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Small scale kinematics of massive star-forming cores



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Small scale kinematics of massive star-forming cores

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Dedicated to my parents

Cover: Hunting for massive disks. Figure by the author.

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Chapter 1

Introduction

1.1 Massive star formation

1.1.1 What are massive stars?

Stars are the “atoms” of our universe. By mass, they are classified as low-mass stars ($M \sim 0.05 - 2 M_{\odot}$), intermediate-mass stars ($M \sim 2 - 8 M_{\odot}$), and, the major focus of this thesis, massive stars ($M \geq 8 M_{\odot}$) which are defined by their mass exceeding the Chandrasekhar limit (core mass $\sim 1.4 M_{\odot}$), so that during their death with catastrophic core collapse they become neutron stars ($M \sim 8 - 25 M_{\odot}$) or black holes ($M > 25 M_{\odot}$). Unlike low-mass stars, which dominate the stellar population, massive stars are relatively rare, according to the high-mass end (about $\geq 1 M_{\odot}$) of the initial mass function (IMF; Salpeter 1955; Kroupa 2001; Chabrier 2003, see Bonnell et al. (2007) for more discussion) formulated as

$$\frac{dN}{dM} \propto M^{-2.35}, \quad (1.1)$$

or

$$\frac{dN}{d\log M} \propto M^{-1.35}, \quad (1.2)$$

where dN is the number count per mass bin dM . The Salpeter IMF implies that for a stellar population with massive stars, most of the mass is in low-mass stars (total mass $\sim \int M dN$), while most of the luminosity comes from massive stars (assuming¹ $L \propto M^3$, total luminosity $\sim \int L dN$). Therefore, the rare massive stars can influence the evolution of interstellar medium (ISM), galaxies, and our universe. In Table 1.1, we classify main-sequence massive stars by their mass or spectral type. In this thesis, we focus on the early B-type to late O-type stars. The rarity of these stars can be seen in Table 1.1 if the IMF follows Eq. (1.1).

¹c.f. Salaris & Cassisi (2005) for stellar mass greater than about $2 M_{\odot}$

Table 1.1. Classification of main-sequence massive stars

Mass	Designation	Spectral Type	N ^a
8–16 $M_{\odot}$	early B-type	B3V to B0V	17
16–32 $M_{\odot}$	late O-type	O9V to O6V	7
32–64 $M_{\odot}$	early O-type	O5V to O2V	3
64–128 ^b $M_{\odot}$	O/WR-type	WHL–H	1

Note. — Adopted from Table 1 and Table 2 of Zinnecker & Yorke (2007). ^aNumber of stars according to the initial mass function $dN/dM \sim M^{-2.35}$ if the number count of the highest mass range is normalized to unity. ^b A more realistic upper limit of this mass range is $\sim 150 M_{\odot}$ (Figer 2005).

Although rare, massive stars are the main factories that synthesize atoms up to iron during their main-sequence lifetime and produce heavier elements during their supernova phase. This ISM enrichment is a very fast process at cosmic timescales since the typical lifetime of a massive star is only a few Myrs. Within this short period, massive stars provide strong feedback to the ISM through intense and massive outflows, dissociative UV radiation, powerful stellar winds, expanding HII regions, and supernova explosions. A combination of this feedback provides a source of turbulence² in the ISM of galaxies, which is thought to be an important mechanism controlling star formation (McKee & Ostriker 2007) and galaxy evolution (Kennicutt & Evans 2012).

1.1.2 Where are the birthplaces of massive stars?

The birthplaces of massive stars may be found by looking at the location of the end-product of their formation — the main sequence OB stars. OB stars are found in clusters and associations (Blaauw 1991; Lada & Lada 2003; Portegies Zwart et al. 2010), which are different in size scales ($\sim 1 - 10$ pc for clusters, and $\sim 10 - 100$ pc for associations). Note that OB star clusters can also be members of OB associations. If the current morphology of the two distributions does not change much due to dynamical interactions of stars after their formation, the different size scales imply that massive star formation can happen at very different scales in molecular clouds (relatively local or global). One interesting finding is that in clusters, massive stars are usually located near the center and

²Extraction of ordered kinetic energy from galactic rotation, mediated via spiral density waves or cloud collisions is also a possible source of turbulence (e.g., Tan 2000; Tasker & Tan 2009).

surrounded by numbers of lower-mass stars (e.g., Hillenbrand & Hartmann 1998). This mass segregation in clusters again implies that either massive stars tend to be directly formed near the densest part of cluster-forming cores (Bonnell & Davies 1998), or they are formed first in parts of clusters and cascade down to the center by dynamical relaxation (Binney & Tremaine 1987).

Clusters containing massive stars can have very different total stellar masses and numbers of OB stars, likely linked to the total masses of the original molecular clouds (Williams & McKee 1997). For example, the probability of finding a single O9.5 star in a cloud with mass of $10^5 M_{\odot}$ is about 50%. If the cloud mass is $10^6 M_{\odot}$, it is highly probable to form at least one late O-type star. The nearest cluster containing O-type stars is the Orion Nebula Cluster (ONC) at distance of 414 ± 7 pc (Menten et al. 2007). Its total stellar mass is about $10^3 M_{\odot}$, including a few O-type stars. NGC 3603 (in the Carina region at ~ 7 kpc) with about a few dozen O-stars and R136 (in the 30 Doradus region in Large Magellanic Cloud at 55 kpc) with a few hundred O-stars are other examples of massive clusters, which have stellar masses of 10^4 and $10^5 M_{\odot}$, respectively. It is expected that their original cloud masses must be higher by one or two orders of magnitude.

There is a third type of massive star that is not found in either clusters or associations, but in the field. From observations, de Wit et al. (2004, 2005) conclude that about 50% of field massive stars can be directly traced back to nearby OB clusters or associations. They are dynamically ejected with velocities more than 40 km s^{-1} from the regions where they formed (e.g., Blaauw 1961). Typical proper motions of OB stars are only a few km s^{-1} . However, the birthplace of a few % of known field OB stars cannot be identified, leading to the question of how they formed in field. A remarkable example is the O9.5 star HD93521, which is located at ~ 1 kpc above the galactic plane and is believed to have formed in the galactic halo (Irvine 1989). In the 30 Doradus region of Large Magellanic clouds, the evidence of isolated massive star formation is also found (Bressert et al. 2012). To understand this, the formation of massive stars in clusters and (relative) isolation needs to be uncovered.

1.1.3 How do massive stars form?

Compared to the formation of their low-mass counterparts, our understanding of the formation and early evolution of massive stars is still sketchy (Zinnecker & Yorke 2007; Beuther et al. 2007). We begin with an outline of the stages of low-mass star formation and later point out the main differences and difficulties for massive star formation. Followed by the observational classification of massive star-forming cores, we outline possible scenarios of massive star formation.

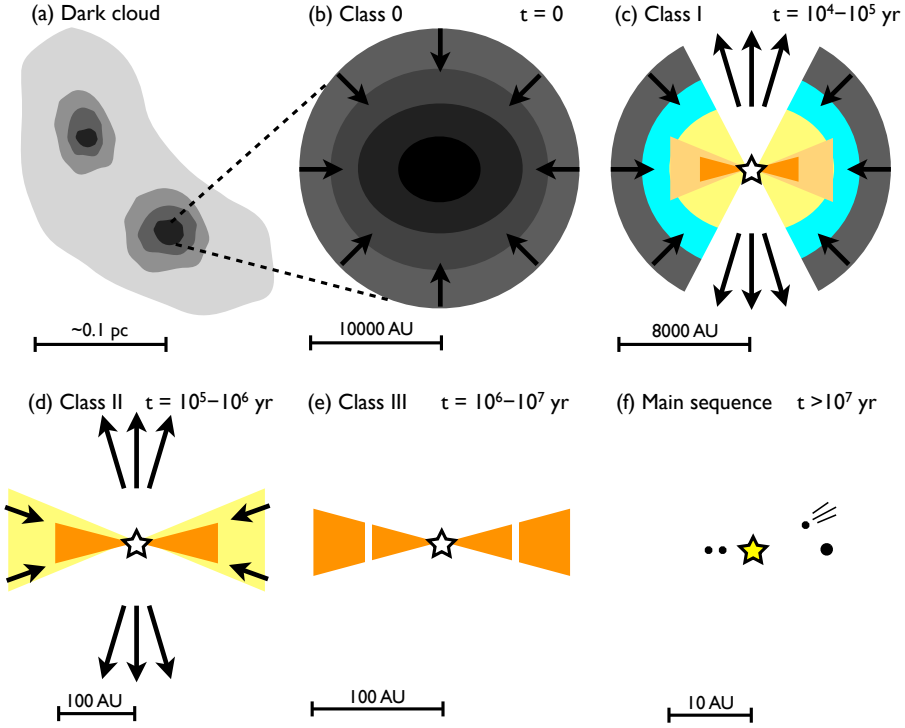


Figure 1.1 Evolutionary stages of low-mass star formation.

1.1.3.1 Low-mass star formation

For an isolated low-mass star, the formation process is summarized by Shu et al. (1987) and McKee & Ostriker (2007) and is presented graphically by Wilking (1989) (Fig. 1.1). Low-mass star formation happens in dense cores (size: 0.03–0.2 pc, density: 10^4 – 10^5 cm $^{-3}$) of molecular clumps (size: $\sim 0.3 - 3$ pc, density: 10^3 – 10^4 cm $^{-3}$) embedded in dark molecular clouds (size: $\sim 2 - 15$ pc, density: 50–500 cm $^{-3}$; Bergin & Tafalla 2007, and reference therein). The temperature reaches its local minimum of ~ 10 K for a prestellar core before global infall. Once gravitational collapse happens (Class 0), the core is heated inside-out and may drive a high temperature chemistry with rich emission from complex organic molecules (e.g., the hot corino: IRAS 16293–2422; Kuan et al. 2004; Bottinelli et al. 2004; Bisschop et al. 2008; Caux et al. 2011; Jørgensen et al. 2011). The conservation of angular momentum of infalling cores results in the formation of circumstellar disks in Keplerian rotation (Class I or earlier). At this stage, mass transfer happens from envelope to disk and then from disk to star, while in the meantime the excess of angular momentum can be removed via bipolar outflows. Most of the final stellar mass is acquired at this stage (accretion timescale $t_{\text{acc}} \sim$

few $\times 10^5$ yr; Evans et al. 2009). In a later less embedded phase with little mass transfer from any remaining envelope to disk (Class II), a pre-main-sequence star is surrounded by a protoplanetary disk and may still be driving a weak bipolar outflow. Later, the bipolar outflow ceases and the pre-main-sequence star contracts slowly toward the main sequence (Class III). Typical timescales of 10^7 yr for contraction of a low-mass protostar are estimated via the Kelvin-Helmholtz time,

$$t_{\text{KH}} = \frac{GM^2}{RL}, \quad (1.3)$$

where M , R , and L are stellar mass, radius, and luminosity, respectively. Therefore, for low-mass star formation, t_{acc} is smaller than t_{KH} , meaning that there is a well-defined pre-main sequence phase. The total amount of time to form a mature planetary system, like our Solar system, from the onset of the collapse of prestellar core is more than 10^7 yr. The formation time of a low-mass star is about 0.1% of its total lifetime.

1.1.3.2 Massive star formation: difficulties

The difficulties of massive star formation come from the fact that forming massive stars are not only rare (according to the IMF) but they evolve very fast over $\sim 10^5$ yr or a few % of their total lifetime (few 10^6 yr; Churchwell 2002) while still highly embedded ($A_V > 100$ mag). Most importantly, the Kelvin-Helmholtz time for massive stars is only $10^4 - 10^5$ yr, meaning that massive stars enter the main sequence phase while collapse of the dense core and subsequent accretion still happen. A distinct difference between low- and high-mass star formation is that massive stars generate intense and dissociative UV radiation, leading to radiation pressure that is strong enough to halt accretion and generate HII regions. Early studies show that if massive stars form through spherical accretion, an upper-limit on the stellar mass of $\sim 40 M_\odot$ is found (highly depends on dust properties; Kahn 1974; Wolfire & Cassinelli 1987), which also sets a cutoff to the IMF. However, from observations, a cutoff of about $150 M_\odot$ is more likely (e.g., Figer 2005), implying that formation schemes other than spherical accretion must exist. Through 2D axi-symmetric simulations following massive star formation from a collapsing core to an accretion disk including radiation feedback, Yorke & Sonnhalter (2002) found that the radiation problem is less severe since the disk in the equatorial plane around the forming massive star helps to redirect the stellar radiation to the polar direction allowing accretion in the equatorial regions (see also Nakano et al. 1995; Jijina & Adams 1996). This is the so-called “flashlight effect”. The cavities created by bipolar outflows also enhance the flashlight effect (Krumholz et al. 2005b). Radiation may not always be destructive since massive stars may form through radiatively driven Rayleigh-Taylor instabilities (Krumholz et al. 2005a). Alternatively, the radiation problem

can be solved by introducing a high accretion rate of the order of 10^{-3} to $10^{-4} M_{\odot} \text{ yr}^{-1}$ which is high enough to sustain inward motion (McKee & Tan 2003). We note that if massive stars form through accretion, the requirement of high accretion rates is implicitly implied by their short lifetime. The high accretion rates also enable accretion through ionized flows (Keto 2007).

Our understanding of massive star formation is not only limited by theoretical difficulties, but also by observational limits. Massive star-forming regions are typically at a few kpc from our Sun, thus high-angular resolution observations are required. Apart from their distance, massive star-forming cores are highly embedded, which only centimeter, millimeter, submillimeter, and mid/far-infrared wavelengths can penetrate. In addition, the rapid evolution of massive star-forming cores makes the target selection difficult. The mixture of stellar feedback and high column densities of star-forming materials make the interpretation of observational data non-straightforward.

1.1.3.3 Massive star formation: observational phases

Although it is difficult to observe massive star-forming regions, modern techniques at the above mentioned wavelengths allow us to classify massive star-forming cores observationally (Churchwell 1999; Beuther et al. 2007; Zinnecker & Yorke 2007). In the following, we highlight the various components of this classification one by one, as shown in Fig. 1.2.

High-mass starless core (Fig. 1.2 a)

Massive star formation starts in high mass starless cores (HMSC) within molecular clumps where the density reaches a local maximum ($> 10^6 \text{ cm}^{-3}$) and the temperature is a local minimum ($< 20 \text{ K}$). The typical masses of these clumps, with typical sizes of 0.25–0.5 pc, are a few 100 to a few 1000 $M_{\odot}$ (e.g., Beuther et al. 2002a; Williams et al. 2004). The mean density is about 10^5 cm^{-3} . Infrared Dark Clouds (IRDC), identified as dark filaments against bright infrared backgrounds (Simon et al. 2006), are one type of objects that satisfy the above conditions. High-mass starless cores are rare, suggesting that their timescales may be very short (e.g., Ragan et al. 2012).

High-mass protostellar object (Fig. 1.2 b)

This type of source is classified based on the detection of infall signatures, non-detection of cm-wave emission from ionized gas, and non-detection or weak detection of emission from complex molecules. The absence of free-free emission indicates that the forming stars have not yet reached the limit for hydrogen fusion. The forming stars may be still low-mass to intermediate-mass. The non-detection of the emission from complex molecules may be due to limited sensitivity of observations, since the hot core is still small in size. Hot dense gas confined close to forming stars is expected to be present inside any HMPO.

Hot molecular core (Fig. 1.2 c)

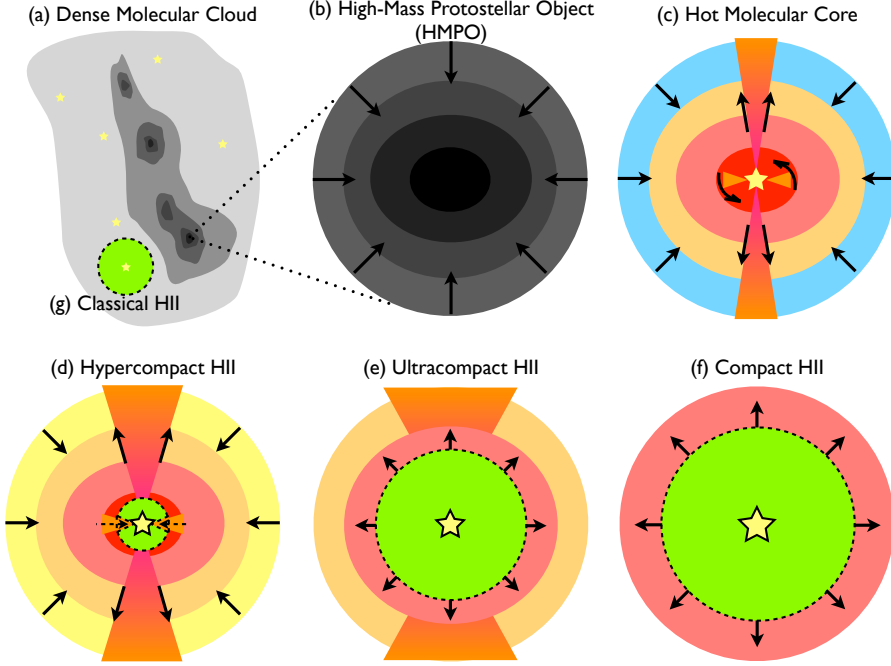


Figure 1.2 Observational classification of massive star-forming cores.

This type of source is characterized by its rich emission from complex organic molecules such as CH_3OH , HCOOCH_3 , and $\text{C}_2\text{H}_5\text{CN}$, etc. (e.g., Kurtz et al. 2000; Cesaroni 2005), as an indication that a significant part of the star-forming core has been heated up, leading to evaporation of ice on dust grains and further high-temperature gas-phase chemistry (Herbst & van Dishoeck 2009).

Hypercompact and ultracompact HII regions (Fig. 1.2 d and e)

Once the forming massive stars start fusion at their central regions, the intense UV radiation can ionize the surrounding gas, leading the formation of hypercompact or ultracompact HII regions (Kurtz 2005; Hoare et al. 2007). The difference between the two is their size. Typical sizes are few 100 AU to few 1000 AU. These small HII regions are spatially confined to their host stars. Hypercompact HII regions are suggested as the remnant of photoevaporating disks (Keto 2007), while ultracompact HII regions contain no disk and photoionize their surrounding molecular cocoon.

Compact and classical HII regions (Fig. 1.2 f and g)

Ionization happens globally (pc scales) in these type of sources (Mezger et al. 1967; Yorke 1986). They expand hydrodynamically and disrupt the parent molecular cloud. At this stage, embedded massive stars with their surrounding low-mass stellar population can be observed at optical and near infrared wavelengths.

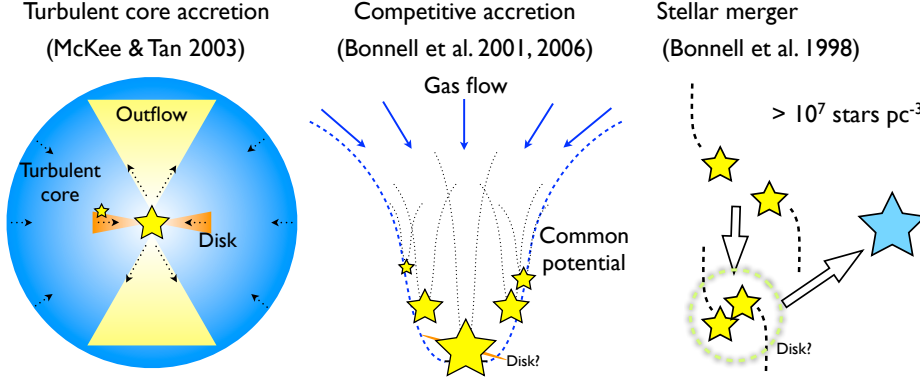


Figure 1.3 Theories of massive star formation.

The above observationally defined classes of objects may be linked in an evolutionary ordering. We note that the sequence presented in Fig. 1.2 does not necessarily represent one according to evolution. In fact, the evolution of a forming massive star is so fast that it is hard to construct a distinct evolutionary sequence and it is observationally difficult to distinguish evolution from luminosity differences. The above different phases may be coexisting. A possible formation sequence of a single massive star or a small cluster may be as follows: HMPO (Fig. 1.2 (b)), hypercompact HII (Fig. 1.2 (d)), ultracompact HII (Fig. 1.2 (e)), compact HII (Fig. 1.2 (f)), and classical HII (Fig. 1.2 (g)). The hot molecular core phase (Fig. 1.2 (c)) may coexist with hypercompact and ultracompact HII regions.

1.1.3.4 Massive star formation: theories

The formation of massive stars may follow two very different scenarios: by accretion, or by coalescence (merger). The latter model provides a brute-force solution to avoid the radiation problem by allowing direct collision of stellar components in dense clusters (Bonnell & Davies 1998). The former can be further classified into two different accretion mechanisms: turbulent core accretion (McKee & Tan 2003) and competitive accretion (Bonnell et al. 2001; Bonnell & Bate 2006). These three different concepts of massive star formation are summarized in Fig. 1.3.

The turbulent core accretion model or monolithic collapse model is similar to the formation of isolated low-mass stars as outlined in Sect. 1.1.3.1, but with modification in the strength of turbulence and accretion rates. In this model, core density and velocity dispersion follow power-laws as functions of radius. The turbulence is strong enough to provide ram pressure to support the core against fragmentation before massive star formation proceeds. The star-forming

core can also be supported by large-scale magnetic fields. The high accretion rates ($10^{-4} - 10^{-3} M_{\odot} \text{ yr}^{-1}$) are able to sustain accretion in an environment with strong radiation pressure. Accretion can proceed through a disk, which also helps to redirect radiation in the polar direction. The final stellar mass is correlated with the initial mass of the star-forming core. In other words, the accretion happens locally. The overall picture of massive star formation resembles its low-mass counterpart. (i.e., a collapsing core with formation of a disk and outflows)

Competitive accretion relies on the physics of gravity and the observational fact that massive stars usually form in clustered environments. The initial star-forming cloud (pc scales) does fragment down to thermal Jeans mass ($\approx 1 M_{\odot}$). For regions with higher (proto)stellar density, further run-away growth can proceed by Bondi-Hoyle accretion (Bondi 1952), which describes the accretion process of a spherical object traveling in the interstellar medium, or tidal accretion enabled by the joint gravitational potential of star clusters. The relatively massive stars (not necessarily yet $> 8 M_{\odot}$) sitting at the bottom of the joint gravitational potential well have the highest chance to become more massive stars ($> 8 M_{\odot}$). Accretion happens globally at cloud scales down to core scales (i.e., the mass for a given massive star may come from any part of the parent cloud and depends on how the infalling material is distributed over the most massive cluster members). In addition, this type of formation mechanism is able to reproduce the full IMF similar to the observed one (Bonnell et al. 2007).

The most dramatic mechanism of forming a massive star is through coalescence of lower-mass protostars or main sequence stars in the center of dense clusters with stellar densities higher than $\sim 10^7 \text{ pc}^{-3}$. This merger scenario is a violent process during which circumstellar disks will be destroyed, outflows will be disrupted, and stars may be ejected.

1.1.4 Why do kinematics at small scales ($\leq 0.1 \text{ pc}$) matter?

Among the three dominant theories of massive star formation, disks and outflows are essential components, but with different properties. In the turbulent core accretion model, these structures are more long-lived, while in the other two formation schemes, these structures should be perturbed and likely short-lived. The high occurrence of collimated massive bipolar outflows observed toward massive star-forming cores (Zhang et al. 2001; Beuther et al. 2002b) provides a strong hint that the formation of massive stars may follow the disk accretion process similar to the turbulent core accretion model. However, to date, the presence of circumstellar “disks” is reported only toward about few tens or so young early B-type stars, via (sub)millimeter observations (summarized by Cesaroni et al. 2007) and direct imaging in infrared wavelengths (e.g., Kraus et al. 2010; Boley et al. 2012). These disk-like structures are found to be large ($\sim 10^{2-4} \text{ AU}$)

and massive ($M_{\text{disk}} \leq M_{\star}$), which is quite different from the disks around low-mass protostars ($M_{\text{disk}} \ll M_{\star}$). On the contrary, only large “toroids” undergoing solid-body rotation with masses greater than stellar masses are found toward young O-type stars (e.g., Beltrán et al. 2005; Furuya et al. 2008). These rotating structures show diverse characteristics. Therefore, it is interesting to study massive star-forming cores on small scales (≤ 0.1 pc scales) with high-angular resolution observations and focus on the gas motions including turbulence, infall, outflow, and especially *rotation*. Furthermore, the presence of disks open up the possibility of planet formation around massive stars.

1.2 Methodology

1.2.1 Millimeter and submillimeter observations

Observations at millimeter and submillimeter wavelengths are important in the field of star formation. At these wavelengths, cold and warm dust can be probed by measuring its thermal emission. Physical conditions, such as temperature, density, kinematics, as well as chemical conditions, such as chemical abundances and distributions, can be studied through rotational transitions of interstellar molecules. With the advent of millimeter and submillimeter interferometric facilities such as the Submillimeter Array (SMA), Combined Array for Millimeter Astronomy (CARMA), and Plateau de Bure interferometer (PdBI), it is now possible to investigate the physical and chemical conditions of massive star forming cores on small scales in detail. Interferometric observations are especially important for hunting for massive disks since typical massive star-forming regions are located at a few kpc from the Sun and the typical sizes of massive disks are a few 1000 AU or less, corresponding to $\sim 1''$ or less.

The basic idea of (sub)millimeter interferometry is that instead of building a single huge single element telescope to achieve high angular resolution following $\theta_{\text{HPBW}} \sim \lambda/D$, where θ_{HPBW} is the half-power beam width, λ is the observing wavelength, and D is the size of the dish, a set of small dishes is distributed over an area and linked together to simulate an equivalent big single-dish telescope. The signal from the sky is correlated for each pair of antennas, with the correction of the geometric delay and instrumental delay. At an instantaneous moment, different pairs of antennas have different spatial sensitivity formulated as $\theta_{ij} \sim \lambda/B_{ij}$, where θ_{ij} is the spatial resolution for a given antenna pair ij , and B_{ij} is the length of the baseline ij . Due to the Earth rotation, the spatial sensitivity of each baseline changes due to the projection effect. An ensemble of different correlations with different projections forms a spatial sampling in the Fourier plane or (u,v) plane. In principle, samples with small uv -distances ($\sqrt{u^2 + v^2}$) probe signal from large scales, while samples with large uv -distances are more sensitive to signal from small scales. We note that uv -data or “visibility” data

are the real output from interferometers, not direct images. Images are reconstructed by performing Fourier transformation of the visibility and subsequent image processing.

Although through interferometric techniques, high angular resolution can be obtained at (sub)millimeter wavelengths, there are caveats. The largest spatial sensitivity is set by the smallest uv sampling. Therefore, interferometers are blind to signals coming from scales greater than the scales set by the shortest baselines. This is the so-called “missing flux” problem. This potential problem may be solved by filling the uv gap with single dish (total power) observations. So far, full image synthesis (combining single-dish and array data) is still not a routine observing strategy. In this thesis, we use both single dish observations and (sub)millimeter interferometric observations to individually study the gas kinematics of massive star-forming cores at different scales.

1.2.2 Observing dust emission and molecular line emission

Dust and molecules are essential components of star-forming cores. At a temperature of 10–100 K, dust is a strong emitter at (sub)millimeter wavelengths. By measuring its continuum emission, one can estimate the total dust mass of the source by assuming a dust temperature and a dust opacity. Ossenkopf & Henning (1994) provides a good reference of dust opacities for star-forming cores. With an additional assumption on the gas-to-dust ratio, one can also derive the total H_2 mass and column density of the source.

Molecular transitions are classified in terms of electronic transitions, vibrational transitions, and rotational transitions. The former two transitions correspond to UV/optical and mid-infrared wavelengths, respectively. Rotational transitions of molecules mainly fall in the (sub)millimeter wavelength regime. The physical conditions associated with star-forming regions are especially suitable for excitation of rotational levels of molecules. By measuring molecular rotational emission lines, one can estimate the physical and chemical conditions of the star-forming cores. In addition, molecular lines carry kinematical information. Therefore, observing molecular lines at (sub)millimeter wavelengths is well suitable to probe infall and rotation near forming massive stars.

Hot molecular cores are associated with massive star-forming regions (Sect. 1.1.3.3). The evaporation of icy mantles from the surfaces of dust grains plus high-temperature gas-phase reactions result in rich complex organic molecules. The first model of hot core chemistry was proposed by Brown et al. (1988) who followed the gas-phase chemistry of cold gas during the core collapse, including the accretion and subsequent surface reactions on dust grains, until the heating mechanism drives the icy mantles back to the gas phase. Later Charnley et al. (1992) demonstrated that a realistic mixture of ices containing H_2O , NH_3 and CH_3OH , as observed in cold clouds, could reproduce the observed molecular

abundances in the Orion KL hot molecular core by high temperature chemistry following evaporations. The hot core chemistry has been further extended to include S-bearing (Charnley 1997), Si-bearing (Mackay 1995) and P-bearing (Charnley & Millar 1994) species. Because of new insights into gas phase chemistry, however, more recent models suggest that most of the complex molecules are formed on the grain surfaces (Garrod & Herbst 2006). As the result of rapid change of physical conditions in massive star-forming regions, chemical ingredients could be classified into three kinds: (1) molecules which are formed in the pre-collapse phase and released from the icy mantles on dust grains (e.g., C_2H_2 , CO); (2) molecules that are made on the surface of dust grains and released back to gas phase (e.g., NH_3 , CH_3OH); and (3) molecules that are formed in the gas phase after mantle evaporation. Hot core observations are thus important to provide constraints on the chemical ingredients both in the gas phase and solid phase of hot core models. In this thesis, we utilize the emission from hot core molecules as the diagnostics of physical conditions including kinematics.

1.2.3 Radiative transfer and molecular excitation

The signal from the sky observed by telescopes is described by the equation of radiative transfer,

$$\frac{dI_\nu}{dz} = -\kappa_\nu I_\nu + j_\nu, \quad (1.4)$$

where I_ν is the specific intensity, z is the coordinate system along the line of sight, κ_ν is the absorption coefficient and j_ν is the emission coefficient (Fig. 1.4). Both κ_ν and j_ν are macroscopic parameters. Microscopically, these two parameters are related to the atomic or molecular properties. The microscopic interplay between radiation and matter is conveniently described by the Einstein coefficients A and B . Collisions, determined by temperature and density, happen between particles and are described by the collisional rate coefficient C . Here we focus on the rotational transitions of interstellar molecules, which millimeter and submillimeter observations are sensitive to. Every molecule has its own unique “pattern” of discrete energy levels based on quantum theory (c.f., Townes & Schawlow 1955). For simplicity, we assume a two-level system (Fig. 1.4). This two-level system can be de-excited via spontaneous emission, stimulated emission, and collisions with transition probabilities of A_{ul} , $\frac{4\pi}{c} I_\nu B_{ul}$, and $n_{\text{col}} C_{ul}$ respectively, while the system can be excited via absorption of radiation and collision with transition probabilities of $\frac{4\pi}{c} I_\nu B_{lu}$ and $n_{\text{col}} C_{lu}$, respectively (n_{col} is the volume density of the collisional partner). The observed spectral lines are the results of detailed balance between radiation and collision, and the integration over the emitting medium along the line of sight based on the radiative transfer equation (Eq. 1.3).

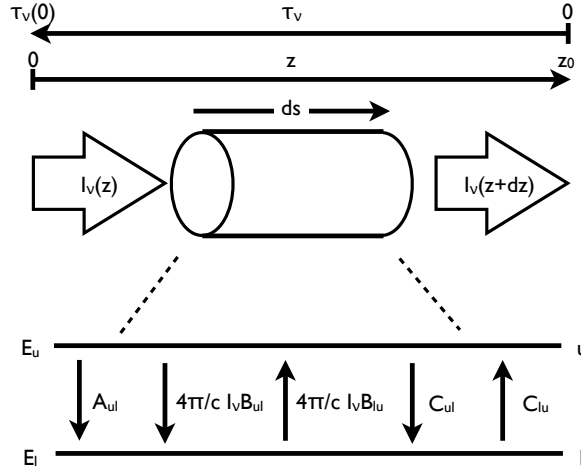


Figure 1.4 A sketch of radiative transfer process including molecular excitation.

In general, solving the equation of radiative transfer to understand the excitation conditions for a given molecule is a complicated task (van der Tak 2011). This requires good assumptions of temperature, density, and velocity distribution, as well as source geometry. Most importantly, the collisional rate coefficients of molecules are needed, which so far have been tabulated for only few molecules and limited levels (c.f., Schöier et al. 2005). However, it is still possible to derive some basic quantities, such as excitation temperature T_{ex} and total molecular column density N_{tot} , from the observed line intensities, without solving the radiative transfer equation. The most straightforward and frequently used method is the “rotation diagram” (e.g., Turner 1991), which assumes that the observed transitions are all optically thin and follow a single Boltzmann distribution at T_{ex} . If the observed target has high enough gas density to fully thermalize the energy levels via collisions, the derived T_{ex} is a good approximation of the kinetic temperature (T_{kin}). If, however, some transitions are optically thick, or the energy levels are subthermally excited, this method results in highly uncertain T_{ex} as well as N_{tot} . For molecules with known collisional rate coefficients, this problem may be solved by using approximated methods to solve to detailed balance of energy levels and radiative transfer, such as the large velocity gradient (LVG) approximation (Goldreich & Kwan 1974) or escape probability method (Rybicki 1985). In this thesis, we use the computer program RADEX (van der Tak et al. 2007) to perform this type of analysis. This approach still assumes that the source is homogeneous and characterized by a single T_{kin} , a single N_{tot} , and an uniform gas density. To fully solve the equation of radiative transfer including detailed balance of energy levels as a function of space with varying temperature

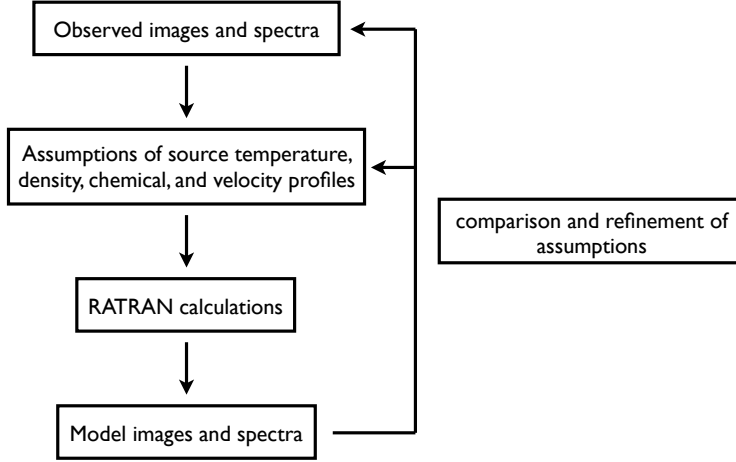


Figure 1.5 Steps of radiative transfer modeling of kinematics with RATRAN.

and density, we utilize the state-of-art code RATRAN (Hogerheijde & van der Tak 2000), which employs an accelerated Monte Carlo approach.

1.2.4 Radiative transfer modeling of kinematics

In this thesis, we mainly focus on the observed molecular line profiles which carry kinematical information of massive star-forming cores. Although a molecular transition has a well defined transition frequency ($\nu = (E_u - E_l)/h$, with h the Planck constant), the observed line profile is usually not a delta function. The finite width of the observed line profiles is a superposition of many aspects. Due to the uncertainty principle of quantum theory, the line is broadened naturally. This effect, however, is negligible for rotational lines, compared to thermal Doppler broadening, which is the result of thermal random motion. In the warm (≥ 100 K) massive star-forming cores, the thermal linewidth is about a few 0.1 km s^{-1} only. The typical broad linewidth (few to several km s^{-1}) observed toward massive star-forming cores implies that non-thermal Doppler broadening effects, such as motions like infall, outflow, rotation, and turbulence, dominate the observed line profiles. To extract the kinematical information hidden in the observed line profiles, we use the radiative transfer code RATRAN (Hogerheijde & van der Tak 2000) as an engine to generate model line profiles with the above non-thermal motions and compare with observations. In Fig. 1.5, we visualize the steps of RATRAN modeling of the kinematics. The analysis of the kinematics in this thesis is performed on a qualitative basis, limited by the data.

1.3 Components of this thesis

In this thesis, the diagnostics provided by molecular line emission and dust emission are used to understand the physical conditions associated with massive star-forming cores at various scales (few 100 AU to few 10000 AU). Kinematics on these scales is the focus of this work. In the following chapters, one survey and three case studies are presented.

1.3.1 Chapter 2

In this chapter, we present single-dish observations with the James Clerk Maxwell Telescope (JCMT) toward 17 massive star-forming cores in lines of C^{17}O , C^{34}S , and CH_3CN near 345 GHz. We aim to establish if these species are indeed robust tracers of disks as suggested by interferometric observations in the literature. We compare the observed spectra with generic radiative transfer models including infall, rotation, and turbulence to have an idea on the origin of the observed linewidth. We conclude that C^{17}O 3–2 best traces turbulence at scales of a few 10000 AU, while C^{34}S mainly traces turbulence at scales of a few 1000 AU. CH_3CN 18–17 lines are the best disk tracer at 1000 AU scales or less, compared to the other two transitions. Further detailed radiative transfer modeling of individual sources is required to disentangle these single-dish line profiles. This chapter will be submitted to A&A.

1.3.2 Chapter 3

In this chapter, we present interferometric observations with the Submillimeter Array (SMA) at 354 GHz toward the proto-Trapezium cluster forming region W3 IRS5. The $1''$ – $3''$ resolution continuum and line data allow us to study the structure, kinematics, and chemistry at 2000–6000 AU scales. The continuum observations show five emission peaks with two forming massive stars and the other three as either starless cores or low-mass star-forming cores with the potential to become massive stars in the future. The kinematics are found to be very complex in the clustered environment of W3 IRS5. From this dataset, we suggest that the proto-Trapezium cluster W3 IRS5 is an ideal test case to discriminate between models of massive star formation. Either the massive stars accrete locally from their local cores; in this case the small core masses imply that W3 IRS5 is at the very end stage (~ 1000 yr) of infall and accretion. Alternatively, the stars may be still accreting from the global collapse of a massive, cluster forming core. Observations that reliably probe infall from large to small scales are needed answer this question. This chapter is published in A&A, 2013, 558, A69.

1.3.3 Chapter 4

In this chapter, we present arcsecond to subarcsecond resolution interferometric observations with the Plateau de Bure interferometer (PdBI) in the 1.3 mm and 3 mm bands toward a forming late O-type star AFGL 2591–VLA3. Through radiative transfer modeling of the HDO $1_{1,0}$ – $1_{1,1}$ and H₂¹⁸O $3_{1,3}$ – $2_{2,0}$ line profiles, we propose that there is a layered disk-like structure undergoing subKeplerian rotation and radial expansion around AFGL 2591–VLA3. The subKeplerian motion may be due to magnetic braking in the disk regions, while the expansion may be the signature of outflow or disk wind activities. Our observations imply that late O-type stars may form following the turbulent core accretion model. This chapter is published in A&A, 2012, 543, A22.

