared structure, with a geometrical thickness that increases with radius (Kenyon & Hartmann 1987). Gas-poor, or debris disks, may well have a much more flattened geometry.

Based on such physical models, the current picture of the general disk chemical structure is schematically shown in Figure 2. At $r \gtrsim 100$ AU, the disk can be divided into three layers: the photon dominated region (PDR), the warm molecular layer, and the midplane freeze-out layer. The disk is irradiated by UV radiation from the central star and ISM that drives ionization and dissociation in the surface layer. In the midplane the temperature is mostly lower than the freeze-out temperature of CO (~ 20 K), one of the most abundant and volatile molecules in the ISM. Since the timescale of adsorption onto grains is short at high density ($\sim 10\,(10^9 \mathrm{cm}^{-3}/n_{\mathrm{H}})$ yr), heavy-element species are significantly depleted onto grains. At intermediate heights, the temperature is several tens of K, and the density is sufficiently high ($\gtrsim 10^6$ cm^{-3}) to ensure the existence of molecules even if the UV radiation is not completely attenuated by the upper layer (Aikawa & Herbst 1999; Aikawa *et al.* 2002). Here water is still frozen onto grains, trapping much of the oxygen in ices. Thus, the warm CO-rich gas layers will have C/O ~ 1, leading to a rich and extensive carbon-based chemistry (Willacy & Langer 2000).

Do such models provide a good match to observed abundances? The observational challenges of answering this question are highlighted in Figure 3, in which it can be seen that even the strongest lines from the most optically thick species are strongly beam diluted by the resolution achievable with single-dish telescopes that can operate over a wide frequency range. The combination of millimeter-wave imaging, described next, with submillimeter-wave spectroscopy forms a powerful means of constraining the temperature, density, and molecular abundances in disks (van Zadelhoff *et al.* 2001). Work in this area began with the pioneering observations of DM Tau and GG Tau with the IRAM 30-m telescope (Dutrey *et al.* 1997) and TW Hya with the JCMT (Kastner *et al.* 1997). Further detections of the higher-J lines of high dipole moment species such

