

Unravelling the Chemical Structure of Young Stellar Objects with ALMA

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Abstract. The importance of ALMA to quantitatively trace the evolution of gas and dust from interstellar clouds to planetary systems is discussed and illustrated with recent observational studies of molecules in low- and high-mass young stellar objects. Line surveys using single-dish submillimeter telescopes reveal large chemical variations between different sources, which are likely related to their evolutionary state. A chemical scenario is presented in which molecules produced by grain-surface chemistry during the cold collapse phase are returned to the gas once the young star has formed, leading to an active high-temperature gas-phase chemistry. Both thermal evaporation and release of icy mantles in shocks plays a role. Current observational facilities lack the spatial resolution and image quality to distinguish these different physical and chemical regimes. Exploratory observations of the excitation and distribution of molecules in circumstellar disks are presented, but only ALMA can study the chemistry in the planet-forming zones of circumstellar disks.

1. Introduction

The star-formation process is accompanied by orders of magnitude changes in physical state, with temperatures ranging from <10 K in the collapse phase to >1000 K in outflow regions, and densities from 10^4 cm^{-3} in pre-stellar cores to 10^{11} cm^{-3} in circumstellar disks. The chemistry and excitation of the molecules respond to these changes. One of the aims of astrochemistry is to establish which species and lines are particularly good diagnostics of different evolutionary stages. This is not only important for understanding the chemistry of star- and planet-forming regions, but also for determining their physical structure: molecular lines are the only means to trace the velocity fields and dynamics of highly-obscured gas and to constrain the density and temperature structure. A second, related goal of astrochemistry is to trace the evolution of the abundances of the molecules from the interstellar clouds to circumstellar disks, since it provides the raw material from which new planetary systems are made.

The typical sizes of the physical components associated with young stellar objects (YSOs) range from ~ 5000 AU for the outer collapse envelope to ~ 100 AU for the circumstellar disks. At the distances of the nearest low-mass star-

forming clouds (~ 150 pc), this corresponds to $< 1''$ to $\sim 30''$. Thus, all of these physical components are ‘blurred’ together by the $15''$ – $30''$ beams of most single-dishes, and even interferometers at a few $''$ resolution have limited success because of their poor spatial sampling. ALMA at $\sim 0.1''$ resolution with good uv -plane coverage will be essential to disentangle the different physical and chemical regimes. When combined with more sophisticated 2-D and 3-D radiative transfer models, ALMA imaging will be able for the first time to address quantitatively the chemical evolution during star- and planet-formation.

In this brief paper, selected observational results of molecules in the envelopes and disks around low- and high-mass young stars are presented, and areas for future ALMA observations are emphasized. A more detailed overview can be found in the proceedings of IAU Symposium 197 on ‘Astrochemistry: From Molecular Clouds to Planetary Systems’ (eds. Minh & van Dishoeck 2000).

2. Chemical Scenario

Existing single-dish and interferometer observations have revealed large chemical variations between YSOs at different evolutionary stages (see van Dishoeck & Blake 1998, van Dishoeck & Hogerheijde 1999, Langer et al. 2000 for recent reviews). The prototypical sources are Orion-KL and SgrB2, where thousands of molecular lines have revealed a rich chemistry with large abundances of complex, saturated organic molecules. Not all YSOs show such a wealth of lines, however. Some of them show spectra dominated by sulfur-bearing species whereas others mostly have lines due to simple molecules such as radicals and ions. Figure 1 shows an example of a line survey in the 335–365 GHz range of three massive YSOs in the W 3 giant molecular cloud with different chemical characteristics (see also Menten et al., this volume).

The most successful models for explaining the observed chemical differentiation start with the accretion of species into an icy mantle during the cold (pre-)collapse phase, where grain-surface chemistry produces new molecules. In particular, O, C, N and CO are expected to be hydrogenated to H_2O , CH_4 , NH_3 , H_2CO and CH_3OH , respectively, whereas oxidation of CO may lead to CO_2 . Recent mid-infrared observations with the *Infrared Space Observatory* (ISO) and from the ground have confirmed this picture and produced a complete inventory of the ices (see Ehrenfreund & Schutte 2000 for an overview).

