Chapter 1

Introduction

"The interesting question is not why – but how!"

1.1 Low-mass star formation

"Stars are formed from contraction out of dense cores in molecular clouds" is basically the statement which characterizes our understanding of low-mass star formation. This area of research has undeniably had a significant boost from the early eighties up through the nineties with infrared observations, in particular, with the IRAS and ISO satellites, and millimeter and submillimeter studies. Simultaneously the increase of computer power has lead to a deepened theoretical understanding of phenomena such as turbulence in molecular clouds, detailed continuum and line radiative transfer in protostellar cores, and the physics of the ubiquitous protostellar jets and outflows as well as accretion onto circumstellar disks. For recent reviews of these topics see the proceedings of the "Protostars and Planets IV" (Mannings et al. 2000) and "The Origins of Stars and Planetary Systems" (Lada & Kylafis 1999) conferences.

Despite all these efforts serious holes in our understanding of star formation still exist. Just to mention a few: is the star formation process dynamic or quasi-static, do magnetic fields or turbulence dominate core support and on what timescales does collapse occur? What are the initial conditions for star formation, for example, what is the importance of the parental cloud structure and mass on the emerging protostars? What are the main mechanisms responsible for the dispersal of the protostellar envelopes once the young protostar has formed, including the relative importance of the ongoing accretion versus the outflows?

Studies of the star formation process can be divided into two groups depending on whether they address the "forward" or "backward" time arrow before or after the star is formed. In the first group studies of molecular cloud structure, its relation to turbulence and magnetic fields, and the importance for triggering core formation and protostellar collapse constrains the "forward" direction. Studies of the properties and evolution of emerging young stellar objects and their relation to the ambient environment in contrast approach star formation "backwards", by pushing down to the earliest stages just after the core collapse. Both have interesting and wider ranging applications, e.g., for understanding the formation and dynamical evolution of molecular clouds in the first case or the subsequent formation of disks and planets in the latter case. A unified theory of star formation eventually has to address both aspects in a continuous sequence from the earliest cloud stages to the resulting (most likely binary) stellar and planetary system.

1.1.1 The evolution of young stellar objects

The focus of this thesis is to constrain the properties of low-mass young stellar objects (YSOs) in their earliest stages. After collapse, a young stellar object is deeply embedded in a thick envelope which is gradually dispersed partly through the continued accretion onto the central star-disk system, partly through the action of the powerful outflows driven by the young stellar object. Fig. 1.1 illustrates such a young stellar object schematically. An evolutionary sequence based on the classification of the spectral energy distributions (SEDs) of the embedded protostars was suggested by Lada (1987) dividing the young stellar objects into three groups, class I, II and III. In this scheme, class I objects represent the embedded protostellar phase with SEDs peaking in the mid-tofar infrared. The class II group includes objects with emission both in the visible and infrared that can be modeled as originating in a typical revealed star-disk system, whereas the class III objects show nearly pure blackbody emission with little or no infrared excess. Before the collapse and formation of the central protostar, the clumps seen in maps of, e.g., ammonia (NH₃) or (sub)millimeter dust continuum emission without associated infrared sources (Myers et al. 1983; Ward-Thompson et al. 1994) are good candidates for preprotostellar cores (often, and in this thesis, just referred to as pre-stellar cores).

Much emphasis has been put into finding and characterizing "the earliest protostars". André et al. (1993) suggested the so-called class 0 objects, consisting of objects with strong submillimeter emission relative to their overall bolometric luminosity ($L_{\rm submm}/L_{\rm bol} \gtrsim 0.5\%$) or equivalently a bolometric temperature¹ less than 70–100 K. These objects have subsequently been found to be associated with the more energetic outflows, which has been suggested to reflect higher mass accretion rates in the earlier stages (e.g., Bontemps et al. 1996). Still, the distinction between class 0 and I objects is not unambiguous: as pointed out by Jayawardhana et al. (2001), the more deeply embedded objects are found in the more dense environments and the distinction in terms of circumstellar mass and outflow energetics may reflect an environmental rather than chronological difference. Likewise the classical distinction between class II and class III objects (i.e., classical and weak-lines T-Tauri stars) may also be less clear-cut than suggested by the SED classification scheme alone. Naturally searches for other distinguishing tracers of the evolution of young stellar objects are warranted.