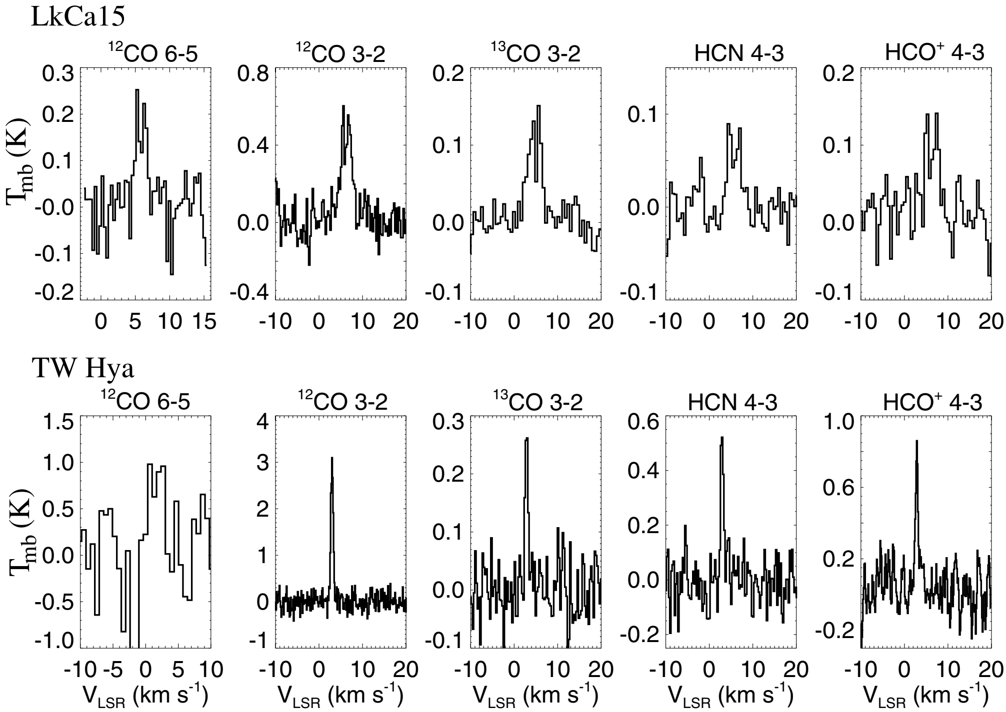

Figure 3. Submillimeter-wave emission lines from the LkCa 15 and TW Hydra circumstellar disks, observed with the JCMT and CSO (van Zadelhoff *et al.* 2001). The double-peaked nature of the emission lines from LkCa 15 is consistent with Keplerian rotation in an inclined disk ($i \sim 60°$); while TW Hydra is thought to be viewed nearly face on ($i \sim 7°$), hence the narrow lines.

as HCN and HCO^+ along with statistical equilibrium analyses demonstrated that the line emission indeed arises from the warm molecular layer with $n_{H_2} \approx 10^6$–10^8 cm^{-3}, $T \gtrsim 30$ K (van Zadelhoff *et al.* 2001). In agreement with theory, the gas-phase abundances are generally lower than in dense clouds, but the CN/HCN ratio is higher (see also Thi *et al.* 2004). The low molecular abundance is caused by depletion in the midplane, and the high CN/HCN ratio originates in the surface PDR (*cf.* Figure 2), as seen in PDR's in the ISM (Rodríguez-Franco *et al.* 1998).

At $r \lesssim 100$ AU, the midplane temperature is high enough to sublimate various ice materials that formed originally in the outer disk radius or parental cloud core (e.g., Markwick, this volume). This sublimation will be species dependent with the "frost line" for a given species appearing at different radii. For, example in the solar nebula the water ice frost line appeared near 3–5 AU, while the CO snow line would appear at greater distances where the midplane dust temperatures drop below ~20 K. Within these species-selective gaseous zones, sublimated molecules will be destroyed and transformed to other molecules by gas-phase reactions. In this fashion, the chemistry is similar to the so-called "hot core" chemistry, which appears in star-forming cores surrounding protostars (e.g., Hatchell *et al.* 1998; Liu, Hollis contributions to this volume). For example, sublimated CH_4 is transformed to larger and less volatile carbon-chain species, which can then accumulate onto grains (Aikawa *et al.* 1999). The very deepest single-dish integrations have begun to reveal more complex species (Thi *et al.* 2004), though the larger organics often seen toward hot cores/corinos remain out of reach of existing single-dish telescopes.

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3. (Sub)Millimeter-wave Imaging Spectroscopy of Disks

From studies such as those outlined above, a suite of disks have been identified that are many arcseconds in diameter, either because they are nearby (TW Hya) or are intrinsically large (AB Aur). The evolutionary status of the individual objects can be difficult to obtain, but is pivotal to a proper interpretation of the molecular observations. As first argued by Hogerheijde (2002) and described further in the posters by Brinch *et al.*, Guilloteau *et al.*, and Semenov *et al.* at this meeting, the very large structures seen in dust and molecular line emission around L1489 and AB Aur (see Figure 4) may provide examples of sources in which the dynamic accretion that characterizes embedded protostars is giving way to the centrifugal support that dominates more mature star+disk systems. Such systems would not only provide estimates of the 'initial conditions' for studies of disk chemistry, at high spatial resolution they would provide stringent constraints on the mechanisms of angular momentum redistribution in star and planet formation.