Once the YSO has begins to heat its surroundings, the icy mantles evaporate back into the warm gas, where they subsequently drive a rapid high-temperature gas-phase chemistry for $\sim 10^4 - 10^5$ yr, resulting in complex, saturated organic molecules (e.g., Charnley et al. 1992, 1995; Charnley 1997; Caselli et al. 1993, see review by Millar 1997). The abundance ratios of species such as $\text{CH}_3\text{OCH}_3/\text{CH}_3\text{OH}$ and $\text{SO}_2/\text{H}_2\text{S}$ show strong variations with time, and may be used as ‘chemical clocks’ for a period of 5,000–30,000 yr since evaporation.

The heating can occur either through radiation —resulting in thermal evaporation of the ices – or through the interaction of the outflow with the envelope – resulting in shocked regions where ice mantles are liberated and grain cores partially sputtered, leading to enhanced gas-phase Si. The former process probably dominates in high-mass YSOs, whereas the latter is more important in low-mass YSOs (van Dishoeck & van der Tak 2000). Once part of the envelope has

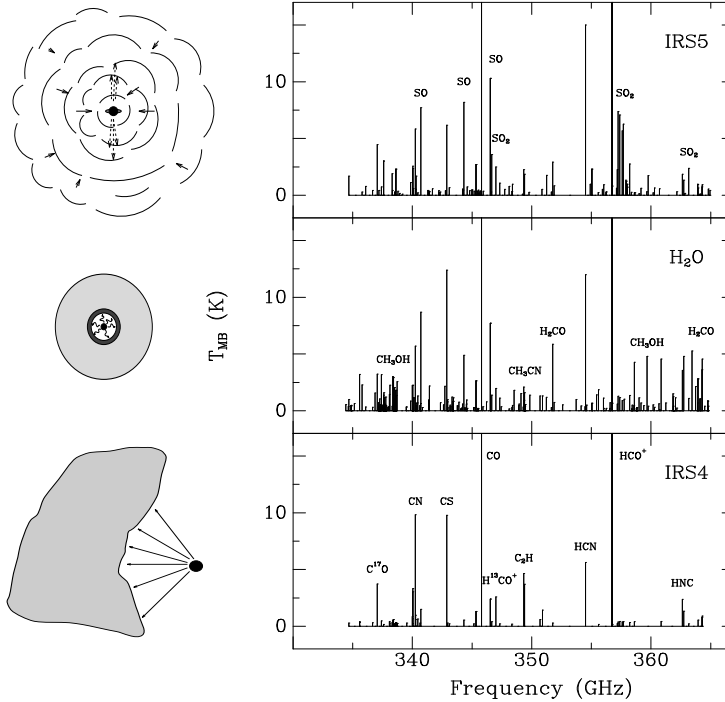


Figure 1. JCMT 335–365 GHz line survey of three massive YSOs in the W 3 molecular cloud. Large chemical and physical differences are found between the three regions, which are likely linked to their different evolutionary states (based on Helmich & van Dishoeck 1997).

cleared and ultraviolet radiation can escape, a photon-dominated region (PDR) is formed, dissociating molecules into radicals (e.g., $\text{HCN} \rightarrow \text{CN}$).

Table 1 summarizes the sizes of various physical components at the distances of the Taurus and Orion clouds, together with some of their chemical characteristics. Even though the existing facilities do not resolve them, such data highlight the dominant component in the beam. Combined with the above chemical scenario, one may then attempt to establish an evolutionary sequence. ALMA, together with future mid-infrared spectroscopy on SIRTf and NGST to probe the ices, will be needed to truly unravel the chemical structure.

Note that the physical distinction between the ‘hot core’ and the warm inner envelope listed in Table 1 is currently not clear: does the ‘hot core’ represent a separate physical component found only for high-mass YSOs, or is it simply the inner warm envelope at a different stage of chemical evolution? Observationally, there do appear to be different types of hot cores: some are internally heated by the young star (e.g., W 3(H₂O)), whereas others may simply be externally heated dense clumps (e.g., the Orion compact ridge) (Watt & Mundy 1999).

