Chapter 1

Introduction

Abstract

The ongoing radial velocity searches for extrasolar planets have resulted in the detection of >120 planets around other main sequence stars, and also around pulsars and white dwarfs (Dorminey, 2002[1]). The vast majority of exoplanetary systems appear to be very different from our own solar system, possessing large gaseous planets, similar to Jupiter, which orbit with high eccentricities, close to the star (most at < 3 AU). If these systems are representative of extrasolar planets (and not largely due to selection effects of the detection mechanisms)[2], then the diversity of planetary systems most likely arises from differences in conditions during the planet-forming phase. Specifically, the composition of gas, dust and ices in each stage of star formation plays a major role in determining what kind of planetary system, if any, can be formed. Observations tracing the evolution of material in young stellar objects (YSOs) are thus essential for addressing these issues. Such observations can additionally shed light on the formation of comets and the development of prebiotic molecules and planets that can sustain life. For example, similarities between comets and older "debris" disks, in particular the dust composition, indicate that comets are assembled in the later stages of star formation; observations of saturated molecules in hot cores and production of organic molecules by laboratory photolysis of "astronomical" ices indicate that the development of prebiotic molecules may be highly dependent on the energetic processing of grain mantles.

1.1 Star formation, chemistry and SEDs

Within the interstellar medium there exist clouds with sufficiently high densities (n = 10^2–10^6 molecules/cm^3) that the gas phase is dominated by H_2 and CO, which, once synthesized, are self-shielding from photodissociation by UV. Stars are formed from the gravitational collapse of cores within such clouds. The radiation of the star+dust system ranges from the UV (dominated by

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[1] http://exoplanets.org/science.html

[2] Jupiter sized planets located at 5 AU are just now becoming detectable using standard radial velocity methods.

stellar blackbody emission) to the infrared and millimeter (dominated by dust emission) regions. The spectral energy distribution (SED) of the emergent radiation changes with the morphology of the YSO and is often used to classify the stages of stellar evolution (as shown in Figure 1.1).