1.3.4 Chapter 5

In this chapter, we present subarcsecond resolution interferometric observations with the expanded Submillimeter Array (eSMA) at 345 GHz in both molecular lines and dust continuum toward the early B-type star S255IR–SMA1. The 345-GHz continuum of SMA1 is resolved at $\sim 0.3''$ resolution (500 AU) for the first time. We find that massive star formation activity is highlighted by the presence of the emission from complex hot core molecules. In addition, a disk-like structure is found in CH₃OH lines which shows a clear velocity gradient perpendicular to large scale outflows. Through a comparison with radiative transfer models, the observed velocity gradient cannot be characterized by Keplerian rotation with the expected stellar mass. Through luminosity analysis, we find that S255IR–SMA1 is a young ($10^3 - 10^4$ yr) forming early B-type star with a high accretion rate (few $10^{-4} M_{\odot} \text{ yr}^{-1}$). Our observations also act as supporting evidence that an early B-type star may form following the turbulent core accretion scenario. This chapter is submitted to A&A.

1.4 General conclusion and Outlook

In this section, we highlight our general conclusions drawn from chapters 2 to 5 of this thesis. The central goal of this thesis is to characterize the kinematics of massive star-forming cores at scales of 0.1 pc or less. We especially focus on the properties of the rotational component, i.e., massive disks, in massive star-forming cores. Through single-dish and interferometric observations at millimeter and submillimeter wavelengths, we conclude:

- (1) C¹⁷O 3–2 and C³⁴S 7–6 are good tracers of turbulence in massive star-forming cores at scales of a few 10000 AU and a few 1000 AU, respectively. Typical turbulent linewidths are $\sim 2\text{--}4 \text{ km s}^{-1}$ at these scales, suggesting that massive star-forming cores are highly turbulent. (Chapter 2)

- (2) Hot core molecules such as CH_3OH and CH_3CN , are good lines to hunt for disks at scales of ~ 1000 AU or less around massive forming stars. (Chapter 2 and 5)
- (3) Hot core molecules are good tracers for massive star formation activity. (Chapter 2, 3, and 5)
- (4) Late O-type stars may also form through disk accretion. (Chapter 4)
- (5) Fossil molecules, such as deuterated species which formed in the cold prestellar phase, are potentially good probes for rotation in massive star-forming cores. (Chapter 4)
- (6) Around very young forming early B-type stars, disks may not be Keplerian. Magnetic fields at scales of few 100 AU may regulate the kinematics of the disk. (Chapter 5)
- (7) Supporting evidence for the turbulent core accretion model and the competitive accretion model is found in our case studies. (Chapter 3, 4, and 5)

With the main conclusions outlined above, we will continue our hunt for massive disks with the Atacama Large Millimeter/sub-millimeter Array (ALMA). Its superior sensitivity at subarcsecond resolution is the best tool for this research. With ALMA, the speed of hunting for massive disks can be boosted by factors of 10–100, compared to current (sub)millimeter interferometers. Sensitive line observations are essential for detailed radiative transfer modeling with better constraints. Wideband line observations are also very powerful to select potential good disk tracers in an uniform way. We believe that ALMA can provide answers to the ultimate question of this thesis: how do massive stars form?

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Kinematics of massive star-forming cores: a JCMT study of infall, outflows, rotation, and turbulence

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in preparation for journal submission

Abstract

Context. Like low-mass stars, massive stars may form via disk accretion, although more observational evidence is required to assess how general this phenomenon is.

Aims. Molecules like C^{17}O , C^{34}S , and CH_3CN are claimed in the literature to trace disks around massive protostars, based on interferometric data. We aim to establish if these species are indeed robust tracers of disks.

Methods. We obtain single-dish observations with the James Clerk Maxwell Telescope toward 17 massive star-forming cores in lines of C^{17}O , C^{34}S , and CH_3CN near 345 GHz. We compare the line profiles to radiative transfer models that include rotation, infall, and turbulence.

Results. The C^{17}O 3–2 emission toward all sources is extended in the $2' \times 2'$ maps, while C^{34}S 7–6 and CH_3CN 18–17 lines remain largely unresolved in the $14''$ beam. Three different types of C^{17}O 3–2 line profiles are found: single Gaussian, narrow+broad Gaussians, and two Gaussians with comparable FWHM. The C^{34}S 7–6 and CH_3CN 18–17 lines are mostly single-peaked and Gaussian-like. The broad component of C^{17}O 3–2 (FWHM linewidths $\sim 3.5\text{--}9.0 \text{ km s}^{-1}$) likely traces outflow activity, judging from the distribution of the high velocity gas. We speculate that the small observed linewidths of C^{17}O (narrow components: $2.5 \pm 0.7 \text{ km s}^{-1}$) and C^{34}S ($3.5 \pm 0.7 \text{ km s}^{-1}$) sets an upper limit to the strength of turbulence at scales of a few 10,000 AU to a few 1000 AU, respectively. From the narrow C^{34}S lines we find that the core's density profile is likely flatter than the assumed $\propto r^{-1.5}$ power-law. The broader CH_3CN lines

($6.5 \pm 1.8 \text{ km s}^{-1}$) hint at infalling motions, or more likely, rotation, on scales below $\sim 1000 \text{ AU}$. Further detailed modeling of individual cores is required to confirm this result.

Conclusions. Our observations and comparisons to models suggest that C^{17}O 3–2 and C^{34}S 7–6 are good tracers of turbulence on scales of 10,000–1000 AU in massive star forming cores, while the broader CH_3CN 18–17 lines are promising tracers of rotation on $\lesssim 1000 \text{ AU}$ scales for our entire sample. Turbulent motions may increase toward smaller radii inside these cores.

2.1 Introduction

Compared to Solar-type stars, the formation of massive stars ($M_\star \geq 8 M_\odot$) is less understood both observationally and theoretically (Beuther et al. 2007; Zinnecker & Yorke 2007; McKee & Ostriker 2007). It is challenging to observe high-mass young stellar objects (YSOs) because they are rare and usually form in groups at large distances (typically a few kpc). More significantly, their formation occurs in much denser regions with high extinction, where only radiation at radio, (sub)millimeter and far-infrared wavelengths can escape. A key difference with low-mass star formation is that massive stars initiate hydrogen fusion while still accreting mass from their surroundings (Palla & Stahler 1993). The resulting large luminosities ($\sim 10^{3-5} L_\odot$), especially in the ultraviolet, affects the infalling material, ionizes the gas, and disrupts continued accretion. This interaction makes it much more difficult to unambiguously follow the formation process of massive stars, while, at the same time, the energetic feedback may play a fundamental role in regulating or shutting off the accretion. To understand massive star formation it is therefore essential to study the kinematics of massive star-forming cores, which provides clues on how massive stars accumulate their final mass.

Infall motions toward massive star-forming cores have been observed at both single-dish and interferometric scales in various molecular lines at centimeter and (sub)millimeter wavelengths, such as ^{13}CO , C^{18}O , CS, NH_3 , HCO^+ and HCN, etc. (e.g., Beltrán et al. 2006; Birkmann et al. 2007; Klaassen & Wilson 2007, 2008; Furuya et al. 2011; Liu et al. 2011a,b; Wyrowski et al. 2012; Rygl et al. 2013). The observed optically-thick line signatures such as the ‘blue-skewed’ line profiles and the inverse P-Cygni profiles provide supporting evidences for infall motions (Myers et al. 1996; Evans 1999). Outflow motions, usually observed in CO lines, are also ubiquitous in massive star-forming cores (e.g., Zhang et al. 2001; Beuther et al. 2002; López-Sepulcre et al. 2009, 2011), which provide an efficient way to remove the excess of angular momentum of an accreting star (Arce et al. 2007), and also provide a channel to re-direct strong radiation

pressure from massive stars (e.g., Krumholz et al. 2005).

Due to conservation of angular momentum, a flattened rotating structure, perhaps a circumstellar disk, should form around a young star with large scale infall motions (Ulrich 1976; Terebey et al. 1984). The high detection rates of bipolar outflows toward massive star-forming cores (e.g., Zhang et al. 2001; Beuther et al. 2002) imply that disk-like structures around forming massive stars should be present, similar to the standard disk-outflow geometry observed in low-mass star-forming cores (Shu et al. 1987). However, to date, the presence of circumstellar “disks” is reported only toward few tens of young early B-type stars in a variety of tracers like radio (sub)millimeter emission lines (such as C^{17}O , C^{34}S , HDO , H_2^{18}O , H^{13}CN , H^{13}CO^+ , NH_3 , and CH_3CN) as well as infrared lines and polarization measurements (e.g., Cesaroni et al. 2007, and reference therein). These “disk-like” structures are found to be large ($\sim 10^{2-4}$ AU) and massive ($M_{\text{disk}} \leq M_\star$), which is quite different from the disks around low-mass stars ($M_{\text{disk}} \ll M_\star$). On the contrary, only large “toroids” undergoing solid-body rotation with masses greater than stellar masses are found toward young O-type stars (Beltrán et al. 2005; Furuya et al. 2008). Although not yet statistically significant, it seems that the formation of massive stars through disk accretion could be applied up to early B-type star as predicted in turbulent core accretion models (e.g., McKee & Tan 2003; Krumholz et al. 2009). However, the formation of O-type stars may follow different scenarios such as competitive accretion in clustered environment (e.g., Bonnell et al. 2001). As a result, studying the physical properties of these disks/toroids is an important step toward understanding the mass transport from envelopes to forming massive stars.

From (sub)millimeter interferometric observations, a collection of “disk” molecular line tracers can be made as listed above. An intermediate question one may ask is whether one disk tracer applicable to a certain source can also be applied to other sources for disk identification? We note that interferometric observations have spatial filtering effects which on the one hand are helpful for disk hunting, but on the other hand miss the large scale structure where infall and outflow happen, preventing us from making unambiguous disk identifications. In addition, the strong turbulence (typical FWHM $\geq 2 - 3 \text{ km s}^{-1}$) toward massive star-forming cores makes the interpretations of kinematics even more difficult.

To investigate these issues, we initiated a survey of 17 massive star-forming cores in the C^{17}O 3–2, C^{34}S 7–6, and CH_3CN 18–17 lines with the James Clerk Maxwell Telescope¹ (JCMT). The selection of the first nine sources in our sample is based on the literature which reports possible detections of massive circumstellar disks through millimeter interferometric observations and infrared

¹The James Clerk Maxwell Telescope is operated by the Joint Astronomy Centre on behalf of the Science and Technology Facilities Council of the United Kingdom, the National Research Council of Canada, and (until 31 March 2013) the Netherlands Organisation for Scientific Research.

observations. The other eight sources are selected based on the survey by Sridharan et al. (2002) and Beuther et al. (2002), which satisfy the following criteria: (1) weak centimeter-wave emission and strong millimeter-wave emission (ensuring the source is less evolved with no or little hot ionized gas), (2) presence of line wings and SiO emission (as the indication of outflow/shock gas, implying the potential existence of disk predicted by theoretical models), (3) presence of CH₃OH, CS and CH₃CN emission (tracing warm and compact molecular gas), and (4) kinematic distance less than 5 kpc. The basic characteristics of the selected sources are summarized in Table 2.1. The potentially optically thin C¹⁷O 3–2 and C³⁴S 7–6 lines allow us to probe deeper into star-forming cores, while the highly excited CH₃CN 18–17 lines can trace the densest and warmest central regions of star-forming cores. The spectroscopic properties of the observed lines are summarized in Table 2.2. We aim to test if these lines are really promising as tracers of rotation and to see what the effect of turbulence is in the interpretation of the kinematics of massive star-forming cores including infall, outflows, and rotation.

We organize this paper as follows. In Sect. 2.2, we describe the JCMT observations and data reduction. In Sect. 2.3, we present the molecular images and spectra of our JCMT observations. Followed by molecular excitation and kinematics analysis in Sect. 2.4, we provide a general discussion of the kinematics in massive star-forming cores in Sect. 2.5. We conclude this paper in Sect. 2.6.

2.2 Observations and data reduction

The survey observations were taken with the 16-element Heterodyne Array Receiver Programme B (HARP-B²) and the Auto-Correlation Spectral Imaging System (ACSIS) correlator at the JCMT on the summit of Mauna Kea, Hawaii (Buckle et al. 2009). The 16 receptors of the HARP receiver are distributed in a 4×4 pattern with regular separations of $30''$. The survey was conducted in three semesters from 2009 to 2011 (Table 2.3).

In 2009 (project ID: M09BN07) and 2010 (M10BN06), we observed all 17 sources (Table 2.1) in C¹⁷O 3–2, C³⁴S 7–6, and CH₃CN 18–17 (Table 2.2) with HARP-B in jiggle-chop mapping mode. The spectrometer was configured to operate in single sideband (SSB) mode with 250 MHz bandwidth to observe C¹⁷O 3–2 and C³⁴S 7–6 simultaneously. The jiggle pattern of HARP4 was adopted to image a $\sim 2' \times 2'$ region with a pixel size of $7.5''$ which slightly under-samples the beam ($\sim 14''$). In the 2009 run, the integration time per jiggle position was 40 seconds, resulting a total observing time per source per line of ~ 90 minutes. In the 2010 run, the integration time per jiggle position was 34 seconds, result-

²http://www.jach.hawaii.edu/JCMT/spectral_line/Instrument_homes/HARP/HARP.html

2.2. OBSERVATIONS AND DATA REDUCTION

Table 2.1. List of sample sources

Source	RA(J2000) (hh:mm:ss.s)	Dec(J2000) (dd:mm:ss)	d^a (kpc)	L^b ($L_\odot$)	V_{LSR}^c (km s $^{-1}$)
AFGL 490	03:27:38.4	+58:47:04	1.0	2.0×10^3	−13.0
05358+3543	05:39:10.4	+35:45:19	1.8	6.3×10^3	−17.6
05553+1631	05:58:13.9	+16:32:00	2.5	6.3×10^3	+5.7
S255IR	06:12:54.0	+17:59:23	1.6	2.0×10^4	+7.0
18089−1732	18:11:51.3	−17:31:29	3.6	3.2×10^4	+34.0
18151−1208	18:17:57.1	−12:07:22	3.0	2.0×10^4	+32.8
18182−1433	18:21:07.9	−14:31:53	4.5	2.0×10^4	+59.1
18264−1152	18:29:14.3	−11:50:26	3.5	1.0×10^4	+43.6
19410+2336	19:43:11.4	+23:44:06	2.1	1.0×10^4	+22.4
20126+4104	20:14:25.1	+41:13:32	1.7	1.0×10^4	−4.0
AFGL 2591	20:29:24.9	+40:11:21	3.3	2.2×10^5	−6.0
20293+3952	20:31:10.7	+40:03:10	2.0	6.3×10^3	+6.3
S140 IRS1	22:19:18.2	+63:18:47	0.8	8.5×10^3	−7.0
Cepheus A	22:56:17.9	+62:01:49	0.7	2.5×10^4	−3.0
23033+5951	23:05:24.8	+60:08:14	3.5	1.0×10^4	−53.0
NGC 7538S	23:13:44.8	+61:26:51	2.7	1.5×10^4	−56.0
23139+5939	23:16:09.3	+59:55:23	4.8	2.5×10^4	−44.7

Note. — ^{a} Distance. ^{b} Bolometric luminosity. ^{c} LSR velocity.

Table 2.2. List of observed molecular lines

Molecule	Transition	Frequency (MHz)	E_u^a (K)	n_{crit}^b (cm $^{-3}$)
C ^{17} O	3–2	337061.1	32	3.4×10^4
C ^{34} S	7–6	337396.5	65	1.9×10^7
CH $_3$ CN	18 $_0$ –17 $_0$	331071.5	151	1.5×10^7
	18 $_1$ –17 $_1$	331065.2	158	1.4×10^7
	18 $_2$ –17 $_2$	331046.1	180	1.4×10^7
	18 $_3$ –17 $_3$	331014.3	215	1.5×10^7
	18 $_4$ –17 $_4$	330969.8	265	1.5×10^7
	18 $_5$ –17 $_5$	330912.6	329	1.4×10^7
	18 $_6$ –17 $_6$	330842.8	408	1.4×10^7
	18 $_7$ –17 $_7$	330760.3	501	1.4×10^7

Note. — ^{a} Upper level energy. ^{b} Critical density at 100 K, derived using collisional rate coefficients from Yang et al. (2010), Turner et al. (1992), Green (1986), as summarized by Schöier et al. (2005).

Table 2.3. Summary of the JCMT observations

	M09BN07	M10BN06	M11BN08
Target line	C ¹⁷ O 3–2 C ³⁴ S 7–6 CH ₃ CN 18–17	C ¹⁷ O 3–2 C ³⁴ S 7–6 CH ₃ CN 18–17	CH ₃ CN 18–17
Bandwidth	250 MHz	250 MHz	1000 MHz
Observing mode	Mapping Jiggle-chop	Mapping Jiggle-chop	Stare
Observing time ^a	90 mins	60 mins	75 mins
Typical $\tau_{225\text{GHz}}$	0.05–0.08	0.05–0.08	0.08–0.12
Target source	AFGL 490 S255IR 18089–1732 20126+4104 AFGL 2591 Cepheus A 23033+5951 NGC 7538S	05358+3543 05553+1631 18151–1208 18182–1433 18264–1152 19410+2336 20293+3952 S140 IRS1 23139+5939	AFGL 490 05358+3543 05553+1631 S255IR 19410+2336 20126+4104 20293+3952 S140 IRS1 23033+5951 NGC 7538S 23139+5939

Note. — The CH₃CN 18–17 single pointing spectrum of IRAS 18089–1732 is taken from the JCMT archive with project code M09BN10 (Isokoski et al. 2013). ^aObserving time per source per line.

ing a total observing time per source per line of ~ 60 minutes. In the 2011 run (M11BN08), we observed 11 sources in CH₃CN 18–17 with HARP–B in single pointing mode for better signal-to-noise (S/N) ratio. The spectrometer was configured to operate in SSB mode with 1000 MHz bandwidth. The integration time was 450 seconds per offset position and the total observing time per source was ~ 75 minutes. The typical atmospheric opacities at 225 GHz in 2009/2010 and 2011 were 0.05–0.08 and 0.08–0.12, respectively. In all observing runs, the receptor R15 (H14) was offline, resulting a $30'' \times 30''$ blank area in final images.

The raw time-series data are processed with the Starlink³ software package. Each scan is inspected for bad receptors, baseline issues, and spikes, which are flagged out before time summation and transforming into image cubes. Baselines are removed by selecting line-free channels as reference. The intensity is scaled from the corrected antenna temperature T_A^* to the main beam temperature

³<http://starlink.jach.hawaii.edu/starlink>

T_{MB} by adopting a main beam efficiency of 0.61 ± 0.03 (Buckle et al. 2009). The final calibrated image cubes were exported to FITS file and we use the MIRIAD software package (Sault et al. 1995) for further analysis. A Gaussian-like emission spike close to the $K=2$ transition was found in the CH_3CN 18–17 spectrum, which is a ghost signal from the receptor R06 (H05). Therefore, we did not use the $K=2$ transition for further analysis.

In addition to the line observations, we obtained the SCUBA 850 μm images from the database presented by Di Francesco et al. (2008). The images are re-gridded to match the pixel size of line images ($7.5''$). The 850 μm image of IRAS 20293+3952 is partly corrupted.

2.3 Results

2.3.1 Molecular distribution

In Fig. 2.1, we present the integrated intensity maps of C^{17}O 3–2 (blue contours) and C^{34}S 7–6 (yellow contours) toward all 17 sources. The SCUBA 850 μm continuum emission (peak intensity is normalized to unity) taken from the archive published by Di Francesco et al. (2008) is also shown in grey scale. In all cases except IRAS 05358+3543, the C^{17}O 3–2 emission peak ($\text{S/N} > 10$) is spatially correlated with the 850 μm continuum peak, suggesting that gas and dust are coupled well at core scales (a few 0.1 pc). The “Main” source toward IRAS 05358+3543 shows stronger 850 μm emission and weaker C^{17}O 3–2 emission, while the “SW” source behaves in the opposite way. Toward all 17 sources, C^{34}S 7–6 emission is detected, which is also spatially correlated with the 850 μm emission. The C^{34}S 7–6 emission is more compact than the C^{17}O 3–2 emission, likely because C^{34}S 7–6 requires much higher gas densities than C^{17}O 3–2 for collisional excitation (Table 2.2). The different excitation conditions and the good spatial correlation with the 850 μm emission make C^{17}O 3–2 and C^{34}S 7–6 good tracers of gas kinematics from the large envelope to the central, dense part of star-forming cores.

Gaussian fits are performed to further study the morphology of the extended C^{17}O 3–2 emission and the SCUBA 850 μm continuum. In Fig. 2.1, the C^{17}O 3–2 emission shows the complex morphologies in our sample, such as elongated (e.g., AFGL 490), compact (e.g., IRAS 05553+1631), and multiple-core (e.g., IRAS 05358+3543). To have a rough estimate of emission sizes, we assume that the emission can be approximated as a single elliptical Gaussian peaking at emission peak (i.e., the center position is fixed in the fit). We note that the fit may be affected by the boundary of our maps ($\sim 2' \times 2'$) and the presence of multiple local emission peaks. The purpose here is to have an idea of the differences of the spatial distributions of C^{17}O 3–2 and 850 μm continuum at a few 0.1 pc scales. We fit all the C^{17}O 3–2 and 850 μm continuum maps and

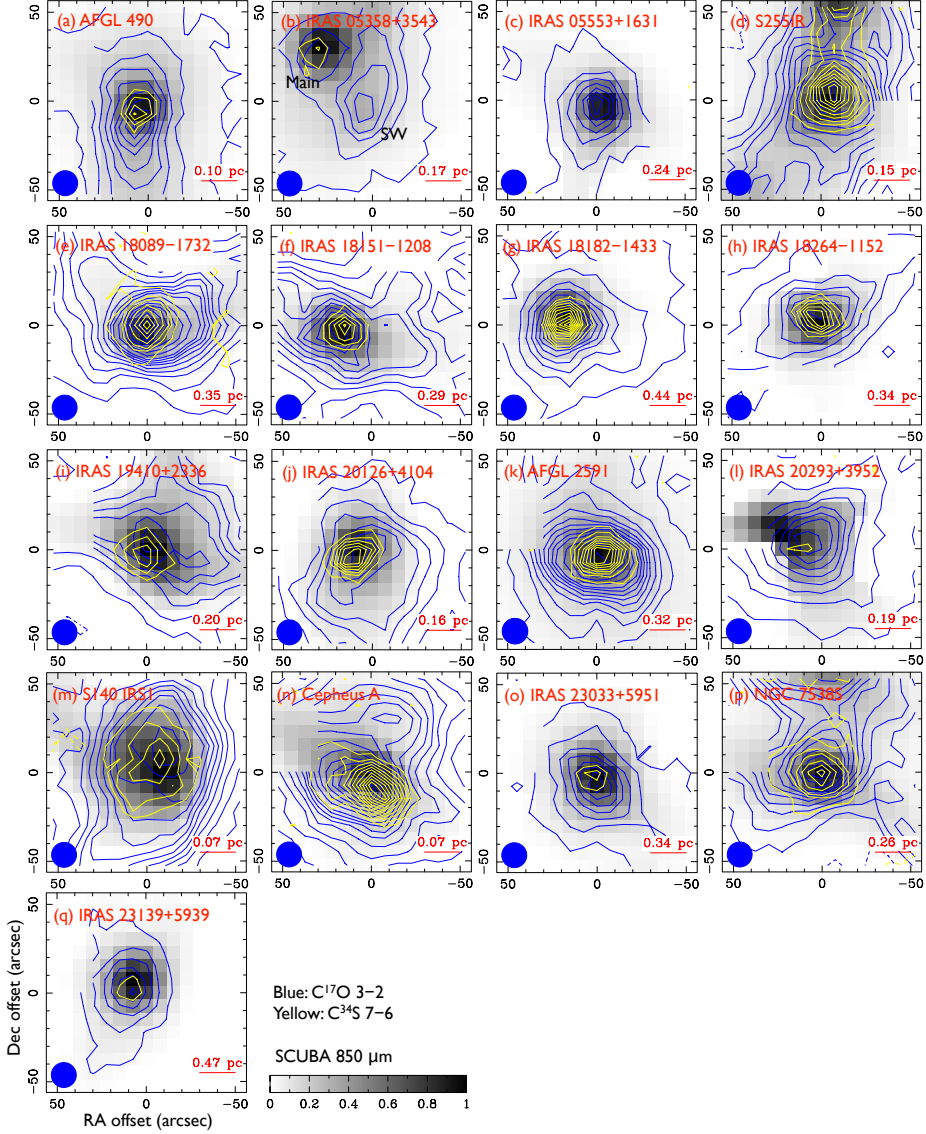


Figure 2.1 Integrated intensity maps ($\int T_{\text{MB}} dV$) of C^{17}O 3–2 (blue contours) and C^{34}S 7–6 (yellow contours) toward our sample massive star-forming cores. The image in grey is the SCUBA 850 μm emission (peak intensity is normalized to unity) taken from Di Francesco et al. (2008). The blue circle represents the $\sim 14''$ resolution of the JCMT HARP-B observations. The bar in red gives the linear scale in pc. The (0,0) position of each map is our pointing center and its absolute coordinate is given in Table 2.1. The $1\text{-}\sigma$ noise levels of C^{17}O 3–2 from panel (a) to (q) are 0.14, 0.14, 0.15, 0.11, 0.15, 0.14, 0.18, 0.16, 0.14, 0.12, 0.14, 0.14, 0.19, 0.18, 0.13, 0.14, and 0.17 K km s^{-1} . The contour levels of C^{17}O in all panels are 3, 8, 13, ... , 43, 53, 63, ... σ . The $1\text{-}\sigma$ noise levels of C^{34}S 7–6 from panel (a) to (q) are 0.09, 0.13, 0.15, 0.11, 0.18, 0.13, 0.22, 0.17, 0.11, 0.13, 0.11, 0.10, 0.17, 0.19, 0.12, 0.17, and 0.11 K km s^{-1} . The contour levels of C^{34}S in all panels are 3, 5, 7, ... σ .

summarize the results in Table 2.4. We found that in all sources, the geometric mean sizes derived from the 850 μm continuum images are all smaller than the sizes derived from the C^{17}O 3–2 images. Likely this is because C^{17}O 3–2 partly traces outflows which would naturally enlarge the sizes of overall distributions (See Sect. 2.3.3), or because of the fact that C^{17}O is more sensitive to lower density gas than the 850 μm continuum is. Therefore, we suggest that the effect of outflows in shaping the C^{17}O 3–2 line profiles cannot be neglected in massive star-forming cores.

We tried to image CH_3CN 18–17 transitions in our sample but only AFGL 2591 and Cepheus A show detections with point source morphology (not shown here). A further attempt was made in single pointing mode to detect the lines. We expect the CH_3CN 18–17 emission to be point-source like in a $\sim 14''$ beam since it usually arises in a hot core of a few arcsecond in size. We present the CH_3CN 18–17 spectra in Sect. 2.3.2. Excitation analysis of CH_3CN lines and the determination of emission size are given in Sect. 2.4.1.

2.3.2 Molecular spectra

We present a collection of C^{17}O 3–2 and C^{34}S 7–6 spectra in Fig. 2.2. The beam-averaged spectra are taken at the emission peak based on the integrated intensity maps (Fig. 2.1). To enhance the S/N and minimize the effect of under-sampling of HARP-B maps, we averaged 3×3 pixels ($22.5'' \times 22.5''$) centered at the emission peak to derive the spectra. The typical line profiles of C^{17}O 3–2 and C^{34}S 7–6 are Gaussian-like, suggesting that turbulence may dominate the kinematics of our source sample. Exceptions can be seen in C^{34}S 7–6 toward IRAS 20126+4104 and Cepheus A, which shows double-peaked profiles. A detailed check of the high S/N ratio spectra of C^{17}O 3–2 shows that some line profiles contain an additional broad component (FWHM linewidths $\sim 3.5\text{--}9.0 \text{ km s}^{-1}$) at low intensity level (e.g., IRAS 18264–1152 and IRAS 20126+4104). The presence of this broad low-level component implies that C^{17}O 3–2 may trace part of outflow motions near the source.

We performed Gaussian fits to decompose different kinematical components and summarize the results in Table 2.5 and Fig. 2.2. We adopted a rule to determine the total number of Gaussian components in the decomposition process of a line profile. For a pure Gaussian line profile, the full width at p % of maximum intensity (ΔV_p) follows $\Delta V_p = 2 \times \text{FWHM} \times \sqrt{\ln(p/100)/-4 \ln 2}$. In other words, ΔV_{50} is exactly $\sqrt{1} \times \text{FWHM}$ linewidth, ΔV_{25} is $\sqrt{2} \times \text{FWHM}$ linewidth, and $\Delta V_{12.5}$ is $\sqrt{3} \times \text{FWHM}$ linewidth, etc. This forms a very useful test to determine if the observed line profile is a single Gaussian or a superposition of multiple Gaussians. If there is a low-level emission line wing in the observed line profile, through a series of tests with different p , we can quantitatively determine how many Gaussians are needed to decompose the line

Table 2.4. Gaussian decomposed size of C¹⁷O 3–2 and SCUBA 850 μ m emission

Source	C ¹⁷ O 3–2 Angular			C ¹⁷ O 3–2 Linear			850 μ m Angular			850 μ m Linear		
	θ_a ($''$)	θ_b ($''$)	P.A. ($^\circ$)	θ_a (pc)	θ_b (pc)	θ_{mean} (pc)	θ_a ($''$)	θ_b ($''$)	P.A. ($^\circ$)	θ_a (pc)	θ_b (pc)	θ_{mean} (pc)
AFGL 490	75	34	0	0.38	0.17	0.25	52	34	0	0.26	0.17	0.21
05358+3543	111	78	53	0.94	0.66	0.79	54	49	73	0.46	0.42	0.44
05553+1631	39	25	–5	0.47	0.30	0.37	29	25	–24	0.35	0.30	0.32
S255IR	106	48	–18	0.80	0.36	0.53	69	41	–22	0.52	0.31	0.40
18089–1732	46	33	90	0.81	0.58	0.68	31	23	–89	0.54	0.40	0.47
18151–1208	129	50	76	1.87	0.73	1.16	35	22	69	0.51	0.32	0.40
18182–1433	33	29	–77	0.73	0.64	0.68	26	22	–81	0.57	0.48	0.53
18264–1152	73	35	–58	1.24	0.60	0.86	28	21	–73	0.48	0.36	0.41
19410+2336	98	53	74	0.98	0.53	0.72	45	35	62	0.45	0.35	0.40
20126+4104	68	55	19	0.54	0.44	0.49	35	28	–11	0.28	0.22	0.25
AFGL 2591	43	30	76	0.69	0.48	0.57	46	36	50	0.74	0.58	0.65
20293+3952	59	49	–70	0.56	0.47	0.51	50	32	81	0.48	0.30	0.38
S140 IRS1	115	69	–29	0.40	0.24	0.31	52	44	49	0.18	0.15	0.17
Cepheus A	81	60	22	0.28	0.21	0.24	51	31	54	0.18	0.11	0.14
23033+5951	48	31	44	0.82	0.53	0.66	34	27	23	0.58	0.46	0.52
NGC 7538S	58	46	–56	0.75	0.60	0.67	43	35	79	0.56	0.46	0.50
23139+5939	36	25	–7	0.85	0.59	0.70	27	23	–32	0.63	0.54	0.59

Note. — The uncertainties in θ_a (major axis) and θ_b (minor axis) are all less than 7.5'' (one pixel size). θ_{mean} is the geometric mean size. The uncertainty in source distance is not considered in converting angular size to linear size.

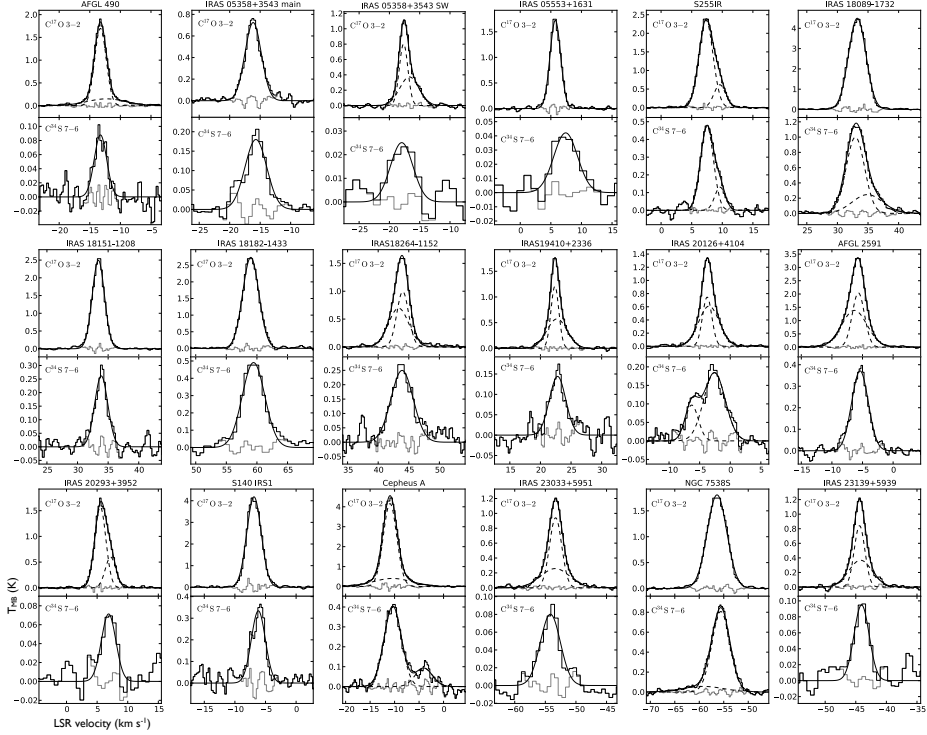


Figure 2.2 Beam-averaged C^{17}O 3–2 and C^{34}S 7–6 spectra taken at emission peaks of all sample sources. The observed spectra are plotted in black histogram. The Gaussian fit is plotted in solid lines, while each Gaussian component (if any) is shown in dashed lines. The fitting residual is plotted in grey histogram.

profile. We applied this test to the observed C^{17}O 3–2 line profiles and allowed a 10% tolerance when comparing the apparent FWHM linewidth with the apparent ΔV_p . Through this analysis, the C^{17}O 3–2 line profiles can be classified into three categories: single Gaussian (e.g., IRAS 05553+1631), narrow+broader Gaussians (e.g., IRAS 19410+2336), and two Gaussians with comparable FWHM linewidth (e.g., S255IR). Similar to C^{17}O 3–2, the C^{34}S 7–6 line profiles can also be classified in these three categories in spite of their lower S/N ratios.

Table 2.5. Beam-averaged line properties of C¹⁷O 3–2 and C³⁴S 7–6

Source	W^a (K km s ⁻¹)	ΔV^b (km s ⁻¹)	V_{LSR}^c (km s ⁻¹)	Note
C ¹⁷ O 3–2				
AFGL 490	4.02 ± 0.06	2.23 ± 0.02	-13.26 ± 0.01	Narrow component
	1.20 ± 0.07	7.48 ± 0.41	-12.28 ± 0.16	Broad component
05358+3543 Main	2.44 ± 0.15	3.16 ± 0.22	-16.15 ± 0.09	Single component
05358+3543 SW	1.42 ± 0.28	1.66 ± 0.16	-17.66 ± 0.05	Narrow component
	1.48 ± 0.29	3.72 ± 0.35	-16.71 ± 0.28	Broad component
05553+1631	3.73 ± 0.12	2.03 ± 0.07	5.73 ± 0.03	Single component
S255IR	6.76 ± 0.15	2.70 ± 0.04	7.35 ± 0.03	Component I
	1.48 ± 0.15	2.25 ± 0.10	9.60 ± 0.08	Component II
18089–1732	16.00 ± 0.05	3.34 ± 0.01	33.24 ± 0.01	Single component
18151–1208	6.25 ± 0.11	2.35 ± 0.05	33.40 ± 0.02	Single component
18182–1433	9.12 ± 0.13	3.13 ± 0.05	59.00 ± 0.02	Single component
18264–1152	2.40 ± 1.13	2.27 ± 0.34	44.01 ± 0.10	Narrow component
	2.89 ± 1.13	3.91 ± 0.42	43.34 ± 0.32	Broad component
19410+2336	1.97 ± 0.39	1.53 ± 0.15	22.36 ± 0.04	Narrow component
	2.37 ± 0.38	3.89 ± 0.47	22.70 ± 0.15	Broad component
20126+4104	1.43 ± 0.15	1.80 ± 0.07	-3.77 ± 0.02	Narrow component
	2.59 ± 0.14	3.99 ± 0.13	-3.46 ± 0.04	Broad component
AFGL 2591	5.12 ± 1.05	2.36 ± 0.19	-5.68 ± 0.05	Narrow component
	7.19 ± 1.04	4.88 ± 0.34	-6.33 ± 0.15	Broad component
20293+3952	3.60 ± 1.44	2.15 ± 0.36	5.53 ± 0.34	Component I
	1.30 ± 1.43	2.05 ± 0.83	7.20 ± 0.81	Component II
S140 IRS1	12.35 ± 0.10	2.74 ± 0.03	-6.88 ± 0.01	Single component
Cepheus A	14.42 ± 0.18	3.26 ± 0.02	-10.93 ± 0.01	Narrow component
	3.99 ± 0.18	9.23 ± 0.37	-10.43 ± 0.10	Broad component
23033+5951	2.35 ± 0.14	2.35 ± 0.06	-53.32 ± 0.01	Narrow component
	1.54 ± 0.14	5.61 ± 0.35	-53.38 ± 0.08	Broad component
NGC 7538S	9.08 ± 0.03	4.72 ± 0.02	-56.37 ± 0.01	Single component
23139+5939	1.83 ± 0.79	2.04 ± 0.35	-44.38 ± 0.07	Narrow component
	1.77 ± 0.76	4.51 ± 1.16	-44.23 ± 0.26	Broad component
C ³⁴ S 7–6				
AFGL 490	0.22 ± 0.02	2.40 ± 0.28	-13.25 ± 0.12	Single component
05358+3543 Main	0.80 ± 0.04	4.20 ± 0.24	-15.70 ± 0.10	Single component
05358+3543 SW	0.12 ± 0.03	4.36 ± 1.18	-17.97 ± 0.49	Single component
05553+1631	0.21 ± 0.04	4.58 ± 0.96	7.42 ± 0.41	Single component
S255IR	1.26 ± 0.12	2.50 ± 0.16	7.50 ± 0.11	Component I
	0.28 ± 0.12	2.05 ± 0.42	9.64 ± 0.30	Component II
18089–1732	3.75 ± 1.01	3.52 ± 0.30	32.94 ± 0.08	Component I*
	1.54 ± 1.03	5.87 ± 1.03	34.92 ± 1.45	Component II*
18151–1208	0.71 ± 0.16	2.53 ± 0.65	33.87 ± 0.28	Single component
18182–1433	2.28 ± 0.06	4.36 ± 0.14	59.45 ± 0.06	Single component
18264–1152	1.14 ± 0.25	4.29 ± 1.09	43.91 ± 0.47	Single component

Table 2.5 (cont'd)

Source	W^a (K km s ⁻¹)	ΔV^b (km s ⁻¹)	V_{LSR}^c (km s ⁻¹)	Note
19410+2336	0.48 ± 0.12	3.14 ± 0.94	22.80 ± 0.40	Single component
20126+4104	0.81 ± 0.07	4.12 ± 0.40	-2.57 ± 0.18	Component I*
	0.26 ± 0.07	2.54 ± 0.46	-6.29 ± 0.23	Component II*
AFGL 2591	1.26 ± 0.09	3.19 ± 0.27	-5.40 ± 0.12	Single component
20293+3952	0.21 ± 0.03	2.78 ± 0.46	6.88 ± 0.20	Single component
S140 IRS1	0.96 ± 0.15	2.69 ± 0.48	-6.17 ± 0.20	Single component
Cepheus A	0.41 ± 0.05	4.18 ± 0.59	-4.04 ± 0.23	Component I*
	1.79 ± 0.05	4.15 ± 0.14	-10.37 ± 0.05	Component II*
23033+5951	0.33 ± 0.03	3.85 ± 0.35	-54.17 ± 0.15	Single component
NGC 7538S	3.70 ± 0.13	4.31 ± 0.07	-55.59 ± 0.02	Component I*
	0.60 ± 0.14	9.85 ± 1.17	-59.20 ± 1.08	Component II*
23139+5939	0.30 ± 0.03	2.92 ± 0.32	-44.05 ± 0.14	Single component

Note. — Components with * listed in the C³⁴S 7–6 part represent different gaussian fit compared to C¹⁷O 3–2 (See Fig. 2.2). ^aBeam-averaged integrated intensity: $W = \int T_{\text{MB}} dV$, where T_{MB} is the main beam temperature. ^bGaussian FWHM linewidth. ^cGaussian line center LSR velocity.