¹The bolometric temperature is defined as the temperature of a blackbody radiating with the same mean frequency as the observed source.



Figure 1.1. A typical embedded young stellar object. The object consist of a central protostar surrounded by a ~ 100 AU circumstellar disk both inside a larger scale ~ 10,000 AU centrally condensed envelope. This is a highly simplified figure: it does not include the presence of the bipolar outflows driven by most objects. It indicates a simple 1D geometry of the envelope, whereas in reality it is most likely flattened due to the effects of, e.g., rotation and magnetic fields. Finally, it suggests sharp boundaries for the envelope, outwards to the surrounding cloud medium and inwards to an inner cavity harboring the circumstellar disk: these transition regions are most likely much more complex, depending on the physical evolution of the cloud, envelope, disk, and central protostar.

A candidate for such a chronological tracer may be the chemistry. Since the timescales for many key chemical processes are comparable to the typically inferred timescales for protostellar evolution at the densities and temperatures characteristic for star-forming regions, the chemistry must reflect the changing conditions (see, e.g., van Dishoeck & Blake 1998). The problem with directly using the chemistry is that the physical structure itself also needs to be well-understood in order to interpret, e.g., the molecular excitation. Vice versa, the chemistry may seriously affect the physical evolution, through cooling of the gas, regulation of the ionization balance, etc. Finally, the chemistry established early in the evolution of young stellar objects is likely reflected directly in the molecular composition of their circumstellar disks and thus eventual planetary

systems. A good understanding of the chemical structure and evolution of protostellar objects is therefore an integral part of any complete theory of low-mass star formation.

1.2 Techniques

1.2.1 Observations

A number of fundamentally different observational techniques are applied in studies of the gas and dust around young low-mass stars. In the infrared, extinction of background stars can be used to probe the amount of material in a targeted pre- or protostellar core with high spatial resolution to constrain, e.g., their density profile (see, e.g., the work of Alves et al. 2001). Similar studies of absorption lines toward infrared sources, either the protostellar object itself or background stars, constrain the solid state chemistry along the line of sight. A problem with these techniques is that they require bright background sources, which is why the most deeply embedded stages remain elusive. Also the observed chemistry is an average along the line of sight often with multiple components or varying temperature/density regimes present, and it is not possible to directly disentangle these from single pointed infrared observations.

In the (sub)millimeter regime, a new window opens up since continuum emission and rotational transitions of molecules probe low temperature dust and gas, respectively. The submillimeter cameras and receivers are very sensitive and thus allow mapping of clouds at low column densities, and molecular species with low abundances. Moreover (sub)millimeter receivers provide spectral resolution of 0.1 km s^{-1} or $\lambda/\Delta\lambda = c/\Delta v \sim 3 \times 10^5/0.1 = 3 \times 10^6$, significantly higher than what can be obtained with infrared spectrometers. This allows for detailed maps with important information about the line of sight components through the obtained velocity information. A drawback is that data on multiple transitions of the same molecule typically require observations in different frequency windows, which have to be covered by different telescopes and/or receivers with different efficiencies, etc.

The biggest problem with radio observations is the diffraction limit, which ranges from $\approx 10-15''$ in the submillimeter up to $\sim 1'$ at wavelengths of a few millimeters for typical radio telescopes, such as the 15 m James Clerk Maxwell Telescope (JCMT), the Institut de Radio Astronomie Millimètrique (IRAM) 30 m telescope and the Onsala Space Observatory 20 m telescope. A well-known way to improve the spatial resolution is through aperture synthesis observations. A radio interferometer in its simplest description utilizes the rotation of the Earth to introduce a phase difference between the signals received by two different telescopes varying with time. In effect, it functions as a large radio telescope with a spatial resolution of a single telescope of size equal to the largest distance between the two telescopes in the array.