For stars that are closer to the main sequence (GM Aur, LkCa 15, DM Tau), the age, large size, and masses of their surrounding disks make them important for further study since they may represent an important transitional phase, in which viscous disk spreading and dispersal competes with planetary formation processes. At present, aperture synthesis observations can only sense the line emission from the outer disk ($r > 30 - 50$ AU; see Dutrey & Guilloteau 2004; Dutrey *et al.* 2005) for stars in the nearest molecular clouds. Thus, the *chemical* imaging of disks is rarer still, with studies concentrating on a few of the best characterized T Tauri and Herbig Ae stars. Imaging studies of LkCa 15, for example, have detected a number of isotopologues of CO along with the molecular ions HCO^+ and NNH^+ and the more complex organics formaldehyde and methanol (Duvert *et al.* 2000; Qi *et al.* 2003). For this disk at least, molecular depletion of molecules onto the icy mantles of dust grains near the disk midplane is found to be extensive, but the fractional abundances and ionization in the warm molecular layer are in line with those seen toward dense PDRs. While the lines from the less abundant species can be detected (*cf.* Figure 4), they were too weak to image with good signal-to-noise. Thus, while millimeter-wave rotational line emission is a good tracer of the outer disk velocity field it is not a robust tracer of the mass unless the chemistry is very well understood.

The detection of ions such as HCO^+ is of particular interest thanks to the appreciation of the Magneto-Rotational Instability (MRI) as a potential mechanism for disk angular momentum transport (e.g., Stone *et al.* 2000). Chemistry should therefore be linked to disk dynamics as the presence of ions is necessary to couple the gas to the magnetic field. As shown by Figures 1 and 2, since most of the ionization processes are active on the surface, there exists the potential that accretion may only be active near the surface (Gammie 1996).

A central question, much discussed at this meeting, is whether cosmic rays penetrate through the possibly intense winds from young stars to reach the inner disk. Within our own planetary system, the Solar wind excludes ionizing cosmic rays. If cosmic rays do penetrate, the primary charge carriers range from metal ions or grains at small radii ($\sim$1 AU) to molecular ions for $r >$ a few AU with $x_e \sim 10^{-13}$ near the midplane. If ionizing cosmic rays are excluded, radionuclides can produce $x_e \sim 1.3\times10^{-8}(T/20\ \mathrm{K})^{-0.5}/\sqrt{n_H}$ (assuming H_3^+ as the dominant ion). In dense protostellar cores, models and observations now suggest near total freeze-out of volatiles that results in D_3^+ and other forms of deuterated H_3^+ becoming important charge carriers (Roberts *et al.* 2004; Walmsley *et al.* 2004). The disk midplane should present a similar environment. The detection of H_2D^+ by Ceccarelli *et al.* (2004) in the outer disks of TW Hya and DM Tau supports this view, and is consistent with cosmic ray ionization.