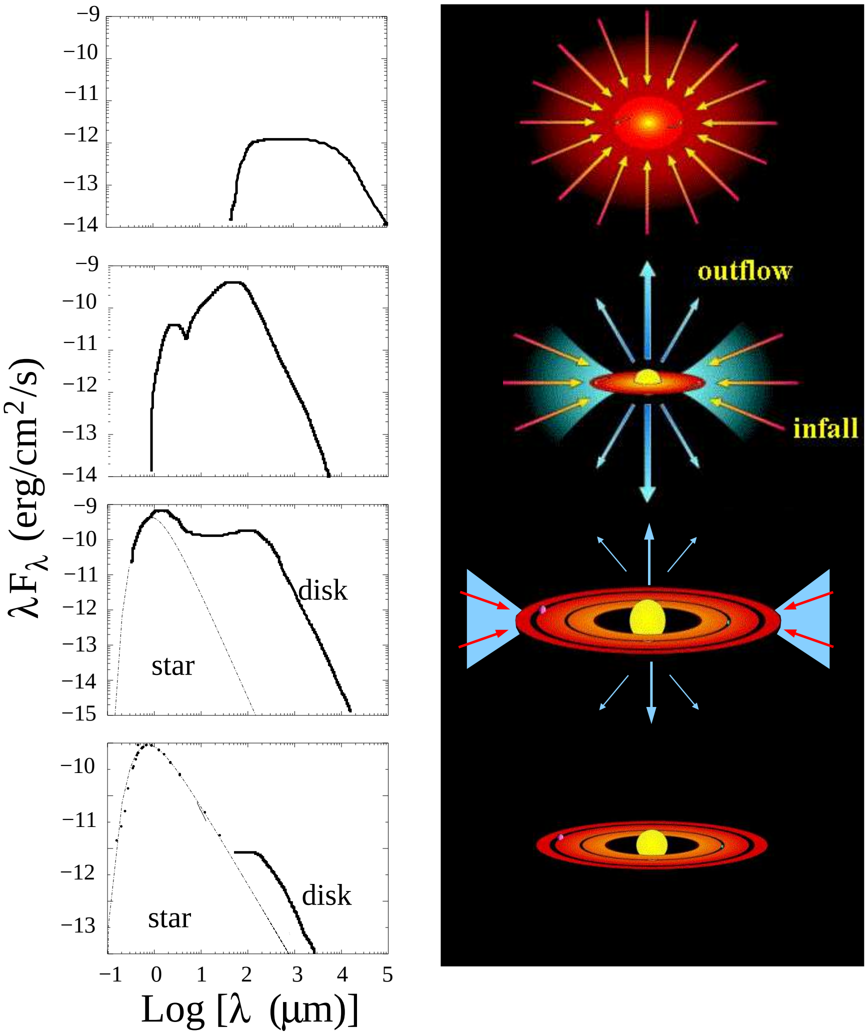

Figure 1.1 Evolution of YSOs and their SEDs, adapted from a figure by McCaughrean (private communication). The right panel shows a cartoon of the evolution of YSOs from a Class 0 embedded protostar to a Class III optically thin disk. The left panel shows the corresponding changes in the SED.

The initial collapse phase (the so-called Class 0 phase) is identified by radiation at millimeter and far-IR wavelengths that is typical of cool dust (T = 10–40 K). At these low temperatures, gaseous species (atoms and molecules) rapidly accrete onto the dust grain surfaces at roughly the collision rate (at densities of $\gtrsim 10^4$ cm^{-3}, this is $\gtrsim$ one H_2 molecule per day; Tielens & Allamandola, 1987) forming ice mantles with thicknesses of $\sim$1 μm. Class 0 objects are therefore associated with ice absorption bands from several species including CO, CO_2, H_2O, and X-CN, indicating a rich grain mantle chemistry. As the core collapses, the forming star illuminates the surrounding dust and gas, evaporating the ices and increasing the chemical complexity in the gas phase. Angular momentum is largely conserved during collapse, and so the infalling matter forms a disk around the star, and a fraction of this material is funneled along magnetic field lines into an outflow perpendicular to the plane of the disk. The outflow clears a cavity in the core and reveals warm dust close to the forming star, leading to emission at shorter wavelengths. Objects in this phase form Class I. The high densities and velocities within the outflow in this phase lead to increased collisions between grains resulting in the evaporation of ices from grain mantles and the sputtering of metals from grain cores. For this reason, the outflows of Class I objects are characterized by gas-phase emission from species such as H_2CO, CH_3OH and SiO, which are thought to be formed on grain surfaces or require atoms located in grain cores. As material from the disk slowly moves toward the star on the path to accretion, what is left of the original cloud core either falls onto the disk, accretes onto the star, or is removed from the system by the outflow. As the outer envelope begins to clear ($\sim 10^6$ yr), the star becomes visible. The SED at this stage is characterized by emission from the star in the optical and UV and radiation from circumstellar dust at $\lambda > 1$ μm (Class II). The chemistry in the circumstellar disk is a complex function of the temperature and density variations with distance from the star, and the surface chemistry within the disk is the main focus of this thesis. Over time, this outer envelope is eventually cleared away, leaving only the disk, and because there is no material left to fuel it, the outflow ceases. As the gas is cleared, increased grain collisions in the Keplerian velocity field lead to grain growth and the disk becomes optically thin (Class III). It is these circumstellar disks that are the site of planetary formation (c.f. Pollack et al., 1996).