Different kinematical components hidden in line profiles can be decomposed by multiple Gaussians as described above only if the line emission is optically thin. To quantify the opacities of the observed C¹⁷O 3–2 and C³⁴S 7–6 lines, we use the Eq. (27) of Goldsmith & Langer (1999) as an estimate. Assuming an H₂ column density of 3×10^{23} cm⁻² (c.f., Hatchell et al. 2000) and a Gaussian line profile with a FWHM linewidth of 4.0 km s⁻¹, the line center opacities of C¹⁷O 3–2 are ~ 0.5 and ~ 0.1 at 40 K and 100 K, respectively, if we adopt a fractional abundance of 1×10^{-7} as derived from Lacy et al. (1994) and Wilson & Rood (1994). The line center opacities of C³⁴S 7–6 are ~ 0.2 and ~ 0.08 at 40 K and 100 K, respectively, assuming a fractional abundance of 3×10^{-10} based on van der Tak et al. (2000) and Wilson & Rood (1994). The real line opacities of the C¹⁷O 3–2 and C³⁴S 7–6 lines of each source may vary by a factor of few, but in all cases we suggest that these two lines are optically thin and it is safe to perform line decompositions with Gaussians.

In Fig. 2.3, we present the 8 sources with detections of CH₃CN 18–17. Due to limited S/N, we do not apply the Gaussianity test outlined above. In deriving the line center velocity, FWHM linewidth, and integrated intensity, we assume that the line profile of each K component is Gaussian. We further assume that the FWHM linewidth and line center velocity of each K component are the same in the fitting process. For sources with low S/N, we fit their linewidth by eye and keep it fixed in the fit. We summarize the line properties of CH₃CN 18–17 in

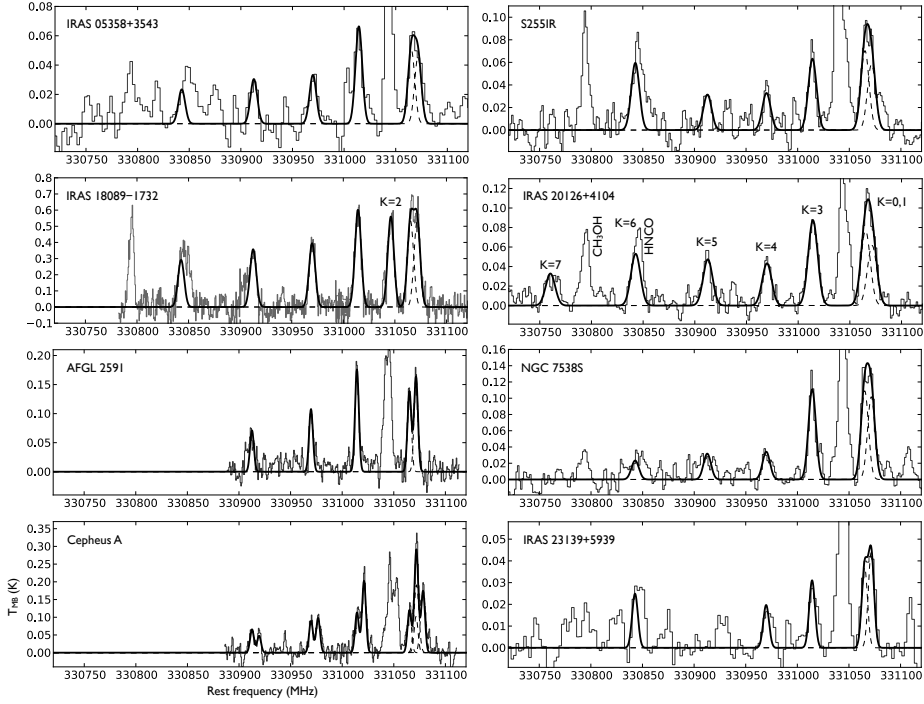


Figure 2.3 Beam-averaged CH_3CN 18–17 spectra toward 8 massive star-forming cores. The observed spectra are plotted in histogram, while the thick lines represent the best-fit spectra with each K component in dashed lines. We label the K components and other molecular lines in the panels of IRAS 18089–1732 and IRAS 20126+4104. The spectral feature near the $K = 2$ component of all sources except IRAS 18089–1732 is a superposition of the target signal and the ghost signal from receiver (See Sect. 2.2).

Table 2.6. Toward Cepheus A, the line profile of each K component is double-peaked, implying that likely there are two velocity components along the line of sight, also known from other species (e.g., CH_3OH ; Torstensson et al. 2011). Therefore, we used two sets of Gaussians to decompose the observed spectrum. From the fit, the assumption of similar line center velocity and FWHM linewidth of all K components is valid.

Apparently, the observed linewidths of C^{17}O 3–2, C^{34}S 7–6 and CH_3CN 18–17 form an interesting sequence with C^{17}O 3–2 the narrowest and CH_3CN 18–17 the broadest. To quantify this, we averaged the FWHM linewidth of the narrow component of all three lines. If the line profile is classified as two Gaussians with comparable FWHM, we use the strongest one. We note that the broad component seen in C^{17}O 3–2 may come from outflow motions (see Sect. 2.3.3). As a result, we found that the mean FWHM linewidths are $2.5 \pm 0.7 \text{ km s}^{-1}$, $3.5 \pm 0.7 \text{ km s}^{-1}$,

Table 2.6. Beam-averaged line properties of CH₃CN 18–17

	IRAS05358	S255IR	IRAS18089	IRAS20126	AFGL2591	NGC7538S	CepA-1	CepA-2	IRAS23139
V_{LSR}^a	-16.5 ± 0.4	5.0 ± 0.4	33.4 ± 0.1	-4.3 ± 0.3	-5.1 ± 0.1	-56.4 ± 0.2	-4.4 ± 0.1	-10.6 ± 0.1	-42.6 ± 0.3
ΔV^b	7.0 (fixed)	8.5 ± 0.7	6.4 ± 0.2	9.7 ± 0.4	4.0 (fixed)	7.7 ± 0.4	4.0 (fixed)	5.0 (fixed)	6.0 ± 0.5
W^c									
$K=0$	0.34 ± 0.07	0.53 ± 0.10	3.60 ± 0.20	0.64 ± 0.09	0.70 ± 0.03	0.83 ± 0.07	0.43 ± 0.21	0.93 ± 0.05	0.28 ± 0.04
$K=1$	0.37 ± 0.07	0.63 ± 0.10	3.61 ± 0.20	0.79 ± 0.09	0.59 ± 0.03	0.89 ± 0.07	0.51 ± 0.04	1.02 ± 0.23	0.24 ± 0.04
$K=2$	ghost	ghost	3.80 ± 0.19	ghost	ghost	ghost	ghost	ghost	ghost
$K=3$	0.50 ± 0.06	0.57 ± 0.07	4.08 ± 0.19	0.91 ± 0.06	0.75 ± 0.03	0.91 ± 0.05	0.48 ± 0.04	1.08 ± 0.04	0.20 ± 0.04
$K=4$	0.25 ± 0.06	0.30 ± 0.07	2.68 ± 0.19	0.45 ± 0.06	0.46 ± 0.03	0.28 ± 0.05	0.38 ± 0.04	0.52 ± 0.04	0.13 ± 0.04
$K=5$	0.23 ± 0.06	0.28 ± 0.07	2.42 ± 0.19	0.49 ± 0.06	0.30 ± 0.03	0.26 ± 0.05	0.28 ± 0.04	0.25 ± 0.04	...
$K=6$	0.17 ± 0.06	0.54 ± 0.10	1.98 ± 0.35	0.55 ± 0.12	...	0.19 ± 0.09	...	...	0.16 ± 0.05
$K=7$	...	...	...	0.34 ± 0.06	...	...	...	...	...
δW^d	0.12	0.12	0.26	0.10	0.07	0.10	0.10	0.10	0.11
RADEX excitation analysis in LVG approximation ^e									
T_{kin}^f	200	240	110	370	180	110	80	140	130
N_{mol}^g	7×10^{15}	5×10^{16}	2×10^{17}	3×10^{16}	2×10^{16}	3×10^{15}	2×10^{17}	4×10^{15}	5×10^{16}
$n(\text{H}_2)^h$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$	$\geq 10^6$
f^i	6.0×10^{-4}	6.0×10^{-4}	6.4×10^{-3}	4.0×10^{-4}	2.1×10^{-3}	2.5×10^{-3}	1.7×10^{-3}	2.7×10^{-3}	5.0×10^{-4}
θ_s^i	0.3	0.3	1.1	0.3	0.6	0.7	0.6	0.7	0.3
$\theta_{s, \text{linear}}^i$	620	550	4000	480	2100	1900	400	510	1500

Note. — The $K=2$ component of all listed sources except IRAS18089 has a ghost emission from the receptor. We do not derive the line properties of the $K=2$ component. ^aLSR velocity in km s^{-1} . We assume that all K components have the same velocity in the Gaussian fitting process. ^bFWHM linewidth in km s^{-1} . We assume that all K components have the same linewidth in the Gaussian fitting process. ^cIntegrated intensity in K km s^{-1} . ^dThe $3\text{-}\sigma$ upper limit of the integrated intensity ($3 \times 1.064 \times \sigma \sqrt{\delta V \Delta V}$) in K km s^{-1} . ^eOnly the best-fit solution is listed. The uncertainty of each free parameter is presented graphically in Fig. 2.9 and 2.10. ^fKinetic temperature in K. ^gTotal molecular column density in cm^{-2} . ^h H_2 volume density in cm^{-3} . A lower-limit value is listed since this parameter is less constrained (Fig. 2.9 and 2.10). ⁱAssuming a Gaussian beam and a Gaussian source geometry, the filling factor f is $\theta_b^2/(\theta_b^2 + \theta_s^2)$, where θ_b and θ_s are the beam size and source size in arcsecond, respectively. The linear source size in AU $\theta_{s, \text{linear}}$ is calculated by adopting the distance listed in Table 2.1.

and $6.5 \pm 1.8 \text{ km s}^{-1}$ for C^{17}O 3–2, C^{34}S 7–6 and CH_3CN 18–17, respectively. This result suggests that if turbulence dominates the observed line profiles, there should be a gradient in the strength of turbulence throughout the star forming core, with turbulence stronger close to the forming stars. However, it is also possible that the apparent larger mean FWHM linewidths seen in C^{34}S 7–6 and CH_3CN 18–17 come from other kinematics such as infall and/or rotation, or interaction of outflows with dense inner envelopes, that are more pronounced at the smaller scales probed by these lines. We further investigate this aspect in Sect. 2.4.

2.3.3 Distributions of high-velocity gas

In the previous section, we found that line emission wings can be seen in the C^{17}O 3–2 spectra toward some sources (Fig. 2.2). It is therefore interesting to investigate the spatial distributions of the high velocity gas traced by C^{17}O 3–2. To do so, we use the spectra presented in Fig. 2.2 as the reference and integrate over the velocity ranges set by the $3\text{-}\sigma$ intensity and 50 % peak intensity. Results are plotted in red and blue contours in Fig. 2.4. We find that toward many sources, the apparent positional offsets in the peak positions of the blue- and red-shifted components imply that the high-velocity gas traced by C^{17}O 3–2 likely follows outflow motions. It is possible that the apparent positional offset near the forming star is due to cloud rotation at $\sim 0.1 \text{ pc}$ scales. However, this would require a very large central stellar mass (violating the total luminosity) unless self-gravity of the entire core cannot be ignored. We suggest that the typical broad line component seen in C^{17}O and other CO isotopologues in single-pointing single-dish observations is an indication of outflow motions. In later analysis (Sect. 2.4), we therefore focus on the narrow component and look for its origin.

2.4 Analysis

2.4.1 CH_3CN $J=18\text{--}17$ excitation analysis and emission size

For sources with multiple detections of the CH_3CN $J=18\text{--}17$ K components, we perform excitation analysis in order to study the physical conditions where CH_3CN originates. We use “rotation diagrams” (c.f., Turner 1991) to visualize the level populations derived from the observed line intensities (Table 2.6). In such plots, the natural logarithmic value of upper state column density (N_u) per statistical weight (g_u) calculated as

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{3kW}{8\pi^3\nu S\mu^2 g_I g_K}\right), \quad (2.1)$$

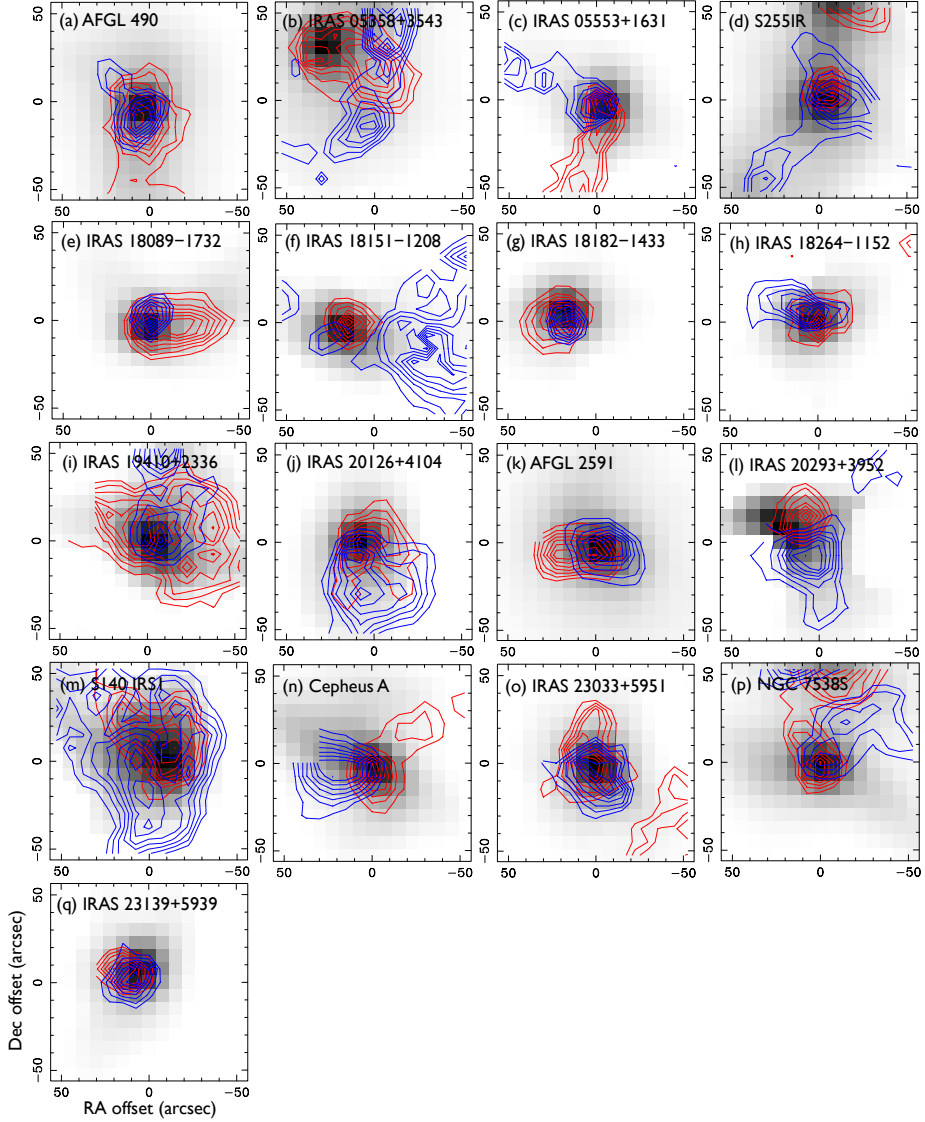


Figure 2.4 High-velocity gas traced by C^{17}O 3–2 toward all 17 sources. The red and blue contours represent the red-shifted and blue-shifted components. The image in grey color represents the normalized SCUBA 850 μm continuum emission. The position offsets in their peak positions near the forming stars suggest that these high-velocity gases trace most likely outflows. In other words, the “board” components seen in Fig. 2.2 likely do not trace infall or rotation motions.

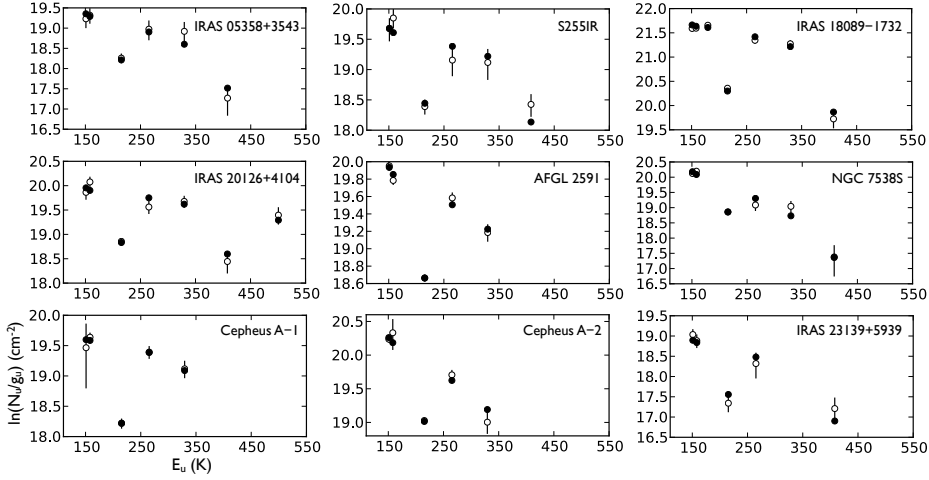


Figure 2.5 Rotation diagrams of the $\text{CH}_3\text{CN } J=18-17$ transitions. A set of open circles with error bars represents the observed values, while the filled circles are the best-fit RADEX model. The best-fit physical conditions are summarized in Table 2.6.

where k is Boltzmann constant, W is integrated intensity, ν is the rest frequency of transition, S is line strength, μ is electric dipole moment, g_I is spin degeneracy, and g_K is projected rotational degeneracy, is plotted versus the upper state energy E_u (Fig. 2.5). If all observed transitions are optically thin and characterized by a single excitation temperature, the points in the rotation diagram should lie on a straight line. In Fig. 2.5, the observed points are fairly scattered (especially the $K = 3$ and 6 transitions), suggesting that some transitions may be optically thick, and/or the excitation is not in local thermodynamic equilibrium (LTE). Therefore we do not perform a rotation diagram fit (Turner 1991) to our data. Instead, we use the code RADEX (van der Tak et al. 2007) to analyze the $\text{CH}_3\text{CN } J=18-17$ excitation. The code calculates the level population with the considerations of collisional and radiative excitation, and line opacities. We assume that the large velocity gradient (LVG) regime can be applied to our sources. We further assume that the source is characterized by a single kinetic temperature (T_{kin}), a total column density (N_{mol}), and an H_2 volume density ($n(\text{H}_2)$). We perform χ^2 optimization of a grid of models to obtain the best-fit solution to the above variables. In addition, we apply a beam filling factor (f , between 0 and 1) to scale the model intensities before calculating χ^2 , assuming all transitions have the same source size. The best-fit solutions are plotted in the form of rotation diagram in Fig. 2.5 (filled circles) and summarized in Table 2.6. The χ^2 distribution of each free parameter is plotted in Fig. 2.9 and 2.10.

With the simplified “point-source” RADEX model, we obtain physical con-

ditions of each source with detections of CH_3CN $J=18-17$. The lower- K transitions are indeed optically thick. In general, the kinetic temperatures are all ≥ 80 K, suggesting that the $J=18-17$ transitions originate from a warm region in the star-forming core. The column densities vary between sources ($\sim 10^{15-17} \text{ cm}^{-2}$). The H_2 volume densities cannot be well constrained by our RADEX model (Fig. 2.9 and 2.10), but generally speaking the $J=18-17$ transitions probe a region with density greater than 10^6 cm^{-3} . This is consistent with the high critical densities required for collisional excitation of the transitions ($\sim 10^7 \text{ cm}^{-2}$; Table 2.2). The observed level population may be slightly sub-thermalized. Interestingly, we find that the filling factors of all sources are very small ($\sim 10^{-4} - 10^{-3}$), corresponding to source sizes of a few $0.1''$ to $1''$. We assume a Gaussian beam (θ_b) and a Gaussian source (θ_s) to derive the source angular size ($f = \theta_s^2/(\theta_s^2 + \theta_b^2)$). A linear source size of few 100 AU to few 1000 AU is also derived. The estimation of source size is consistent with the point source structure observed in AFGL 2591 and Cepheus A (imaging observations; Sect. 2.2). With this result, we suggest that CH_3CN $J=18-17$ transitions trace an unresolved region toward all sources (with detections) at the $\sim 14''$ resolution of JCMT beam. The inferred source sizes, gas densities, and kinetic temperatures support the idea that CH_3CN traces warm and dense rotating structures toward massive star-forming cores (e.g., Beltrán et al. 2006; Cesaroni et al. 2006).

2.4.2 Toy models of kinematics

In this section, we analyze the observed C^{17}O 3–2, C^{34}S 7–6, and CH_3CN 18–17 line profiles toward our sample of massive star-forming cores through a comparison with toy radiative transfer models. We do not perform detailed radiative transfer modeling of the observed line profiles toward the individual sources because this procedure requires information from multiple transitions per molecule and knowledge of temperature/density/velocity profiles as well as chemistry. Instead, we introduce a simplified source configuration and focus on how different kinematics affect the synthetic line profiles. The aim is to have an idea on what kinematical component, such as infall, rotation, or turbulence, dominates the observed linewidth. We exclude outflow motion in the analysis due to its complexity (orientation, opening angle, chemistry, etc.). For some sources, the outflow contribution can be extracted by analyzing their observed C^{17}O 3–2 line profile (Sect 2.3.2) and spatial distribution of high velocity gas (Sect. 2.3.3). We therefore focus on the narrow component only.

2.4.2.1 Model setup and model line profiles

We use the 2D radiative transfer code RATRAN (Hogerheijde & van der Tak 2000) as an engine to generate model line profiles with different kinematics.

We assume the model source is spherically symmetric with an outer boundary of $r_{\text{out}} = 50,000$ AU for C^{17}O models and $r_{\text{out}} = 5000$ AU for $\text{C}^{34}\text{S}/\text{CH}_3\text{CN}$ models. The use of different model source sizes follows from the very different critical densities of the molecules (Table 2.2). The assumption of spherical symmetry may not be true at small scales (few 1000 AU) due to conservation of angular momentum and subsequently the formation of disk-like structure or the formation of a small cluster. In the $\sim 14''$ JCMT beam, the substructures mentioned above are unresolved. The density and temperature profiles are chosen as $n(r) = 10^5(r/10000 \text{ AU})^{-1.5} \text{ cm}^{-3}$ and $T_{\text{kin}}(r) = 100(r/10000 \text{ AU})^{-0.5} \text{ K}$, respectively. The above physical conditions are sampled in 208 adaptive grid cells (Fig. 2.6 (a)–(d)). The enclosed gas masses within $r_{\text{out}} = 50,000$ AU and $r_{\text{out}} = 5000$ AU sampled by our model grid cells are about $54 M_{\odot}$ and $1.7 M_{\odot}$, respectively.

With these fixed density and temperature profiles, we consider two different velocity profiles: (1) free-fall motion ($v_{\text{ff}}(r) = \sqrt{2GM_{\star}/r}$, where r is the distance to the central star), and (2) Keplerian rotation ($v_{\text{Kep}}(R) = \sqrt{GM_{\star}/R}$, where R is the distance to the rotation axis). We note that these two different motions are the extreme cases for a star-forming core. In reality the gas motion in the envelope can be a mixture of infall and rotation. The stellar mass $M_{\star}$ is set at 8, 12, 16, 20, 30, and $40 M_{\odot}$. For the Keplerian rotation models, we consider three different inclination angles (the angle between the rotation axis and the line of sight) at 15° , 45° , and 75° . The turbulent FWHM linewidths of all models are set at 1.0, 2.0, and 3.0 km s^{-1} . The fractional abundances of C^{17}O , C^{34}S , and CH_3CN are assumed to be 1×10^{-7} , 3×10^{-10} , and 3×10^{-8} respectively.

In Fig. 2.6 (e) to (g), we show the relative level population of the C^{17}O $J=3$ level, the C^{34}S $J=7$ level, and the CH_3CN $J_K = 18_3$ level, respectively. The models are calculated assuming a turbulent linewidth of 2.0 km s^{-1} , a stellar mass of $20 M_{\odot}$, and a core with free-fall motion. The population plots are similar to those in Fig. 2.6 if the core is in Keplerian rotation. We found that C^{17}O 3–2 emission traces the entire core except the very inner part, while the C^{34}S 7–6 and CH_3CN 18_3 – 17_3 transitions originate only from the very inner part of the core at few 1000 AU scales (unresolved in $14''$ beam at a source distance of 4 kpc). The CH_3CN $J=18$ – 17 emission is more compact compared to C^{34}S 7–6, consistent with its high upper level energy (215 K).

To simulate the model line profiles observed with a $14''$ beam, we assume a distance of 4 kpc. We chose this distance is because most of our sample sources are within 4 kpc (15 out of 17) and we use this distance as the reference to compare the observed line profiles with the modeled ones (See next section). In Fig. 2.7, we show a sample of C^{17}O 3–2, C^{34}S 7–6, and CH_3CN 18_3 – 17_3 line profiles with free-fall motion or Keplerian rotation (with 45° inclination) with different stellar masses and turbulent linewidths. As expected, the line profile becomes broader if turbulent linewidth and stellar mass increase. Stronger

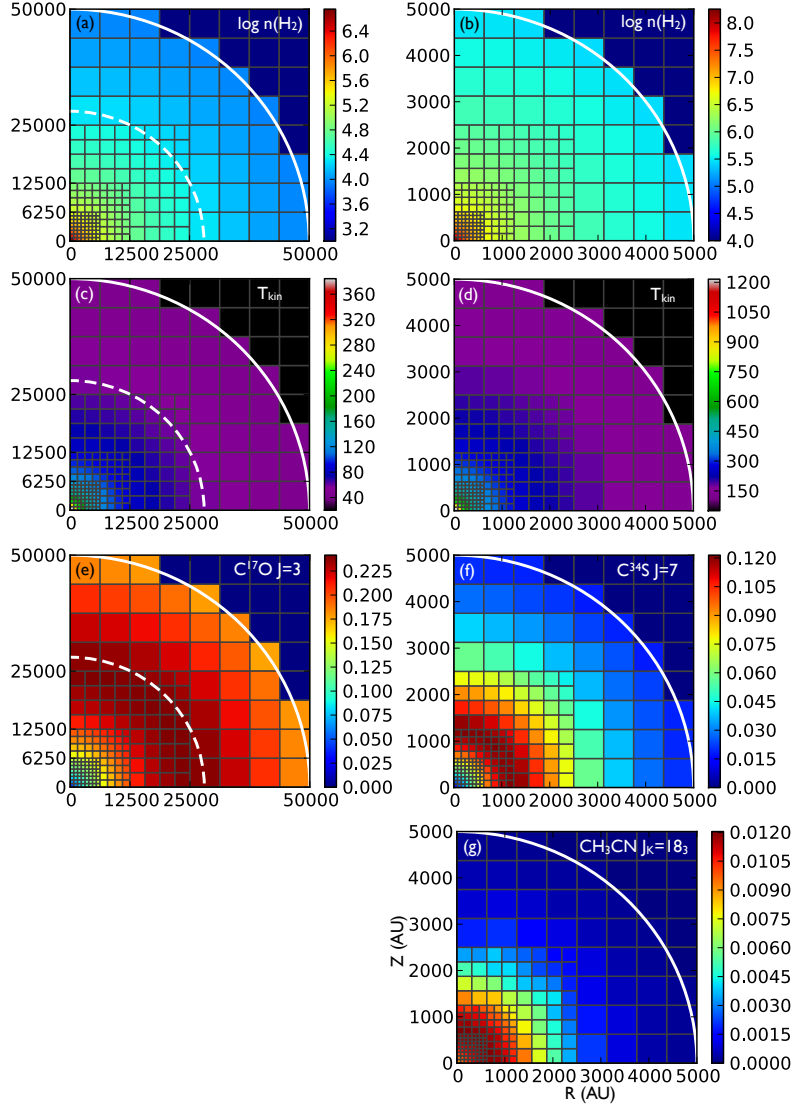


Figure 2.6 RATRAN model distributions of gas density in cm^{-3} (a)/(b), kinetic temperature in K (c)/(d), $\text{C}^{17}\text{O } J=3$ relative population (e), $\text{C}^{34}\text{S } J=7$ relative population (f), and $\text{CH}_3\text{CN } J_K=18_3$ relative population (g). The relative population shown here was calculated assuming a stellar mass of $20 M_{\odot}$, a turbulent linewidth of 2 km s^{-1} , and a free-fall motion. We use adaptive mesh to sample the models (grey grids). The solid line in white is the outer boundary of the model source, while the dashed line in white is the JCMT beam coverage at a source distance of 4 kpc. We use the same grid layout to sample the model but set the outer boundary to be different for C^{17}O ($r_{\text{out}} = 50000 \text{ AU}$), and for $\text{C}^{34}\text{S}/\text{CH}_3\text{CN}$ ($r_{\text{out}} = 5000 \text{ AU}$).

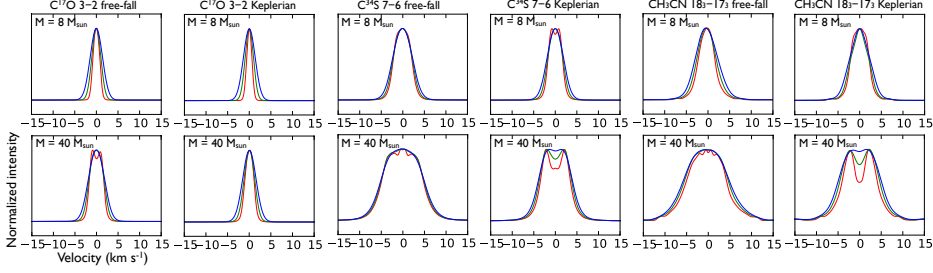


Figure 2.7 Sample RATRAN line profiles of C^{17}O 3–2, C^{34}S 7–6, and CH_3CN 18₃–17₃ with different stellar masses and turbulent linewidths (red: 1 km s^{-1} , green: 2 km s^{-1} , blue: 3 km s^{-1}). The inclination angle of the Keplerian rotation models is 45° .

turbulence smears out the double-peaked signature seen in the free-fall and the Keplerian models. For lower stellar masses, the line broadening due to the increase of the turbulent linewidth is more noticeable. However, for high stellar masses, the increase in turbulence does not change the linewidth significantly, which is dominated by either the infalling motions or the rotation.

2.4.2.2 Comparison with observations

With a grid of models comprising different kinematics, stellar masses, and turbulent linewidths, we now compare the observed line FWHM linewidths with the modeled ones (Fig. 2.8). We plot the FWHM linewidth (measured from observations and models) versus the stellar mass. The stellar mass of each source in our sample is calculated based on the zero-age main-sequence luminosity listed by Mottram et al. (2011) and assuming no contribution from accretion luminosity to the total luminosity. The inferred stellar mass is therefore an upper limit of the real mass. We present the models with three different turbulent FWHM linewidths (blue: 3 km s^{-1} ; green: 2 km s^{-1} ; red: 1 km s^{-1}). In the plots of Keplerian models, each curve (inclination angle = 45°) is overplotted with a colored region. The upper and lower boundaries of the colored regions represent the FWHM linewidth measured at 75° and 15° , respectively.

Since all models are calculated assuming a source distance of 4 kpc, we need to consider the effect of different source distances in our sample when comparing observations with models. To check if the distance changes the linewidth significantly, we integrated over an effective linear area covered by a $14''$ beam at 4 kpc for sources within 4 kpc to derive the effective linewidth. We found that the difference between the linewidth at the real distances and at an effective 4 kpc is generally small (± 0.1 – 0.3 km s^{-1}) in both C^{17}O 3–2 and C^{34}S 7–6. Therefore the difference in source distance should not be a dominant factor when

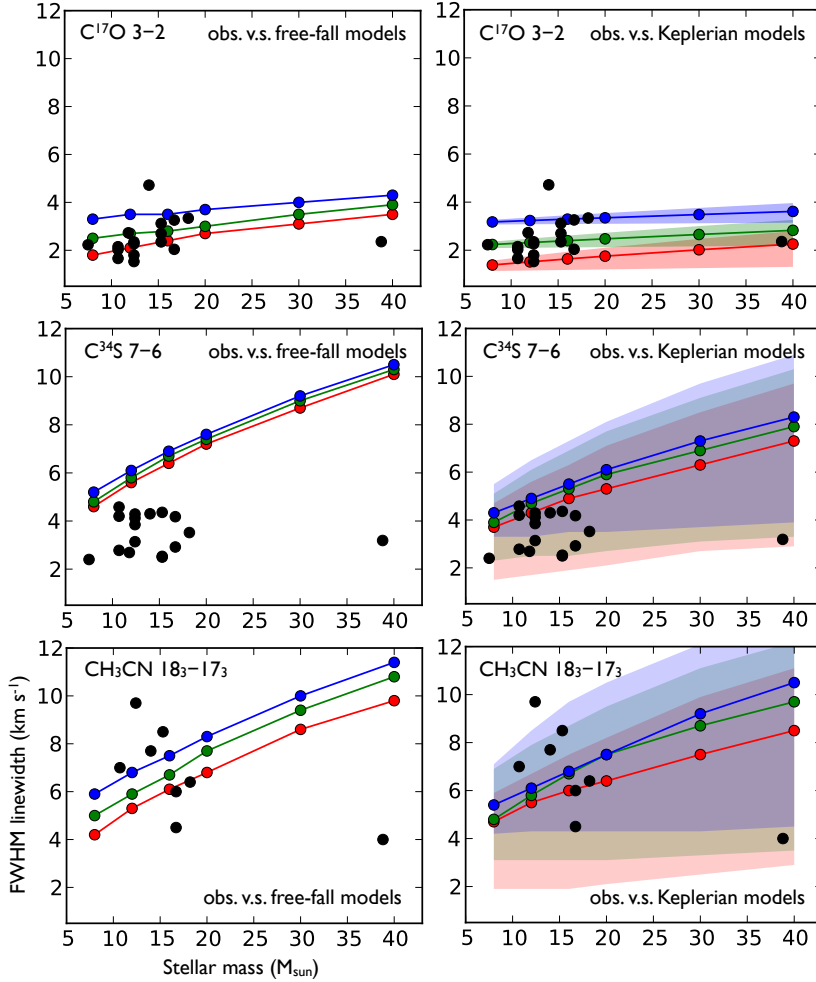


Figure 2.8 Comparison of observed FWHM linewidth with model FWHM linewidth. In all panels, the three curves represent the models with different turbulent FWHM linewidths (blue: 3 km s^{-1} ; green: 2 km s^{-1} ; red: 1 km s^{-1}). In the panels of Keplerian models, additional colored regions are overplotted for each curve. The upper boundary and lower boundary are the model FWHM linewidths measured at 75° and 15° inclination angles, respectively. The curve is the linewidth at 45° inclination. The black circles are the observed line FWHM linewidths plotted versus the inferred upper limit main-sequence masses (based on Mottram et al. (2011)).

comparing the ensemble of the observed linewidths with the models at 4 kpc.

The observed C^{17}O 3–2 linewidths agree well with the models. However, as is shown in Fig. 2.8, the model linewidths do not depend strongly on the stellar mass but do reflect the adopted turbulence. This is explained by the fact that the C^{17}O 3–2 emission originates from large radii, where the infall and/or rotation is small compared to the adopted turbulence of $1\text{--}3\text{ km s}^{-1}$. We therefore conclude that the narrow component of C^{17}O 3–2 line predominantly traces the turbulence on large scales.

For C^{34}S 7–6 we find that the models do not depend strongly on the adopted turbulence but do depend on the stellar mass. This is explained by the fact that the emission originates from relatively small radii where the infalling or rotating motions are much larger than the adopted turbulence. Interestingly, the observed C^{34}S 7–6 linewidths are well below the model curves. Even in the absence of turbulence, rotation or infall would generate wider lines. This could mean that the core is static, but in the light of the CH_3CN results discussed below, we prefer the interpretation that the C^{34}S line originates from larger radii than suggested by our model. A flatter density profile could reproduce such behavior.

The observed CH_3CN $18_3\text{--}17_3$ linewidths show a fairly large scatter but agree well in magnitude with both infalling and rotating models. Like the models for C^{34}S , these mostly depend on the stellar mass, indicating that in the models the emission originates from small radii. The observations and their scatter can be well explained by models with rotation where differences in inclination cause the scatter. The fact the CH_3CN shows broader lines than C^{34}S in spite of similar critical densities is attributed to the larger upper-level energies (265 K v.s. 65 K, respectively), limiting the region of efficient excitation to small radii even in the presence of a flatter density profile as implied above.

In summary, we find the C^{17}O 3–2 traces the turbulence on 10,000 AU scales, that C^{34}S 7–6 traces turbulence on a few 1000 AU scales, and that CH_3CN $18_3\text{--}17_3$ may trace rotation on <1000 AU scales. We confirm that this transition may indeed be an excellent tracer of disk-like structure around massive stars, but stress that detailed modeling of individual sources and high resolution observations are required to confirm this.

2.5 Discussion

2.5.1 Caveats of our qualitative comparison

In our comparison of the observed linewidth with toy radiative transfer models, there are some caveats that need to be pointed out. Firstly, we have assumed that all sources in our sample can be characterized by a spherical core with fixed temperature and density profiles regardless the central stellar mass. In reality, the temperature and density profiles may vary with respect to the stellar mass. Once

the central star becomes more massive, the surrounding core should be warmer. In addition, the temperature and density profiles should also depend on the evolutionary stages of the forming star. Different profiles could change the excitation condition significantly and hence the observed linewidth. The C^{34}S results already imply that a flatter density profile than the adopted $r^{-1.5}$ powerlaw may be appropriate.

Also, we have assumed uniform turbulence in our model star-forming core regardless of stellar mass. In reality, powerful outflows and stellar radiation from the forming massive stars could provide the source of turbulence in star-forming cores. The strength of turbulence may also vary as a function of radius. If the variation of turbulence is considered in our toy models, the model linewidths change accordingly.

In future work, we will explore the caveats listed above by studying the sensitivity of the synthetic line profile to the free parameters in our model. More realistic models including both infall and rotation (Ulrich 1976) will also be generated and compared to our observations.