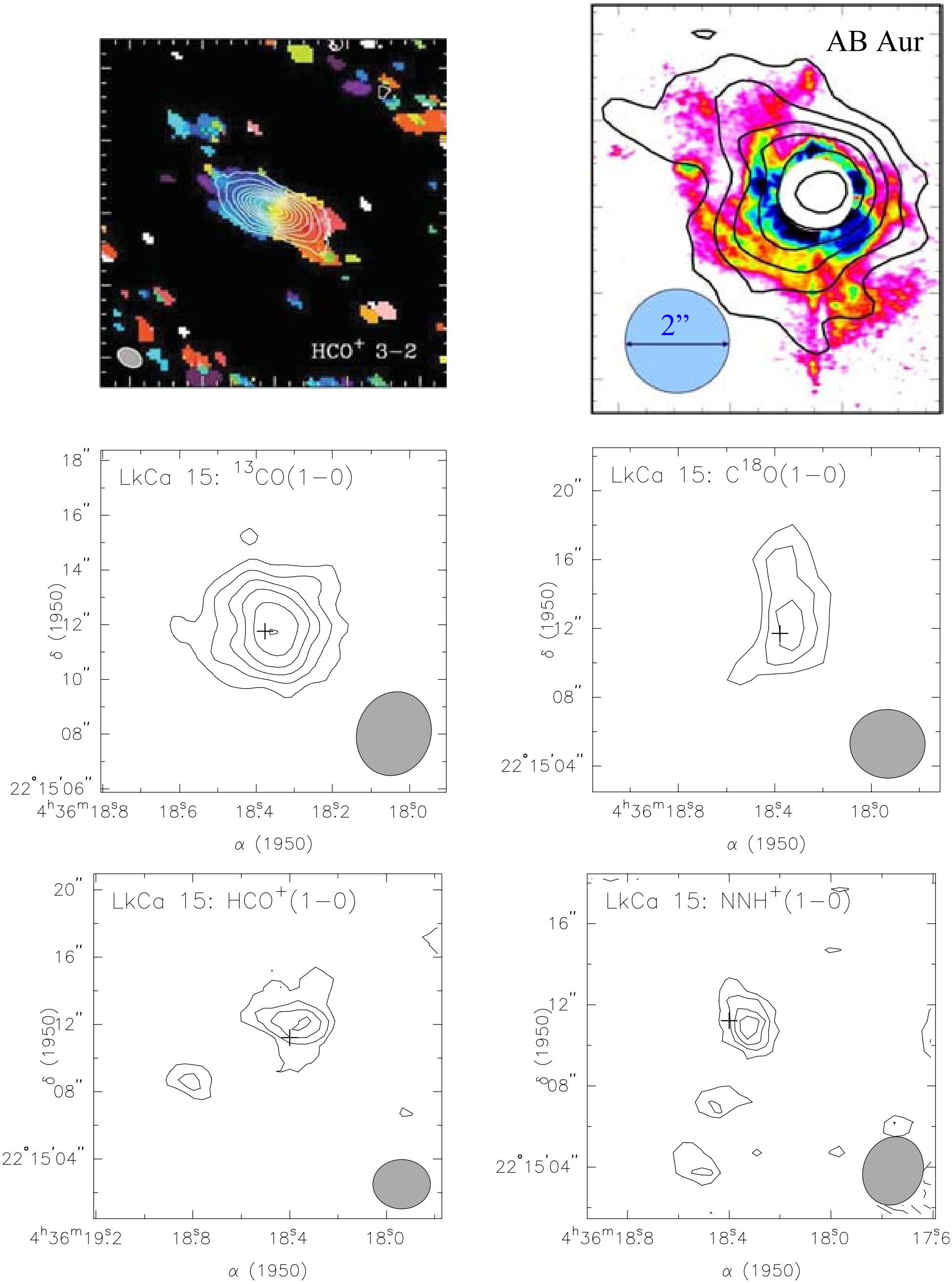

Figure 4. Integrated intensity millimeter-wave images of several disk systems. *Top:* BIMA HCO^+ J=3–2 image of L1489, and an OVRO image of the 3 mm dust continuum from AB Aur (contours) overlaid on the H-band scattered light image of Fukagawa *et al.* (2004). Figures adapted from Hogerheidje (2002) and Corder *et al.* (2005), respectively. *Bottom:* OVRO Millimeter Array aperture synthesis images of the ^{13}CO, $C^{18}O$, HCO^+, and N_2H^+ J=1–0 emission from the disk encircling LkCa 15 (Qi *et al.* 2003). Hatched ellipses at lower right present the synthesized beams.