Nothing comes for free and there is a trade-off: the radio interferometer only measures the Fourier transform of the sky brightness distributions at discrete points, namely those frequencies corresponding to the projected baselines of the interferometer. To reconstruct the actual sky brightness distribution of the source, one has to rely on deconvolution and image restoration techniques. As a specific example, there is a limit to the minimum baselines one can measure, given by the size of the individual dishes and how closely these can be packed. This conversely translates to a lack of sensitivity of extended structures and is a serious problem for studies of, e.g., protostellar envelopes that may extend over scales of 10,000 AU (or 50–100" for nearby star-forming regions). This problem has to be addressed either by including missing short-spacings from corresponding single-dish mapping observations or by direct comparison between the interferometer observations and models for the source structure.

1.2.2 Radiative transfer modeling

The interpretation of any of the described astronomical observations relies on understanding the equation of radiative transfer:

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}\tau_{\nu}} = -I_{\nu} + S_{\nu} \tag{1.1}$$

with the formal solution:

$$I_{\nu}(\tau_{\nu}) = \int_{0}^{\tau_{\nu}} S_{\nu}(\zeta_{\nu}) \exp[-(\tau_{\nu} - \zeta_{\nu})] d\zeta_{\nu} + I_{\nu}(0) \exp(-\tau_{\nu})$$
(1.2)

This basically says that the radiation along a line of sight at a given optical depth, τ_{ν} , consist of two terms: 1. the background radiation, $I_{\nu}(0)$, suffering the extinction $\exp(-\tau_{\nu})$ and 2. the sum of intensities, S_{ν} , of the radiation originating at positions, ζ_{ν} , along the line of sight, suffering extinction according to the optical depth separation $\tau_{\nu} - \zeta_{\nu}$.

This simple statement contains a large amount of physics and is naturally more complicated. For example, for a spherical protostellar envelope with a given density profile, Eq. 1.2 cannot be applied directly, since the source function, S_{ν} , depends on the unknown temperature profile and the optical depth, τ_{ν} , depends on the absorption coefficient, κ_{ν} , possibly varying with radius. For line observations of a given molecule, in particular, κ_{ν} depends on the level populations and thus conversely on the incident radiation field. It is therefore necessary to establish detailed radiative transfer models that can both explicitly account for the temperature and density dependencies with radius and solve the line radiative transfer including the molecular excitation. This then has to be coupled with "virtual observing packages" that produce not only a theoretical sky brightness distribution but also simulate the observations, e.g., convolve with the telescope beam, apply instrument profile(s), etc. Again this illustrate a common problem: to interpret the observations and derive a description of the source, a priori assumptions about its structure have to be made. This requires in many instances a number of iterations through a number of modeling steps, simulations of the observations, etc. and it is therefore



Figure 1.2. The evolution of the number of class 0 objects from 1992 to 2000, when this Ph.D. thesis research was initiated. All young stellar objects designated "class 0" protostars in literature, irrespective of parameters such as luminosity and distance, have been counted.

important to establish a systematic (and relatively unbiased) framework for the interpretation.

1.3 This thesis

1.3.1 Context

The focus of this thesis is on the physical and chemical properties of deeply embedded low-mass young stellar objects, i.e., typical class 0 objects. The cornerstone of this thesis is a large molecular line survey of a sample of 18 preand protostellar sources. Previous studies have focused on either just a few individual sources or on a small number of selected molecular species. A study such as this has only become feasible in recent years due to an improvement of observational techniques, in particular improved heterodyne receivers and high sensitivity bolometer continuum cameras such as SCUBA and MAMBO. The latter developments, in particular, have made it possible to map larger star-forming regions (see, e.g., Motte et al. 1998) and have lead to the discovery of a large number of deeply embedded objects (see Fig. 1.2).

The main goals of this thesis are: 1. To establish the physical and chemical structure of low-mass protostars in the earliest deeply embedded stages. 2. To determine observational diagnostics of the different protostellar components, such as different regions of the envelope and the circumstellar disks. 3. To use the chemical structures to test basic chemical networks in protostellar environ-

ments, in particular the interaction between the gas and the grains, and 4. To address if, and how, it is possible to use the chemistry as a "protostellar clock".

1.3.2 Outline and conclusions

The work in this thesis falls in three closely related parts. Chapters 2–4 describe the single-dish survey of the physical and chemical properties of 18 low-mass pre- and protostellar objects. Chapters 5–7 apply the derived physical and chemical models to the interpretation of high resolution interferometer observations for specific sources. Chapter 7, together with Chapters 8 and 9, discusses some of the important chemical effects related to shocks and heating around low-mass protostars. Fig. 1.3 illustrates the different steps taken in this thesis.