1.2 Planet formation, the solar system and the solar nebula

What is known about the process of planet formation within such disks is based primarily on knowledge of our own solar system and in particular the chemical and physical properties of the planets, Kuiper Belt Objects (KBOs), comets and meteorites. The terrestrial planets (Mercury, Venus, Earth, and Mars) are located less than two astronomical units from the Sun (1 AU = 1.5×10^{13} cm). They have dense (3.9–5.5 g/cm^3) cores composed of primarily iron- and magnesium-bearing silicates and iron-nickel alloys along with thin atmospheres composed primarily of CO_2 and N_2, which are thought to have originated from partial outgassing of the planets' interiors. These rocky planets also have small numbers of satellites, typically only one or two. In contrast, the giant planets (Jupiter, Saturn, Uranus, and Neptune), located greater than 5 AU from the Sun, are lower in bulk density (0.7–1.7 g/cm^3) and possess thick atmospheres (8–21 g/cm^3), which constitute a up to 95% of the planetary mass. These atmospheres differ from those of the terrestrial planets in that they are composed of predominantly H_2 and He (at $\sim$solar proportions) and reduced species,

Table 1.1. Properties of the planets. From Encrenaz (2001).

Planet	Helioc.Distance (AU)	Radius (R_E)	ρ (g/cm^3)	Number of satellites	Atmosph. Composition
Terrestrial planets					
Mercury	0.39	0.38	5.44	0	...
Venus	0.72	0.95	5.25	0	CO_2(96%),N_2(4%)
Earth	1.0	1.0	5.52	1	N_2(77%),O_2(21%)
Mars	1.52	0.53	3.91	2	CO_2(95%),N_2(3%)
Giant Planets					
Jupiter	5.20	11.19	1.31	16	H_2(91%),He(9%)
Saturn	9.55	9.41	0.69	21	H_2(96%),He(4%)
Uranus	19.22	3.98	1.21	15	H_2($\sim$90%),He($\sim$10%)
Neptune	30.11	3.81	1.67	8	H_2($\sim$90%),He($\sim$10%)
Pluto	39.44	0.18	2	1	CH_4,N_2?

CH_4 and NH_3 (Table 1.1). Unlike the rocky planets, large numbers (8–21) of satellites have been found around the gas giant planets. The orbits of all planets (except Pluto) are quasi-circular in the ecliptic plane and rotate in the same direction, with the planet often in direct rotation around its axis (except Venus) in a manner similar to the rotation of planets around the sun. Gas giants also possess rings of ice and rock, similar in composition to their satellites.

The orbits of the planets and satellites can be explained by formation from a flattened primordial disk, which revolved around the protosun. A lower bound to the mass of the protoplanetary nebula (10^{-2} $M_\odot$) is often obtained from the current masses of the planets, adding enough hydrogen and helium to establish solar elemental abundances (the so called Minimum Mass Solar Nebula model, or MMSN). The accepted model of formation of the solar system is that planets form from accretion of planetesimals and nebular gas (Encrenaz, 2001). In this model, grains evaporate near the protostar during the gravitational collapse of a high-density region of an interstellar cloud. As the nebula cooled, material was condensed and the composition of this material varied as a function of distance from the star, with metals and silicates condensing close to the star and ices forming in the outer regions of the nebula.

This theory is supported by studies of ^{26}Mg ($t_\lambda = 7\times10^5$ yr) which suggest that most (but not all) grains were formed very early in the solar system. These initial grains were micron-sized and thoroughly mixed with the gas, and grain growth proceeded through the freezout of ices onto grain surfaces, increasing the sticking probability of grain-grain collisions and resulting in the formation of fluffy grain aggregates. As these particles grew (in size), they settled to the disk midplane, where accretion was accelerated by high gas and particle densities. In the outer nebula (R > 5 AU) colder temperatures and increased abundances of ices led to the formation of large cores ($M = 15$ M_E). These cores then attracted large amounts of gas from the nebula, forming precursors to the gas giants.

Table 1.2. Properties of the giant planets

	Sun	Jupiter	Saturn	Uranus	Neptune
Total mass[a](M_E)	...	318.1	95.1	14.6	17.2
Envelope mass (M_E)	...	288.1–303.1	72.1–79.1	1.3–3.6	0.7–3.2
Core mass (M_E)	...	15–30	16–23	11–13.3	14–16.5
Atmospheric composition[b]					
C/H	4.7×10^{-4}	2.9±0.5	2–6	25	25
N/H	9.8×10^{-3}	3.2±1.4	2–4	$\ll$1	$\ll$1
O/H	8.3×10^{-4}	0.033±0.015	...	...	...
D/H	2×10^{-5}	0.35-6.5	3.0	3.0	...