3. Chemistry in the envelopes around YSOs

3.1. The pre-collapse and deeply-embedded phases

Dark, cold cores prior to collapse show a differentiated chemical structure on arcsec to arcmin scales. Some cores (e.g., TMC-1) have exceptionally high

Table 1. Physical sizes and chemical characteristics of YSOs

Component	Size (AU)	Taurus (")	Orion (")	Chemical Characteristics
Pre-stellar core	>10,000	> 70	> 20	Ions, Long-chains (HC ₅ N, DCO ⁺ , ...)
Cold envelope	5000	35	10	Simple species, Heavy depletions (CS, N ₂ H ⁺ , ...)
Warm inner envelope	500	3	1	Evaporated species, High- <i>T</i> products (CH ₃ OH, HCN, ...)
Hot core (high-mass?)	500	...	2	Complex organics (CH ₃ OCH ₃ , CH ₃ CN, ... vib. excited mol.)
Outflow: direct impact	<100–500	<0.7–4	<0.2–1	Si- and S-species (SiO, SO ₂ , ...)
Outflow: walls, entrainment	100–1000	0.7–7	0.2–2	Evaporated ices (CH ₃ OH, ...)
Disk	100	0.7	0.2	Ions, D-rich species, Photoproducts (HCO ⁺ , DCN, CN, ...)
PDR, compact H II regions (high-mass)	100–3000	...	0.2–7	Ions, Radicals (CN/HCN, CO ⁺)

abundances of long carbon-chain molecules such as C₂S and HC₅N, whereas other sources (e.g., L1544) show evidence for large depletions in the center and high deuterium fractionation (e.g., Kuiper et al. 1996, Caselli et al. 1999, see also Ohashi, this volume). In the first case, the cores may still be assembling material from the surrounding lower-density, atomic C-rich gas, whereas in the second case, the cores are centrally condensed and appear on the verge of collapse. ALMA is needed to trace the origin of these variations on arcsec scales, as well as the ionization fraction which controls the dynamics.

In the earliest stages after collapse, observations show a rapid evolution of the chemistry in the protostellar phase. Toward NGC 1333 4A and 4B, depletions of more than an factor of 10 have been inferred in the quiescent envelope for all molecules including CO (Blake et al. 1995). One of the few exceptions may be N₂, which has an evaporation temperature of only 13 K and can be traced by N₂H⁺ emission (di Francesco et al. 2000). Serpens SMM1 is an intermediate case, where only mild depletions of at most a factor of 3 are found (Hogerheijde et al. 1999, see Figure 2). Finally, IRAS 16293 –2422 has a rich spectrum of lines, with no significant depletions (van Dishoeck et al. 1995). Since all three sources are classified as ‘class 0’ YSOs with estimated ages of less than 10⁵ yr, this suggests that the phase of heavy depletions is short-lived.

In the early protostellar phase, the envelope mass exceeds that of the star and its circumstellar disk, and separation of the inner envelope and disk is difficult with current instrumentation. In the subsequent ‘class I’ phase, such separation has proven possible through careful analysis of interferometric data (e.g., Keene & Masson 1990, Hogerheijde et al. 1997). A good model of the envelope is a prerequisite before any statements about the disk can be made.