2.5.2 Molecular tracers of kinematics in massive star-forming cores

In this study, we use the optically thin C^{17}O 3–2 and C^{34}S 7–6 transitions and the optically thick CH_3CN 18–17 lines as diagnostics of kinematics of massive star-forming cores. We found that CH_3CN 18–17 is a good potential tracer of rotation in the inner core, although the Gaussian line shapes indicate that turbulence is important. We also found that C^{34}S 7–6 and C^{17}O 3–2 probe turbulence on a few thousand to a few 10,000 AU scales. C^{17}O 3–2 also shows a broad line component (FWHM linewidth $\sim 3.5\text{--}9.0 \text{ km s}^{-1}$) which likely traces outflow activity.

As a consequence of infall onto star-forming cores, the formation of circumstellar disks and bipolar outflows provides a way to transport and release excess angular momentum of an accreting object (Shu et al. 1987). Outflows, usually observed in low- J CO transitions and SiO, toward massive star-forming regions are found to be ubiquitous as they are in dense cores forming low-mass stars (e.g, Zhang et al. 2001; Beuther et al. 2002; Klaassen & Wilson 2007). The large mass loss rates ($\sim \text{few times } 10^{-4} M_{\odot} \text{ yr}^{-1}$) serve as an indication that the central disk-like structure should accrete gas from the envelope and transport it to the forming star at similar strength. In this study, we found that C^{17}O 3–2 can trace outflows as seen in the broad line wings and the narrow component traces turbulence. In CH_3CN 18–17, we do not see large scale outflow signature in our maps. Instead, speculated from our modeling of the observed linewidth, we suggest that this line traces rotation, though small-scale ($< 14''$) outflows cannot be ruled out. From high-resolution interferometric observations, rotation signatures have been found in C^{34}S and CH_3CN toward some massive star-forming

cores (e.g., Beltrán et al. 2006; Cesaroni et al. 2006). In the case of C^{34}S this implies that emission from rotating regions may be a small fraction of the total line emission picked up by our single-dish measurements. We suggest that future high-resolution survey of massive star-forming cores in C^{34}S and CH_3CN may help in enlarging the detection rate of massive disks. We also suggest that hot core molecules (HCOOH , CH_3CN , HCOOCH_3 , etc.) may be good tracers of massive disks as some authors already pointed out from their high-resolution observations (e.g., Beuther et al. 2004; Wang et al. 2011).

2.6 Conclusion and future work

In this work, we observed C^{17}O 3–2, C^{34}S 7–6, and CH_3CN 18–17 toward 17 massive star-forming cores with the JCMT, aiming at testing what kind of kinematics these lines can trace. We found that CH_3CN 18–17 is a good potential tracer of rotation in the inner core, although the Gaussian line shapes indicate that turbulence is important. We also found that C^{34}S 7–6 and C^{17}O 3–2 probe turbulence on a few 1000 AU to a few 10,000 AU scales. C^{17}O 3–2 also shows a broad line component which likely traces outflow activity.

In the future, we will study how different core temperature and density profiles can affect the synthetic linewidth, which will allow us to better establish the robustness of the line tracers as probes of rotation of star-forming cores. We will also construct a more realistic model including a self-consistent density and velocity profiles of a infalling and rotating star-forming core.

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2.7 Supplementary material

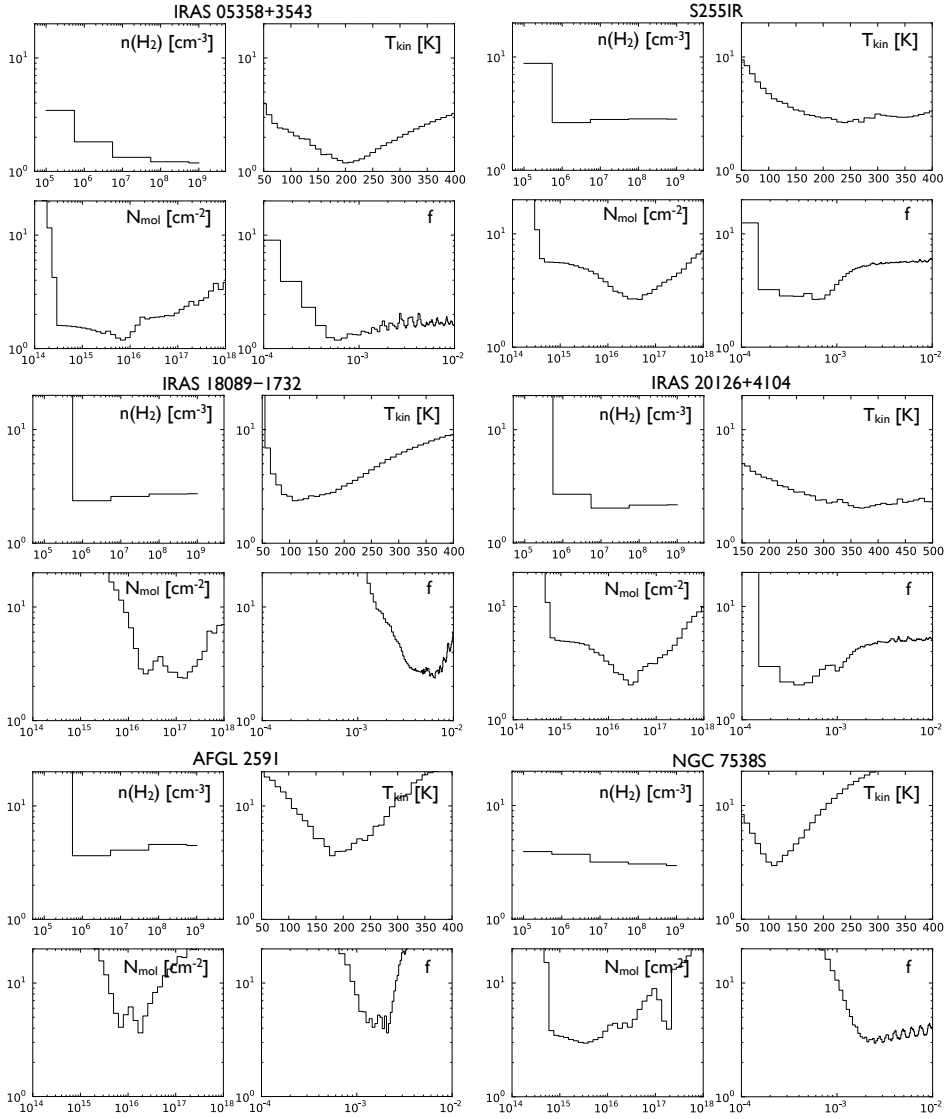


Figure 2.9 χ^2 value (y-axis of each panel) versus each free parameter in RADEX excitation analysis of CH_3CN lines. Only the lower-bound of χ^2 distribution is plotted.

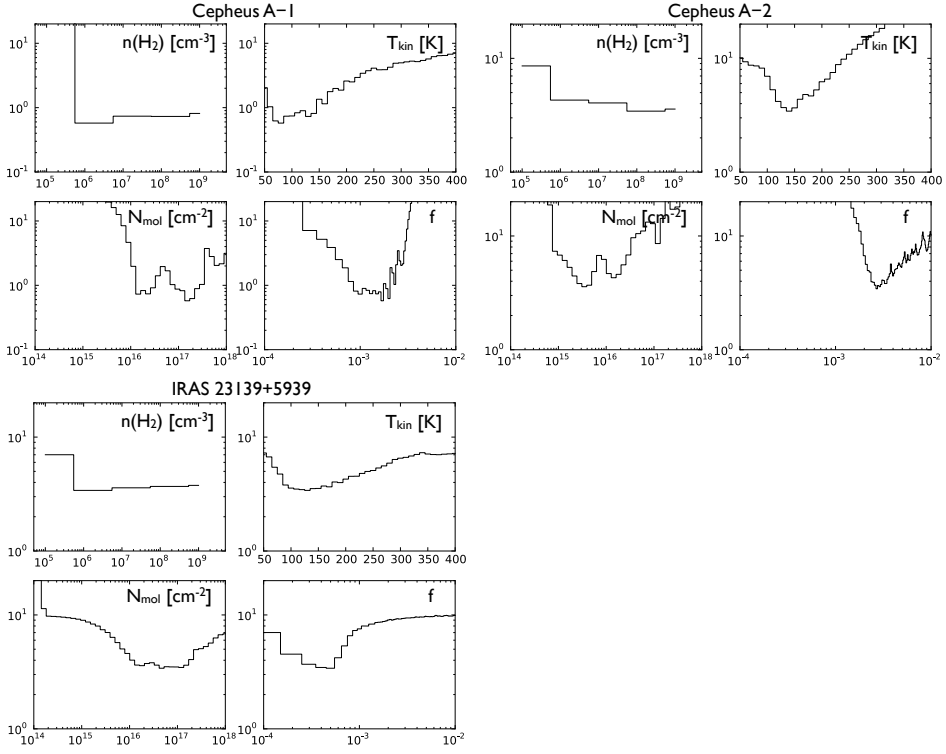


Figure 2.10 χ^2 value (y-axis of each panel) versus each free parameter in RADEX excitation analysis of CH_3CN lines. Only the lower-bound of χ^2 distribution is plotted.

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Chapter 3

Dense molecular cocoons in the massive protocluster W3 IRS5: a test case for models of massive star formation

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Abstract

Context. Two competing models describe the formation of massive stars in objects like the Orion Trapezium. In the turbulent core accretion model, the resulting stellar masses are directly related to the mass distribution of the cloud condensations. In the competitive accretion model, the gravitational potential of the protocluster captures gas from the surrounding cloud for which the individual cluster members compete.

Aims. With high resolution submillimeter observations of the structure, kinematics, and chemistry of the proto-Trapezium cluster W3 IRS5, we aim to determine which mode of star formation dominates.

Methods. We present 354 GHz Submillimeter Array observations at resolutions of $1''$ – $3''$ (1800–5400 AU) of W3 IRS5. The dust continuum traces the compact source structure and masses of the individual cores, while molecular lines of CS, SO, SO₂, HCN, H₂CS, HNCO, and CH₃OH (and isotopologues) reveal the gas kinematics, density, and temperature.

Results. The observations show five emission peaks (SMM1–5). SMM1 and SMM2 contain massive embedded stars ($\sim 20 M_{\odot}$); SMM3–5 are starless or contain low-mass stars ($< 8 M_{\odot}$). The inferred densities are high, $\geq 10^7 \text{ cm}^{-3}$, but the core masses are small, $0.2 - 0.6 M_{\odot}$. The detected molecular emission reveals four different chemical zones. Abundant ($X \sim \text{few } 10^{-7} \text{ to } 10^{-6}$) SO

and SO_2 are associated with SMM1 and SMM2, indicating active sulfur chemistry. A low abundance (5×10^{-8}) of CH_3OH concentrated on SMM3/4 suggest the presence of a hot core that is only just turning on, possibly by external feedback from SMM1/2. The gas kinematics are complex with contributions from a near pole-on outflow traced by CS, SO, and HCN; rotation in SO_2 , and a jet in vibrationally excited HCN.

Conclusions. The proto-Trapezium cluster W3 IRS5 is an ideal test case to discriminate between models of massive star formation. Either the massive stars accrete locally from their local cores; in this case the small core masses imply that W3 IRS5 is at the very end stages (1000 yr) of infall and accretion, or the stars are accreting from the global collapse of a massive, cluster forming core. We find that the observed masses, densities and line widths observed toward W3 IRS 5 and the surrounding cluster forming core are consistent with the competitive accretion of gas at rates of $\dot{M} \sim 10^{-4} M_\odot \text{ yr}^{-1}$ by the massive young forming stars. Future mapping of the gas kinematics from large to small scales will determine whether large-scale gas inflow occurs and how the cluster members compete to accrete this material.

3.1 Introduction

In contrast to low-mass star formation, there is no single agreed upon scenario for the formation of massive stars (Zinnecker & Yorke 2007). Current models either predict that a turbulent core collapses into a cluster of stars of different mass (e.g. McKee & Tan 2003), or that multiple low-mass stars compete for the same mass reservoir, with a few winning and growing to become massive stars while most others remain low-mass stars (e.g. Bonnell et al. 2001; Bonnell & Bate 2006). Both theories are supported by observations (e.g. Cesaroni et al. 1997; Pillai et al. 2011), suggesting that there may be two different modes of massive star formation (Krumholz & Bonnell 2009). However, it is challenging to observe massive star-forming regions since they are at large distances (a few kpc), requiring high-angular resolution to resolve the highly embedded complex structures in which gravitational fragmentation, powerful outflows and stellar winds, and ionizing radiation fields play influence the star-formation processes (Beuther et al. 2007).

Although observationally challenging, progress in testing the models of massive star formation has been made recently with at centimeter, and (sub)millimeter wavelengths. Based on observations of the protocluster NGC 2264 with the IRAM 30m telescope, Peretto et al. (2006) proposed a mixed type of star formation as proposed by Bonnell et al. (2001) and Bonnell & Bate (2006), and McKee & Tan (2003), where the turbulent, massive star-forming core is formed

by the gravitational merger of lower mass cores at the center of a collapsing protocluster. Observations of G8.68–0.37 with the Submillimeter Array (SMA) and the Australia Telescope Compact Array (ATCA) imply that to form an O star, the star-forming core must continuously gain mass by accretion from a larger mass reservoir since protostellar heating from the low-mass stars is not sufficient to halt fragmentation (Longmore et al. 2011). Multi-wavelength observations of G29.96–0.02 and G35.20–1.74 suggest that the mass of massive star-forming cores is not limited to the natal cores formed by fragmentation and turbulence is not strong enough to prevent collapse, which favors the competitive accretion model (Pillai et al. 2011). On the other hand, Very Large Array (VLA) observations of IRAS 05345+3157 (Fontani et al. 2012) suggest that turbulence is an important factor in the initial fragmentation of the parental clump and is strong enough to provide support against further fragmentation down to thermal Jeans masses.

W3 IRS5 is a massive star-forming region located in the Perseus arm at a distance of 1.83 ± 0.14 kpc (Imai et al. 2000) with a total luminosity of $2 \times 10^5 L_{\odot}$ (Campbell et al. 1995). A cluster of hypercompact (< 240 AU) H II regions are found from high-resolution cm-wavelength observations (Claussen et al. 1994; Wilson et al. 2003; van der Tak et al. 2005). Based on observations at near-IR wavelengths, Megeath et al. (1996, 2005, 2008) found a high stellar surface density of $\sim 10000 \text{ pc}^{-2}$ and proposed that W3 IRS5 is a Trapezium cluster (Abt & Corbally 2000) in the making. A high protostellar number density exceeding 10^6 protostars pc^{-3} is also concluded by Rodón et al. (2008) from their 1.4 mm observations with the Plateau de Bure Interferometer (PdBI). The proximity and the dense protostellar environment make W3 IRS5 an excellent target to study massive star formation in a highly clustered mode.

(Sub)millimeter observations show that the molecular structure of W3 IRS5 is physically and chemically complex. Multiple bipolar outflows with various orientations are reported via different tracers (e.g. Mitchell et al. 1992; Ridge & Moore 2001; Gibb et al. 2007; Rodón et al. 2008; Wang et al. 2012). Although the outflow driving sources are not determined unambiguously, the infrared pair NIR1 and NIR2 (Megeath et al. 2005) are likely candidates. The detection of near-IR and X-ray emission toward W3 IRS5 (Megeath et al. 2005; Hofner et al. 2002) likely benefits from an outflow oriented near the line of sight. A velocity gradient in the NW–SE direction on scales of a few arcseconds is seen in SO_2 , which may indicate rotation of the common envelope of NIR1 and NIR2 (Rodón et al. 2008; Wang et al. 2012). At $14''$ resolution, many molecular species are detected toward W3 IRS5, especially sulfur-bearing molecules (Helmich et al. 1994; Helmich & van Dishoeck 1997), implying active hot-core chemistry (e.g. Charnley 1997) or shocks (e.g. Pineau des Forets et al. 1993). The sulfur-bearing species SO and SO_2 peak near NIR1/NIR2, while complex organic molecules such as CH_3CN and CH_3OH peak at offset positions (Rodón et al. 2008; Wang

et al. 2012).

This paper presents Submillimeter Array (SMA) observations of W3 IRS5 at 354 GHz with an angular resolution of $1''$ – $3''$, revealing the complex molecular environment of the proto-Trapezium cluster and tracing the star formation processes in the dense cluster-forming core. The observations and data calibration are summarized in Sect. 3.2. We present the observational results in Sect. 3.3, followed by data analysis in Sect. 3.4. We discuss our findings in Sect. 3.5, and conclude this paper in Sect. 3.6.

3.2 Observations and Data reduction

W3 IRS5 was observed with the SMA¹ (Ho et al. 2004) on 2008 January 7 in the compact configuration and on 2006 January 15 in the extended configuration. Both observations were conducted with 7 antennas and were centered on $\alpha(2000) = 02^{\text{h}}25^{\text{m}}40^{\text{s}}.78$, $\delta(2000) = 62^{\circ}05'52''.50$. The weather conditions were good with $\tau_{225\text{GHz}} \sim 0.1$. The reference V_{LSR} was set to -39.0 km s^{-1} . The receiver was tuned to 353.741 GHz in the upper sideband, covering frequencies from 342.6 to 344.6 GHz and from 352.6 to 354.6 GHz. The correlator was configured to sample each spectral window by 256 channels, resulting a velocity resolution of $\sim 0.35 \text{ km s}^{-1}$ per channel. For the compact configuration dataset, 3C454.3 was observed as bandpass calibrator. Gain calibration was performed by frequent observations of two quasars, 0136+478 ($\sim 16^{\circ}$ away from the source) and 3C84 ($\sim 22^{\circ}$ away from the source). Uranus was adopted as absolute flux calibrator. For the extended configuration dataset, 3C273, 3C84 and 3C273 were observed, respectively, as bandpass, gain and flux calibrators. The adopted total flux density of 3C273 is 9.6 Jy, which is the mean value reported for five observations² during 2006 January 13–30. We estimate that the uncertainty in absolute flux density is about 20%. The uv -range sampled by the combined dataset is $10 \text{ k}\lambda$ ($21''$) to $210 \text{ k}\lambda$ ($1''$).

Data reduction was conducted by using the MIR package (Scoville et al. 1993) adapted for the SMA, while imaging and analysis were performed in MIRIAD (Sault et al. 1995). To avoid line contamination, line-free channels were selected to separate the continuum and line emission in the visibility domain. The continuum visibilities for each dataset were self-calibrated using the brightest clean components to enhance the signal-to-noise ratio. Self-calibrated datasets were combined to image the continuum. To optimize sensitivity and angular resolution, a robust weighting³ parameter of 0.25 was adopted for the con-

¹The Submillimeter Array is a joint project between the Smithsonian Astrophysical Observatory and the Academia Sinica Institute of Astronomy and Astrophysics and is funded by the Smithsonian Institution and the Academia Sinica.

²<http://sma1.sma.hawaii.edu/callist/callist.html>

³<http://www.atnf.csiro.au/computing/software/miriad/userguide/node107.html>

tinuum imaging, resulting in a 1σ rms noise of 10 mJy per $1''$ beam. Line identification was conducted by using the compact configuration dataset only with the aid of spectroscopy databases of JPL⁴ (Pickett et al. 1998) and CDMS⁵ (Müller et al. 2005). For those lines that were also clearly detected in the extended-configuration dataset, we imaged the combined compact+extended dataset.

3.3 Observational results

3.3.1 Continuum emission

Figure 3.1 shows the continuum image and visibilities at 353.6 GHz. At a resolution of $1''.1 \times 0''.8$ and P.A. -14° , five major emission peaks, SMM1 to SMM5, were identified based on their relative intensities and a cutoff of 9σ . We note that irregular, extended emission is also observed around the identified peaks. More emission peaks may be present in the diffuse surroundings, which requires better sensitivity, angular resolution, and image fidelity for confirmation. The total flux density recorded by the SMA is about 2.5 Jy which is about 6% of the flux contained in the SCUBA image at $850\ \mu\text{m}$ (Wang et al. 2012). To derive the positions and flux densities of the emission peaks, we fitted the data with five point sources in the visibility domain (Fig. 3.1 (b)). The properties of the five sources are summarized in Table 3.1. With this simplified model, about half of the observed flux originates from the unresolved sources, while the extended emission detected in baselines of 10–25 k λ contributes the other half. The fit deviates significantly from the data at long baselines ($> 150\ \text{k}\lambda$) and on short baselines ($< 20\ \text{k}\lambda$). The former corresponds to fine image detail that we could fit by adding more point sources, but we find that the S/N does not warrant additional “sources”. The latter indicates that on scales $> 8''$ there is significant emission that our 5-point model does not represent properly. An extended, Gaussian envelope could match these observations. However, on even larger spatial scales our uv sampling misses even larger amounts of emission. Therefore, we do not aim to model this extended emission, but instead refer to the SCUBA $850\ \mu\text{m}$ emission to trace this component.

Table 3.1 lists the cm-wave, (sub)mm and IR sources associated with SMM1–5 (Claussen et al. 1994; Wilson et al. 2003; van der Tak et al. 2005; Megeath et al. 2005; Rodón et al. 2008; Wang et al. 2012). In Fig. 3.1 (a), we see that the emission decreases between SMM1/SMM2 and SMM3/SMM4/SMM5, dividing the cloud into two regions with the eastern part containing clusters of IR and cm-wave emission as well as X-ray emission (Hofner et al. 2002), while the western part shows no IR and cm-wave sources. This dichotomy implies that the east-

⁴<http://spec.jpl.nasa.gov/>

⁵<http://www.astro.uni-koeln.de/cdms/>

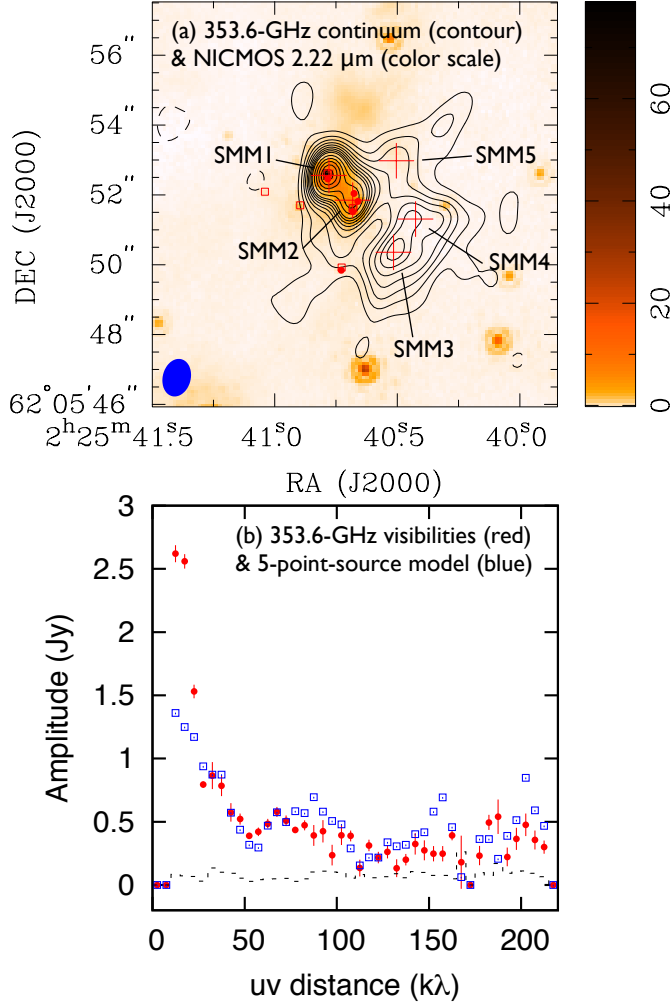


Figure 3.1 (a) Continuum emission of W3 IRS5 region at 353.6 GHz (black contours) overplotted with the NICMOS 2.22 μm emission (color scale). The synthesized beam size is $1''.1 \times 0''.8$, P.A. -14° . The contour levels are -3, 3, 5, 7, ..., 19, 23, 27, ... σ with 1σ of 10 mJy beam^{-1} . The red crosses mark the positions of the five point sources derived from the visibility fit. The red open squares are the positions of near-infrared sources identified by Megeath et al. (2005) while the red filled circles represent the positions of cm-wave sources from van der Tak et al. (2005). (b) Vector-averaged 353.6 GHz continuum visibilities. The red filled circles with error bars are the observed data. The expected zero amplitude is shown as a dashed histogram. The model consisting of five point sources is plotted with open blue squares.

Table 3.1. Characteristics of the continuum emission in W3 IRS5 at 353.6 GHz

Source	$\alpha(2000)$ (hh mm ss)	$\delta(2000)$ (dd mm ss)	I_ν^a (Jy beam $^{-1}$)	S_ν^b (Jy)	$N(\text{H}_2)^c$ ($\times 10^{23}$ cm $^{-2}$)	$M(\text{H}_2)^d$ ($M_\odot$)	$n(\text{H}_2)^e$ ($\times 10^7$ cm $^{-3}$)	Associated cm-wave, IR, or mm source
SMM1	02 25 40.779	+62 05 52.55	0.41	0.43	4.4	0.6	3.2	D2 ^{f} , Q5 ^{g} , K7 ^{g} , MIR1 ^{g} , NIR1 ^{h} , MM-1 ^{i} , SMS1-MM1 ^{j}
SMM2	02 25 40.679	+62 05 51.89	0.30	0.39	3.2	0.5	2.9	B ^{f} , Q1-3 ^{g} , K2-4 ^{g} , MIR2 ^{g} , NIR2 ^{h} , MM-2/3 ^{i} , MM-5 ^{i}
SMM3	02 25 40.509	+62 05 50.41	0.16	0.24	1.7	0.3	1.8	SMS1-MM2 ^{j}
SMM4	02 25 40.431	+62 05 51.36	0.14	0.22	1.5	0.3	1.6	SMS1-MM2 ^{j}
SMM5	02 25 40.504	+62 05 52.99	0.09	0.13	1.0	0.2	1.0	

Note. — ^{a} Peak intensity measured from the image. ^{b} Point source flux density measured from the visibility fit. ^{c} H $_2$ column density. We assume $T_d = 150$ K for all submillimeter sources. ^{d} H $_2$ mass. We assume $T_d = 150$ K for all submillimeter sources. ^{e} H $_2$ volume density. We assume $T_d = 150$ K for all submillimeter sources. A spherical source with a diameter of 1'' or 1830 AU is assumed. ^{f} Claussen et al. (1994) and Wilson et al. (2003). ^{g} van der Tak et al. (2005). ^{h} Megeath et al. (2005). ^{i} Rodón et al. (2008). ^{j} Wang et al. (2012).

ern part of the source is more evolved and less embedded than the western part. We note that the projected positions of SMM1, SMM2 and SMM3 are aligned nearly in a straight line which could be the result of fragmentation at the scale of $1''$ – $2''$ (~ 1800 AU– 3600 AU), although this may be a projection effect.

Because SMM1 and SMM2 contain cm-wave sources, the observed submillimeter flux may contain non-thermal contributions. We estimate the free-free contribution from VLA observations at 5, 15 and 22.5 GHz (Tieftrunk et al. 1997). For SMM1 and SMM2, the extrapolated free-free contributions at 353.6 GHz are 8 mJy and 0.4 mJy, respectively, much smaller than the observed fluxes (SMM1: 0.43 Jy, SMM2: 0.39 Jy). We therefore conclude that the 353.6 GHz emission is dominated by thermal emission from dust and ignore any contribution of free-free emission toward SMM1 and SMM2.

3.3.2 Line emission

3.3.2.1 Molecular distribution

Within the passbands (342.6–344.6 GHz and 352.6–354.6 GHz), we identify 17 spectral features from 11 molecules (Table 3.2). Most emission features come from sulfur-bearing molecules such as CS, SO, ^{33}SO , SO_2 , $^{33}\text{SO}_2$, $^{34}\text{SO}_2$ and H_2CS . Others come from HCN, HC^{15}N , HNCO and CH_3OH . This set of lines covers upper level energies from 43 K to 1067 K and high critical densities (10^7 – 10^8 cm^{-3}). Figure 3.2 shows a sample of molecular emission images toward W3 IRS5 using the compact-configuration data and natural weighting (panels (a) to (l), with a resolution of $3''.3 \times 1''.8$, P.A. -12°) and with uniform weighting (panels (m) to (r), with a resolution of $1''.1 \times 0''.7$, P.A. -17°).

Most of the emission from SO and SO_2 and their isotopologues peaks toward the continuum peaks SMM1 and SMM2, while weaker emission is seen toward SMM3 and SMM4. However, other sulfur-bearing molecules such as CS and H_2CS show a very different spatial distribution, and mainly peak to the north-west of SMM1–5 (Fig. 3.2 (i) and (m)). Most of the emission from HCN and its isotopologues comes from SMM1 and SMM2 (Fig. 3.2 (g), (h) and (n)). Additional emission can be seen toward SMM3 and SMM4, as well as east and north-west of the SMM sources. The typical hot-core molecule CH_3OH exclusively peaks toward SMM3 and SMM4 (Fig. 3.2 (k)). HNCO is detected toward SMM1 and SMM2 only (Fig. 3.2 (j)). Combining all these observational facts, the overall molecular emission toward W3 IRS5 can be classified into four zones (A: SMM1/SMM2; B: SMM3/SMM4; C: north-west region; may be associated with SMM5; and D: east of SMM1–5), and summarized in Figure 3.3.

3.3. OBSERVATIONAL RESULTS

Table 3.2. Detected molecular transitions in W3 IRS5

Molecule ^a	Frequency (MHz)	Transition	E_u^b (K)	n_{crit}^c (cm ⁻³)
CS	342883.0	$J=7-6$	66	2.0×10^7
SO	344310.6	$N_J=8_8-7_7$	87	1.2×10^7
³³ SO	343086.1	$N_J=8_9-7_8, F=15/2-13/2$	78	1.4×10^7
	343087.3	$N_J=8_9-7_8, F=17/2-15/2$	78	1.4×10^7
	343088.1	$N_J=8_9-7_8, F=19/2-17/2$	78	1.4×10^7
	343088.3	$N_J=8_9-7_8, F=21/2-19/2$	78	1.4×10^7
SO ₂	342761.6	$J_{K_a, K_c}=34_{3,31}-34_{2,32}$	582	^d
	343923.8	$J_{K_a, K_c}=24_{2,22}-23_{3,21} v_2=1$	1038	^d
³³ SO ₂	353741.0	$J_{K_a, K_c}=19_{4,16}-19_{3,17}, F=39/2-39/2$	213	2.5×10^7
	353741.1	$J_{K_a, K_c}=19_{4,16}-19_{3,17}, F=37/2-37/2$	213	2.5×10^7
	353741.6	$J_{K_a, K_c}=19_{4,16}-19_{3,17}, F=41/2-41/2$	213	2.5×10^7
	353741.6	$J_{K_a, K_c}=19_{4,16}-19_{3,17}, F=35/2-35/2$	213	2.5×10^7
³⁴ SO ₂	344245.3	$J_{K_a, K_c}=10_{4,6}-10_{3,7}$	88	3.4×10^7
	344581.0	$J_{K_a, K_c}=19_{1,19}-18_{0,18}$	167	4.8×10^7
	353002.4	$J_{K_a, K_c}=14_{7,7}-15_{6,10}$	212	1.5×10^7
	354277.6	$J_{K_a, K_c}=34_{3,31}-34_{2,32}$	580	^d
	354397.8	$J_{K_a, K_c}=19_{8,12}-20_{7,13}$	326	2.9×10^7
HCN	354505.5	$J=4-3$	43	1.8×10^8
	354460.5	$J=4-3 v_2=1$	1067	^d
HC ¹⁵ N	344200.3	$J=4-3$	43	1.2×10^8
H ₂ CS	342944.4	$J_{K_a, K_c}=10_{0,10}-9_{0,9}$	91	^d
HNCO	352897.9	$J_{K_a, K_c}=16_{1,15}-15_{1,14}, F=17-16$	187	3.0×10^7
	352897.9	$J_{K_a, K_c}=16_{1,15}-15_{1,14}, F=16-15$	187	3.0×10^7
	352897.9	$J_{K_a, K_c}=16_{1,15}-15_{1,14}, F=15-14$	187	3.0×10^7
CH ₃ OH	342729.8	$J_K=13_1-13_0 A$	227	4.8×10^7

Note. — ^aSpectroscopy data taken from JPL molecular spectroscopy and CDMS. ^bUpper level energy. ^cCritical density at 100 K derived from LAMDA (Schöier et al. 2005). The critical densities for ³³SO, ³³SO₂ and ³⁴SO₂ are quoted from their main isotopologues. ^dCollisional rate coefficient is not available for this transition.

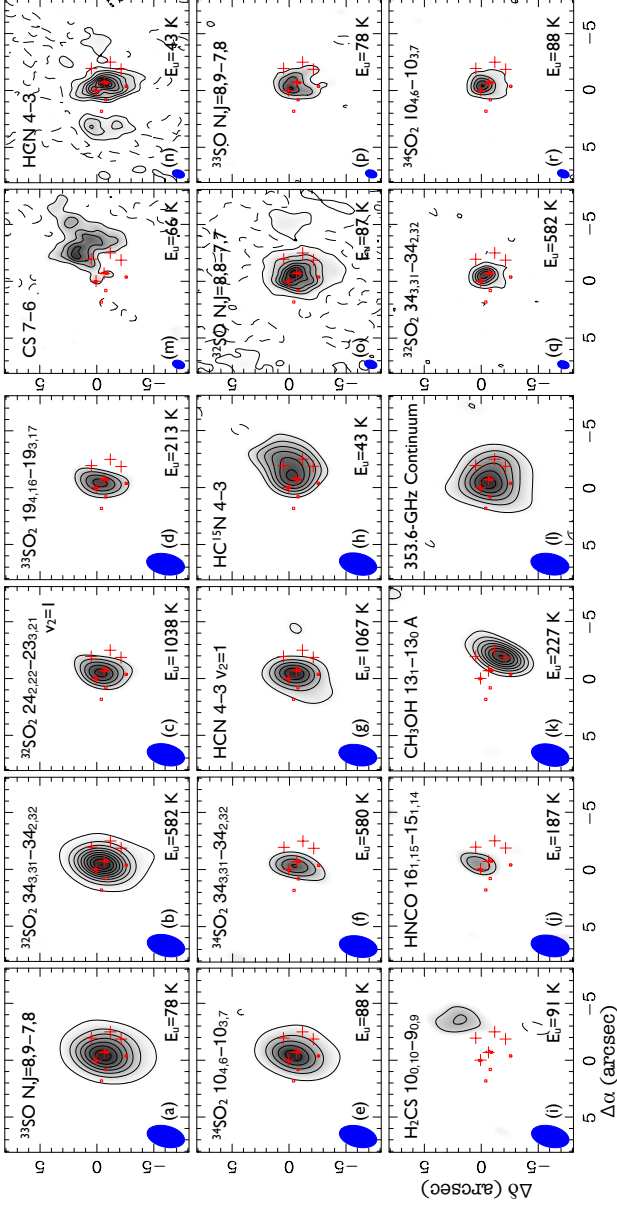


Figure 3.2 Moment 0 maps of molecular emission toward W3 IRS5. The 353.6-GHz continuum emission is also presented for comparison. In panels (a) to (l), the compact dataset is imaged using natural weighting, resulting in a resolution of $3''.3 \times 1''.8$ (P.A. -12°) shown as the filled ellipse in the bottom-left corner of each panel. In panels (m) to (r), the combined dataset is imaged using uniform weighting, resulting in a resolution of $1''.1 \times 0''.7$ (P.A. -17°). The five crosses represent the positions of SMM1 to SMM5 (c.f. Fig. 3.1). Open squares are the positions of IR sources taken from Megath et al. (2005), while filled circles are the positions of cm-wave sources reported by van der Tak et al. (2005). The (0, 0) position corresponds to the reference phase center (Sect. 3.2). In all panels, contour levels start at 3σ (solid line) and -3σ (dashed line). The contour units are $\text{Jy beam}^{-1} \text{ km s}^{-1}$ for panel (a)–(k) and (m)–(r), and Jy beam^{-1} for panel (l). The 1σ noise levels from (a) to (r) are 1.0, 0.9, 0.35, 0.39, 0.72, 0.46, 1.0, 0.45, 0.22, 0.45, 0.36, 0.04, 0.47, 0.94, 0.66, 0.68, 0.84 and 0.68 respectively. The contour steps from (a) to (r) are 10, 10, 2, 2, 10, 2, 4, 2, 1, 1, 2, 4, 5, 20, 5, 6 and 5, respectively.

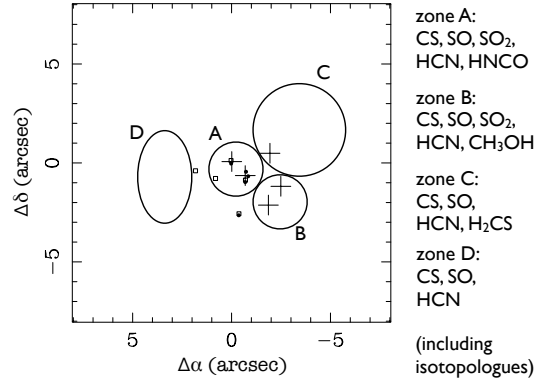


Figure 3.3 The main molecular zones identified toward W3 IRS5. The representative molecular species including their isotopologues are listed. The crosses, filled circles and open squares represent the same sources as in Fig. 3.2.

3.3.2.2 Velocity channel maps

Among the detected spectral features, most of the emission is compact (in zones A and B). Only CS $J=7-6$, SO $N_J=8_8-7_7$ and HCN $J=4-3$ are extended and trace the large scale gas kinematics. Figure 3.4 shows the channel maps of these molecules from -49 km s^{-1} to -30 km s^{-1} and from -41 km s^{-1} to -35 km s^{-1} , using robust weighting (robust = 0). These three molecules show emission over a broad velocity range. The emission at extreme velocities is mainly concentrated toward zone A. Weaker emission is seen toward zone B. Zone C is best traced by CS with some emission from SO, HCN, and H₂CS as well. At velocities ranging from -49 to -42 km s^{-1} , the emission from all three molecules can be seen toward zone D.