[a] In units of the Earth's mass = 5.98×10^{27}g

[b] Planetary elemental ratios ×solar

The inner nebula consisted of primarily metals and silicates and ices were less abundant, therefore only small, dense cores were formed in $\gtrsim10^7$ years and atmospheres were generated by secondary processes. Due to accretion of gas onto the giant planets and other forms of gas loss, the nebula is expected to have dissipated in $\sim 10^6$–10^7 yr. Thus, the relative amounts of atmospheric material present in the gas giants, namely, Jupiter $\geq$ Saturn $>$ Uranus $>$ Neptune, are often explained by early formation of Jupiter and Saturn (t $\sim 10^6$ yr) followed by formation of Uranus and Neptune (t = 10^7 yr) at a point where little gas was left in the nebula.

Trends in the composition of the giant planets also provide important information about their formation mechanism and the nature of the protoplanetary nebula. The MMSN model discussed above indicates that carbon should be in the form of CO or CH_4, nitrogen as N_2 or NH_3 and additional oxygen in the form of H_2O. Table 1.2 (compiled by Gautier, 1988) shows the elemental ratios of the giant planets, which are all enriched in C, N and O compared to the Sun. The enhancement in C, N, O is indicative of the formation mechanism for these planets. There is a marked increase in the C/H and D/H ratios from Jupiter to Neptune, which can be explained by a temperature gradient in the disk. (Additional support for a temperature gradient is that the core size of the planets is approximately constant with varying atmospheric masses that are approximately solar.) The D/H increase as a function of heliocentric distance occurs because deuterium fractionation is increased at low temperatures, and thus in the core ices, with the larger atmospheres of the inner gas giants diluting the overall D/H ratio. The increase of C/H with heliocentric distance can be explained in a similar manner, but requires that the initial cores were composed primarily of CH_4 as opposed to CO, decreasing the gas-phase C/H ratio. The C/H ratio is then smaller in Jupiter because the gas:ice ratio is larger than that of Neptune.

Table 1.3. Observed exoplanet properties, August 2003

Property	value
R_{sep}	0.38–3 AU
$M_P \sin i$	0.16–17 M_J
period	3–2300 days
ϵ	0.0–1.0

1.3 Extrasolar planet formation and protoplanetary disks

Observations of extrasolar planets indicate that the process of planet formation have not been as straightforward for other planetary systems as it was for the Solar System. Among the >120 planets found orbiting other stars, many are in extrasolar planetary systems which appear to be quite different from our own (see Table 1.3). Large numbers of very close-in Jupiter mass planets have been detected and the radius of one such planet, HD 209458, indicates a very low density, corresponding to a temperature 10 times warmer than Jupiter, T = 1300–1400 K. The presence of these "hot Jupiters" can be explained by the formation of these planets farther out ($R \approx 5$ AU), followed by migration inward at later times, which is stopped by dissipation of nebular gas. However, current models of gas accretion result in migration faster than the timescale for nebular dissipation and the planets are accreted into the star. Additionally, the orbital eccentricities (ϵ; see Table 1.3) observed for extrasolar planets are much larger than those of Solar System planets, and those produced by early accretion disk models ($\epsilon \approx 0$). Recent models of planet-disk interactions (Goldreich & Sari, 2003) indicate, however, that eccentricities may be enhanced as the planet clears a gap in the disk. Another anomaly in the observations of extra solar planets is the paucity of large planets with $M_P \sin i > 20\ M_J$. This mass cutoff is likely related to the relative timescales for planetary formation and dissipation of molecular gas from the protoplanetary disk, but its exact nature is not yet understood.