Statistical studies of the physics and chemistry of protostellar envelopes

In order to model and understand the chemistry of protostellar environments, the physical conditions such as temperature and density have to be established. In chapter 2 the physical models for the studied sample of pre- and protostellar objects are established based on their submillimeter dust continuum emission observed by SCUBA on the JCMT. The density structure is constrained and the temperature distribution is calculated self-consistently for each envelope through 1D radiative transfer modeling. It is found that all envelopes can be fit with density power-law profiles ($n \propto r^{-p}$) with values of p in the range 1.5–2, in agreement with typical collapse models. No trend is seen between density profile and class of object (i.e., class 0 or I) although the "bluer" objects are found to have less massive envelopes.

For each object the CO abundance structure is furthermore constrained through Monte Carlo line radiative transfer modeling. The objects with the more massive envelopes clearly have lower CO abundances, whereas the less embedded objects have abundances close to those inferred for general molecular clouds. This likely reflects the freeze-out of molecules at low temperatures and high densities. Interestingly the CO desorption temperature is found to be higher than previously thought ($T \gtrsim 35$ K) which may reflect the properties of the dust ice-mantles as suggested by recent laboratory experiments.

Chapter 3 presents a large molecular line survey of the entire sample of objects performed at the JCMT from 2001 to 2003. Molecular abundances are constrained using Monte Carlo line radiative transfer. Clear trends are found between a number of different molecular species. For example, CO and HCO⁺ are very closely correlated as expected from the formation of HCO⁺ through reactions between H_3^+ and CO. Vice versa, the N_2H^+ abundances are found to be anti-correlated with those of CO, reflecting that this molecule is destroyed through reactions with CO when it evaporates from dust grains at higher temperatures. An empirical chemical network is constructed on basis of the complete set of abundances, illustrating also the relations between the sulfur-bearing species or within the group of nitrogen-bearing species.



Figure 1.3. Overview of path toward a complete picture of the physical and chemical evolution of low-mass protostars. Continuum observations and modeling are discussed in Chapters 2, 5, 6 and 7. A large single-dish line survey constraining the chemical structure of each source is described in Chapters 2, 3 and 9. Interferometer observations constraining the small scale physical and chemical properties of the protostars are discussed in Chapters 5–7 and specific chemical models in Chapters 4 and 6. Finally the use of mid-infrared observations to constrain the properties of embedded protostars is briefly addressed in Chapter 10. The discussion about ices in low-mass protostars form a very large and important aspect of interstellar chemistry, but is not included here. Also studies of the importance of outflows in shaping the properties of low-mass protostars, as discussed in Chapter 8 and 9, are not indicated.

Time- and density dependent freeze-out in protostellar envelopes

Chapter 4 further explores the important conclusion from Chapters 2 and 3 that the abundances vary with envelope mass. A simple empirical chemical model is introduced in which the derived constant abundances probe the size of the region where a given molecule is frozen out. This is similar to the known situation for pre-stellar cores: such cores have low temperatures at all radii and one should therefore expect CO to be completely frozen out. However, as the density varies with radius so does the timescale for freeze-out. Only in the innermost dense region is the timescale for a given (e.g., CO) molecule short enough that significant depletion occurs within the lifetime of the core. In the exterior regions no depletion occurs and the abundances stay high there. In the protostellar stages the central object heats the envelope and the temperature becomes high enough toward the center that molecules start to evaporate. The abundance thereby shows a characteristic "drop structure" with high abundances in the inner- and outermost regions of the envelope and a drop at intermediate radii. As argued in Chapter 4, this is a good probe of the thermal and dynamical evolution of the core and thus, in principle, an age indicator for the pre- and protostellar stages. Fig. 1.4 illustrates the different density, temperature and abundance structures for pre- and protostellar objects from Chapter 4.