Of these three molecules, the image quality near the systemic velocity ($\sim -39.0 \text{ km s}^{-1}$) is poor due to the missing flux of extended emission. However, some additional emission features can be seen near the systemic velocity. Figure 3.4 shows the channel maps of CS, SO and HCN at velocities ranging from -41 km s^{-1} to -35 km s^{-1} . The emission of HCN is much weaker than the other species near -39 km s^{-1} suggesting that HCN is much more extended, and therefore more heavily filtered out by the interferometer, or that the emission is self-absorbed. Additional extended emission in the N-S and NW-SE directions can be seen in the CS channel maps from -41 km s^{-1} to -38 km s^{-1} , which might delineate two collimated outflows or a single wide-angle outflow in the NW-SE direction. The small velocity range suggests that the outflow may be in the plane of sky. In the SO channel maps, a bar-like structure can be seen from -41 km s^{-1} to -37 km s^{-1} . Our data suggest that CS, SO and HCN trace

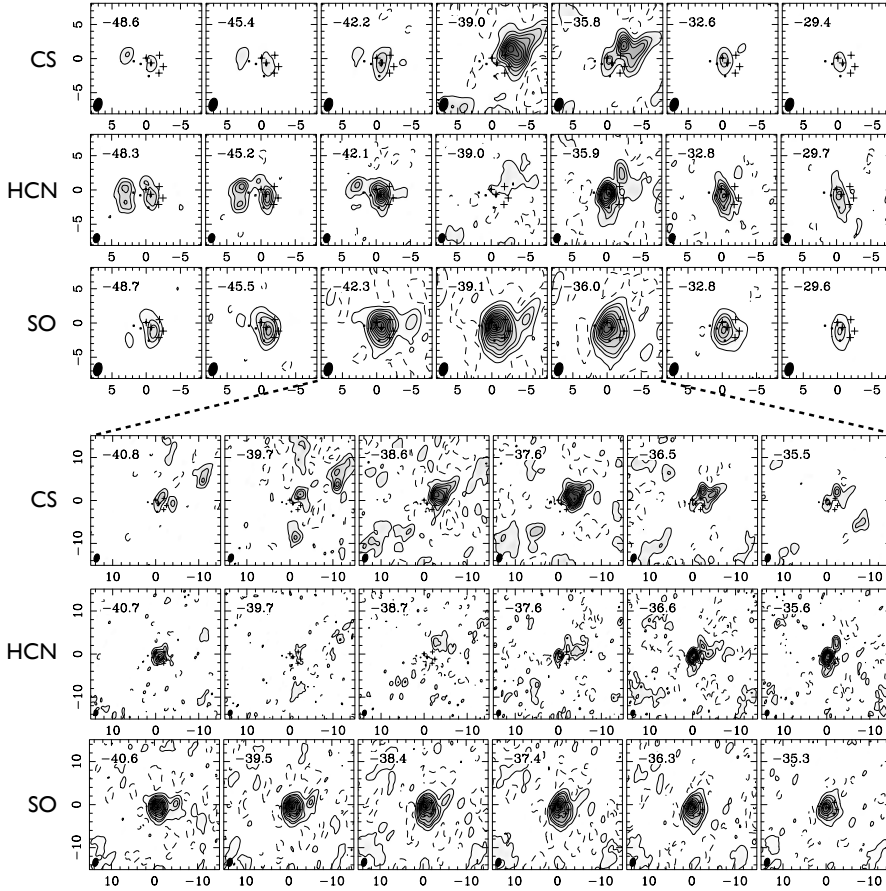


Figure 3.4 Velocity channel maps of CS $J=7-6$, SO $N_J=8_8-7_7$ and HCN $J=4-3$ toward W3 IRS5. Robust weighting (robust = 0) is used for the imaging, resulting resolutions of $1''.9 \times 1''.2$, P.A. -15° , $1''.3 \times 0''.9$, P.A. -13° , and $1''.9 \times 1''.2$, P.A. -14° , for CS, HCN and SO, respectively. The x - and y -axes are R.A. offset and DEC offset relative to the phase center $\alpha(2000) = 02^h25^m40^s.78$, $\delta(2000) = 62^\circ05'52''.50$ in arcseconds, respectively. The upper three rows shows the velocity range between -49 km s^{-1} to -30 km s^{-1} . The lower three rows show a narrower velocity range from -41 km s^{-1} to -35 km s^{-1} . The markers are identical to Fig. 3.2. Solid and dashed contours represent positive and negative intensities, respectively. The absolute contour levels for CS in the upper panel are 3, 8, 13,... σ ($1 \sigma = 0.11 \text{ Jy beam}^{-1}$). The absolute contour levels for HCN in the upper panel are 3, 8, 13,... σ ($1 \sigma = 0.12 \text{ Jy beam}^{-1}$). The absolute contour levels for SO in the upper panel are 3, 13, 23, 43, 63... σ ($1 \sigma = 0.11 \text{ Jy beam}^{-1}$). The absolute contour levels for CS in the lower panel are 3, 8, 13,... σ ($1 \sigma = 0.18 \text{ Jy beam}^{-1}$). The absolute contour levels for HCN in the lower panel are 3, 7, 11,... σ ($1 \sigma = 0.16 \text{ Jy beam}^{-1}$). The absolute contour levels for SO in the lower panel are 3, 13, 23, 43, 63,... σ ($1 \sigma = 0.14 \text{ Jy beam}^{-1}$).

different parts of the molecular condensation in W3 IRS5 and show a complex morphology in velocity space.

3.3.2.3 Line profiles

Figure 3.5 presents the hanning-smoothed spectra toward zone A (thick line; offset position $-0.42''$, $-0.43''$) and B (thin line; offset position $-1.89''$, $-1.78''$) where most of the detected molecules peak. The compact-configuration dataset and natural weighting is used for all molecules except CS, SO and HCN, which are imaged with the combined dataset in natural weighting and convolved to the same resolution as the other images.

SO shows a flat-top line profile at both positions, implying the line may be optically thick or is a blend of multiple velocity components. If SO is fully thermalized, optically thick, and fills the beam, the peak brightness temperatures indicate kinetic temperatures of ~ 70 K and ~ 45 K for zone A and B, respectively. These values are lower limits to the kinetic temperature if the beam filling factor is not unity. In addition, a blue-shifted spectral feature is seen at zone B.

CS and HCN show broad line profiles with a dip near the systemic velocity due to missing flux of extended emission. Single-dish JCMT observations of the same transitions (Helmich & van Dishoeck 1997) show single-peaked profiles and rule out self absorption. The line profiles at zone A are comparable with more emission in the blue-shifted line wing, suggesting both species trace similar cloud components. At zone B, both lines also show broad line wings. Near systemic velocity, HCN shows a wider dip than CS, suggesting that the spatial distributions of both lines are different. Vibrationally excited HCN peaks mainly toward zone A and shows an asymmetric line profile. HC^{15}N is present toward both zones; its smaller line width toward zone B implying that this zone is more quiescent than zone A.

The line profiles of all the other molecules presented in Fig. 3.5 are Gaussian toward both zones. There is no significant velocity shift between the two zones. We note that the apparent velocity shift seen in ^{33}SO and $^{33}\text{SO}_2$ is due to the blending of multiple hyperfine transitions; we have defined the velocity axis with respect to the hyperfine component with the lowest frequency (Table 3.2).

We derive the line center LSR velocity (V_{LSR}), FWHM line width (dV) and integrated line intensity (W) of the line profiles in zones A and B using Gaussian decomposition (Table 3.3). Since the CS and HCN line profiles are highly non-Gaussian, we do not attempt to derive the line parameters. For molecules with hyperfine transitions such as ^{33}SO , $^{33}\text{SO}_2$ and HNCO , we assume that each component has the same FWHM line width and LSR velocity. The relative intensity of hyperfine components are calculated assuming LTE and we fit the combined profile to the data. The results are summarized in Table 3.3. From the Gaussian fit, we do not find significant differences in LSR velocity between zones A and

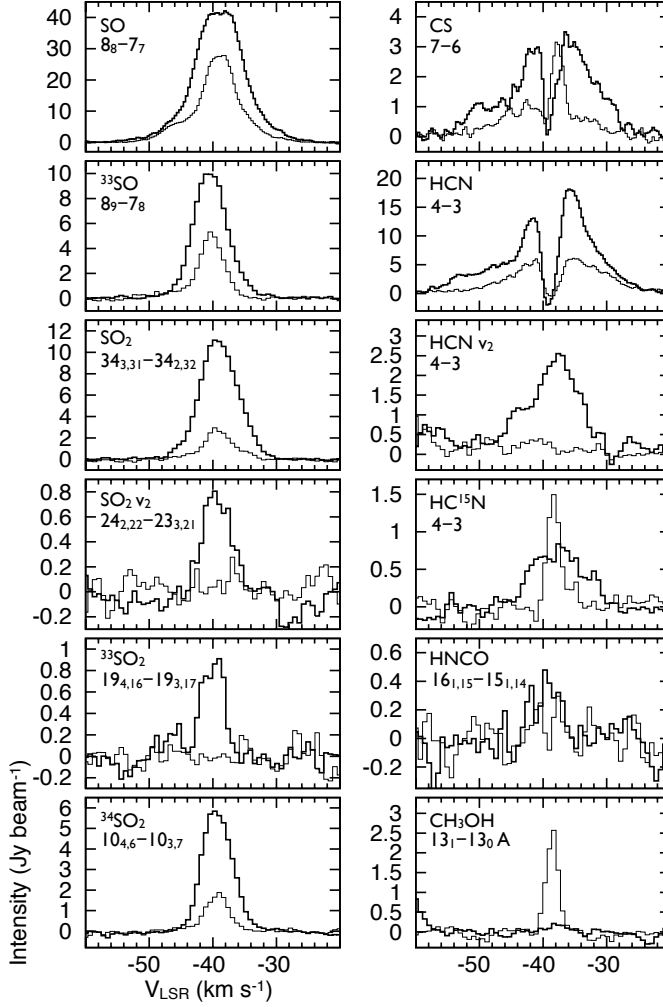


Figure 3.5 Hanning-smoothed molecular spectra toward molecular zone A (thick line; offset position $(-0.42'', -0.43'')$) and B (thin line; offset position $(-1.89'', -1.78'')$). The compact-configuration dataset and natural weighting is used for all molecules except CS 7–6, SO $N_J=8_8-7_7$ and HCN 4–3 which are taken from the combined dataset using natural weighting but convolved to the beam size of the compact dataset ($3''.3 \times 1''.8$, P.A. -12°). The apparent offset in velocity seen in ^{33}SO and $^{33}\text{SO}_2$ is due to the blending of hyperfine transitions for which the reference velocity is set to the transition with lowest frequency (see Table 3.2).

B. Different line widths are derived in both zones depending on the molecular transitions but the general trend is that the lines are broader in zone A, suggesting a more turbulent environment.

We estimate the amount of missing flux of CS 7–6, SO 8₈–7₇, HCN 4–3, and ³²SO₂ 34_{3,31}–34_{2,32} by comparing our SMA observations with the JCMT observations (Helmich & van Dishoeck 1997). Our SMA observations miss $\sim 70\%$, $\sim 40\%$, and $\sim 80\%$ flux for CS, SO, and HCN, respectively. Given the excitation of these lines, the derived missing flux is consistent with the large amount missing flux at 850 μm ($\sim 94\%$; Sect. 3.3.1). The SMA observation of ³²SO₂ 34_{3,31}–34_{2,32} likely recovers all emission, because this transition has a high upper level energy (corresponding to 582 K), and the emission therefore preferentially traces the dense, warm, and compact part of W3 IRS5.

3.4 Analysis

3.4.1 Mass and density of the submillimeter sources

We estimate the H₂ column density and mass of each point source based on the continuum at 353.6 GHz. The H₂ column density at the emission peak can be estimated as

$$N(\text{H}_2) = \frac{I_\nu a}{2m_{\text{H}}\Omega_b\kappa_\nu B_\nu(T_{\text{d}})}, \quad (3.1)$$

where I_ν is the peak flux density, a is the gas-to-dust ratio (100), Ω_b is the beam solid angle, m_{H} is the mass of atomic hydrogen, κ_ν is the dust opacity per unit mass and $B_\nu(T_{\text{d}})$ is the Planck function at dust temperature T_{d} . We apply the interpolated value of $\kappa_\nu(845\mu\text{m}) \approx 2.2 \text{ cm}^2 \text{ g}^{-1}$ as suggested by Ossenkopf & Henning (1994) for gas densities of 10^6 – 10^8 cm^{-3} and coagulated dust particles with thin ice mantles. The dust temperature of all five submillimeter sources is assumed to be 150 K (see excitation analysis, Sect. 3.4.2). The gas mass for each continuum peak is estimated from the total flux derived from the visibility fit (Table 3.1) via

$$M_{\text{gas}} = \frac{S_\nu d^2 a}{\kappa_\nu B_\nu(T_{\text{d}})}, \quad (3.2)$$

where S_ν is the total flux density of dust emission and d (1.83 kpc) is the distance to the source. Assuming a spherical source with $1''$ in size, the H₂ number density is also derived. We summarized the results in Table 3.1.

From the density and mass estimates, we find beam-averaged H₂ column densities, masses and volume densities toward SMM1 and SMM2 of about 3 – $4 \times 10^{23} \text{ cm}^{-2}$, $0.5 M_\odot$ and $3 \times 10^7 \text{ cm}^{-3}$, respectively. Toward SMM3, SMM4 and SMM5 values smaller by factors 2–3 are found. The derived H₂ column densities and masses are sensitive to the adopted dust opacity and temperature.

Table 3.3. Gaussian decomposition of the line profiles in W3 IRS5

Molecule	Transition	Zone A:SMM1/SMM2			Zone B:SMM3/SMM4		
		W^a (Jy beam ⁻¹ km s ⁻¹)	ΔV^b (km s ⁻¹)	V_{LSR}^c (km s ⁻¹)	W^a (Jy beam ⁻¹ km s ⁻¹)	ΔV^b (km s ⁻¹)	V_{LSR}^c (km s ⁻¹)
CS ^d	7-6	...	...	...	...	...	...
SO	8 ₈ -7 ₇	412.9 ± 2.2	9.0 ± 0.1	-39.0 ± 0.1	207.8 ± 2.5	7.4 ± 0.1	-39.0 ± 0.1
³³ SO ^e	8 ₉ -7 ₈	68.9 ± 0.5	6.0 ± 0.1	-39.1 ± 0.1	25.7 ± 0.6	4.4 ± 0.1	-38.9 ± 0.1
SO ₂	3 _{43,31} -3 _{42,32}	83.8 ± 0.6	7.1 ± 0.1	-39.1 ± 0.1	15.6 ± 0.5	5.6 ± 0.2	-39.1 ± 0.1
	2 _{42,22} -2 _{33,21} v ₂ =1	4.4 ± 0.3	5.1 ± 0.4	-39.4 ± 0.2	...	...	...
³³ SO ₂ ^e	19 _{4,16} -19 _{3,17}	4.1 ± 0.3	4.1 ± 0.4	-39.8 ± 0.2	...	...	...
³⁴ SO ₂	10 _{4,6} -10 _{3,7}	35.1 ± 0.4	5.5 ± 0.1	-39.3 ± 0.1	8.3 ± 0.3	4.3 ± 0.2	-39.3 ± 0.1
	19 _{1,19} -18 _{0,18}	63.0 ± 0.5	6.1 ± 0.1	-39.3 ± 0.1	14.8 ± 0.4	4.1 ± 0.1	-39.4 ± 0.1
	14 _{7,7} -15 _{6,10}	2.1 ± 0.3	6.0 ± 1.0	-39.2 ± 0.4	...	...	...
	3 _{43,31} -3 _{42,32}	4.4 ± 0.4	4.8 ± 0.5	-38.3 ± 0.2	...	...	...
	19 _{8,12} -20 _{7,13}	1.2 ± 0.2	2.2 ± 0.4	-39.2 ± 0.2	...	...	...
HCN ^d	4-3	...	...	...	...	...	...
	4-3 v ₂ =1	24.5 ± 1.0	10.2 ± 0.5	-38.2 ± 0.2	...	...	...
HC ¹⁵ N	4-3	7.8 ± 0.4	9.5 ± 0.5	-37.7 ± 0.2	3.7 ± 0.2	2.3 ± 0.2	-38.3 ± 0.1
H ₂ CS ^f	10 _{0,10} -9 _{0,9}	...	...	...	...	...	...
HNCO ^e	16 _{1,15} -15 _{1,14}	2.0 ± 0.3	4.9 ± 1.0	-39.4 ± 0.4	...	...	...
CH ₃ OH	13 ₁ -13 ₀ A	0.7 ± 0.2	3.4 ± 1.3	-37.7 ± 0.5	6.1 ± 0.2	2.3 ± 0.1	-38.5 ± 0.1

Note. — The beam size for all transitions listed in this table is about $3''.3 \times 1''.8$, P.A. -12° . ^aIntegrated intensity. ^bFWHM line width. ^cLine center LSR velocity. ^dNot attempted to perform Gaussian decomposition due to missing flux and complex line profile. ^eWith hyperfine transitions. Total W is reported. ^fPeaked toward zone C.

If a bare grain model is adopted (Ossenkopf & Henning 1994), the derived values are reduced by a factor of <3 . For dust temperatures between 100 and 200 K, the derived values change by a few ten% only. If the dust temperature is 30 K, the reported H_2 column densities and masses increase by factors of ~ 5 . The excitation analysis of Sects. 4.2.1 and 4.2.2 suggest such low temperatures are unlikely. The estimated H_2 volume density is sensitive to the assumed source size as size^{-3} . For example, the densities toward SMM1 and SMM2 increase to $2.4 \times 10^8 \text{ cm}^{-3}$ if the source size decreases to $0''.5$. Since the submillimeter continuum peaks are unresolved, we treat the H_2 volume densities of Table 3.1 as lower limit. We note that the core masses are all small ($<1 M_\odot$).

3.4.2 Excitation analysis: temperatures

The detected molecular transitions, covering E_u from 43 K to 1067 K and critical densities of $\sim 10^7\text{--}10^8 \text{ cm}^{-3}$ (Table 3.2), form an useful dataset for the diagnostics of the physical conditions toward W3 IRS5. Among these molecular lines, multiple detections of the transitions from SO_2 and $^{34}\text{SO}_2$ toward zones A and B allow us to perform excitation analysis. Multiple detections of $\text{CH}_3\text{CN } J=12\text{--}11$ transitions reported by Wang et al. (2012) form another useful dataset for additional constraints of the excitation conditions toward zone B. We describe the details in the following two sections.

3.4.2.1 Rotational diagram

The molecular excitation conditions can be estimated via rotation diagram analysis assuming all the transitions are optically thin and the emission fills the beam. In a rotation diagram, the column density of the upper state N_u is given by

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N_{\text{tot}}}{Q}\right) - \frac{E_u}{kT_{\text{rot}}}, \quad (3.3)$$

where g_u is the total degeneracy of the upper state, N_{tot} is the total molecular column density, Q is the partition function, E_u is the upper level energy, k is the Boltzmann constant and T_{rot} is the rotational temperature. The left-hand side of equation 3.3 can be derived from the observations via

$$\ln\left(\frac{N_u^{\text{obs}}}{g_u}\right) = \ln\left(\frac{2.04 \times 10^{20}}{\theta_a \theta_b} \frac{W}{g_I g_K \nu_0^3 S \mu_0^2}\right) \text{ cm}^{-2}, \quad (3.4)$$

where θ_a and θ_b are the major and minor axes of the clean beam in arcsec, respectively, W is the integrated intensity in $\text{Jy beam}^{-1} \text{ km s}^{-1}$, g_I and g_K are the spin and projected rotational degeneracies, respectively, ν_0 is the rest frequency in GHz, S is the line strength and μ_0 is the dipole moment of the transition in Debye. Figure 3.6 plots the logarithm of the column densities from our data

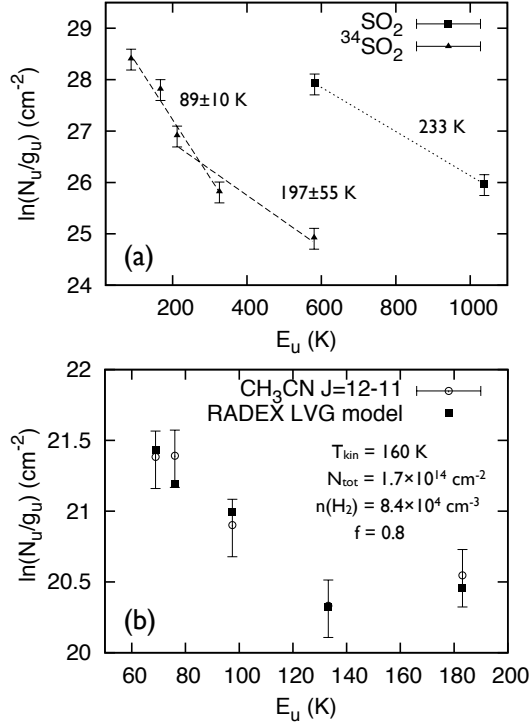


Figure 3.6 (a) Rotation diagram of SO₂ (filled squares) and ³⁴SO₂ (filled triangles) toward zone A. The straight lines are the model fit. The derived rotational temperatures are indicated. (b) Rotation diagram of CH₃CN $J=12-11$ toward zone B (open circles) taken from Wang et al. (2012). The best-fit model from the RADEX LVG analysis is overplotted for comparison (filled symbols).

(Eq. 3.4) versus E_u/k (Eq. 3.3) and a fitted straight line with T_{rot} and N_{tot} as free parameters. We adopt a 20% uncertainty of the integrated intensity in the analysis.

Figure 3.6 (a) shows the rotation diagrams of SO₂ and ³⁴SO₂ toward zone A, which sample level energies from 88 K to 1038 K (Table 3.2). ³⁴SO₂ is detected in five transitions with E_u ranging from 88 to 580 K, and indicates a T_{rot} of 141 ± 25 K. However, the curvature in the distribution of the points implies that there might be a cooler and a warmer component along the line of sight. A two-component fit to the data gives $T_{\text{rot}} = 89 \pm 10$ K and $T_{\text{rot}} = 197 \pm 55$ K. The gas component traced by SO₂ ($E_u = 582$ and 1038 K) implies a rotational temperature of 233 K, compatible with the temperature of the warm component derived from ³⁴SO₂ but obviously less well constrained because only two data points are available.

The curvature in the ³⁴SO₂ rotation diagram (Fig. 3.6 (a)) may also be due

to line opacity (unlikely for the $^{34}\text{SO}_2$ isotopologue) or subthermal excitation (see next section). The relatively abundant main-isotope SO_2 may have optically thick lines, leading to an overestimate for T_{rot} . However, we detected the $34_{3,31} - 34_{2,32}$ transition of both SO_2 and $^{34}\text{SO}_2$. Equation 3.4 yields a $N_{\text{u}}(\text{SO}_2)/N_{\text{u}}(^{34}\text{SO}_2)$ ratio of ~ 20 at $50 - 300$ K, consistent with the $^{32}\text{S}/^{34}\text{S}$ ratio of 22 in the interstellar medium (Wilson & Rood 1994), suggesting that the $34_{3,31} - 34_{2,32}$ transition of SO_2 (and its isotopologues) is optically thin. The $24_{2,22} - 23_{3,21}v_2 = 1$ transition of SO_2 is also likely optically thin since its Einstein-A coefficient is only about a factor of 2 greater than that of the $34_{3,31} - 34_{2,32}$ transition. These considerations suggest the a temperature gradient in zone A explains the rotation diagrams, with a cooler region at $\sim 100\text{K}$ and a warmer region of $\geq 200\text{K}$ (Table 3.4).

We do not have enough data to obtain a reliable temperature estimate toward zone B (Table 3.3). Only the lowest two transitions of $^{34}\text{SO}_2$ in level energy are detected here, and imply a rotational temperature of about 133 K. To have a better constraint of the excitation conditions toward zone B, we took the CH_3CN $J = 12 - 11$ lines obtained by Wang et al. (2012) with the SMA at a resolution of $4.0'' \times 2.6''$. This molecule peaks toward zone B exclusively and shows a much narrower FWHM line width ($\sim 1.6 \text{ km s}^{-1}$) compared to $^{34}\text{SO}_2$ ($\sim 4 \text{ km s}^{-1}$), suggesting a different molecular condensation in zone B. Figure 3.6 (b) shows the CH_3CN $J = 12 - 11$ $K=0-4$ rotation diagram. The scatter in the data indicates that the lines are not optically thin. Therefore, we can not carry out rotation diagram analysis on the CH_3CN lines, and instead perform an LVG analysis in Sect. 3.4.2.2.

3.4.2.2 RADEX LVG model

To further investigate the physical conditions such as kinetic temperature (T_{kin}), column density (N_{tot}) and H_2 volume density (n_{H_2}) toward zone A and B, we performed statistical equilibrium calculations to solve the level populations inferred from the observations. The purpose here is to have a crude estimate. Detailed analysis of temperature and density profiles in W3 IRS5 is beyond the scope of this work. We used the code RADEX (van der Tak et al. 2007) which solves the level populations with an escape probability method in the large-velocity-gradient (LVG) regime. Limited by the available observed data and collisional rate coefficients (Schöier et al. 2005), we perform calculations only for the $^{34}\text{SO}_2$ lines and CH_3CN $J = 12 - 11$ lines (Wang et al. 2012). For $^{34}\text{SO}_2$, we adopted the collisional rate coefficients from SO_2 (Green 1995)⁶ as an approximation since both species have similar molecular properties. The

⁶Recent calculations by Spielfiedel et al. (2009) and Cernicharo et al. (2011) show that the collisional rate coefficients calculated by Green (1995) are lower by a factor 3–5. The listed critical densities in Table 3.2 may be 3–5 times smaller.

Table 3.4. Molecular excitations in W3 IRS5

Molecule	Zone A:SMM1/SMM2		Zone B:SMM3/SMM4		Note
	T (K)	N_{tot} (cm $^{-2}$)	X^a	X^b	
Rotation diagram: $T = T_{\text{rot}}$					
SO $_2$	233	6.6×10^{16}	4.4×10^{-7}	...	zone A: 2 trans.
$^{34}\text{SO}_2$	89 ± 10	$6.1^{+3.2}_{-2.2} \times 10^{15}$	$4.1^{+2.1}_{-1.5} \times 10^{-8}$	2.0×10^{-8}	zone A: lowest 4 trans, zone B: 2 trans.
	197 ± 55	$3.7^{+5.9}_{-2.4} \times 10^{15}$	$2.5^{+3.9}_{-1.6} \times 10^{-8}$	...	zone A: highest 3 trans.
RADEX LVG model: $T = T_{\text{kin}}$					
$^{34}\text{SO}_2$	85	7.3×10^{15}	4.9×10^{-8}	...	zone A: $f = 0.9$, $n_{\text{H}_2} \geq 10^9 \text{ cm}^{-3}$
CH $_3$ CN ^{c}	...	...	...	1.7×10^{14}	zone B: $f = 0.8$, $n_{\text{H}_2} = 8.4 \times 10^4 \text{ cm}^{-3}$
Column densities at $T = T_{\text{rot}} = 150 \text{ K}$					
SO	150	$> 1.3 \times 10^{16}$	$> 8.7 \times 10^{-8}$	$> 6.6 \times 10^{15}$	opacities ($\sim 0.3 - 0.5$) in both zones
^{33}SO	150	9.7×10^{15}	6.5×10^{-8}	3.6×10^{15}	
SO $_2$	150	1.4×10^{17}	9.4×10^{-7}	2.5×10^{16}	
$^{33}\text{SO}_2$	150	9.5×10^{14}	6.4×10^{-9}	$< 9.5 \times 10^{13}$	
$^{34}\text{SO}_2$	150	6.1×10^{15}	4.1×10^{-8}	1.9×10^{15}	
HC ^{15}N	150	1.7×10^{13}	1.1×10^{-10}	8.1×10^{12}	
HNCO	150	1.1×10^{14}	7.4×10^{-10}	$< 3.0 \times 10^{13}$	
CH $_3$ OH	150	4.9×10^{14}	3.3×10^{-9}	4.5×10^{15}	

Note. — ^aFractional abundance. $N(\text{H}_2)=1.5 \times 10^{23} \text{ cm}^{-2}$ is derived from our data. ^bFractional abundance. $N(\text{H}_2)=8.9 \times 10^{22} \text{ cm}^{-2}$ is derived from our data. ^cData taken from Wang et al. (2012).

collisional rate coefficients of CH_3CN are taken from Green (1986). To find the best-fit solution, we applied χ^2 minimization to the 4-dimensional parameter space (T_{kin} , N_{tot} , n_{H_2} and f , the beam filling factor).

Figure 3.7 shows the χ^2 surfaces near the best-fit solution on each parameter axis, and Table 3.4 summarizes the results. Toward zone A, we use four $^{34}\text{SO}_2$ lines (excluding the transition with $E_{\text{u}} = 580$ K) in the calculations due to the limited table of collisional rate coefficients. The RADEX calculations suggest that the kinetic temperature traced by the $^{34}\text{SO}_2$ lines is about 90 K, consistent with the temperature derived from rotation diagram analysis and suggesting the excitation is thermalized. This requires a high H_2 volume density ($> 10^{9-10} \text{ cm}^{-3}$) toward zone A. Apparently, the cool component toward zone A is very dense. Toward zone B, our RADEX calculations indicate a kinetic temperature of 160 K. Interestingly, the H_2 volume density traced by CH_3CN is only about 10^5 cm^{-3} , lower than the critical density of a few 10^6 cm^{-3} , implying subthermal excitation. The beam filling factor is about 0.8. The best-fit model for CH_3CN is plotted as filled squares in Fig. 3.6 (b).

Alternatively, the excitation conditions toward zone A and B can be estimated via the line ratio of the $19_{1,19} - 18_{0,18}$ over the $10_{4,6} - 10_{3,7}$ transition of $^{34}\text{SO}_2$ of 1.8. We assume that both transitions have the same filling factor. Using a FWHM line width of 5.0 km s^{-1} (the average FWHM line widths in zones A and B are 6.0 km s^{-1} and 4.0 km s^{-1} , respectively) in the RADEX calculations, we calculate the intensity ratio as function of T_{kin} and N_{tot} for four different values of n_{H_2} (Fig. 3.8). We again assume that the two transitions in the RADEX calculations have the same filling factor. These calculations suggest a high density of $> 10^9 \text{ cm}^{-3}$ traced by $^{34}\text{SO}_2$ toward zone A and B. The kinetic temperatures are ≥ 150 K, depending on the H_2 volume density.

Combining the results from the rotation diagram analysis and the RADEX LVG calculations, we conclude that the gas traced by $^{34}\text{SO}_2$ is dense ($n_{\text{H}_2} \geq 10^9 \text{ cm}^{-3}$) in zones A and B. There is a temperature gradient along the line of sight in zone A, characterized by a cool region of ~ 100 K and a warm region of ≥ 200 K. Toward zone B, the temperature gradient is less prominent. However, a quiescent (FWHM line width 1.6 km s^{-1}) and less dense region ($n_{\text{H}_2} \sim 10^5 \text{ cm}^{-3}$) traced by CH_3CN is also present in zone B.

3.4.2.3 Molecular column density

We estimate the beam averaged ($3''.3 \times 1''.8$) molecular column density of each detected molecule toward zone A and B via Eq. 3.5 by assuming optically thin emission and a single rotational temperature of 150 K which is a representative value in W3 IRS5 (see previous two sections).

$$N_{\text{tot}} = \frac{N_{\text{u}}^{\text{obs}}}{g_{\text{u}}} \times Q e^{E_{\text{u}}/kT_{\text{rot}}} \quad (3.5)$$

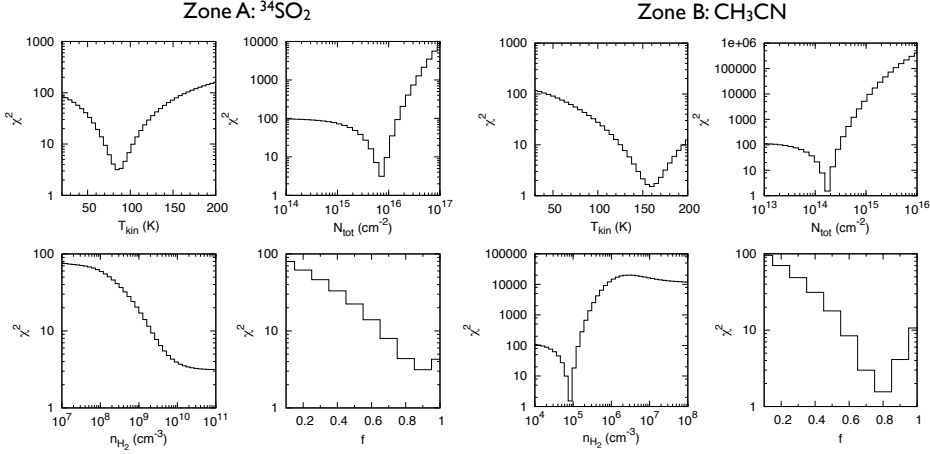


Figure 3.7 RADEX excitation analysis toward zone A traced by $^{34}\text{SO}_2$ (left four panels) and zone B traced by CH_3CN (right four panels). The χ^2 surfaces near the best-fit solution on each parameter axis are displayed.

We only use the ground vibrational state for the estimates. If multiple transitions of a given molecule are detected, we adopt the averaged value. The uncertainty of the exact rotational temperature results in an error in the column density of a few 10% (for T_{rot} from 100 K to 200 K). As a consistency check, we estimate the line center opacity of each transition via

$$\tau = \frac{c^3}{8\pi\nu_0^3} \frac{A_{\text{ul}}}{\Delta V} \frac{g_u N_{\text{tot}}}{Q} e^{-E_u/kT_{\text{rot}}} (e^{h\nu_0/T_{\text{rot}}} - 1), \quad (3.6)$$

where c is the speed of light, A_{ul} the Einstein-A coefficient, and ΔV the FWHM line width. All lines are consistent with the optically thin assumption ($\tau \ll 1$); only SO has line center opacities as large as $\tau \sim 0.3\text{--}0.5$). Therefore, a lower limit of SO column density is derived. A more representative value for SO can be derived from ^{33}SO by assuming the isotopic ratio $^{32}\text{S}/^{33}\text{S}$ of ~ 132 (Wilson & Rood 1994; Chin et al. 1996). To convert the molecular column densities into fractional abundances with respect to H_2 , we adopt H_2 column densities of $1.5 \times 10^{23} \text{ cm}^{-2}$ and $8.9 \times 10^{22} \text{ cm}^{-2}$ toward zone A and B, respectively (derived from the continuum image in Fig. 3.2 (l) with the same assumptions described in Sect. 3.4.1). We summarize the results in Table 3.4. Toward zone A and zone B, SO and SO_2 are very abundant with fractional abundances up to few 10^{-6} , several orders of magnitude higher than found in dark clouds (few 10^{-9} , Ohishi et al. 1992). This is indicative of active sulfur chemistry. Among the detected molecules, we do not see significant differences in fractional abundance between zones A and B, except for CH_3OH which is a factor of 10 more abundant in zone B.

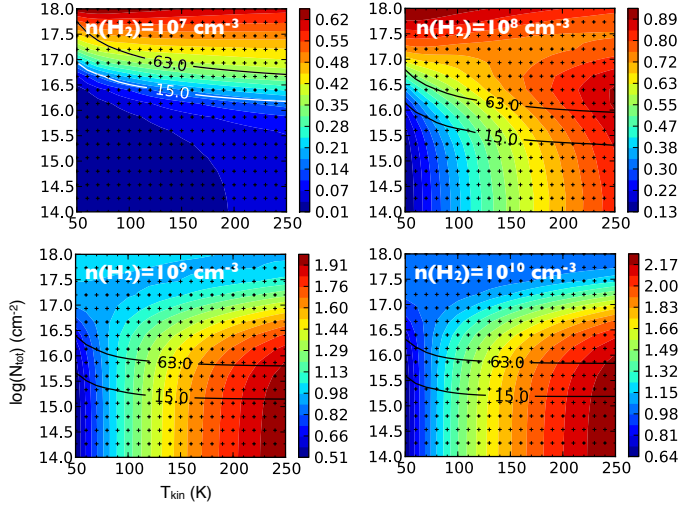


Figure 3.8 RADEX analysis of the $^{34}\text{SO}_2$ line ratios toward zone A and B assuming a FWHM line width 5.0 km s^{-1} . The intensity ratios $19_{1,19} - 18_{0,18}/10_{4,6} - 10_{3,7}$ are plotted in color scale. The observed integrated intensities of the $19_{1,19} - 18_{0,18}$ transition are plotted in curves (zone A: $\sim 63 \text{ Jy beam}^{-1} \text{ km s}^{-1}$, zone B: $\sim 15 \text{ Jy beam}^{-1} \text{ km s}^{-1}$). Toward both zones, the line ratio is about 1.8 (Table 3.3). Our results suggest that a high H_2 volume density ($> 10^9 \text{ cm}^{-3}$) is needed to reproduce the observed line ratios.

3.4.3 Kinematics

Complex velocity fields in W3 IRS5 are observed in various molecules. Figure 3.9 shows several first moment maps derived from different molecules. The upper four maps are made from the compact-configuration dataset using natural weighting, while the bottom ones are derived from the combined dataset with uniform weighting. Different velocity gradients are observed in $^{34}\text{SO}_2$ (NW–SE), HC^{15}N (E–W) and $\text{HCN } v_2 = 1$ (NE–SW). CH_3OH shows an interesting velocity distribution with a slightly blue-shifted emission peak (SMM3 and SMM4). Comparing the velocities near SMM3 and SMM4 derived from $^{34}\text{SO}_2$ and CH_3OH , we suggest that there are two distinct regions along the line of sight. Indeed, the line widths of these two molecules are very different (Table 3.3). At one-arcsecond resolution (combined dataset with uniform weighting), $^{34}\text{SO}_2$ peaks toward SMM1 and SMM2, and shows a velocity gradient consistent with the NW–SE gradient found from lower angular resolution observations. For the three strongest lines, CS, SO and HCN, we adopted uniform weighting to form the images in order to minimize the strong sidelobes which otherwise corrupt the images. CS and HC^{15}N show similar velocity patterns with some patchy velocity shifts. The velocity field traced by SO is very different from the ones seen from other molecules in Fig. 3.9, which is likely due to opacity

effects. Near SMM1 and SMM2, HCN and its vibrationally excited transition show similar velocity patterns. The velocity components traced by CS and HCN toward zone C are red-shifted with respect to the systemic velocity ($\sim -39 \text{ km s}^{-1}$). However, a clear velocity jump is seen near SMM5 if we compare the maps of $^{34}\text{SO}_2$ to CS and HCN, implying that the gas component in zone C is not closely related to the ones in zones A and B. Another velocity jump is seen in the HCN map if we compare the velocities in zones A and D, suggesting that the gas component in zone D is also not closely related to zones A and B.

In Fig. 3.9, we see that the velocity gradients seen in $^{34}\text{SO}_2$ and HCN $v_2 = 1$ are roughly perpendicular to each other. To confirm this, we fit the emission of HCN $4-3 \ v_2 = 1$ ($E_u = 1067 \text{ K}$) and $\text{SO}_2 \ 34_{3,31} - 34_{2,32}$ ($E_u = 582 \text{ K}$) (compact configuration with natural weighting) channel-by-channel with a Gaussians to determine the movement of the peak positions. In Fig. 3.10, the velocity gradient seen in SO_2 is roughly perpendicular to the line joining SMM1 and SMM2, while the velocity gradient observed in the vibrationally excited HCN is parallel to this line. The vibrationally excited HCN may trace outflow or jet emission since the observed velocity gradient is parallel to the free-free emission knots observed by Wilson et al. (2003). We suggest that SO_2 traces a rotating structure orthogonal to this outflow axis.