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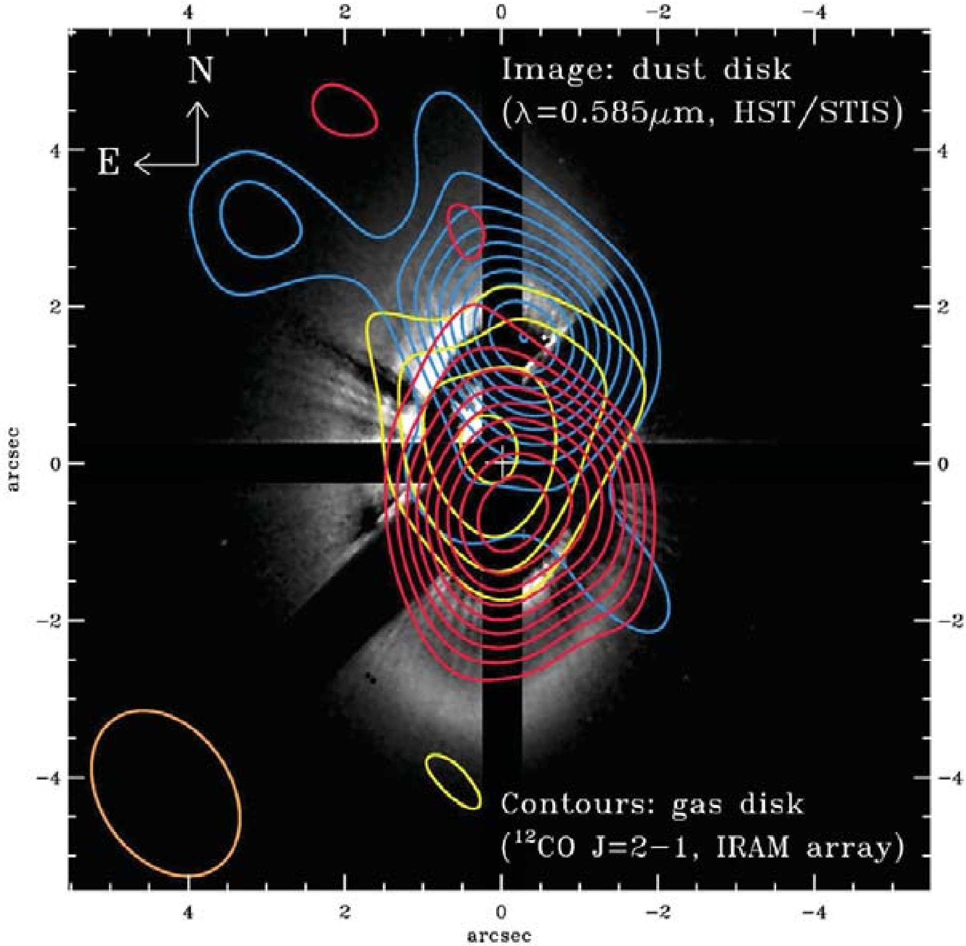

Figure 5. Plateau de Bure image of the CO emission from the transitional disk candidate HD 141569A (greyscale image from HST). Yellow contours trace gas at the systematic velocity, those in red and blue trace the expected offsets along the major axis for a disk in Keplerian rotation (from Dutrey *et al.* 2005).

At still later evolutionary stages, disk dissipation will eventually leave a young star surrounded by an optically thin, dust dominated disk. Just how this process occurs, and over what timescale, is pivotal to the development of planetary systems. The inner disk can be drained by accretion, while photoevaporation is more likely important in the outer disk – especially for stars that are members of young clusters (Hollenbach *et al.* 2000). If holes are opened in the inner disk due to the combination of planet formation and accretion onto the central star, the near- through mid-IR SED can modified substantially. A number of these potentially transitional disks are known, and more are being discovered through extensive surveys being undertaken with the Spitzer Space Telescope. High-resolution imaging and spectroscopy of these putative transitional disks is pivotal, and Figure 5 illustrates the power of millimeter-wave aperture synthesis studies through Plateau de Bure observations of one such Herbig Ae star, HD 141569A (Dutrey