High-resolution studies of the physics and chemistry of low-mass protostellar envelopes

A problem with the single-dish observations presented in Chapters 2 and 3 is the poor spatial resolution which can be reached at (sub)millimeter wavelengths. Chapter 5 presents millimeter wavelength aperture synthesis observations of the protostar NGC 1333-IRAS2. Both the millimeter continuum emission and lines of optically thin species such as $H^{13}CO^+$ and $C^{34}S$ are well reproduced by the larger-scale envelope models constrained by the single-dish data. This has two important implications: 1. The structure on scales of a few thousand AU or more derived from single-dish observations can be successfully extrapolated to the smaller (~ 500 AU) scales probed by interferometer data, and 2. the envelope models can be used to address the problem of missing short-spacings from the interferometer observations.

The source itself shows interesting structure on smaller scales: the observations reveal compact continuum emission from two sources separated by ≈ 7000 AU. This emission is unaccounted for by the envelope model, but could originate in circumstellar disks around each of the components. N₂H⁺ only shows emission around one of these sources but is very strong toward a nearby third submillimeter clump, possibly a pre-stellar core without a central source of heating and a large degree of CO depletion. These three objects thereby illustrate the progressive evolution of CO abundances and mass from the pre-stellar through protostellar stages. Outflows in the system are probed by the main isotopic species of HCO⁺, CS and HCN. These molecules show characteristic emission around the dominant component of the binary, forming two sets of outflow lobes perpendicular to each other, indicating that this component may itself be a close (≤ 65 AU) unresolved binary.

Chapter 6 explores a number of the chemical effects discussed in the previous chapters by further high-resolution millimeter interferometer observations of another class 0 protostar, L483-mm. The anti-correlation between CO and N_2H^+ abundances is directly imaged: CO is seen to come off the dust grains close to central protostar whereas N_2H^+ avoids this region and peaks where CO freezes out. The "drop abundance" structure of CO is constrained by direct comparison between the observed and modeled source structure. CN



Figure 1.4. Density, temperature and abundance profiles for pre- and protostellar objects. The left column gives the temperature and density as functions of radius (black solid and grey dashed lines, respectively) for three archetypical low-mass pre- and protostellar objects: L1544 (pre-stellar core), N1333-I2 (class 0, $M_{\rm env} > 0.5M_{\odot}$ protostar) and TMR1 (class I, $M_{\rm env} < 0.5M_{\odot}$ protostar). The black dotted line indicate the derived abundance structure. The right column gives the depletion signature for each class of object with, going from the outside to the inside, the dark grey indicating the region where the density is too low for depletion ($n < n_{\rm de}$), the black indicating the region where the molecules deplete and the light grey indicating the region where they evaporate ($T > T_{\rm ev}$).

emission is found to probe a boundary between quiescent material in the envelope traced by N_2H^+ and outflowing material probed by HCO^+ . A scenario is suggested in which CN is enhanced in outflow cavities in the envelope, possibly due to UV radiation escaping from the central star-disk system creating spatially unresolved photo-dissociation regions in the outflow cavity walls.

Shocks and passive heating in envelopes and clouds

Freeze-out and evaporation of other molecules such as H_2CO and CH_3OH also provide interesting puzzles for the studies of low-mass protostellar envelopes. Chapter 7 presents a high angular resolution study of 1 mm H_2CO observations of two protostars, L1448-C and IRAS 16293-2422. In particular, the question whether these objects have "hot inner regions" in their envelopes is addressed with these data. Again, the density dependent freeze-out is important in the interpretation and the interferometer observations can in fact be explained without the need for an abundance increase at small scales.

Chapter 8 presents a combined interferometer and single-dish study of the shock from the outflow associated with the class 0 protostar NGC 1333-IRAS2A also discussed in Chapter 5. The morphology of the interferometer emission clearly reveals the chemistry of the shock with large enhancements of, e.g., SiO and CH₃OH close to the shock front due to sputtering and evaporation of grain-mantles. Other species such as HCO⁺, which are destroyed through reactions with H₂O simultaneously released in the shock, are seen to be absent. The physical properties in the shocked and quiescent gas and the column densities/abundances are derived through statistical equilibrium calculations complementing the interpretation from the interferometer maps.

The enhancements of CH₃OH in shocks become relevant in further studies of the protostellar sample covered by the JCMT survey. Chapter 9 concludes the chemistry discussion of this thesis by presenting and discussing abundances of CH₃OH and H₂CO derived for the full sample. Whereas the H₂CO abundances are related to the other species discussed in Chapter 3, the CH₃OH data show large line widths and abundance jumps which indicate that it is enhanced through the outflows in the envelopes close to the central protostar. This is further supported by, e.g., high frequency observations of CS transitions originating in the innermost envelopes.