In our data, only the CS $7-6$, HCN $4-3$ and SO $N_J=8-7_7$ emission show a wide velocity range (about $30-40 \text{ km s}^{-1}$; Fig. 3.5), presumably due to outflow activity in W3 IRS5. To study the distribution of the high velocity components (Fig. 3.11), we integrate the emission over three different velocity ranges (blue: -50 to -43 km s^{-1} , green: -43 to -35 km s^{-1} and red: -35 to -28 km s^{-1}). We took the combined-configuration dataset and used natural weighting for the analysis. The images are plotted with contours starting well above 3σ to minimize the impact of sidelobes, especially for the green component. As seen in Fig. 3.11, the high-velocity components of all three molecules peak near zone A and close to SMM2, suggesting a bipolar outflow with an inclination close to the line of sight. The existence of a line-of-sight outflow also implies a rotating structure in the plane of the sky, in which SMM1 and SMM2 form a binary system. Therefore, the small scale velocity gradients (Fig. 3.10) seen in HCN $4-3 \ v_2 = 1$ and SO_2 may highlight the kinematics of the envelope. Additional blue-shifted components are seen toward zone D. The green component of CS highlights the gas in zone C. In the HCN map, the emission in zone D together with the emission peaking near the offset position ($-8'', 0''$) may form another bipolar outflow in the E-W direction since the line connecting these peaks passes through zone A which contains star-forming cores. In this case, the one-arcsecond scale velocity gradients seen in Fig. 3.10 imply a complex motion (rotation plus expansion or contraction) in the common envelope of SMM1 and SMM2. To summarize, the kinematics in W3 IRS5 is very complex and requires additional observations at high resolution with good image fidelity for further analysis.

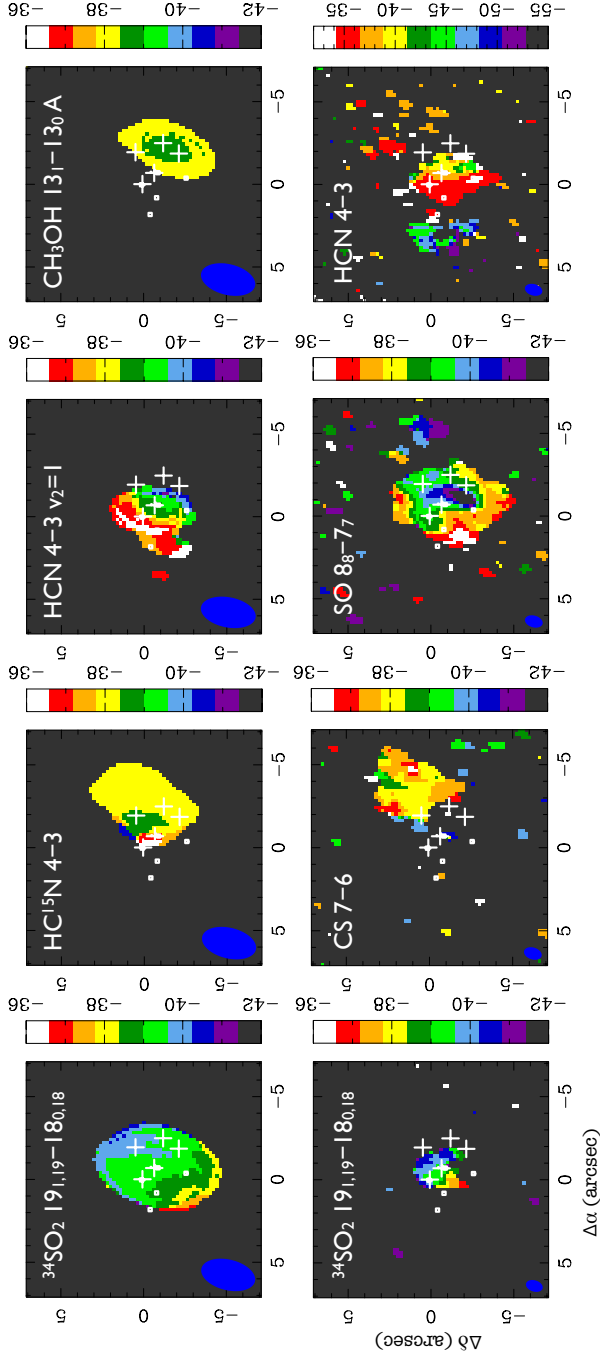


Figure 3.9 First moment maps of different molecules observed toward W3 IRS5. The upper four maps are derived from the compact-configuration dataset with natural weighting, while the bottom four maps are made from the combined dataset using uniform weighting. The markers are identical to the ones in Fig. 3.1. The zero position is the phase center. We note that the velocity ranges are the same for all maps except HCN 4-3.

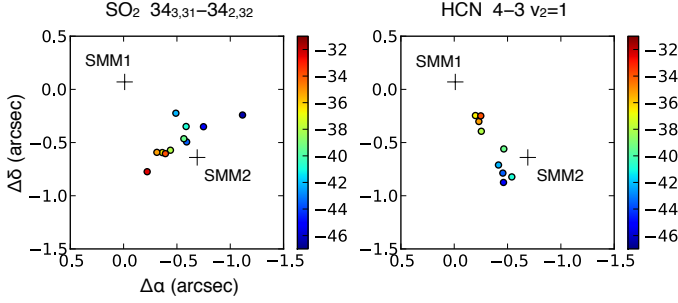


Figure 3.10 Channel-by-channel locations of the emission peaks of the SO_2 $34_{3,31} - 34_{2,32}$ and HCN $4-3$ $v_2 = 1$. The emission peaks are color-coded with respect to their V_{LSR} in km s^{-1} shown in the color wedge. Two distinct, orthogonal velocity gradients are seen.

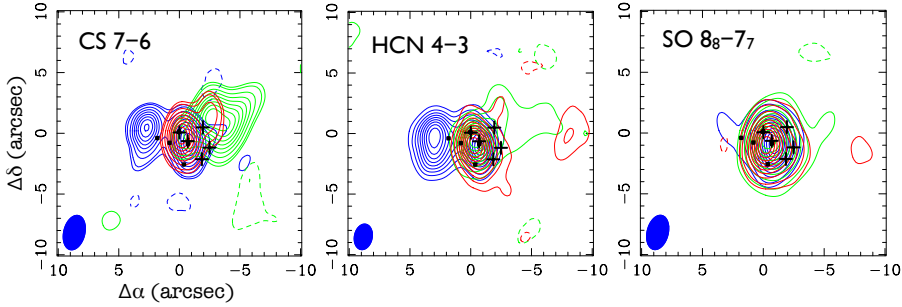


Figure 3.11 Integrated intensity maps at different velocity ranges (blue: -50 to -43 km s^{-1} ; green: -43 to -35 km s^{-1} ; red: -35 to -28 km s^{-1}). We adopted the combined-configuration dataset in natural weighting in order to show the additional weak emission features. The contour levels of each Doppler-shifted component for CS, HCN and SO are 15, 20, 30, 40,...%, 10, 20, 30,...% and 5, 10, 20, 30,...% of the emission peak, respectively. We note that the first contours are all $\geq 3 \sigma$ noise level. The markers are identical to the ones in Fig. 3.1.

3.5 Discussion

3.5.1 Star formation in W3 IRS5

3.5.1.1 Different evolutionary stages within W3 IRS5

Based on the continuum image at 353.6 GHz, we identified five compact sources (SMM1 to SMM5) toward W3 IRS5 (Fig. 3.1 and Table 3.1). SMM1 and

SMM2 also show compact cm-wave emission (Wilson et al. 2003; van der Tak et al. 2005) indicating that stars sufficiently massive to ionize their surroundings have formed ($>8 M_{\odot}$). The non-detection of compact cm-wave emission toward SMM3, SMM4 and SMM5 implies that currently those cores have not (yet) formed massive stars. By comparing the 353.6-GHz continuum with the NICMOS 2.22 μm emission and cm-wave emission (Fig. 3.1(a), Megeath et al. 2005; Wilson et al. 2003; van der Tak et al. 2005), we suggest that the eastern part (SMM1 and SMM2) of the source is more evolved than the western part (SMM3, SMM4 and SMM5). The small core mass ($\sim 0.3 M_{\odot}$) suggests that SMM3–5 may be forming low-mass stars or are starless cores.

For a virialized star-forming core ($M_{\text{core}} + M_{\text{star}} \approx M_{\text{vir}}$), the 1D virial velocity dispersion (σ_{vir} ; c.f. McKee & Ostriker (2007)) is

$$\sigma_{\text{vir}} = \sqrt{\frac{GM_{\text{vir}}}{5r}}, \quad (3.7)$$

where r is the radius of the source, G is the gravitational constant, and M_{vir} is the virial mass. Assuming a core radius of $0.5''$, core gas masses of $\sim 0.3 M_{\odot}$, and stellar masses of SMM3–5 less than $8 M_{\odot}$, the 1D virial velocity dispersions should be no more than 1.3 km s^{-1} . From our observations of CH_3OH line toward SMM3/4 and CS line toward SMM5, the inferred 1D velocity dispersions ($\sigma = \Delta V / \sqrt{8 \ln 2}$) are 1.0 km s^{-1} and 1.4 km s^{-1} . The large observed line widths suggest that either these cores contain stars just under 8 solar masses, or the clumps may have smaller mass stars, and the large velocities may be the influence of outflows from SMM1/2. In the latter, case, it is not clear if the gas in the cores is gravitationally bound. Subarcsecond observations of dust continuum and outflow tracers should tell if SMM3–5 are low-mass starless leftover cores after the formation of SMM1–2 or harbor low-mass protostars under the influence of outflows from SMM1–2.

3.5.1.2 Fragmentation and Jeans analysis

From the continuum analysis, we found the core masses of the identified SMM sources are small ($0.2\text{--}0.6 M_{\odot}$) and the projected distance between the SMM sources are about $1'' - 2''$ ($1800 \text{ AU} - 3600 \text{ AU}$). This observed structure, in the meantime, is still embedded in a large massive core with size about $1'$ and mass of several hundred $M_{\odot}$ (W3-SMS1 in the SCUBA 850 μm image, Di Francesco et al. 2008; Wang et al. 2012). At $1'$ scale, Megeath et al. (1996) found that there are ~ 300 low-mass stars in the core surrounding W3 IRS5 with a stellar density of few 1000 pc^{-3} . Therefore, it is interesting to investigate the cloud structure from $1'$ scale to $1''$ to see what determines the overall core/stellar mass distribution and their spatial distribution. To study this question, we perform Jeans analysis in W3 IRS5 based on our SMA continuum image and the JCMT

SCUBA 850 μm image (Di Francesco et al. 2008; Wang et al. 2012). The Jeans length and Jeans mass are expressed as (c.f. Stahler & Palla 2005, Eq. (9.23) and (9.24)):

$$\lambda_J \approx 0.19 \left(\frac{T}{10 \text{ K}} \right)^{1/2} \left(\frac{n_{\text{H}_2}}{10^4 \text{ cm}^{-3}} \right)^{-1/2} \text{ pc}, \quad (3.8)$$

and

$$M_J \approx 1.0 \left(\frac{T}{10 \text{ K}} \right)^{3/2} \left(\frac{n_{\text{H}_2}}{10^4 \text{ cm}^{-3}} \right)^{-1/2} M_\odot, \quad (3.9)$$

where T is the kinetic temperature and n_{H_2} is the H_2 volume density. These two quantities are more sensitive to the adopted H_2 volume density. To estimate the $1'$ scale H_2 density, we measured the total flux density in a $1'$ by $1'$ box centered toward W3 IRS5 using the SCUBA 850 μm image. Using the same prescription outlined in Sect. 3.4.1, a total flux density of 160 Jy corresponds to a mass of 950 $M_\odot$ assuming a dust temperature of 40 K. The mean H_2 volume density is $2.4 \times 10^5 \text{ cm}^{-3}$. Therefore, at $1'$ we derived the Jeans length and Jeans mass to be 16000 AU ($\sim 9''$) and 2 $M_\odot$, respectively. Interestingly, these two characteristic quantities seem to match the observed spatial separations of low-mass stars (18000–12000 AU, Megeath et al. 1996), implying that the spacing of the young low mass stars are consistent with gravitational fragmentation. The Jeans masses are greater than the mean stellar mass for a standard initial mass function ($0.5 M_\odot$), which is expected given a typical efficiency of low-mass star formation $\sim 30\%$ (Alves et al. 2007). Toward the central regions of W3 IRS5, the temperature ($\sim 140 \text{ K}$) and density (few 10^7 cm^{-3}) are higher than the values on the scale of the entire core. The corresponding Jeans length and Jeans mass are 2700–3800 AU ($1.5''$ – $2.1''$) and $\sim 1 M_\odot$, respectively. The Jeans length is consistent with the observed spacing of the SMM cores, implying that gravitational fragmentation may be occurring in the dense, warm center of the cluster. On the other hands, the implied Jeans masses are much smaller. This immediately leads to the question how the massive stars in SMM1/2 accreted their current masses.

3.5.1.3 Accretion rates

The largest accretion rate that an object can sustain is essentially given by its mass divided by its free-fall time,

$$\dot{M}_{\text{star}} \approx M_{\text{core}}/t_{\text{ff}}, \quad (3.10)$$

where $t_{\text{ff}} = \sqrt{3\pi/32G\bar{\rho}}$ and $\bar{\rho}$ is the mean density. The masses of the SMM1–5 cores come from Table 3.1. We use the observed size for the SMM1–5 cores, which are set to $1''$ in diameter based on Fig. 3.1 (a). We adopt stellar masses of 20 $M_\odot$ for SMM1 and SMM2 based on the total luminosity of $2 \times 10^5 L_\odot$. We use the combined stellar and core masses and the core radii to determine the

average baryonic density; the corresponding free-fall times are ~ 1000 yr for SMM1/2, and > 1700 yr for SMM3–5. These imply mass accretion rates of $5 \times 10^{-4} M_{\odot} \text{ yr}^{-1}$ for SMM1/2, and $< 2 \times 10^{-4} M_{\odot} \text{ yr}^{-1}$ for SMM3–5. The upper limits for the latter follow from the upper limit on the embedded stellar masses of $8 M_{\odot}$. The accretion rates are consistent with those expected for the formation of massive stars (Keto 2003). The combination of small core masses and high accretion rates imply very short time scales of a few thousand years. If the massive stars in SMM1/2 form from accretion of the local cores ($1''$ scales), the low core masses imply that they are now in a stage that most of core mass has been accrete onto the stellar components. On the other hand, the SMM cores may be accreting material that have been resolved out by the interferometers on scales $> 1''$. In this case, the reservoir of material from which the cores are accreting is larger than the observed projected spacing of the protostars, implying that the accretion is coming from a global collapse of the molecular core in which the proto-Trapezium is embedded.

To determine whether it is possible that the massive stars in W3 IRS5 are being fed from the collapse of the surrounding core, we estimate the potential accretion rates from this accretion. The free-fall time for the central $1'$ W3–SMS1 condensation, with a total mass of $950 M_{\odot}$ and an embedded stellar mass of $\lesssim 50 M_{\odot}$, is 72000 yr and the free-fall mass accretion rate is $1 \times 10^{-2} M_{\odot} \text{ yr}^{-1}$. We note that the derived accretion rate is the maximum rate of infall assuming free-fall collapse. In the central region, the amount of gas accreted by each star is given by

$$\dot{M} = \rho \pi R_{\text{acc}}^2 v_{\text{inf}} \quad (3.11)$$

(Bonnell et al. 2001), where v_{inf} is the infall gas velocity, ρ is the density of the gas surrounding the proto-Trapezium, and R_{acc} is the radius within which the infalling gas is accreted onto a specific star. We assume $n_{\text{H}_2} = 10^6 \text{ cm}^{-3}$ to compute ρ , which is intermediate between the density of the surrounding $1'$ diameter core (10^5 cm^{-3}) and the core of the inner $1''$ (10^7 cm^{-3}). Given FWHM line widths of $2\text{--}5 \text{ km s}^{-1}$, we adopt a v_{inf} equal to the 3D gas velocity dispersion implied by the FWHM line width ($\sqrt{3}\Delta V/\sqrt{8 \ln 2}$), which is $1.5\text{--}3.7 \text{ km s}^{-1}$ with a mean value of 2.6 km s^{-1} . The uncertainty of v_{inf} gives a factor of < 3 in error of accretion rate. The possible values for R_{acc} are the radius set by the the motions of the stars through the gas (Bondi-Hoyle radius) and the radius set by tidal interaction of the stars with the gravitational potential of the cluster core (tidal radius). The actual accretion rate is given by the minimum of these two radii (Bonnell et al. 2001). To estimate R_{acc} due to tidal interactions, we use the equation from Bonnell et al. (2001) and rewrite in terms of the gas density around the star,

$$R_{\text{acc}}^{\text{tidal}} = 0.5 \left(\frac{M_{\text{star}}}{4/3\pi\rho} \right)^{1/3}. \quad (3.12)$$

In this case, $R_{\text{acc}}^{\text{tidal}}$ are 4700 AU and 3500 AU for a $20 M_{\odot}$ and $8 M_{\odot}$ central star embedded in a core with gas density 10^6 cm^{-3} , respectively. The accretion rates are then $2 \times 10^{-4} M_{\odot} \text{ yr}^{-1}$ and $1 \times 10^{-4} M_{\odot} \text{ yr}^{-1}$ for the $20 M_{\odot}$ and $8 M_{\odot}$ stars, respectively. Alternatively, the motions of the stars through the cloud can limit the gas accretion; only the gas within a radius where the escape velocity is less than the velocity of the star relative to the gas can be accreted. The R_{acc} in this case can be approximated by the Bondi-Hoyle radius:

$$R_{\text{acc}}^{\text{BH}} \approx \frac{2GM_{\text{star}}}{\sigma_{3\text{D}}^2}. \quad (3.13)$$

The resulting $R_{\text{acc}}^{\text{BH}}$ are 5200 AU and 2100 AU for the $20 M_{\odot}$ and $8 M_{\odot}$ stars, and the mass infall rates are $3 \times 10^{-4} M_{\odot} \text{ yr}^{-1}$ for a stellar mass of $20 M_{\odot}$ and $4 \times 10^{-5} M_{\odot} \text{ yr}^{-1}$ for a stellar mass of $8 M_{\odot}$.

As a result, from our basic analysis, global collapse of the core and subsequent accrete of the material from the collapse onto the stars can sustain infall rates in excess of $10^{-4} M_{\odot} \text{ yr}^{-1}$ for SMM1/2 and are sufficient to sustain high mass star formation. For SMM3–5, the rates are 10 times lower. However, the local density around SMM3–5 is closer to 10^7 cm^{-3} , the actual densities and the accretion rates may be higher. The fact that the stellar accretion rates is two orders of magnitude less than the free-fall accretion rate for the large cores suggests that there is sufficient infall of material to feed the accretion of the individual stars, even if the actual collapse times is ten free fall times.

In summary, we find two alternatives. Either the massive stars accrete locally from their local cores; in this case the small core masses imply W3 IRS5 is at the very end stages (1000 yr) of infall and accretion. Alternatively, the stars are accreting from the global collapse of a massive, cluster forming core. This later scenario is similar to the competitive accretion models of massive star formation (e.g., Bonnell & Bate 2006). For the two massive objects SMM1/2, the observed densities and velocity widths are consistent with those needed for the global collapse to feed accretion onto the massive stars at rates of $\sim 10^{-4} M_{\odot} \text{ yr}^{-1}$. For the remaining objects, SMM 3–5, a lower infall rate is estimated; perhaps these are forming intermediate mass stars, although the rate of accretion may rise as they increase in mass as precede by the models of competitive accretion. However, a clear detection of the infall of gas has not yet been observed. This makes the W3 IRS5 cluster a perfect region to further test the competitive accretion model, if the kinematics of the gas motions can be traced on scales from $1'$ down to $< 1''$. Future single-dish and interferometric observations of this region, e.g., combining SMA or PdBI observations with IRAM 30m measurements, are required to fully map the gas flow across these scales.

3.5.2 The molecular environment of W3 IRS5

3.5.2.1 Distinct molecular zones

A JCMT spectral line survey characterized W3 IRS5 as a remarkable massive star-forming region with rich spectral features from sulfur-bearing molecules (Helmich et al. 1994; Helmich & van Dishoeck 1997). Helmich et al. (1994) also reported that the CH_3OH abundance is remarkably low, even compared to typical dark clouds. From our SMA data, and the results from Wang et al. (2012), we find that sulfur-bearing molecules such as SO , SO_2 and their isotopologues, strongly peak toward the submillimeter sources SMM1 and SMM2 (zone A) with extended emission toward SMM3, SMM4 and SMM5 (Fig. 3.2). This suggests that SMM1 and SMM2 are the driving center of the sulfur chemistry. Interestingly, typical hot-core molecules such as CH_3OH (Fig. 3.2 (k)) and CH_3CN (Wang et al. 2012) peak toward SMM3/4 (zone B) exclusively, underlining the chemical differences between zones A and B. Moreover, toward zone B, there are two distinct regions along the line of sight with different physical characteristics. The narrow FWHM line widths seen in CH_3OH (2.3 km s^{-1} ; Table 3.3) and CH_3CN (1.6 km s^{-1} ; Wang et al. 2012) suggest that this ‘hot core’ source is less turbulent compared to the gas component traced by SO and SO_2 , which have larger line widths ($\sim 4 - 7 \text{ km s}^{-1}$; Table 3.3). As implied by the excitation analysis (Sect. 3.4.2.2), this ‘hot core’ is less dense ($\sim 10^5 \text{ cm}^{-3}$) than the gas traced by $^{34}\text{SO}_2$ ($\geq 10^9 \text{ cm}^{-3}$). We suggest that this ‘hot core’ may be created by feedback from the star-forming activity associated with SMM1 and SMM2. It is, however, hard to tell if this core is heated internally or externally since we do not find significant temperature differences between $^{34}\text{SO}_2$ and CH_3CN (Sect. 3.4.2.2). In addition, there is another interesting chemical signature in W3 IRS5, where SO and SO_2 are peaked toward zone A, while CS and H_2CS are peaked toward zone C (Fig. 3.2). Although these species are chemically related (e.g. Charnley 1997), this spatial de-correlation implies that different chemical processes are involved, such as hot core versus shock chemistry (Hatchell & Viti 2002).

3.5.2.2 Abundances of SO , SO_2 and CH_3OH

It has been proposed that the abundance ratios of sulfur-bearing species can be used to measure the time elapsed since the start of ice-mantle evaporation in star-forming cores *if* proper physical conditions are applied (e.g. Charnley 1997; van der Tak et al. 2003; Wakelam et al. 2004). Unfortunately, the rough estimates of the SO and SO_2 abundances provided by our data limit us to a qualitative comparison only. SO and SO_2 are abundant toward W3 IRS5. The fractional abundance of SO and SO_2 (Table 3.4) are, respectively, 8.6×10^{-6} and 9.4×10^{-7} toward zone A, and 5.4×10^{-6} and 2.8×10^{-7} toward zone B. This corresponds

to SO_2/SO ratios of 0.1 and 0.05 for zones A and B, respectively. The uncertainty of these ratios are factors of few, and SO_2 is clearly less abundant than SO toward W3 IRS5.

Charnley (1997), Hatchell et al. (1998) and Wakelam et al. (2004) present chemical models that relate the SO_2/SO ratio to the time since the onset of grain-mantle evaporation. Although these models are very sensitive to the initial mantle composition, cosmic ray ionization rate, density and temperature, these models show that the evolution of the fractional abundances of SO and SO_2 peak after roughly 10^4 - 10^5 yr after grain-mantle evaporation. Such time scales are consistent with the free-fall time for the entire cluster calculated in Sect. 3.5.1.3 of $(0.8\text{--}1.4) \times 10^5$ yr.

Toward the emission peak in zone B, we derive a CH_3OH abundance of 5.1×10^{-8} , lower by a factor of 10 – 100 compared to the abundance found toward the Orion Compact Ridge (Menten et al. 1988). This low CH_3OH abundance implies that the ‘hot core’ toward zone B is chemically young since large amounts of CH_3OH are still observed in the solid state (Allamandola et al. 1992). Since zone B does show emission from SO and SO_2 , which is indicative of outflow activity (Fig. 3.11), it is possible that the ‘hot core’ has just been turned on by external heating from zone A.

3.5.3 Non-detection of CO^+ : an indication of FUV origin

Just as much as detected emission can provide information, so can the non-detection of emission tell us something. Molecular ions and radicals like CN, NO, CO^+ , SO^+ and SH^+ , are thought to trace high energy (far-ultraviolet, FUV, and X-ray) radiation toward star-forming regions (Sternberg & Dalgarno 1995; Maloney et al. 1996). Toward W3 IRS5, Stäuber et al. (2007) reported detection of two hyperfine transitions of CO^+ $N=3\text{--}2$, $F=5/2\text{--}3/2$ (353.7413 GHz) and $F=7/2\text{--}5/2$ (354.0142 GHz) with the James Clerk Maxwell Telescope (JCMT) at $14''$ resolution. They concluded that CO^+ is present in FUV-irradiated cavity walls which may be part of the outflows along the line of sight, similar to AFGL 2591 (Stäuber et al. 2007; Benz et al. 2007; Bruderer et al. 2009). However, the detection of X-ray emission toward W3 IRS5 (Hofner et al. 2002) with a luminosity of $\sim 5 \times 10^{30}$ erg s $^{-1}$ implies that CO^+ may have an X-ray origin as well. The geometrical dilution of this X-ray flux down to the cosmic ray ionization level suggests that the source size of CO^+ should be about $0.7''$ if X-rays are the dominant source of CO^+ . Therefore interferometric observations would be helpful to determine if CO^+ can have an X-ray origin.

The same set of CO^+ $N=3\text{--}2$ hyperfine transitions are also covered in our SMA data. Emission at 353.7413 GHz is clearly detected toward zone A and shows a compact structure (c.f. Fig. 3.2 (d)). However, we do not detect the transition at 354.0142 GHz (Fig. 3.12). In LTE the intensity ratio of the CO^+

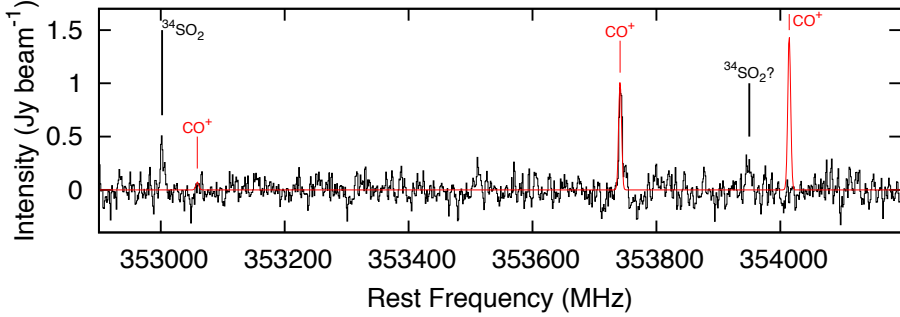


Figure 3.12 Hanning-smoothed spectrum taken from the compact-configuration dataset toward zone A (offset position: $-0.42''$, $-0.43''$). The black lines are the observed data, while the red lines are the model spectrum of CO^+ $N=3-2$, $F=3/2-1/2$ (353.0589 GHz), $5/2-3/2$ (353.7413 GHz) and $7/2-5/2$ (354.0142 GHz) under LTE assumption. The LTE intensity ratio of the hyperfine transitions is $\sim 1:14:20$ (increasing in frequency). The $F=7/2-5/2$ transition at 354.0142 GHz is not detected in our SMA data.

$N=3-2$ hyperfine transitions (including $F=3/2-1/2$ at 353.0589 MHz) is 1:14:20. A similarly compact source at 354.0142 GHz should therefore have been detected. Also, the CO^+ abundance we derive from the 353.7413 GHz intensity ($\sim 1.3 \times 10^{-9}$) is much larger than the prediction from Stauber et al. (2007) and Stauber & Bruderer (2009) ($\sim 10^{-12}$ – 10^{-10}). We therefore rule out CO^+ as the origin of the emission at 353.7413 GHz.

Instead, we assign the line near 353.741 GHz to $^{33}\text{SO}_2$ $19_{4,16} - 19_{3,17}$ transition, as was suggested by Stauber et al. (2007). The anomalous CO^+ line ratio reported by (Stauber et al. 2007) is explained by blending of the CO^+ line with $^{33}\text{SO}_2$ at 353.741 GHz. If this assignment is correct, our SMA data should contain three other lines from $^{33}\text{SO}_2$ (with hyperfine transitions), near 344.031 GHz ($E_u=397$ K), 344.504 GHz ($E_u=232$ K) and 354.246 GHz ($E_u=297$ K). These lines are not detected, but they have either smaller line strengths (344.504 GHz) or decreased intensity due to hyperfine splitting (344.031, 354.246 GHz). In fact, the detected transitions near 353.741 GHz is expected to be the strongest in the passband. The assignment of this line to $^{33}\text{SO}_2$ is further supported by the detection of its $11_{1,11} - 10_{0,10}$ line by Wang et al. (2012). From our data, we find a column density ratio of $^{32}\text{SO}_2/^{33}\text{SO}_2$ of ~ 147 assuming optically thin lines and LTE conditions (Table 3.4). This ratio is consistent with the ISM $^{32}\text{S}/^{33}\text{S}$ ratio of ~ 132 (Wilson & Rood 1994; Chin et al. 1996).

The fact that CO^+ , detected in the JCMT beam, and undetected in our SMA data, suggests an extended ($> 21''$) distribution of the emission consistent with an origin of the emission in the FUV-irradiated cavity walls, and rules out an X-

ray origin. Alternatively, the non-detection of CO^+ in our $\sim 2.5''$ beam may be explained if CO^+ is destroyed rapidly with H_2 or electrons (Stäuber & Bruderer 2009, and the references therein) in the high density ($\geq 10^9 \text{ cm}^{-3}$) material near SMM1 and SMM2 identified by our data.

3.6 Conclusions

Our conclusions can be summarized as follows.

1. The $1''$ resolution continuum image at 353.6 GHz shows 5 compact sub-millimeter sources SMM1–5 (Fig. 3.1). SMM1 and SMM2 have embedded massive stars ($\sim 20 M_\odot$), judging from the detection of compact cm-wave emission. The other sources do not contain massive stars currently, and may be forming low-mass stars or simply be starless.
2. The gas densities of SMM1–5 are high as 10^7 cm^{-3} , but their *core* masses are surprisingly low, $0.2 - 0.6 M_\odot$.
3. If the massive stars in W3 IRS5 accrete locally from the surrounding core, the derived small core masses of the SMM sources imply that the main accretion phase is almost concluded.
4. From Jeans analysis, the cloud structures from $1'$ scales down to $1''$ scales are likely determined by gravitational fragmentation in turbulent environment.
5. The free-fall accretion rates toward SMM1 and SMM2 are about $5 \times 10^{-4} M_\odot \text{ yr}^{-1}$, while SMM3–5 have accretion rates of less than $1-2 \times 10^{-4} M_\odot \text{ yr}^{-1}$ if their stellar masses are $8 M_\odot$ or $2-4 \times 10^{-5} M_\odot \text{ yr}^{-1}$ if they are starless.
6. If star formation in W3 IRS5 follows the competitive accretion model, global collapse of the core and subsequent accretion of the material from the collapse onto the stars can sustain infall rates in excess of $10^{-4} M_\odot \text{ yr}^{-1}$ for SMM1/2 and are sufficient to sustain high-mass star formation.
7. From the molecular line images, we identified four molecular zones (Fig. 3.3). Zone A and B are the major places where sulfur chemistry and hot core chemistry are taking place. Zone C and D, however, seem kinematically unrelated to zone A and B. There is a ‘hot core’ traced by CH_3OH and CH_3CN toward the line of sight of zone B.
8. The large abundances of SO and SO_2 with respect to H_2 (few 10^{-7} to 10^{-6}) derived in zone A and B are indicative of active sulfur chemistry.

9. The low abundance of CH_3OH (5×10^{-8}) in the hot core toward zone B implies that it may be recently heated either internally or externally by feedback from zone A. Zone B seems chemically younger than zone A.
10. The non-detection of $\text{CO}^+ J=3-2$ on small scales supports the idea that CO^+ is formed in the FUV-irradiated outflow cavity walls, and implies that X-rays either do not contribute significantly to the CO^+ production or that this molecule is rapidly destroyed again in the dense material around SMM1 and SMM2.

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Chapter 4

Kinematics of the inner thousand AU region around the young massive star AFGL 2591–VLA3: a massive disk candidate?

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Abstract

Context. Recent detections of disks around young high-mass stars support the idea of massive star formation through accretion rather than coalescence, but the detailed kinematics in the equatorial region of the disk candidates is not well known, which limits our understanding of the accretion process.

Aims. This paper explores the kinematics of the gas around a young massive star with millimeter-wave interferometry to improve our understanding of the formation of massive stars through accretion.

Methods. We use Plateau de Bure interferometric images to probe the environment of the nearby (~ 1 kpc) and luminous ($\sim 20000 L_{\odot}$) high-mass ($10\text{--}16 M_{\odot}$) young star AFGL 2591–VLA3 in continuum and in lines of HDO, H_2^{18}O and SO_2 in the 115 and 230 GHz bands. Radiative transfer calculations are employed to investigate the kinematics of the source.

Results. At $\sim 0.5''$ (500 AU) resolution, the line images clearly resolve the velocity field of the central compact source (diameter of ~ 800 AU) and show linear velocity gradients in the northeast-southwest direction. Judging from the disk-outflow geometry, the observed velocity gradient results from rotation and radial expansion in the equatorial region of VLA3. Radiative transfer calculations suggest that the velocity field is consistent with sub-Keplerian rotation plus Hubble-law like expansion. The line profiles of the observed molecules suggest a layered structure, with HDO emission arising from the disk mid-plane, H_2^{18}O from the warm mid-layer, and SO_2 from the upper disk.

Conclusions. We propose AFGL 2591–VLA3 as a new massive disk candidate, with peculiar kinematics. The rotation of this disk is sub-Keplerian, probably due to magnetic braking, while the stellar wind may be responsible for the expansion of the disk. The expansion motion may also be an indirect evidence of disk accretion in the very inner region because of the conservation of angular momentum. The sub-Keplerian rotation discovered in our work suggests that AFGL 2591–VLA3 may be a special case linking transition of velocity field of massive disks from pure Keplerian rotation to solid-body rotation though definitely more new detections of circumstellar disks around high-mass YSOs are required to examine this hypothesis. Our results support the idea that early B-type stars could be formed with a circumstellar disk from the point of view of the disk-outflow geometry, though the accretion processes in the disk need to be further investigated.

4.1 Introduction

Massive stars play an important role in cycling and mixing material between stars and the interstellar medium in galaxies. However, our understanding of how high-mass stars ($M \geq 8 M_{\odot}$) form is still far from complete (Zinnecker & Yorke 2007). Observationally, it is challenging to gain information from high-mass young stellar objects (YSOs) because high-mass stars usually form in groups at large distances (typically a few kpc), requiring high angular resolution to resolve individual sources. High-mass YSOs are embedded in regions with high extinctions ($\sim 10\text{--}100 A_V$) for $\sim 15\%$ of their lifetime, where complex processes, such as gravitational interaction, powerful outflows and stellar winds, high accretion rates and ionizing radiation fields make the interpretation of observations difficult. Moreover, high-mass YSOs evolve very fast ($\sim 10^5$ yrs) and reach the main sequence while still in the embedded phase. Structures such as circumstellar disks have an even shorter lifetime and are harder to detect.

Accretion via a circumstellar disk is suggested to be the most effective way to overcome radiative pressure and build up a high-mass star (e.g., Krumholz et al. 2009). The detection of massive bipolar outflows with high mass loss rates of $\sim 10^{-4} M_{\odot} \text{ yr}^{-1}$ around young high-mass stars implies the presence of circumstellar disks with comparable mass accretion rates (e.g., Henning et al. 2000; Beuther et al. 2002; Zhang et al. 2005). To date, only a dozen or so B-type young stars have been proposed to have circumstellar disks (e.g., Cesaroni et al. 1997, 1999, 2006; Shepherd & Kurtz 1999; Beuther et al. 2005), with disk masses less than or comparable to the masses of the host stars. In contrast, around young O-type stars, only large rotating toroids are found with masses greater than stellar masses (Beltrán et al. 2005; Furuya et al. 2008).

The presence of circumstellar disks around low-mass young stars is firmly established, and our current observational and theoretical understanding is reviewed by Williams & Cieza (2011) and Armitage (2011), respectively. In contrast, the applicability of a scaled-up version of low-mass star formation via disk accretion for massive stars has not been firmly established (Zinnecker & Yorke 2007), although promising cases have been reported (e.g., Keto & Zhang 2010). Clearly, more observational work is needed to establish the kinematics of material associated with high-mass YSOs.

In this paper, we present observations of massive disk candidate, AFGL 2591–VLA3, a young early B-type star in the Cygnus X region. The distance to this object is uncertain, with reported values ranging from 0.5 to 2 kpc (0.5–2 kpc as discussed in van der Tak et al. 1999) and recent measurements of water masers even suggesting 3.3 kpc (Rygl et al. 2011). In this work, we assume a distance of 1 kpc in order to aid comparison with previous publications and discuss how our conclusions change for a distance of 0.5 or 3 kpc. At 1 kpc, the total luminosity of AFGL 2591 is $\sim 2 \times 10^4 L_{\odot}$ (Lada et al. 1984). Compact radio emission is associated with the source (named as VLA1, VLA2 and VLA3; Campbell 1984; Trinidad et al. 2003). Modeling of its free-free emission implies the stellar mass is about $16 M_{\odot}$ (van der Tak & Menten 2005). An envelope mass of only $40 M_{\odot}$ within 30000 AU around the source is derived through comprehensive radiative transfer modeling of molecular lines by van der Tak et al. (1999).

The geometry of the system can be derived from bipolar ^{12}CO outflows at arcminute scale, which extend in east (red)-west (blue) direction (position angle (P.A.) $\sim 270^{\circ}$ – 325°) observed at resolutions of $14''$ to $21''$ by Mitchell et al. (1992) and Hasegawa & Mitchell (1995). Observations of ^{13}CO at resolution of $14''$ suggests that the P.A. of the outflow is about 280° (van der Tak et al. 1999), confirmed by K -band bispectrum speckle imaging of AFGL 2591 at a resolution of $\sim 0.2''$ showing multiple loops on the western side of the source with P.A. $\sim 260^{\circ}$ (Preibisch et al. 2003). Precession of the outflow axis is also implied. Dense gas in the outflow walls traced by CS and HCN shows a consistent morphology (Bruderer et al. 2009). Based on this orientation of the outflow, a north-south (P.A. $\sim 0^{\circ}$) orientation of the equatorial plane of AFGL 2591–VLA3 is inferred.

Observations of HDO $1_{1,0}$ – $1_{1,1}$, H_2^{18}O $3_{1,3}$ – $2_{2,0}$ and SO_2 $12_{0,12}$ – $11_{1,11}$ with the Plateau de Bure interferometer (PdBI) of the Institut de Radio Astronomie Millimétrique (IRAM)¹ reveal a velocity gradient in the north(east)-south(west) direction across a barely resolved source with a diameter of ~ 800 AU, suggestive of a circumstellar disk (van der Tak et al. 2006). However, the kinematics could not be studied due to the limited angular resolution ($\sim 1''$). Here we present new PdBI observations toward AFGL 2591 at a higher resolution

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of $\sim 0.5''$ (~ 500 AU at 1 kpc), which resolve the kinematics. This paper is organized as follows. Section 4.2 summarizes the PdBI observations and data reduction. Section 4.3 presents the results. In Sect. 4.4, we describe a simple model of the kinematics. Discussions and conclusions are given in Sect. 4.5 and Sect. 4.6, respectively.