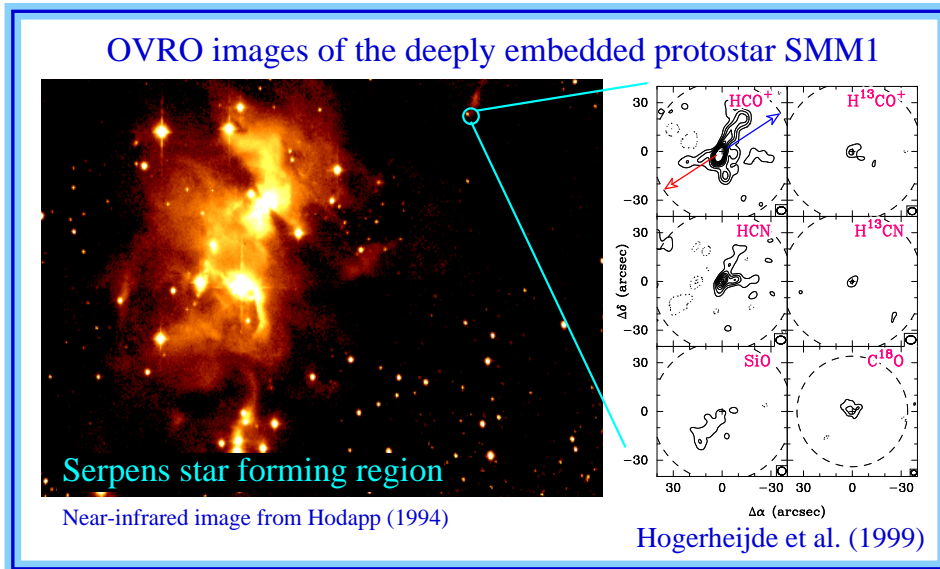


Figure 2. Left: K' image of the Serpens molecular cloud showing a dense cluster of young stars (Hodapp 1994); Right: OVRO images of various molecular lines toward SMM1 (Hogerheijde et al. 1999).

Positional coincidence of the millimeter continuum and line images does not necessarily imply that the molecule resides in a disk, as suggested for CH_3OH toward L1157 by Goldsmith et al. (1999). ALMA observations at subarcsec resolution are needed to study the chemistry as the gas and dust are transported from the envelope to the growing circumstellar accretion disk.

Detailed chemical studies of low-mass ‘class I’ objects are still lacking, since the envelopes around these YSOs have significantly less mass than those surrounding the more deeply-embedded ‘class 0’ protostars. Only ALMA will have the sensitivity to probe the chemistry in this important stage when the envelope is being dispersed and the disk revealed.

Chemical studies of these objects with ALMA require good uv plane sampling, including the short spacings, to image all the flux on $<1'' - 1'$ scales. High spectral resolution ($< 0.1 \text{ km s}^{-1}$) is essential, since the lines are intrinsically very narrow and the molecules may show large abundance variations between velocity components separated by less than 1 km s^{-1} (Langer et al. 1996).

3.2. Hot cores

Hot cores are small clumps of warm gas with temperatures of 100–300 K, densities up to 10^7 cm^{-3} and sizes less than 2000 AU. As discussed in §2, they can either be externally-heated clumps of gas and dust, or they can represent the inner hot part of the envelope at an evolutionary stage when the evaporated molecules drive a complex chemistry. Since their molecular lines are strong with brightness temperatures up to 1000 K, they are prime targets for observations with ALMA at the highest spatial resolution. Because most massive YSOs are at large distances (1–10 kpc), long-baseline observations to reach 30 milli-arcsec resolution ($\sim 100 \text{ AU}$ at $\sim 3 \text{ kpc}$) are essential. The single-dish spectra of these

objects readily reach the confusion limit, but interferometers filter out some of the more extended lines from simple species. Thus, ALMA may push the abundance limits an order of magnitude deeper and thereby reveal the full extent of the chemical complexity of prebiotic molecules (Snyder 1997).

Interferometer observations of W 3 (OH/H₂O) (Wyrowski et al. 1999) and Orion-KL (Blake et al. 1996) have revealed surprising small-scale chemistry variations between sources which are separated by only a few thousand AU. Specifically, variations between O- and N-rich species are found, which are not yet understood. Eventually, chemical studies may be the only way to constrain the time-scales and physical processes associated with the early phases of massive star-formation, which are still poorly characterized observationally and theoretically. ALMA will be essential to disentangle them.

3.3. Outflows

The powerful bipolar outflows that accompany the earliest stages of star formation are thought to originate within the young star/accretion disk boundary region that cannot be directly imaged. The very high velocity of these flows, their complex internal structure, and the inhomogeneous nature of the envelope and molecular cloud surrounding YSOs leads to a wide variety of physical and chemical processes that manifest themselves over a great range of spatial scales. For example, while outflows dissipate their energy and drive high temperature chemistry in *J* (jump) or *C* (continuous) type shock fronts (depending on their velocity and the magnetic field, Drain & McKee 1993, Hollenbach 1997) some 100-10,000 AU in size, mapping of the Orion and NGC 1333 clouds in shock tracers such as vibrationally excited H₂ or high velocity CO reveals that the cloud structure itself may well be regulated by outflows (Yu et al. 1997, Sandell et al. 1994, Warin et al. 1996).