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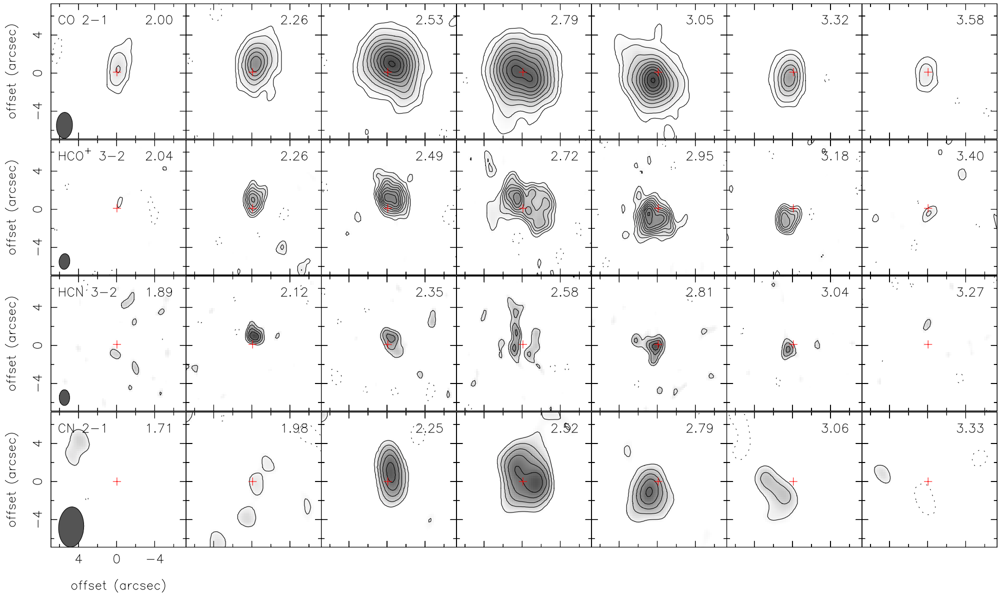

Figure 6. SMA channel maps of the millimeter and submillimeter spectral line emission from the TW Hya circumstellar disk. The ellipses at lower left in each series of panels display the synthesized beam, which for the HCN J=3–2 observations achieves an effective spatial resolution of ∼60 AU. Kindly provided by C. Qi in advance of publication (Qi *et al.* 2006, in preparation).

et al. 2005). For most such systems, however, the holes predicted by analyses of the SEDs lie on angular scales that cannot be studied with current arrays.

3.1. *Observations with New and Upgraded Arrays*

New observational facilities are poised to change our ability to probe the chemistry in disks dramatically, as illustrated by the recent SMA results on the TW Hya disk presented in Figure 6 (Qi *et al.* 2006, in preparation). At a distance of only 56 pc, observations of this source provide nearly 2–3 times the effective linear resolution of disk studies in Taurus. Thus, channel maps such as those presented can be used to derive a great deal about the physical and chemical structure of the disk – its size and inclination (Qi *et al.* 2004), the run of surface density and temperature with radius, the chemical abundance ratios with radius in the outer disk, etc. Ongoing improvements to existing arrays (SMA, PdBI, and CARMA in the north) will soon enable similar studies for a large number of disks, and will push the radii over which chemical studies can be pursued down to 10–20 AU. For transitional disks with large inner holes (or at least zones where dust grains have grown sufficiently large that this part of the disk becomes optically thin), such as that proposed to exist around GM Aur (Calvet *et al.* 2005), sub-arcsecond observations with CARMA should be able to verify the presence of an optically thin inner disk, as Figure 7 demonstrates. Resolving the vertical chemical gradients shown in Figure 2 and studying the chemistry in the 1–10 AU zone of active planet formation will require even greater sensitivity and spatial resolution, and awaits the development of ALMA. Studies of the critical water frost line that complement ongoing IR surveys (see Najita, this volume) are extremely challenging from the ground, but will be possible once SOFIA and Herschel are deployed over the next few years.