Circumstellar disks similar to models of the solar nebula have now been detected around several stars with masses comparable to our sun (0.2–10 $M_\odot$) and are a good environment in which to address the question of planet formation (see Beckwith & Sargent 1996 for review). The distribution of dust with radius affects the frequency of planet formation; the final mass of planets depend on properties of the gas and the occurrence of multiple systems may be dependent on the disk size and mass. Observations of disks indicate that they often extend beyond the size of the current Solar System, with R_{disk} = 10–1000 AU. The timescales for dust agglomeration and gas dissipation in disks provide perhaps the most important observational constraint on the method of planet formation. Near-IR observations indicate that by ~3 Myr half of the disks have lost most of their warm dust (within a radius of 0.1 AU), while ISO 25–60 μm observations indicate that cooler dust is lost, or accreted, by 10 Myr (R = 0.3–3 AU). Timescales for loss of gas from disks are also observed to be on the order of 10^7 yr (Thi et al., 2001). From observation of UV excesses associated with accretion, rates of $\dot{M} = 10^{-8}\ M_\odot/yr$ are derived for disks of age $t \approx 10^6$ yr (Calvet et al., 2002).

1.4 The chemistry of protoplanetary disks

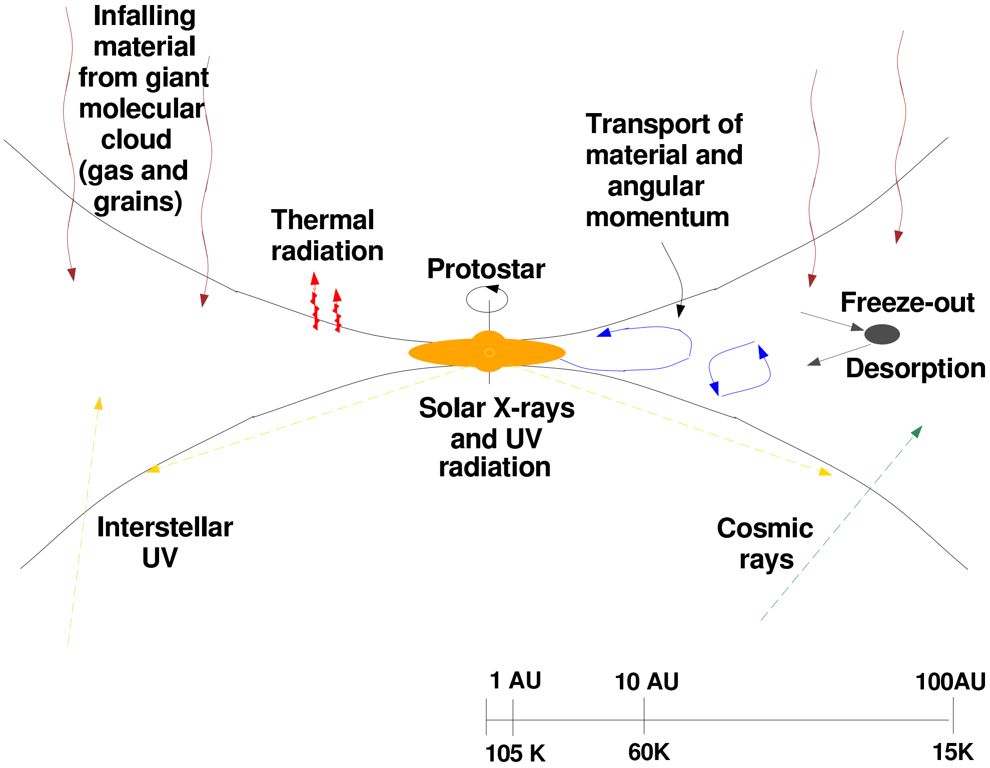

Figure 1.2 The circumstellar environment, modeled after a figure from van Zadelhoff (2002). The solid lines indicate dynamical processes. Infalling material from the molecular cloud likely affects the chemical properties of gas and dust in the outer disk. The transport of material and angular momentum refers to the radial and vertical mixing suggested by disk models. Although the diagram is truncated at a disk radius of 100 AU, observations indicate that disk sizes can be much larger (R∼500 AU) in systems of age $t \geq 10^6$ yr.