4.2 Observations

The source AFGL 2591 was observed with PdBI in 2006–2007 in 4 tracks. The 3 mm receiver was tuned to cover HDO $1_{1,0}-1_{1,1}$ at 80578.3 MHz (hereafter HDO) and the 1.3 mm receiver was tuned to cover H_2^{18}O $3_{1,3}-2_{2,0}$ at 203407.5 MHz (hereafter H_2^{18}O) and SO_2 $12_{0,12}-11_{1,11}$ at 203391.6 MHz (hereafter SO_2). Table 4.1 presents a log of the observations and Table 4.2 summarizes the observed lines. The combined projected baselines range from 26 k λ ($\sim 10''$) to 206 k λ in length at 3 mm and from 48 k λ ($\sim 5''$) to 525 k λ in length at 1.3 mm. The phase tracking center was chosen at $\alpha(2000) = 20^{\text{h}}29^{\text{m}}24^{\text{s}}87$, $\delta(2000) = 40^{\circ}11'19''.50$. The nominal LSR velocity adopted for observations was -5.5 km s $^{-1}$. The quasars 2005+403 and 2013+370, which are about 5° away from AFGL 2591, were frequently observed for phase and gain calibrations in all four observations. 3C273, 3C345 and 3C454.3 were used as the bandpass calibrators, and MWC349 with a total flux density of ~ 1.3 Jy at 203.4 GHz during the time of the observations, as flux calibrator. The flux error is estimated to be within 20%. The spectral resolutions are 39.0625 kHz per channel or 0.145 km s $^{-1}$ per channel at 3 mm band, and 78.125 kHz per channel or 0.115 km s $^{-1}$ per channel at 1.3 mm band. Data reduction was conducted at the IRAM headquarters in Grenoble, using the GILDAS² software.

²<http://www.iram.fr/IRAMFR/GILDAS>

Table 4.1. Log of observations

	03 Feb 2006 ^a	19 Feb 2007	13 Mar 2007	15 Mar 2007
Wavelength	3 mm + 1.3 mm	3 mm	1.3 mm	1.3 mm
On-source time (hours)	5.3	4.5	5.0	4.0
Configuration	6Aq	6Aq	6Bq	6Bq
Bandpass calibrator	3C454.3	3C273	3C345	3C273
Gain calibrator	2005+403, 2013+370	2005+403, 2013+370	2005+403, 2013+370	2005+403, 2013+370
Flux calibrator	MWC349	MWC349	MWC349	MWC349

Note. — ^aAntenna 4 missing due to tuning problems.

Table 4.2. Observed molecular lines

Molecule	Transition	ν^a (MHz)	E_u^b (K)	Beam Size ^c ($'' \times ''$; $^\circ$)
HDO	$1_{1,0}-1_{1,1}$	80578.3	47	1.23×0.72 ; 26
H ₂ ¹⁸ O	$3_{1,3}-2_{2,0}$	203407.5	204	0.51×0.33 ; 22
SO ₂	$12_{0,12}-11_{1,11}$	203391.6	70	0.51×0.33 ; 22

Note. — ^aRest frequency taken from JPL molecular spectroscopy (<http://spec.jpl.nasa.gov/>). ^bEnergy of upper level. ^cSynthesized beam using natural weighting.

4.3 Results

4.3.1 Continuum emission

The natural-weighted continuum images of AFGL 2591–VLA3 at 80.6 GHz and 203.4 GHz are presented in Fig. 4.1. The angular resolutions are $1''.24 \times 0''.72$, P.A. 28° at 80.6 GHz and $0''.51 \times 0''.33$, P.A. 18° at 203.4 GHz. With an arcsecond beam, VLA3 is unresolved at 80.6 GHz. In contrast, at 203.4 GHz VLA3 is well resolved with a subarcsecond beam and shows a diamond shaped morphology in the north-south direction. In addition to VLA3, VLA1 and VLA2 are detected within the field of view at 80.6 GHz. At 203.4 GHz, VLA1 is likely resolved out due to missing short spacings. A previously unknown source (VLA3–NE) located at $\sim 2.5''$ north-eastern to VLA3 is detected at $5\text{-}\sigma$ at 203.4 GHz.

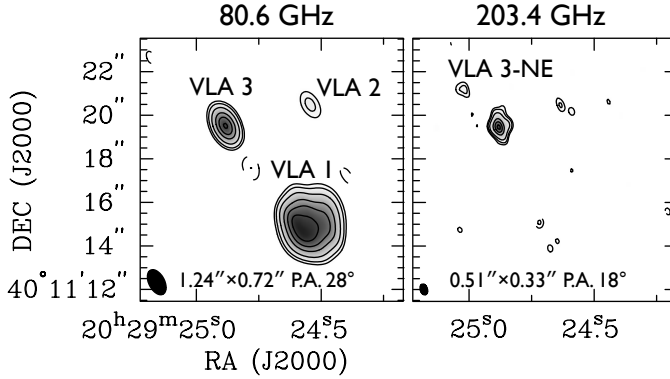


Figure 4.1 Natural-weighted continuum images in the region of AFGL 2591. (Left) 80.6-GHz continuum. Contours are at 3, 5, 10, 20, 30... σ with $1\text{-}\sigma$ of $0.15 \text{ mJy beam}^{-1}$. Sources within the field following Campbell (1984) and Trinidad et al. (2003) are marked on the map. (Right) 203.4-GHz continuum. Contours are at 3, 5, 10, 30, 50... σ with $1\text{-}\sigma$ of $0.4 \text{ mJy beam}^{-1}$.

4.3.1.1 Measurements of positions, sizes and total flux densities

The positions, sizes and total flux densities of the sources in the region of AFGL 2591 are derived in the visibility domain and summarized in Table 4.3. Judging from the images in Fig. 4.1, all sources are fit with point sources, except VLA1 at 80.6 GHz and VLA3 at 203.4 GHz, where Gaussians are used. The vector-averaged visibility plot in Fig. 4.2 shows a compact component on baselines longer than 200 k λ for VLA3 at 203.4 GHz. We therefore fit VLA3 with a 20 mJy point source plus a 65 mJy, $1.0'' \times 0.6''$ ($\sim 800 \text{ AU}$ diameter at 1 kpc) Gaussian source. Including the flux densities of VLA2 and VLA3–NE, the total

Table 4.3. Characteristics of Continuum Emission

Source	$\Delta\alpha^a$ ($''$)	$\Delta\delta^a$ ($''$)	θ_{major}^b ($''$)	θ_{minor}^b ($''$)	P.A. ^b ($^\circ$)	F_ν^c (mJy)	$F_\nu(\text{vdT06})^d$ (mJy)
VLA1	-3.67	-4.49	2.28	2.13	-18 ± 7	62 ± 1	61 ± 1
VLA2	-3.64	1.31	...	...	...	1.1 ± 0.1	9 ± 1
VLA3	0.11	-0.04	...	...	...	7.2 ± 0.1	16 ± 2
203.4 GHz							
VLA1	...	...	...	...	...	...	61 ± 2
VLA2	-2.75	0.94	...	...	...	4.7 ± 0.4	65 ± 4
VLA3 ^e	0.03	0.00	0.96	0.60	6 ± 2	65 ± 2	194 ± 1
	0.16	-0.05	...	...	...	20 ± 1	...
VLA3-NE	1.80	1.82	...	...	...	4.7 ± 0.4	...

Note. — ^aPosition offset with respect to $\alpha(2000) = 20^{\text{h}}29^{\text{m}}24^{\text{s}}.87$ and $\delta(2000) = 40^\circ11'19''.50$. ^bFWHM source size and position angle. ^cTotal flux density. The absolute flux uncertainty is $\sim 20\%$. ^dTotal flux density measured by van der Tak et al. (2006) in the visibility domain. ^eModel with a Gaussian plus a point source. See Fig. 4.2 and text for more discussions.

flux density within the field of view at 203.4 GHz is about 93 mJy which is consistent with the visibility measurement (Fig. 4.2).

Compared to van der Tak et al. (2006), our 80.6-GHz observations measure 100%, 12% and 45% of the total flux densities of VLA1, VLA2 and VLA3, respectively, while the new 203.4-GHz observations detect 0%, 7% and 44% of the total flux densities of VLA1, VLA2 and VLA3, respectively. Considering the different array configurations (limited by the antenna shadowing effect, the shortest baselines of the observations made by van der Tak et al. (2006) are 8 k λ at 3 mm and 20 k λ at 1.3 mm) and the absolute uncertainty of the flux density, the new data are consistent with optically thin free-free emission, optically thick dust or free-free emission and optically thin dust emission for VLA1, VLA2 and VLA3, respectively, as discussed by Trinidad et al. (2003) and van der Tak et al. (1999, 2006). For the newly detected source VLA3-NE, more sensitive high-resolution observations at different frequencies are needed to derive its nature.

4.3.1.2 Estimation of densities and masses

For the “dust” source VLA3, we derive the beam averaged H₂ column density from the measured peak intensity of 30 mJy per beam at 203.4 GHz. The H₂ column density at the emission peak can be estimated as

$$N(\text{H}_2) = \frac{S_\nu a}{2m_{\text{H}}\Omega_{\text{b}}\kappa_\nu B_\nu(T_{\text{d}})}, \quad (4.1)$$

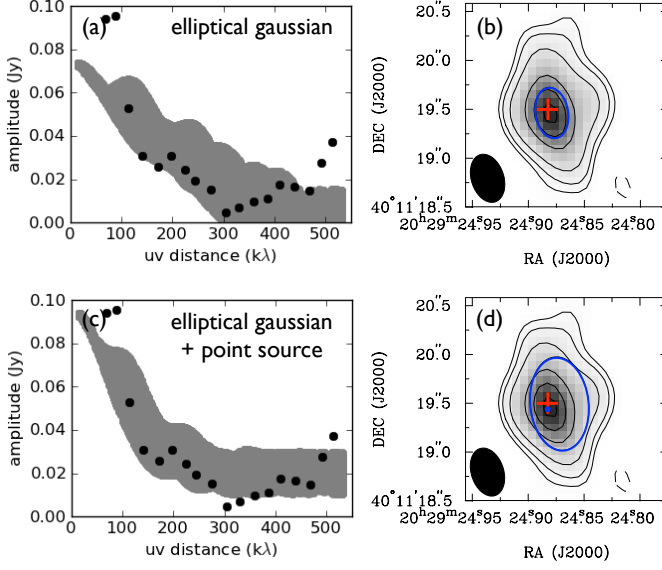


Figure 4.2 Visibility analysis of the continuum at 203.4 GHz. (a) and (c) show the observed visibilities (filled circles) and model visibilities (grey area). The observed data are vector-averaged for the purpose of better visualization. Only the averaged structure in circular symmetry can be observed in the plot. Full model visibilities are plotted in order to show the non-circular symmetric structure of the source. (b) and (d) represent a graphical view of the visibility fits of VLA3 shown in (a) and (c), respectively. The red plus sign is the peak position of the emission. Blue ellipse and filled circle stand for the Gaussian component and the point source.

where S_ν is the peak flux density, a is the gas-to-dust ratio (100), Ω_b is the beam solid angle, m_H is the mass of atomic hydrogen, κ_ν is the dust opacity per unit mass and $B_\nu(T_d)$ is the Planck function at dust temperature T_d . We apply the value of $\kappa_\nu(1.3\text{mm}) \approx 1.0 \text{ cm}^2 \text{ g}^{-1}$ as suggested by Ossenkopf & Henning (1994) for gas densities of $10^6 - 10^8 \text{ cm}^{-3}$ and coagulated dust particles with thin ice mantles. The beam averaged H_2 column densities for T_d from 100 to 300 K (see Sect. 4.3.2.4 for the validity of this assumption) are $0.5 - 1.7 \times 10^{24} \text{ cm}^{-2}$. The gas mass is estimated from the integrated continuum flux density of 85 mJy via

$$M_{\text{gas}} = \frac{F_\nu d^2 a}{\kappa_\nu B_\nu(T_d)}, \quad (4.2)$$

where F_ν is the total flux density of dust emission and d is the distance to the source. At a distance of 1 kpc and temperatures of 100–300 K, the mass is $0.1\text{--}0.3 M_\odot$, significantly less than the stellar mass of VLA3 ($\approx 10\text{--}16 M_\odot$),

Table 4.4. H_2 column density, mass and number density of VLA3

	Dust Temperature			Note
	100 K	200 K	300 K	
$N(\text{H}_2) / 10^{24} \text{ cm}^{-2}$	1.7	0.8	0.5	
$M_{\text{gas}} / M_{\odot}$	0.34	0.16	0.11	$d = 1 \text{ kpc}$
$n(\text{H}_2) / 10^7 \text{ cm}^{-3}$	22.3	10.8	7.2	if size = 800 AU
$M_{\text{gas}} / M_{\odot}$	3.03	1.48	0.98	$d = 3 \text{ kpc}$
$n(\text{H}_2) / 10^7 \text{ cm}^{-3}$	7.5	3.6	2.4	if size = 2400 AU

Lada et al. 1984; van der Tak & Menten 2005). If the distance is 3 kpc, the gas mass is modified to $1\text{--}3 M_{\odot}$, still less than the scaled stellar mass of $> 20 M_{\odot}$. Regardless of the distance, the inferred mass of the surrounding gas around VLA3 is much less than the stellar mass. With the further assumption of a spherical source of $0.8''$ in diameter, as measured from the visibilities of VLA3 at 203.4 GHz, H_2 number densities of $7 - 22 \times 10^7 \text{ cm}^{-3}$ are derived for a distance of 1 kpc, and of $2 - 7 \times 10^7 \text{ cm}^{-3}$ for a distance of 3 kpc. These densities are lower limits if the source structure is flattened. The inferred gas number density is consistent with the envelope density profile within radii of 400 AU (10^{7-9} cm^{-3}) as derived by van der Tak et al. (1999). We summarize these results in Table 4.4.

4.3.2 Line emission

Compact emission of HDO, H_2^{18}O and SO_2 is found toward VLA3 (Fig. 4.3(a)–(c)). With the improved angular resolutions of our new observations (natural weighting; 3mm: $1''.23 \times 0''.72$, P.A. 26° ; 1.3mm: $0''.51 \times 0''.33$, P.A. 22°), all three molecular images are resolved and show a nearly round shape, unlike the diamond shape with a centrally peaked feature seen in the 203.4-GHz continuum. At 1σ noise level, no significant line emission is found toward other sources in AFGL 2591.

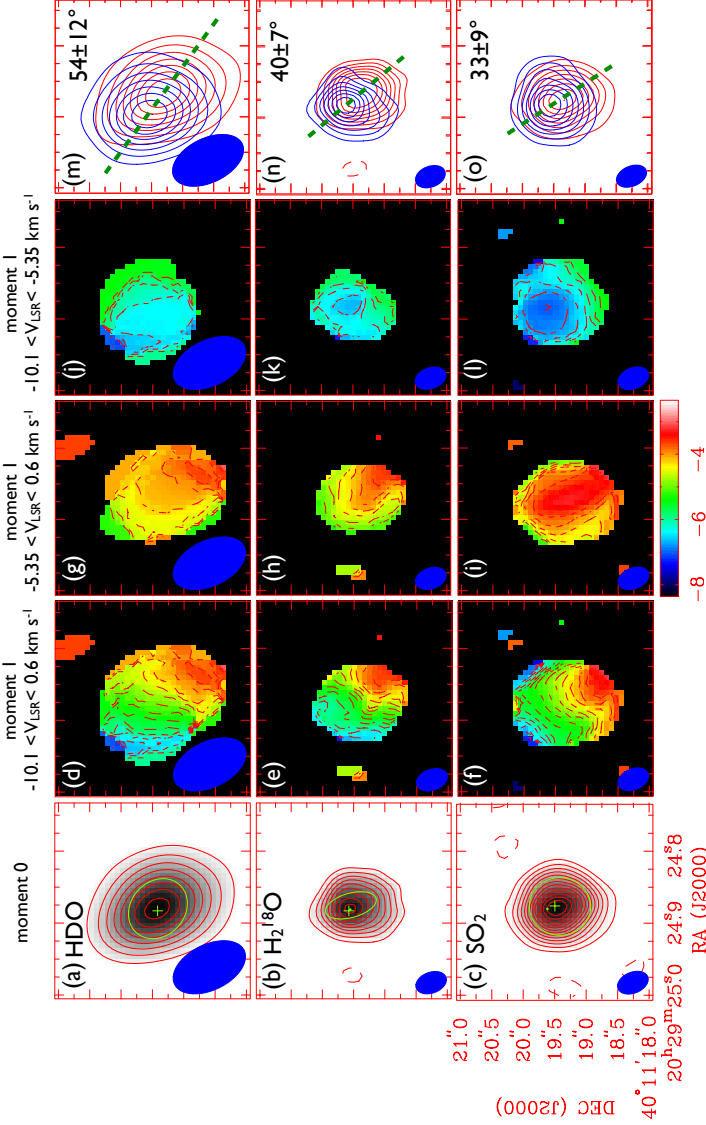


Figure 4.3 (a)–(c) Zero moment maps of HDO, H₂¹⁸O and SO₂ around VLA3, respectively. The contours are at $-3, 3, 6, 9, \dots, \sigma$ for all three maps, where 1σ noise levels are 10, 37 and 65 mJy km s⁻¹ for HDO, H₂¹⁸O and SO₂, respectively. The green crosses mark the positions of emission peaks. The green ellipses represent FWHM sizes derived from visibility fit. The green filled circles indicate the positions of the additional point sources in the visibility fit of H₂¹⁸O and SO₂. The natural-weighted clean beam sizes, shown in blue filled ellipses, of HDO and H₂¹⁸O/SO₂ are $1''.23 \times 0''.72$, P.A. 26° and $0''.51 \times 0''.33$, P.A. 22° , respectively. (d)–(l) First moment maps of HDO, H₂¹⁸O and SO₂ around VLA3, respectively. For all nine maps, the color scales are set to be the same. Dashed lines represent the isovelocity contours with an interval of 0.25 km s^{-1} . (m)–(o) Molecular emission integrated over the velocity ranges of $-5.35 < V_{\text{LSR}} < 0.6 \text{ km s}^{-1}$ (red contours) and $-10.1 < V_{\text{LSR}} < -5.35 \text{ km s}^{-1}$ (blue contours) for HDO, H₂¹⁸O and SO₂, respectively. Contours are plotted with 10% interval of peak value of each velocity component. The inferred position angles of the velocity gradients across VLA3 are plotted as green dashed lines.

Table 4.5. Source positions and size parameters of VLA3 derived from molecular species

Molecule	$\Delta\alpha^a$ ($''$)	$\Delta\delta^a$ ($''$)	θ_{major}^b ($''$)	θ_{minor}^b ($''$)	P.A. ^b ($^\circ$)	V_{grad} P.A. ^c ($^\circ$)
HDO	0.13	−0.08	1.03	0.86	48 ± 15	54 ± 12
$\text{H}_2^{18}\text{O}^d$	0.07	0.05	0.84	0.39	15 ± 7	40 ± 7
	0.14	0.06	...	...	...	...
SO_2^d	0.09	−0.08	0.98	0.92	-2 ± 5	33 ± 9
	0.13	0.12	...	...	...	...

Note. — Positions and source sizes are derived in visibility domain.

^aPosition offset with respect to $\alpha(2000) = 20^{\text{h}}29^{\text{m}}24^{\text{s}}.87$ and $\delta(2000) = 40^\circ11'19''.50$. ^bFWHM source size and position angle. ^cPosition angle of the velocity gradient measured from blue- and red-shifted components. See also Fig. 4.3. ^dModel with a Gaussian plus a point source.

4.3.2.1 Measurements of positions and sizes

We derive the positions and the sizes of the line emission in the visibility domain (Fig. 4.4). In the vector-averaged visibility plots, the amplitude of the visibility decreases up to 200 k λ and is more or less flat onward. This feature is similar to what we observed in the continuum visibility at 203.4 GHz, which implies a point source surrounded by an extended source. As a result, we adopted an elliptical Gaussian plus a point source in the visibility fit of H_2^{18}O and SO_2 . For HDO, we used a Gaussian only in the fit since our baselines at 80.6 GHz only extend to 200 k λ . The source sizes derived in this approach are $0.4''$ – $1.0''$. The lower end of the result is estimated from H_2^{18}O , which could be due to the large dispersion of the visibilities or reflect a smaller source size traced by this higher excitation line ($E_{\text{u}} = 204$ K; 47 and 70 K for HDO and SO_2 , respectively). The size measurements of the molecular lines are consistent with those derived from the continuum, indicating that the dust and the molecular gas have a similar spatial distribution. The locations of the emission peaks differ by much less than the synthesized beam and are negligible. We summarize the results of the visibility analysis in Table 4.5.

4.3.2.2 Velocity gradients across VLA3

The new dataset allows us to spatially resolve the velocity distribution across VLA3. In Fig. 4.3 (d)–(f), velocity gradients in the northeast-southwest direction can be seen with the red-shifted part toward the southwest side and the

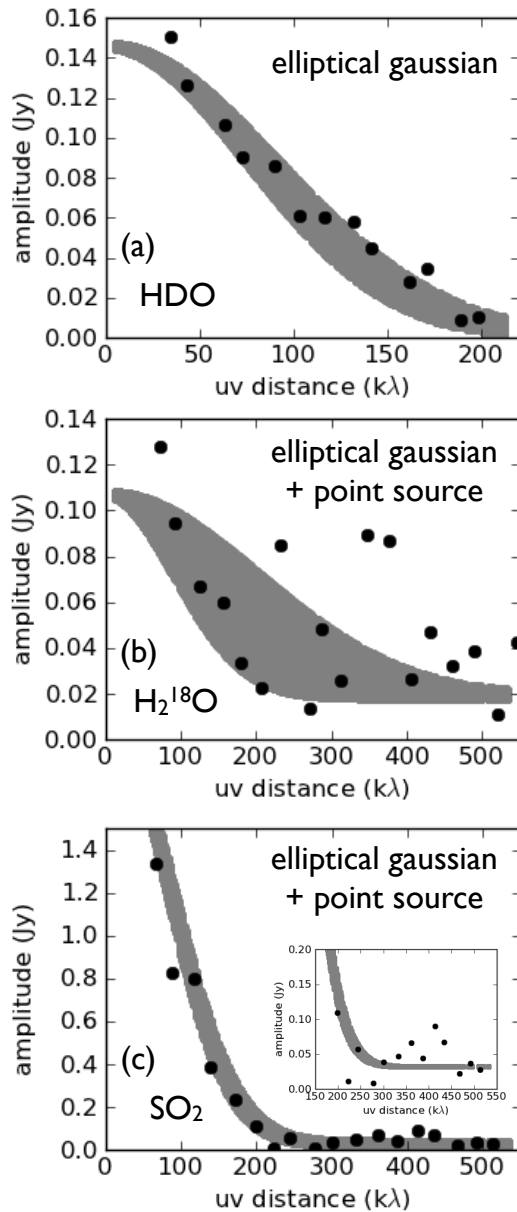


Figure 4.4 Observed visibilities of HDO, $H_2^{18}O$ and SO_2 (filled circles) overplot with model visibilities (grey area). The observed data are vector-averaged corresponding to the circularly symmetric structure. Full model visibilities are plotted in order to show the non-circular symmetric structure of the source.

blue-shifted part toward the northeast side. Apart from the difference in angular resolution, HDO and H_2^{18}O show a similar distribution in isovelocity contours. Detailed investigation of H_2^{18}O image reveals that the isovelocity contours near the systemic velocity (green part) exhibits a mirrored S shape, while SO_2 shows a normal S-shaped distribution of isovelocity contours. The difference implies that HDO/ H_2^{18}O and SO_2 trace different kinematics of VLA3, where SO_2 may be dominated by the east-west outflow. First moment maps plotted in the velocity ranges of $-5.35 < V_{\text{LSR}} < 0.6 \text{ km s}^{-1}$ (Fig. 4.3(g)–(i)) and $-10.1 < V_{\text{LSR}} < -5.35 \text{ km s}^{-1}$ (Fig. 4.3(j)–(l)) support our speculation that SO_2 emission is dominated by the outflow since the extreme velocities originate near the source center, while HDO and H_2^{18}O are less affected by the outflow and presumably dominated by the equatorial motion. We derive the position angles of the velocity gradients across the source seen in Fig. 4.3 (d)–(f) by integrating over the velocity ranges of $-5.35 < V_{\text{LSR}} < 0.6 \text{ km s}^{-1}$ and $-10.1 < V_{\text{LSR}} < -5.35 \text{ km s}^{-1}$ for each line and overplotting them in Fig. 4.3 (m)–(o), respectively. The position angles of velocity gradients are calculated from the emission peaks of the blue- and red-shifted components derived from Gaussian fit. For HDO, H_2^{18}O and SO_2 , the position angles are $54 \pm 12^\circ$, $40 \pm 7^\circ$ and $33 \pm 9^\circ$, respectively (Table 4.5).

The orientation of the observed velocity gradients (northeast-southwest) is not perpendicular to the large scale outflow (east-west) (Mitchell et al. 1992; Hasegawa & Mitchell 1995; van der Tak et al. 1999) with a difference of $\sim 45^\circ$ in position angle. We rule out the possibility of contamination from the bipolar outflow since the red-shifted emission of the molecular emission lies to the southwest, which is inconsistent with the red lobe of the outflow in the east. High-resolution K -band imaging (Preibisch et al. 2003) shows that the orientation of the large-scale outflow remains unchanged on small scales, ruling out contamination by a small-scale outflow to explain the observed velocity pattern. A more likely interpretation for the observed velocity pattern is rotation in the equatorial plane around AFGL 2591–VLA3. For purely azimuthal motion we would expect the velocity gradient to be perpendicular to the bipolar outflow direction. Section 4.4 further explores the effect of radial motion in the equatorial plane that affects the orientation of the velocity gradient.

To further quantify the observed velocity gradients, we plot the position-velocity maps with the position angles defined in Fig. 4.3 (m)–(o) (Fig. 4.5). Clearly, in all cases a *linear* velocity gradient is found, which is very different from the typical Keplerian rotation found in the protoplanetary disks around low-mass stars (e.g., Simon et al. 2000). We derive (projected) velocity gradients of 5.5 ± 0.4 , 10.2 ± 1.3 and $12.4 \pm 0.5 \text{ km s}^{-1} \text{ arcsec}^{-1}$ or km s^{-1} per 1000 AU (at 1 kpc) for HDO, H_2^{18}O and SO_2 , respectively, suggesting that SO_2 is more affected by the east-west outflow while HDO is less affected. To minimize the contamination of the outflow and highlight the motion in the equatorial plane

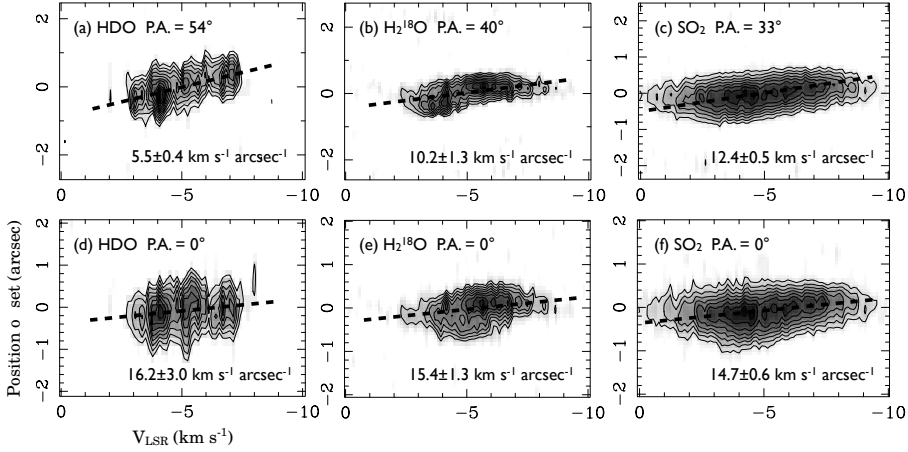


Figure 4.5 (a)–(c) Position-Velocity maps of HDO (P.A. 54° ; see Fig. 4.3 (m)–(o)), H_2^{18}O (P.A. 40°) and SO_2 (P.A. 33°). Linear velocity gradients are fitted to the maps and shown as dotted lines. (d)–(f) Same as (a)–(c) except the position angle of the position-velocity cut for all three molecules is 0° .

of VLA3, we also derive the velocity gradients by taking the position-velocity cut with P.A. = 0° . A consistent strength of linear velocity gradient ($\sim 15 \text{ km s}^{-1} \text{ arcsec}^{-1}$) is derived from all three molecules, indicating that the effect of outflow is indeed minimized.

4.3.2.3 Molecular line profile

Spectra of HDO, H_2^{18}O and SO_2 centered at the mean emission peak ($\Delta\alpha = -0.15''$, $\Delta\delta = 0.02''$) in a single synthesized beam ($1''.23 \times 0''.72$, P.A. 26°) are shown in Fig. 4.6. A triple-peaked line profile is observed for HDO, while the H_2^{18}O and SO_2 line profiles are smooth Gaussians with weak hints of secondary peaks coincident with those seen in HDO. We use three Gaussians to decompose the HDO line profile (Table 4.6) and find that Gaussians with FWHM of $\sim 1.20 \pm 0.05 \text{ km s}^{-1}$ at V_{LSR} of -6.89 ± 0.03 , -5.35 ± 0.34 and $-3.92 \pm 0.26 \text{ km s}^{-1}$ best reproduce the observed spectrum, although significant residuals remain near -8.0 and -3.0 km s^{-1} . The velocity differences between the blue-shifted and systemic components ($1.54 \pm 0.34 \text{ km s}^{-1}$), and, the red-shifted and systemic components ($1.43 \pm 0.43 \text{ km s}^{-1}$) are comparable, which suggest that the red- and blue-shifted components are likely from the same structure undergoing systematic motion, not just a spatial coincidence of three different gas clumps. To decompose the H_2^{18}O and SO_2 line profiles, we fit three Gaussians fixed at V_{LSR} of -6.89 , -5.35 and -3.92 km s^{-1} derived from HDO line profile (Table 4.6). For an FWHM line width of 1.45 km s^{-1} , this fit reproduces most of the

line profile, with only significant residuals at extreme velocities (near -2.5 and -8.5 km s^{-1} for H_2^{18}O , and near -2.0 and -9.0 km s^{-1} for SO_2). Based on the line profiles and the observed velocity gradient across the source, we suggest that the velocity structure of VLA3 consists of three components: two exhibiting motions (azimuthal and radial) in the equatorial plane and one static component.

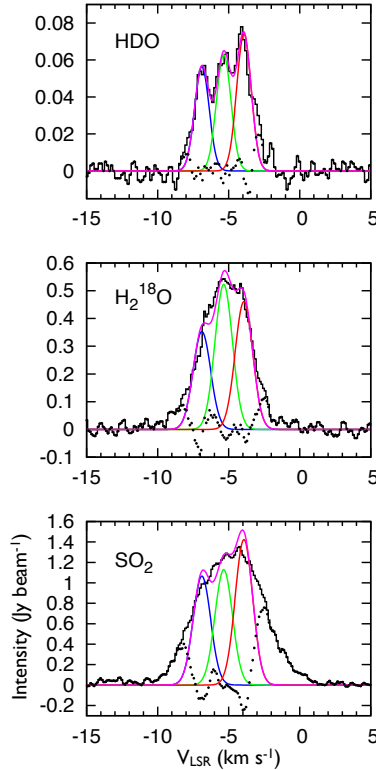


Figure 4.6 Molecular spectra taken at the mean emission peak after convolving all data to the same angular resolution of $1''.23 \times 0''.72$, P.A. 26° . Fitted Gaussians are overplotted in color. Residuals are shown in dots.

4.3.2.4 Molecular excitation

We estimate the excitation conditions of VLA3 based on the line ratios of the chemically related molecules HDO and H_2^{18}O . If we assume optically thin emission and local thermodynamic equilibrium (LTE), the total column density at a given excitation temperature can be derived via

$$N_{\text{tot}} = \frac{2.04W}{\theta_a \theta_b} \frac{Q_{\text{tot}} e^{E_u/T_{\text{ex}}}}{g_I g_K S \mu^2 \nu^3} \times 10^{20} \text{ cm}^{-2}, \quad (4.3)$$

Table 4.6. Line parameters of HDO, H₂¹⁸O and SO₂ derived from fitting of three Gaussian components

Molecule	Blue-shifted			Systemic			Red-shifted		
	V_{LSR}^a (km s ⁻¹)	ΔV^b (km s ⁻¹)	W^c (Jy beam ⁻¹ km s ⁻¹)	V_{LSR} (km s ⁻¹)	ΔV (km s ⁻¹)	W (Jy beam ⁻¹ km s ⁻¹)	V_{LSR} (km s ⁻¹)	ΔV (km s ⁻¹)	W (Jy beam ⁻¹ km s ⁻¹)
HDO	-6.89(3)	1.20 (5)	0.072(3)	-5.35(34)	1.20(5)	0.080(3)	-3.92(26)	1.20(5)	0.094(3)
H ₂ ¹⁸ O	-6.89	1.45	0.544(19)	-5.35	1.45	0.807(19)	-3.92	1.45	0.712(19)
SO ₂	-6.89	1.45	1.64(11)	-5.35	1.45	1.74(12)	-3.92	1.45	2.20(11)

Note. — Errors in units of the last decimal are given in the parentheses. Values without parentheses are fixed in the fitting. ^aLine center velocity. ^bFWHM line width. ^cIntegrated intensity.

where W is the integrated intensity in $\text{Jy beam}^{-1} \text{ km s}^{-1}$, θ_a and θ_b are the FWHM widths of the synthesized beam in arcsec, Q_{tot} is the partition function, E_u is the upper energy level in K, T_{ex} is the excitation temperature in K, g_I and g_K are the spin and K degeneracies, respectively, S is the line strength, μ is the dipole moment in Debye, and ν is the rest frequency in GHz. The source filling factor is assumed be unity and background emission is neglected. In other words, the excitation temperature can be expressed as a (nonlinear) function of the column density ratio of HDO and H_2^{18}O , if HDO and H_2^{18}O share the same excitation temperature. Once the excitation temperature is estimated, the column density can be derived via Equation (4.3).

The column density ratio $N_{\text{tot}}[\text{H}_2^{18}\text{O}]/N_{\text{tot}}[\text{HDO}]$ can be expressed as

$$\frac{N_{\text{tot}}[\text{H}_2^{18}\text{O}]}{N_{\text{tot}}[\text{HDO}]} = \frac{N_{\text{tot}}[\text{H}_2\text{O}]}{N_{\text{tot}}[\text{HDO}]} \times \frac{N_{\text{tot}}[\text{H}_2^{18}\text{O}]}{N_{\text{tot}}[\text{H}_2\text{O}]}. \quad (4.4)$$

For the column density ratio of H_2O and HDO, we adopt the abundance ratio $[\text{H}_2\text{O}]/[\text{HDO}]$ of 1400–2000 for the inner region of the envelope around VLA3 (assuming this ratio can be applied to the observed rotating structure), which is derived based on the “jump” model of 1D radiative transfer calculations (see Table 11 of van der Tak et al. 2006). We assume the column density ratio of H_2^{18}O and H_2O to be 0.002 based on the $[\text{H}_2^{18}\text{O}]/[\text{H}_2\text{O}]$ ratio (Wilson & Rood 1994). Therefore, the column density ratio $N_{\text{tot}}[\text{H}_2^{18}\text{O}]/N_{\text{tot}}[\text{HDO}]$ is 2.8–4.0. The total column densities of HDO and H_2^{18}O as a function of T_{ex} are shown in the upper three panels of Fig. 4.7, while the column density ratio $N_{\text{tot}}[\text{H}_2^{18}\text{O}]/N_{\text{tot}}[\text{HDO}]$ as a function of T_{ex} can be seen in the bottom three panels of Fig. 4.7. From the column density ratio plots, a range of excitation temperatures for a given velocity component can be estimated by finding the intersections of the derived curves of the column density ratio from the new observations (in purple) and the horizontal lines of the adopted column density ratios from Equation (4.4) (in green). We summarize the molecular excitation condition of VLA3 in Table 4.7.

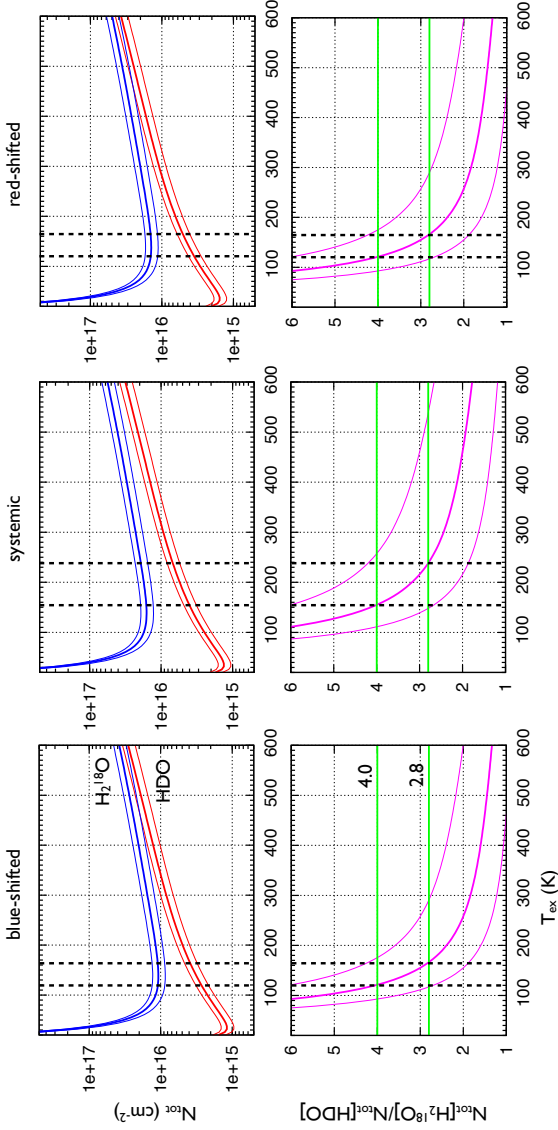


Figure 4.7 H_2^{18}O and HDO column density and column density ratio plots. The left, middle and right columns represent the plots for the blue-shifted, systemic and red-shifted components, respectively. In the first row, total column densities at different excitation temperatures are plotted in blue (H_2^{18}O) and red (HDO) thick curves. Their column density ratios, shown in the second row, are plotted in thick purple curves. The thin curves represent the errors. In addition, the H_2^{18}O over HDO column density ratio, derived from van der Tak et al. (2006) and Wilson & Rood (1994), are plotted as green horizontal lines. The excitation temperatures for a given component can be read out by finding the intersection of the green lines and thick purple lines. The thick vertical dashed lines mark the derived temperatures for ratio 2.8 and 4.0. Here we derive the excitation temperature without considering the error of absolute flux density. Derived temperatures and column densities are summarized in Table 4.7.

We estimate the excitation temperatures for the blue-shifted, systemic and red-shifted components to be 120–165 K, 155–240 K and 120–165 K, respectively, or 90–290 K, 110–540 K and 90–290 K, respectively, if the error in absolute flux calibration is considered. We find that the blue- and red-shifted components have similar excitation temperatures, implying again that both components are from a single source structure such as the observed equatorial gas component around VLA3. There is also an indication that the systemic component might be warmer. The overall column densities counting all three velocity components (without absolute error in flux density) for HDO, H_2^{18}O and SO_2 are 1×10^{16} , 4×10^{16} and $1 \times 10^{16} \text{ cm}^{-2}$, respectively. The fractional abundances are estimated to be 5×10^{-8} , 2×10^{-7} and 6×10^{-8} for HDO, H_2^{18}O and SO_2 , respectively, adopting the 203.4-GHz continuum peak flux at the resolution of $1''.23 \times 0''.72$, P.A. 26° and using $T_d = 200 \text{ K}$ in the calculation of Equation (4.1).