As a final afterthought, Chapter 10 discusses the constraints that can be obtained through mid-IR observations with the Spitzer Space Telescope and ground based observations with 8 m class telescopes such as VLT, Keck, Subaru and Gemini. Chapter 10 presents modeling results from two papers discussing the early results from the Spitzer Space Telescope. In particular, it shows how such observations can constrain the innermost regions of the envelopes and the properties of the embedded source (i.e., star-disk system) itself - complementary to the constraints obtained through the (sub)millimeter observations discussed in the remainder of the thesis.

1.4 Summary and outlook

In summary the main conclusions of this thesis are:

- The dust and gas in envelopes around a sample of 18 embedded lowmass pre- and protostellar objects are constrained through single-dish (sub)millimeter continuum observations and detailed dust radiative transfer modeling. It is found that all protostellar sources are well-described by 1D spherically symmetric power-law density profiles.
- High-resolution (sub)millimeter continuum imaging show that the envelope structures from the single-dish observations sensitive to scales from a few thousand AU up to ≈ 10,000 AU can be extrapolated down to ≈ 500 AU scales. In combination with mid-infrared observations, these data reveal the presence of circumstellar disks around some, but not all, embedded low-mass protostars.
- A large molecular line survey of the same objects constrain the general features of the chemistry in the protostellar envelopes, whereas millimeter interferometer observations directly probe the radial variation of the chemistry for individual sources. The line observations indicate that significant time, density and temperature dependent depletion occurs in protostellar environments. For example, the CO abundances decrease with increasing envelope masses, suggesting that freeze-out takes place in the densest and coldest envelopes. The freeze-out of CO is found to be important for regulating the chemistry of other species and an empirical chemical network can be established by statistical comparisons between the derived sets of abundances.
- An empirical "drop abundance" profile (see Fig. 1.4) provides good fits to both single-dish and interferometer observations of, e.g., CO, HCO⁺ and H₂CO: in these models depletion occur in a zone within the envelope bounded inwards by the radius where the temperature become high so the molecule desorbs and outwards by the radius where the density becomes low (n ≤ n_{de}) so that the timescales for freeze-out become longer than the age of the core. These structures can be used as a tracer of the thermal and dynamical evolution of the cores from their dense pre-stellar through protostellar stages.
- The presence of outflows may dramatically affect the physical and chemical evolution of low-mass protostellar cores, for example by enhancing species such as CH₃OH through grain mantle liberation – or by creating outflow cavities through which UV radiation can escape increasing, for example, the CN abundance.

Observations with near-future facilities will shed further light on the earliest stages of low-mass star formation. In particular, surveys with the Spitzer Space Telescope will increase the number of known mid-infrared sources and thus candidate protostars. At the same time, it will provide high sensitivity studies of the warm dust and ice content in low-mass protostellar envelopes. Such studies will require follow-up at (sub)millimeter wavelengths and in this context the Atacama Pathfinder Experiment (APEX) submillimeter telescope in Chile will be important, providing new opportunities for studies of the Southern sky.

The prospects for more detailed (sub)millimeter studies of low-mass protostars at high angular resolution are likewise promising with the Submillimeter Array (SMA) on Mauna Kea beginning routine operations, the Combined Array for Research in Millimeter Wave Astronomy (CARMA) combining the BIMA and OVRO arrays by late 2005 and, in particular, the 64 antenna Atacama Large Millimeter Array (ALMA) starting operations in late 2007. These facilities will make it possible to image star forming regions at subarcsecond resolution. Since they are located at excellent sites, they allow high frequency studies of high excitation lines originating in the dense and warm material close to the central protostars.

As well as leading to further increases in the known objects and even more detailed studies of protostellar sources, these developments will all push the requirements of our modeling efforts for the interpretation and understanding of the circumstellar environments of young stellar objects. In that context, this thesis also serves as an important development of the approach to observations and modeling of embedded protostars and as a pathfinder for future studies of these crucial stages of low-mass star formation.