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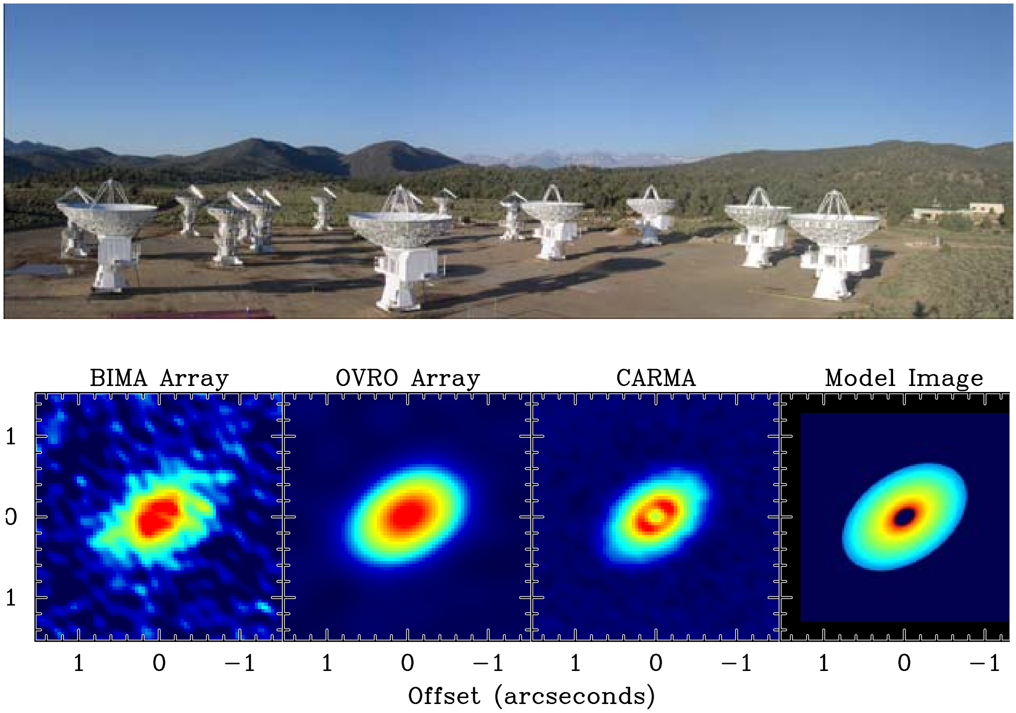

Figure 7. *Top:* Image of the fifteen telescopes of the CARMA array at Cedar Flat, CA in August 2005. The eight 3.5-m telescopes of the University of Chicago Sunyaev-Zel'dovich Array (SZA) will move to the CARMA site in 2007. *Bottom:* Simulated ν=230 GHz dust continuum imaging of a circumstellar disk at 150 pc distance using the BIMA, OVRO, and CARMA arrays in their two highest-resolution configurations, kindly provided by L.G. Mundy. The images are reconstructions of simulated observations of the model disk shown in the right panel, whose mass is 0.01 $M_{\odot}$. The outer radius is 120 AU, and there is an inner hole 20 AU in radius. The simulations included appropriate Gaussian noise levels for each array.

4. Conclusions

High angular resolution (sub)millimeter-wave spectroscopy of circumstellar disks provides a uniquely powerful probe of the chemistry and physics therein. While present instruments can only probe gas beyond the radius of our own Kuiper Belt in the nearest star+disk systems, the ongoing improvements to existing arrays (the SMA, CARMA, and PdBI) and particularly the deployment of ALMA herald a new epoch in which stringent observational tests of chemical and physical models will be possible. Further, the sensitivity of these arrays will be sufficient to trace the gas well into the era of disk dissipation, and will thereby provide an observational context for our emerging understanding of the processes that shape the diverse properties of (extrasolar) planetary systems.

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Discussion

LISEAU: The results you describe pertain mostly to T Tauri stars and Herbig Ae stars with fairly low accretion rates. What is known about the chemical and physical properties of disks in FU Orionis systems for which flow onto the star is much larger?

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Blake: Unfortunately, little is known at present, for a variety of reasons. For example, many such stars lie at distances several times further than for the nearest disk systems in Taurus and Ophiuchus, and so much improved spatial resolution will be needed to characterize FU Orionis disks to the level of detail currently available for T Tauri and Herbig Ae star disks. Some dust and line data are presented for FU Orionis and potential FU Orionis precursor stars in McMuldroch *et al.* (1993, *A. J.* 106, 2477; 1995, *A. J.* 110, 354), but at fairly low spatial resolution. Finally, the linear distances over which the dissipation of accretional energy becomes dominant are sufficiently small that only ALMA can image such regions directly at millimeter wavelengths.

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