On sub-arcsecond scales, studies with HST have produced detailed images of the physical structure in the strongly shock zones traced by the optically visible Herbig-Haro objects (Heathcoate et al. 1996). The chemical manifestations of these shocks include high temperature gas phase products (H₂O, H₂S, etc.) as well as those derived from the sputtering and destruction of grain cores and their mantles (most prominently SiO and SO) that serve as excellent tracers of shock processes in dense, highly extinguished regions (Bachiller 1996). ALMA will be the first instrument capable of fully resolving the shocked regions around low-mass and high-mass YSOs in both high and low-*A_v* regions, especially in very high spatial resolution studies of (sub)millimeter-wave maser activity.

Over the length of the flow, more glancing, or oblique, shocks lead to turbulent layers that mix outflow and ambient cloud material. Such regions can show large enhancements in both shock-created species as well as the those trapped onto grain mantles (HCN, H₂CO, CH₃OH), and as Figure 2 shows these species can be used to trace the walls, or boundaries, of the outflow itself (Hogerheijde et al. 1999, see also studies of L1157 by Bachiller & Pérez Gutiérrez 1997). Imaging with existing interferometers and single dish telescopes has begun to characterize the chemical and physical alterations driven by outflows, but only ALMA will be able to mosaic sufficiently large areas at sufficiently high resolution to fully understand their pivotal role in star formation.

4. Chemistry in circumstellar disks

As the means by which mass is transferred from molecular clouds to young stars and as the birth sites of planets, circumstellar accretion disks are the pivotal link between star formation and exoplanetary science. Planets have now been discovered around some 30 stars, but the diversity of masses and orbits so far uncovered challenges the view that our solar system is typical (Marcy 1999). Protoplanet/disk interactions are the likely means by which planetary migration occurs (Ward & Hahn 2000), and so to place the ongoing extrasolar planet detection programs in perspective it is essential to understand the physical and chemical properties of disks in detail.

Hundreds of disks around T Tauri and Herbig Ae stars have been inferred by their IR excess emission, and over the past several years the presence of disks around many of these stars has been confirmed by detailed (sub)millimeter continuum and line images, which show gas in Keplerian rotation (e.g. Koerner & Sargent 1995, Dutrey et al. 1996, Mannings & Sargent 1997). Disks have also been beautifully resolved by HST scattered light imaging in Orion and Taurus (e.g. McCaughrean & O'Dell 1996, Padgett et al. 1999). Such studies have revealed that the overall masses ($\sim 10^{-3} - 10^{-1} M_{\odot}$) and sizes of (~ 100 AU) of disks are comparable to those inferred for the primitive solar nebula, but provide few constraints on their radial and vertical temperature and density structures or on their chemical composition. A thorough understanding of the physical and chemical structure is important for constraining models of dust processing, settling, and agglomeration to form planetesimals.

Due to radiation from the central star and the liberation of gravitational energy there are strong density and temperature gradients – both radially and vertically – in the disk. These gradients should be reflected in, and ultimately be traceable by, the gas phase chemical composition. In the outer, colder regions much of the (C,N,O,S)-bearing gas should be frozen out onto grains in the disk mid-plane. The surface of the disk is suprathemal due to its interaction with stellar radiation, and a likely site for photochemical processing (Chiang & Goldreich 1997, d'Alessio et al. 1997). As matter accretes inward, the icy mantle evaporates in a differential fashion with the most volatile species released at the largest radii. CO, for example, should remain in the gas phase for $R < 100-200$ AU, while water volatilizes only for $R < 10-20$ AU. This results in complex chemical balance as a function of position in the disk (Willacy et al. 1998, Aikawa & Herbst 1999a,b). The extent to which radial and vertical mixing occurs is very important to the overall chemical balance, but is difficult to predict theoretically and cannot be observed directly with current instrumentation.