As discussed above, the chemical composition of planets are directly related to how and where they formed. The assessment of the chemical composition at each radius of the disk would therefore provide valuable information (i.e., the density, thermal history and composition versus distance) about the initial conditions in the planet-forming zones of the solar nebula and help determine the origin of primitive bodies such as comets. In particular, molecular emission studies of accretion disks can facilitate the quantification of gas-to-dust ratios and the timescales over which they are dissipated (which is important for the process of planet formation) as well as the description of the distribution of volatile species in its outer regions (necessary in the derivation of the evolution of comets and Kuiper Belt Objects).

By means that are not yet fully understood, circumstellar accretion disks radially transport material inward and angular momentum outward. Due to radiation from the central star and the liberation of gravitational energy there are strong density and temperature gradients in the disk. In the outer, colder regions much of the (C,N,O,S)-bearing gas should be frozen out onto an icy mantle on the surfaces of dust grains in the dense mid-plane of the disk (c.f. Figure 1.2). As matter accretes toward the warmer innermost regions, the ice mantle evaporates ($R < 10$ AU), while at radii smaller than $\sim$0.3 AU dust destruction begins (Willacy et al., 1998). This results in complex chemical reactions releasing large, less volatile molecules, into the gas phase in the inner part of the disk (Bauer et al., 1997; Duschl et al., 1996; Willacy et al., 1998). At radii less than 0.05 AU, there exists complete molecular dissociation, leaving only free atoms. The extent to which radial mixing occurs is very important to the overall chemical balance, but is very difficult to predict theoretically, and occurs over such small spatial scales that observational studies are beyond current capabilities.

Current models of the chemistry in the outer regions of circumstellar disks (Aikawa et al., 2002; Willacy & Langer, 2000; Finocchi et al., 1997; Bauer et al., 1997) suggest that at large radii the chemistry is controlled kinetically by two-body gas-phase processes and by adsorption onto and desorption from grains. In the early versions of these models, it was assumed that only thermal desorption occurs. Several models (Aikawa et al., 2002; Willacy & Langer, 2000) are now beginning to apply recently developed self-consistent treatments of the optical/infrared radiative transfer in the disk (Chiang & Goldreich, 1997; Chiang et al., 2001; D'Alessio et al., 1998), instead of using cold mid-plane temperatures. These models include the effects of the processing of radiation by grains near the photosphere, or disk surface, which lead to enhanced disk surface temperatures and a flared geometry. The chemical effects of radiation from the young star and interstellar medium are are thus very important in these surface layers and the likelihood of depletion onto grain mantles is lessened, leading to increased abundances of gas-phase species with respect to early models that had artificially high dust-to-gas ratios. Some models (Glassgold et al., 1997; Finocchi et al., 1997) also take into account the effects of X-rays, short-lived radionuclides, cosmic ray ionization, and photochemistry; but, there are several important processes, such as dust versus gas settling and size sorting, that continue to be neglected.

Advances in molecular modeling of the chemistry of accretion disks are codependent upon the observational study of the disks through molecular line emission. The study of this emission has heretofore been greatly limited by the sensitivity of astronomical instrumentation, however. This has resulted in the primary use of the emission lines of isotopomers of CO and the continuum emission of circumstellar dust for imaging, which allow only the mass and size of disks around young stars to be modeled (Koerner & Sargent, 1995; Koerner et al., 1998; Mannings & Sargent, 1997). The reliance on CO emission, in addition to limiting the scope of the modeling effort, is otherwise problematic in several ways. One main example is that CO emission data sometimes indicate that the masses of gas are much (up to two orders of magnitude) lower than those inferred from the continuum emission (Zuckerman et al., 1995; Dutrey et al., 1996, 1997). There are several proposed explanations for this discrepancy, including loss of gas through freezout of molecules onto grains, inadequate spatial resolution, poor radiative transfer models, and the possibility that the time scale of gas dissipation is shorter than that of dust agglomeration. A more complete assessment of the chemical distribution within the disk could be made with the acquisition of the emission spectra of a greater variety of molecules, specifically species in each chemical family (C-, N-, S-, O-bearing).