Indeed, chemical studies of disks are only just starting. Pioneering single-dish observations have been carried out toward several T Tauri stars by Dutrey et al. (1997) and Kastner et al. (1997), who detected emission from species such as HCN, CN, H₂CO, HCO⁺, CS, ... at intensities similar to that of ¹³CO in sources such as DM Tau and TW Hya. These results suggest that, at least in appropriate disks, chemical studies regarding the nature and variation of the disk composition with radius can be profitably pursued. The data further reveal that both ion-molecule reactions and photon-dominated chemistry must contribute to the observed abundances, since ratios such as CN/HCN are too high to be accounted for by quiescent chemical models alone. The observed line

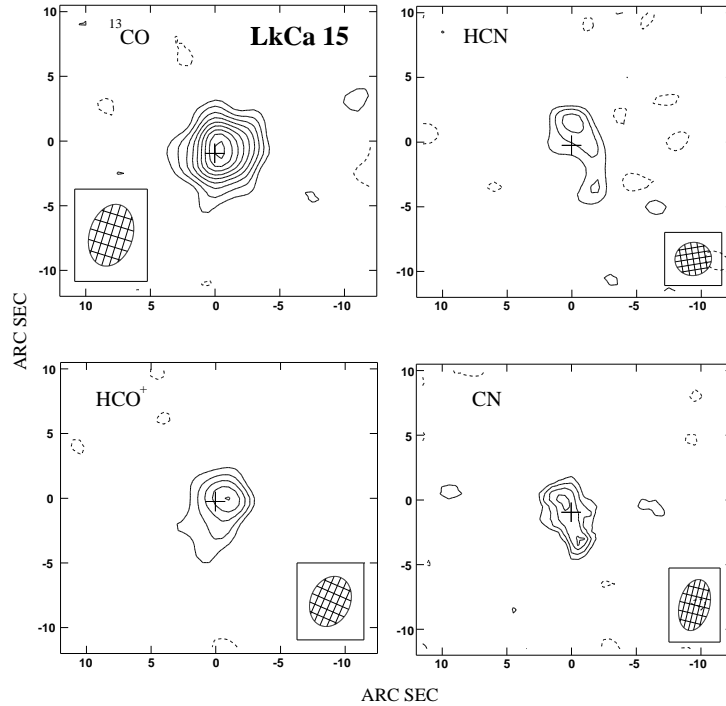


Figure 3. Molecular line emission from the T Tauri star LkCa 15. All maps are of the $J = 1 \rightarrow 0$ transition, while the cross-hatched ellipses at lower right depict the synthesized beams.

fluxes imply that either the heavier molecule abundances are depleted, or, as may be more likely, that the sizes of the emitting regions are strongly species dependent (Dutrey et al. 1997).

A more complete assessment of the chemical distribution within the disk obviously requires high spatial and spectral resolution images of molecules in each chemical family (C-, N-, S-, O-bearing). Present interferometers have the sensitivity to investigate the chemical composition of disks at a resolution of $\sim 1\text{--}3''$. Results from initial 3 mm OVRO observations of the T Tauri star LkCa 15 are shown in Figure 3 (Qi et al. 2000, see also Duvert et al. 2000). Interestingly, different patterns are observed, with species chemically related to CO (e.g. HCO^+) peaking on the stellar position and species influenced by photochemistry, such as HCN and CN, showing more complex gradients.

Reliable chemical abundances can only be derived with the observation of many rotational transitions and once the physical conditions have been reliably determined. In addition, the lines of most simple species are likely to be highly optically thick, and so it is necessary to carry out detailed radiative transfer calculations to accurately model the observed emission. Work along these lines with 1-D and 2-D Monte Carlo routines can now solve the radiative transfer and molecular excitation at each disk radius given a physical structure (van Zadelhoff et al. 2000). The resulting chemical abundances can be compared to those in dense clouds, and can provide critical constraints such as the disk ionization fraction. Eventually, comparison of the chemical gradients observed in disks with the abundances found in comets should yield estimates of the locations in the solar nebula where comets were formed.

These initial exploratory studies serve as an important preparation for full chemical studies with ALMA. The vastly improved imaging sensitivity and resolution of ALMA will enable the first direct observation of chemical gradients in disks, including the pivotal planet-forming region of several to several tens of AU (see Mundy, this volume). As noted above, the chemical structure is of interest in its own right, and reflects both the disk physical profiles and radial/vertical transport timescales important to planet formation.

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