Recently, emission from molecules such as CN, HCN, HNC, CS, HCO^+, C_2H and H_2CO, with intensity comparable to ^{13}CO and $C^{18}O$, has been detected through single dish studies of the disks surrounding TW Hya (Kastner et al., 1997), LkCa 15 (van Zadelhoff et al., 2001), DM Tau and GG Tau (Dutrey et al., 1997). From these pioneering studies, some important conclusions can be made. It is known that the transition optical depths for species such as HCN and HCO^+ are sufficiently large that their emission should be comparable to that of ^{12}CO if the gas is well mixed and interstellar abundances are maintained (M.R. Hogerheijde, private communication). However, it was found in the above studies that they are lower, implying either substantial molecular depletion, or a strong species dependence on the sizes of the emitting regions. In addition, ratios such as CN/HCN and HNC/HCN are too high to be accounted for by quiescent chemical models alone. This suggests that both ion-molecule and photon-dominated chemistry must contribute to the observed abundances (Spaans, 1996; Dutrey et al., 1997; Kastner et al., 1997).

These first detections, in beams large compared to the sizes of the disks, indicate that an initial study of the nature and variation of the chemical composition of disks is now feasible. To this end, the research described here includes the imaging of several molecular emission lines from the circumstellar disks of T Tauri and Herbig Ae stars with the Owens Valley Radio Observatory (OVRO) Millimeter Array. In particular, the distributions of several species around the T Tauri star LkCa 15 have successfully imaged, including HCN, DCN, CN, ^{13}CO, SO, H_2S, CS, SO_2, CH_3OH and HCO^+. The $1''$–$3''$ resolution available at OVRO means that such observations of low excitation transitions are sensitive primarily to the outer ($R > 30$–100 AU) region of the circumstellar disk.

Thus, other tracers must presently be used to examine the warmer, inner regions of the disk. Such tracers would also assist in efforts to constrain the radial and vertical thermal distribution within circumstellar disks. Early models assessed the temperature structure through the use of spectral energy distributions assuming either a flat (Adams et al., 1987) or flaring (Kenyon & Hartmann, 1987) disk geometry. However, the calculations of the mid-plane and surface temperature structure by various groups (Bell et al., 1997; Men'shchikov & Henning, 1997; etc.) differ considerably. Further, in the flared-disk geometry, the surface layer is thought to be heated by the star to temperatures as high as 100 K at radii as large as 100 AU (Chiang & Goldreich, 1997). Accordingly, high spatial resolution observations with 10-meter class telescopes should be able to resolve the silicate dust emission features in the outer layers of disks, and in this way support or discount the existence of a flared geometry. I therefore also describe here the use of Keck Long Wavelength Spectrometer 10 μm long-slit silicate imaging spectroscopy.

The fundamental aim of the research program described here is the quantitative examination of the chemistry of the biogenic elements (C, N, O, S) in circumstellar accretion disks. This was achieved by combining state-of-the-art observational tools at millimeter through infrared wavelengths using various Caltech observatories with state-of-the-art chemical and dynamical codes. As described below, both the observational and theoretical capabilities have only now advanced to the point where such studies are possible, and the results from this research are of interest not only in their own right, but may help pave the way for future ground-based efforts and space-borne missions in the NASA Origins program. An outline of the thesis is as follows. Chapter 2 describes radiative transfer models and the interpretation of molecular line emission from disks. In Chapter 3, a survey of CN, HCN, CO and HCO^+ is presented and the implications for nitrogen chemistry are discussed. Chapter 4 contains a discussion of deuterium fractionation in YSOs and in the solar system, centering on a search for HDO and DCN in three protoplanetary disks. Spectroscopic observations of the 8–13 μm silicate emission feature toward several T Tauri and Herbig Ae stars at various stages of the star formation process are presented in Chapter 5 and an evolutionary trend is suggested. Finally, a summary of the current understanding of disk chemistry (including the results presented in this thesis) and directions for future research are presented in Chapter 6.

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