We note that the line ratio analysis of HDO and H_2^{18}O discussed above is sensitive to the assumed abundance ratios of HDO/ H_2O and $^{16}\text{O}/^{18}\text{O}$. For example, if the assumed $N_{\text{tot}}[\text{H}_2^{18}\text{O}]/N_{\text{tot}}[\text{HDO}]$ is smaller (larger) by a factor of two, the corresponding temperatures would be less than 100 K (greater than 250 K) for all three velocity components. Alternatively, if we adopt a temperature of 100 K (the ice evaporation temperature), the derived column density ratio $N_{\text{tot}}[\text{H}_2^{18}\text{O}]/N_{\text{tot}}[\text{HDO}]$ would be less than 7, consistent with van der Tak et al. (2006). Only observations of multiple transitions of HDO and H_2^{18}O can further constrain the excitation conditions of the inner region of VLA3.

Alternatively, the excitation conditions on large scales near VLA3 can be estimated from the HDO single-dish data published by van der Tak et al. (2006) with the population diagram method (Goldsmith & Langer 1999). Including the effects of beam dilution and line opacity, the excitation temperature, total column density and source size are solved self-consistently. The observed data (red open circles) and best fit model (green crosses) are plotted in Fig. 4.8. The excitation temperature is estimated to be $130 \pm 30 \text{ K}$ with a column density of $\sim (1.0 \pm 0.1) \times 10^{14} \text{ cm}^{-2}$ distributed uniformly in a source with angular size of $17 \pm 2''$. Line opacities of all the transitions used are estimated to be less than 0.006. The excitation temperatures derived from the single-dish data are consistent with the ones derived from our new interferometric data. The total HDO column density including all three velocity components is about $3 \times 10^{13} \text{ cm}^{-2}$ if we observe the same structure (roughly $0.8'' - 1.0''$) seen by the interferometer with a $17''$ beam which is consistent with the value derived from single-dish data if missing flux is considered. As a result, both single-dish and interferometric data imply that HDO is present in both the outer envelope and the inner dense region toward VLA3 with a temperature greater than $\sim 100 \text{ K}$.

Table 4.7. Excitation temperatures and column densities

Component	T_{ex}^a (K)	$N_{\text{tot}}[\text{HDO}]^b$ ($\times 10^{15} \text{ cm}^{-2}$)	$N_{\text{tot}}[\text{H}_2^{18}\text{O}]^b$ ($\times 10^{16} \text{ cm}^{-2}$)	$N_{\text{tot}}[\text{SO}_2]^b$ ($\times 10^{15} \text{ cm}^{-2}$)	$X[\text{HDO}]^c$ ($\times 10^{-8}$)	$X[\text{H}_2^{18}\text{O}]^c$ ($\times 10^{-7}$)	$X[\text{SO}_2]^c$ ($\times 10^{-8}$)
Blue-shifted	120–165	2.7–3.9	1.1	3.0–4.8	...	...	...
Systemic	155–240	4.0–5.5	1.6	4.7–7.3	...	...	...
Red-shifted	120–165	3.5–5.1	1.4	4.0–6.5	...	...	...
Overall	...	10.2–14.5	4.1	11.7–18.6	4.4–6.2	1.7	4.9–7.9

Note. — ^aExcitation temperatures estimated from column density ratios. See Sect. 4.3.2.4 for details. ^bTotal column density derived under LTE and optically thin assumptions. ^cWith respect to H_2 . Assuming a dust temperature of 200 K, $N_{\text{tot}}[\text{H}_2]$ of $2.35 \times 10^{23} \text{ cm}^{-2}$ is derived from the 203.4-GHz continuum at a resolution of $1''.23 \times 0''.72$, P.A. 26° . The uncertainty in $N_{\text{tot}}[\text{H}_2]$ is not considered.

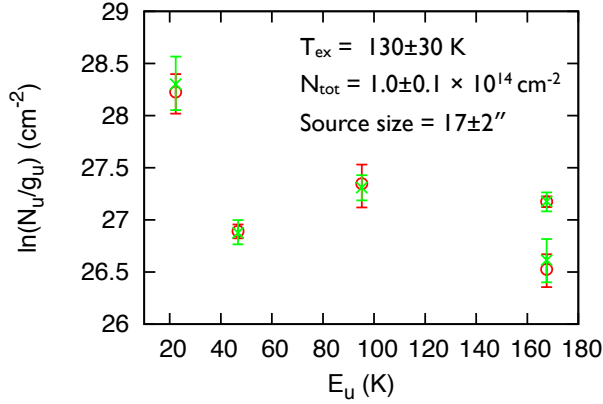


Figure 4.8 HDO rotation diagram plotted with the data published by van der Tak et al. (2006). Red open circles are the data observed with JCMT and IRAM 30m. The green crosses represent the best-fit model from population diagram analysis (Goldsmith & Langer 1999).

4.4 Kinematics of the equatorial region of VLA3

4.4.1 Evidence of rotation and outward radial motions

The new (sub)arcsecond resolution PdBI observations resolve the velocity field in the inner region of AFGL 2591–VLA3. Clear *linear* velocity gradients in the northeast-southwest direction are observed in HDO, H₂¹⁸O and SO₂ lines. Comparison of the distributions of isovelocity contours of these lines reveals that HDO and H₂¹⁸O best reflect the kinematics of the equatorial region of VLA3, while SO₂ is more affected by the east-west outflow. In addition, a triple-peaked line profile is observed in HDO. Given the bipolar outflow geometry in the east-west direction (Mitchell et al. 1992; Hasegawa & Mitchell 1995; Preibisch et al. 2003), which defines a north-south equatorial plane, we propose that the observed lines trace rotation in the inner envelope around VLA3. We suggest that radial motions alter the velocity field’s position angle from the expected north-south direction to the observed northeast-southwest direction. Consider an inclined disk-like structure at P.A. 0°, with rotation and radial motion but without vertical motion (as expected for a model in vertical hydrostatic equilibrium), four possible velocity patterns exist (as shown schematically in Fig. 4.9), depending on whether the rotation appears clockwise or counterclockwise as seen by the observer, and whether the radial motion are inward or outward. Only the combination of counterclockwise rotation and *outward* radial motions reproduce the observed velocity pattern (c.f. Fig. 4.3 and 4.9).

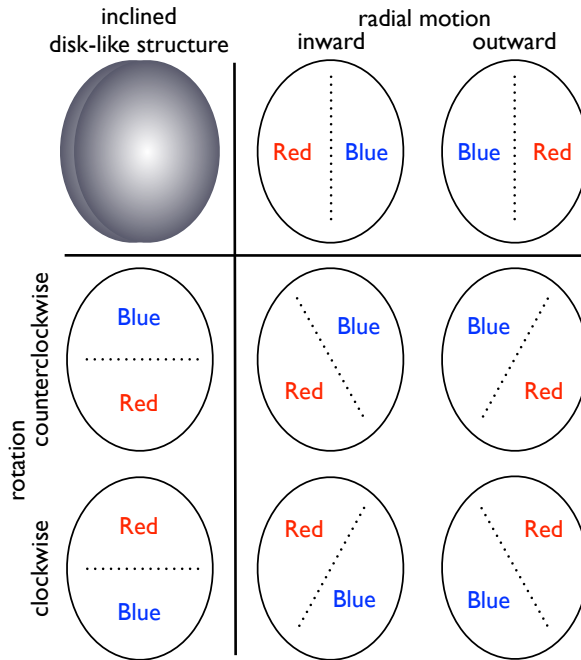


Figure 4.9 Schematic view of the velocity fields combining radial motion and rotation.

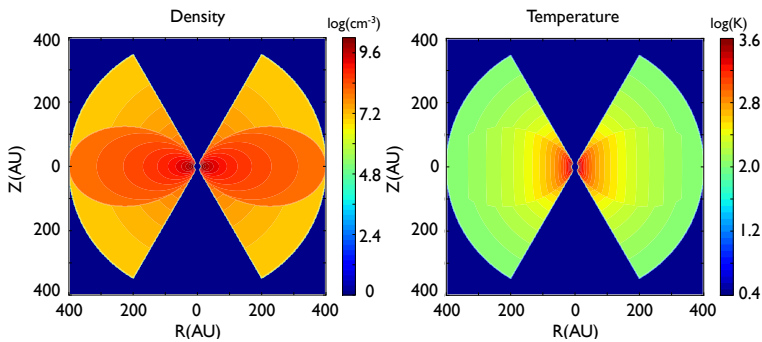


Figure 4.10 Gas density (left) and gas temperature (right) distributions of the source in the radiative transfer models, including a disk-like structure, a spherical turbulent envelope, and an outflow cavity.

4.4.2 A toy model

To explore if a kinematical model as suggested in the previous section can reproduce the observed velocity pattern and molecular line spectra, we constructed a toy model and calculate the resulting emission using the axisymmetric radiative transfer code RATRAN (Hogerheijde & van der Tak 2000). Our model includes a flattened “disk-like” structure surrounded by a static spherical envelope and a bipolar outflow cavity (Fig. 4.10). We adopt a parametrized description of the density, temperature, and velocity field, and assume LTE and optically thin conditions for the line emission. Given the critical densities of the observed transitions (7×10^4 , 3×10^5 and $5 \times 10^6 \text{ cm}^{-3}$ for HDO, H_2^{18}O and SO_2 at 200 K, respectively), and the densities derived in Sect. 4.3.1.2, the excitation is likely in LTE. We scale the model intensity to match the observed line strengths, which means that we can derive conclusions about the velocity field but not the density or temperature. Our only aim is to show that our simple toy model can reproduce the observed velocity pattern and spectral line shapes. We do not perform any global model optimization in density, temperature and velocity profiles. Instead, for fixed sets of density and temperature profiles, we conduct a simplified optimization to the parametrized velocity field. Our derived parameters are therefore not best-fit solutions but rather indicative values.

4.4.3 Details of the model

The density profiles for the disk-like structure (for simplicity, we use “disk” hereafter in this section) and the envelope are assumed to follow power-law distributions, respectively, as $n_{\text{disk}}(r, \theta) = An_{\text{e0}}(r/r_{\text{d}})^{-\alpha} \sin^f(\theta)$ and $n_{\text{env}}(r) = n_{\text{e0}}(r/r_{\text{d}})^{-\alpha}$, where n_{e0} is the density at radius r_{d} (the outer radius of the disk), A is the disk-to-envelope density ratio at r_{d} in the mid-plane, θ is the angle measured from the polar axis, f is the flattening parameter and α is the power-law index. In the disk density profile, regions with densities lower than An_{e0} are set to have zero density, resulting in a dumpling-like, flattened structure. The overall density in the model is the sum of n_{disk} and n_{env} . For the temperature profiles in the disk and the envelope, we assume power-law distributions, respectively, as $T_{\text{disk}}(R) = BT_{\text{e0}}(R/r_{\text{d}})^{-\beta}$ and $T_{\text{env}}(r) = T_{\text{e0}}(r/r_{\text{d}})^{-\beta}$ (i.e., we adopt a vertically isothermal model for the disk) where R denotes the radial direction in cylindrical coordinates, T_{e0} is the temperature at r_{d} , B is the disk-to-envelope temperature ratio, and β is the power-law index. The gas temperature for a given position is the weighted mean of the disk and envelope values: $T = (n_{\text{disk}}T_{\text{disk}} + n_{\text{env}}T_{\text{env}})/(n_{\text{disk}} + n_{\text{env}})$. The distance to the source is assumed to be 1 kpc. The inner radius of the model is set to 12.5 AU (half the size of the HII region; van der Tak & Menten 2005) and the outer radius to 400 AU ($= r_{\text{d}}$, based on the size derived from our 203.4 GHz continuum). In addition,

a bipolar outflow cone with an opening angle of 60° is included in the model by setting the density inside this cone to be zero. We describe the velocity field in the disk by three orthogonal components as radial (v_R), vertical (v_z) and azimuthal (v_a). The velocity field in the static envelope is set to be purely turbulent, inspired by the observed spectra showing emission peaks near systemic velocity. The gas velocity for a given position is the weighted mean of the disk and envelope values: $\vec{v} = (n_{\text{env}}\vec{v}_{\text{env}} + n_{\text{disk}}\vec{v}_{\text{disk}})/(n_{\text{disk}} + n_{\text{env}})$. The inclination of the source is set to be 30° (van der Tak et al. 2006) with the blue-shifted outflow cone pointed to the west. Model parameters are chosen to ensure that the LTE and optically thin assumptions are valid. We adopt $A = 10$, $n_{\text{e}0} = 1 \times 10^7 \text{ cm}^{-3}$, $\alpha = 1.5$, $f = 5$, $B = 1$, $T_{\text{e}0} = 100 \text{ K}$, $\beta = 1$, a molecular fractional abundance of 1×10^{-13} and a turbulent line width of 0.5 km s^{-1} . A detailed description of the parametrized velocity field is given in the next section. We scale the line intensity to the observed values, and only analyze the velocity signatures (moment 1 maps and position-velocity maps) and spectral line profiles. We note that this scaling process makes the exact profiles of density and temperature irrelevant.

4.4.4 Evidence of sub-Keplerian rotation and Hubble-law like radial expansion traced by HDO and H_2^{18}O

The analysis of the position-velocity maps of the observed lines toward VLA3 reveals that the velocity field is characterized by a linear velocity gradient (Fig. 4.5), which suggests that the equatorial region is undergoing solid-body rotation. However, the analysis demonstrated in Fig. 4.9 implies that an extra outward radial component is required to reproduce the observed northeast-southwest velocity pattern (Fig. 4.3 (d)–(f)). Therefore, a direct link between the observed linear velocity gradient and the inferred solid-body rotation may not be trivial. In our toy model, we consider two types of velocity profiles in the azimuthal and radial directions for the disk-like structure: one is proportional to $r^{-0.5}$ and the other follows r^{+1} . Although all the combinations of the velocity field can reproduce the triple-peaked line signature seen in HDO and the linear velocity gradient seen in the position-velocity maps, only Keplerian-like rotation ($v_a \sim r^{-0.5}$) plus Hubble-law like radial expansion ($v_R \sim r^{+1}$) can reproduce the mirrored S-shape isovelocity contours observed in H_2^{18}O , which is less affected by the outflow than SO_2 (Fig. 4.11; c.f., Fig. 4.3(e)). An additional velocity component in the z direction may redistribute the isovelocity contours to match the observed SO_2 moment 1 map. In our toy model, the outflow component is not included due to the complexity of outflow morphology and velocity field. Therefore, we use HDO and H_2^{18}O data to constrain the kinematics of the equatorial region of VLA3. To summarize, we adopt the parametrized velocity for the disk-like

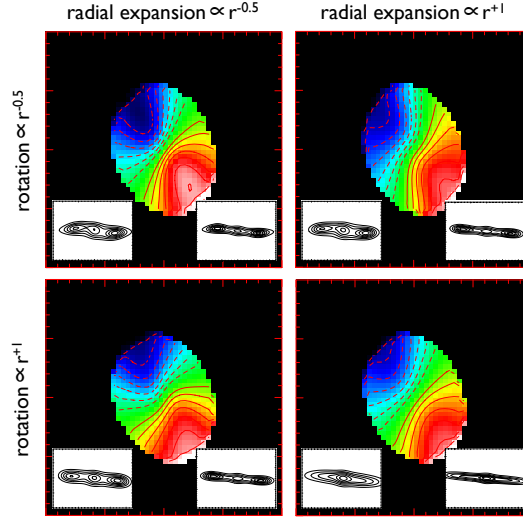


Figure 4.11 Model moment 1 maps of the combined velocity profiles in azimuthal and radial directions. The model position-velocity maps are included in each panel (bottom-left: P.A. 0° , bottom-right: P.A. 45°). In all cases, linear velocity gradient can be inferred. However, only Keplerian-like rotation ($\sim r^{-0.5}$) plus Hubble-law like radial expansion ($\sim r^{+1}$) can reproduce the observed mirrored S-shape isovelocity contours seen in H_2^{18}O (c.f., Fig. 4.3(e)).

structure as:

$$\begin{aligned} v_R &= v_{R0}r \\ v_a &= \xi \sqrt{GM_\star/r} \\ v_z &= 0, \end{aligned} \quad (4.5)$$

where v_{R0} is an analog of the Hubble constant, ξ is a constant between 0 and 1, G is the gravitational constant and $M_\star=16M_\odot$ (van der Tak & Menten 2005) is the stellar mass.

To estimate the strength of the two free parameters v_{R0} and ξ in our kinematic model, we perform a simplified parameter optimization which utilizes the peak velocities of the HDO triple-peaked line profile (-6.7 , -5.4 and -3.9 km s^{-1} for the blue-shifted, systemic and red-shifted components, respectively), and the measured linear velocity gradient of $\sim 15 \text{ km s}^{-1} \text{ arcsec}^{-1}$ at P.A. 0° as the constraints. We constructed a grid of models for HDO with v_{R0} between 4 and 20 km s^{-1} per 1000 AU and ξ between 0.2 and 0.5. For each set of parameters (v_{R0} , ξ), we compute $\Delta^2 = \Sigma(\text{observed peak velocities} - \text{model peak velocities})^2$, which is smaller for a better match. Figure 4.12 shows that the models with the lowest Δ^2 values span a diagonal in (v_{R0}, ξ) -space, indicating that the model is degenerate. To break the degeneracy, we compute the strength of the linear velocity gradient at P.A. 0° in our grid model and plot it as the solid curves

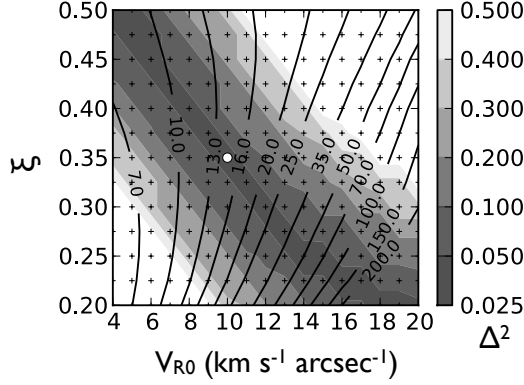


Figure 4.12 Simplified parameter optimization of our kinematic model. The grey scales represent the similarity of model and observed HDO triple-peaked line profile (lower values for better match). The solid curves with values in unit of $\text{km s}^{-1} \text{arcsec}^{-1}$ indicate the measured strength of linear velocity gradient at P.A. 0° in the grid models. The open circle highlights our best matching parameter set ($v_{R0} = 10 \text{ km s}^{-1} \text{arcsec}^{-1}$, $\xi = 0.35$).

in Fig. 4.12. By matching the observed value, we conclude that based on our toy model, the azimuthal motion of the disk-like structure traced by HDO can be characterized by sub-Keplerian rotation (about 1/3 the strength of Keplerian rotation with a stellar mass of $16 M_\odot$) and the radial motion is the accelerated expansion with the analogue Hubble constant of 10 km s^{-1} per 1000 AU at 1 kpc. The best matching model spectrum, moment 1 maps and position-velocity map for HDO can be found in Fig. 4.13 (a)–(e).

To model the H_2^{18}O data, we use the best matching solution for HDO ($v_{R0} = 10 \text{ km s}^{-1} \text{arcsec}^{-1}$, $\xi = 0.35$) as the starting point. Certainly, the turbulent line width of 0.5 km s^{-1} is too narrow for H_2^{18}O since its line profile is Gaussian-like with hints of secondary velocity components. We therefore adopt a turbulent line width of 1.0 km s^{-1} in the model. The best matching model for H_2^{18}O can be seen in Fig. 4.13 (f)–(j). Though not perfectly matching the observations, our toy model of kinematics is able to reproduce both HDO and H_2^{18}O data qualitatively. In our toy model, we found that the kinematics of the proposed disk-like structure around VLA3 is best described by two velocity components: sub-Keplerian rotation and Hubble-law like expansion. We also found that the conclusion of rigid-body rotation across the source judging directly from the linear velocity gradient observed in position-velocity maps may not be made if the observed velocity gradient does not align well with the equatorial plane defined by the outflow.

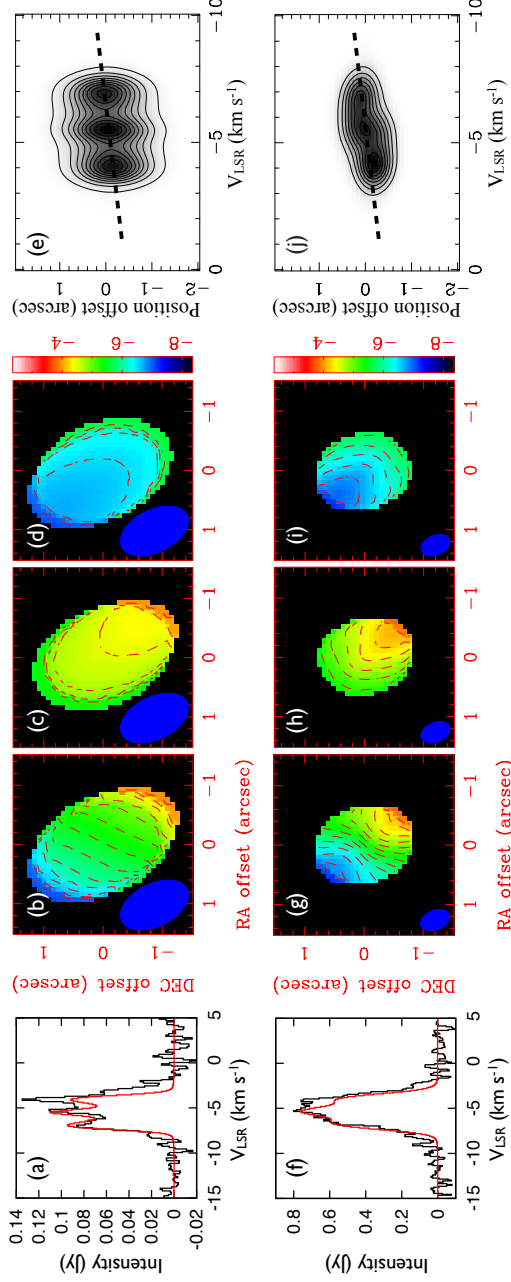


Figure 4.13 (Left) Best matching model spectrum (a), moment 1 maps (b)–(d) and position-velocity map (f) for HDO. The color scales and contour levels for moment 1 maps are identical to Fig. 4.3 (d)–(f). The dashed line in the position-velocity map represents a linear velocity gradient with strength of 15 km s⁻¹ arcsec⁻¹. (Right) Best matching model for H₂¹⁸O.

4.5 Discussion

4.5.1 An embedded disk-like structure in AFGL 2591–VLA3?

Our (sub)arcsecond PdBI images of HDO, H_2^{18}O and SO_2 reveal a clear velocity gradient in the northeast-southwest direction across the source AFGL 2591–VLA3 (Sect. 4.3.2.2). Together with the shape of the HDO line profile (Sect. 4.3.2.3), and the symmetric temperature distribution of the blue- and red-velocity components (Sect. 4.3.2.4), we propose that the source AFGL 2591–VLA3 is surrounded by a disk-like structure undergoing rotation and expansion. The kinematics of the equatorial region is further characterized as sub-Keplerian rotation plus Hubble-law like expansion as shown by radiative transfer modeling of a toy model (Sect. 4.4). In the models for HDO, a microturbulent line width of $\sim 0.5 \text{ km s}^{-1}$ matches the triple-peaked line profile, which appears small for the violent environment of massive star-forming regions (Zinnecker & Yorke 2007). On the other hand, a microturbulent line width of 1.0 km s^{-1} is needed to match the almost single-peaked line profiles seen in H_2^{18}O . We expect that an even larger turbulent line width is required to model SO_2 , judging from the observed SO_2 spectrum. This suggests that these molecules trace different regions within the disk-like structure.

We hypothesize that the disk-like structure has a layered distribution with HDO close to the mid-plane, H_2^{18}O in the warm mid-layer and SO_2 in the upper disk layers (Fig. 4.14). In addition, significant emission from all three molecules originates in a static turbulent envelope surrounding the disk-like structure, especially for H_2^{18}O and SO_2 where it dominates the line profiles (Table 4.7). In the disk-like structure, we find temperatures of about 120–165 K, well above the evaporation temperature of water ice (Fraser et al. 2001). The HDO molecules may be formed on grain surfaces (Tielens 1983; Parise et al. 2005), and released into the gas phase when the disk-like structure is heated by shocks, stellar radiation and winds. Compared to HDO, H_2^{18}O originates from a more turbulent region at larger height with increased turbulence in the disk-like structure. In this picture, the presence of H_2^{18}O but absence of HDO in the mid-layer of the disk-like structure could be due to increased local water formation because of warm gas chemistry as opposed to evaporation of deuterated ices formed at low temperature. SO_2 is a good shock/outflow tracer in massive star-forming regions (Schilke et al. 1997). Judging from the facts that the observed SO_2 line profile has significant emission from line wings, and that a relatively large velocity gradient is measured in SO_2 compared to $\text{HDO}/\text{H}_2^{18}\text{O}$, we suggest that SO_2 traces a part of the disk-like structure where the outflow interacts with the upper layers. The concentric velocity patterns seen both in the blue- and red-shifted part of moment 1 maps of SO_2 (Fig. 4.3(i) and (l)) likely support the idea since the most extreme velocities occur in the region close to the star (unlike HDO and

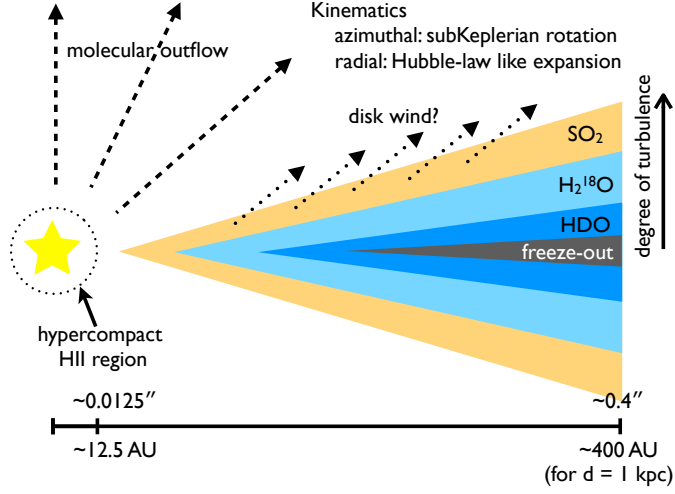


Figure 4.14 A cartoon showing the idea of a layered disk-like structure around AFGL 2591–VLA3. HDO is close to the cooler, quiescent mid-plane. H_2^{18}O is distributed in the warm mid-layer and SO_2 originates in the upper disk layers.

H_2^{18}O) as expected for an outflow origin.

4.5.2 Kinematics of the proposed disk-like structure and comparison to other disk sources

Our toy model suggests that the proposed disk-like structure around VLA3 undergoes sub-Keplerian rotation which cannot be directly inferred from the observed position-velocity maps. We speculate that a magnetic field slows the rotation down below pure Keplerian, which may help to transport the angular momentum outward in VLA3. Similar to the formation of low-mass stars, the magnetic field has been suggested to play an important role in the formation of high-mass stars as well (Girart et al. 2009; Beuther et al. 2010). In strongly magnetized clouds during collapse, magnetic braking is thought to regulate the formation of disks around stars (e.g., Basu & Mouschovias 1994; Allen et al. 2003; Mellon & Li 2008). Certainly in our case, the magnetic field does not fully dominate the kinematics of VLA3, otherwise a solid-body like velocity field would be expected in the inner region of the disk-like structure (c.f. Galli et al. 2006, Fig. 2). From OH maser observations, Hutawarakorn & Cohen (2005) measure a maser disk with radius about 750 AU and the magnetic field strength of a few mG toward AFGL 2591–VLA3, which may be sufficient to slow down the rotation. Subarcsecond dust polarization measurements of the magnetic field toward VLA3 and hence deriving the mass-to-flux ratio would be helpful to test our hy-

pothesis if the magnetic field indeed regulates the kinematics of the equatorial regions of young high-mass stars.

In addition to sub-Keplerian rotation, we found that Hubble-law like expansion occurs in the equatorial region of VLA3. The overall kinematics is similar to the SiO maser disk around Orion–IRc2 in which Keplerian rotation and decelerated expansion characterize the kinematics (Plambeck et al. 1990). The expanding motions in the disk could be due to the interaction between the stellar radiation and winds with the disk-like structure, providing the forces to push the gas outward (e.g., Hollenbach et al. 1994; Yorke & Welz 1996; Richling & Yorke 1997). On the other hand, the presence of an expanding velocity component in the disk-like structure could be the result of accretion through the mid-plane of the very inner region so that the expansion helps to conserve the angular momentum in the equatorial region. The infrared speckle imaging of AFGL 2591 by Preibisch et al. (2003) suggests that the outflow or wind is variable in time thus the accretion in the disk may not be continuous but episodic. In addition, little free-free emission is detected toward the source, indicating an evolutionary stage before the development of an ultracompact HII region (van der Tak & Menten 2005). As a result, the main accretion phase might have ceased although models show that massive young stars can continue to gain mass through the disk even after an ultracompact HII region has been developed (e.g., Keto 2007). Future high-resolution observations of multiple HDO lines and other dense gas tracers, such as N_2D^+ and CH_3CN , would be useful to constrain the physical condition and the kinematics of the disk-like structure around VLA3 better and understand its evolutionary stage of high-mass star formation.

Although massive disks showing pure Keplerian rotation traced by various molecules are reported such as the cases in IRAS 20126+4104 (C^{34}S ; Cesaroni et al. 2005), AFGL 490 (C^{17}O ; Schreyer et al. 2006) and NGC 7538S (H^{13}CN ; Sandell et al. 2003), cases showing non-Keplerian rotation were observed as well such as AFGL 2591 (HDO, H_2^{18}O ; this work) and IRAS 18089–1732 (NH_3 ; Beuther & Walsh 2008). In addition, massive disk candidates have a wide range of mass and size distributions derived via various tracers as summarized by Cesaroni et al. (2007). Despite the fact that the detections of massive disks to date are still limited, Keplerian rotation in the disks is typically found toward young massive stars with masses about $10 M_\odot$ such as the cases quoted above. For stellar masses about $16 M_\odot$, massive disks start to show non-Keplerian motion such as rigid-body rotation reported in the literature. For even higher stellar masses, the rotating structures (toroids) typically show solid-body rotation and are gravitationally unstable (Beltrán et al. 2005; Furuya et al. 2008). The sub-Keplerian rotation discovered in our work suggests that AFGL 2591–VLA3 may be a special case linking transition of velocity field of massive disks from pure Keplerian rotation to solid-body rotation though definitely more new detections of circumstellar disks around high-mass YSOs are required to examine this hypothesis.

4.5.3 Effect of the uncertainty in distance

The distance to AFGL 2591 is uncertain as discussed by van der Tak et al. (1999) and Rygl et al. (2011). In this paper, we assume a distance of 1 kpc with total luminosity of $20000 L_{\odot}$. From the radiative transfer modeling of HDO/H₂¹⁸O with our toy model, we found that the azimuthal motion of the proposed disk-like structure is dominated by sub-Keplerian rotation which is about 1/3 in strength of pure Keplerian rotation with a stellar mass of $16 M_{\odot}$, and the radial motion is consistent with Hubble-law like expansion with the analogue Hubble constant of $10 \text{ km s}^{-1} \text{ arcsec}^{-1}$. For other distances, our results remain unchanged except for the relative strengths of rotation and expansion. In particular, v_{R0} scales as $1/d$ and ξ scales as $1/\sqrt{d}$, so that for $d = 0.5$ and 3.0 kpc, v_{R0} is changed to 20 and $3.3 \text{ km s}^{-1} \text{ arcsec}^{-1}$, while ξ becomes 0.5 (effective Keplerian mass = $4 M_{\odot}$) and 0.2 (effective Keplerian mass = $0.7 M_{\odot}$). We suggest that the disk-like structure cannot undergo pure Keplerian rotation at any of these distances since the effective Keplerian masses are not consistent with the scaled total luminosities.

4.6 Conclusions

Our (sub)arcsecond resolution PdBI observations in millimeter continuum and in lines of HDO $1_{1,0}-1_{1,1}$, H₂¹⁸O $3_{1,3}-2_{2,0}$ and SO₂ $12_{0,12}-11_{1,11}$ successfully resolve the inner thousand AU region of the young high-mass star AFGL 2591–VLA3. We summarize our findings below.

1. From the visibility analysis of millimeter continuum and molecular lines, a compact source with diameter of ~ 800 AU at 1 kpc is found toward VLA3. Depending on the assumptions, the H₂ column density, number density and mass are estimated to be $1 \times 10^{24} \text{ cm}^{-2}$, $1 \times 10^8 \text{ cm}^{-3}$ and $0.2 M_{\odot}$, respectively.
2. A linear velocity gradient in the northeast-southwest direction is found across the source, which has an offset in P.A. by $\sim 40^{\circ}$ to the equatorial region (P.A. 0°) defined by the east-west outflow. We interpret this kinematical signature as a combination of rotation and radial expansion in the equatorial region of VLA3.
3. By introducing a toy model with simplified parameter optimization, we further constrain the rotation to be sub-Keplerian and the radial expansion to be Hubble-law like. This result is independent to the distance of the source.
4. We speculate that sub-Keplerian rotation in the equatorial region could be effect of magnetic field which turns the velocity profile from pure Kep-

lerian to sub-Keplerian. The expansion could be due to the interaction between the stellar radiation/winds and the gas in the equatorial region of VLA3.

5. Based on the molecular line profiles, the chemical structure of the proposed disk appears layered, with HDO near the mid-plane, H_2^{18}O in the mid-layer and SO_2 in the upper layers, judging from their turbulent line widths.

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Chapter 5

A candidate for rotation-regulated massive star formation: S255IR–SMA1

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submitted to A&A

Abstract

Context. It is poorly understood how massive stars form and whether accretion through a disk plays an important role. To study the accretion processes of the innermost regions of massive star-forming cores, high angular resolution observations in appropriate molecular line tracers are required.

Aims. Through subarcsecond resolution observations, we study the kinematics of the equatorial region of a massive star-forming core.

Methods. We observed the massive star forming region S255IR with the expanded Submillimeter Array (eSMA = SMA + JCMT + CSO 10.4m) at $\sim 0.3''$ resolution in a number of molecular lines as well as the continuum at 345 GHz.

Results. The 345-GHz continuum emission reveals a dense (10^9 cm^{-3}) disk-like structure around S255IR–SMA1. Two velocity components are identified with one ($V_{\text{LSR}} \sim 4 \text{ km s}^{-1}$) exclusively showing emission from hot core molecules around the forming massive star S255IR–SMA1. The component at $V_{\text{LSR}} \sim 9 \text{ km s}^{-1}$ likely represents the large scale structure surrounding gas of SMA1 and SMA2. Optically thick CH_3OH lines show a clear velocity gradient roughly perpendicular to the reported jet/maser/outflow emission, implying a rotating disk-like structure. However, the velocities are not Keplerian for the expected stellar mass, but either solid body or subKeplerian with significant turbulence. From accretion luminosity analysis and a comparison of the derived high CH_3OH abundance ($X \sim 10^{-6}$) with chemical models, we suggest that the dynamical age of S255IR–SMA1 is small (10^{3-4} yrs; $> 10\times$ the local free-fall time). The accretion rate is a few times 10^{-5} to a few times $10^{-4} M_{\odot} \text{ yr}^{-1}$.

Conclusions. We suggest that S255IR–SMA1 is a good candidate for massive star formation regulated a rotating, non-Keplerian structure. This structure is likely responsible for transporting gas from the outer envelope to the star. The actual Keplerian disk may hidden within 330 AU and requires at least $0.03''$ resolution observations in optically thin lines to properly resolve the disk kinematics in the equatorial plane of S255IR–SMA1.

5.1 Introduction

Disks and outflows are ubiquitous phenomena during the formation of low-mass stars ($M_{\star} \sim 1M_{\odot}$, Shu et al. 1987). The forming star obtains its mass through accretion from the collapsing envelope to the circumstellar disk and further from the circumstellar disk to the star, while excess angular momentum can be transported away via the bipolar outflow. A similar formation scenario (“turbulent core accretion”) has been proposed for the formation of higher-mass stars ($M_{\star} \approx 8M_{\odot}$, McKee & Tan 2003). The high detection rate of collimated outflows in high-mass star-forming regions (Zhang et al. 2001; Beuther et al. 2002) implies that circumstellar disks may also be common in high-mass star formation, and supports the idea that a scaled-up version of low-mass star formation may be applicable to the formation of higher-mass stars. However, the rare detections of “disks” in high-mass star-forming cores to date (Cesaroni et al. 2007; Kraus et al. 2010; Beuther et al. 2012; Sánchez-Monge et al. 2013) may imply a different formation mechanism for high-mass stars (Zinnecker & Yorke 2007), such as “competitive accretion” in a clustered environment (Bonnell et al. 2001; Pillai et al. 2011). To test different ideas of high-mass star formation, it is therefore essential to study the innermost parts of high-mass star-forming cores to infer accretion signatures at high-angular resolution.

The existence of accretion disks around massive young stars has been shown with varying degrees of confidence around a few objects (Cesaroni et al. 2007). For young B-type stars, the disks are found to be large ($\sim 10^{2-4}$ AU) and massive ($M_{\text{disk}} \leq M_{\star}$), which is quite different from the disks around low-mass stars ($M_{\text{disk}} \ll M_{\star}$). On the other hand, only large toroids undergoing solid-body rotation (appearing as linear features in position-velocity plots) with masses greater than stellar masses are found toward young O-type stars (Furuya et al. 2008; Beltrán et al. 2011). In all cases, the key evidence rests on the presence of velocity gradients (roughly) orthogonal to the direction of large scale outflows. However, this kinematical evidence needs to be interpreted with caution, since unresolved multiplicity, chemical gradients, and the effects of small-scale outflows can conspire to produce a signature masquerading as a velocity gradient of a disk around a single source (e.g., Comito et al. 2007).

In this paper, we present sub-arcsecond resolution observations of the high-mass star-forming cluster S255IR, located between two evolved HII regions S255 and S257 (Sharpless 1959). From the measurements of maser parallaxes, Rygl et al. (2010) estimated a distance of $1.59^{+0.07}_{-0.06}$ kpc. The total bolometric luminosity at 1.6 kpc is about $2 \times 10^4 L_{\odot}$ (corresponding to an single early B-type star), derived from a spectral energy distribution fit (Minier et al. 2005). The adopted luminosity is consistent with the ones derived by Jaffe et al. (1984) and Mezger et al. (1988) within a factor of few. Near the central region of S255IR, Y. Wang et al. (2011) reported two major continuum emission peaks (SMA1 and SMA2) and one blended emission peak (SMA3) at 1.3 mm. A similar continuum map at 1.1 mm is also observed by Zinchenko et al. (2012) with an additional peak (SMA4) $10''$ to the south of SMA1. Among these four sources, only SMA1 is associated with cm-wave emission with a spectral index corresponding to an optically thin HII region (also known as S255-2c, Snell & Bally 1986; Rengarajan & Ho 1996; Ojha et al. 2011). SMA1 is very likely forming a massive star, while the others may be forming low- to intermediate-mass stars. In this paper, we assume that the total bolometric luminosity is associated exclusively with SMA1 for simplicity. We expect that the error of the true bolometric luminosity of SMA1 is much less than a factor of 2.

Outflow signatures in S255IR are observed with different tracers. The CO 2–1 maps presented by Y. Wang et al. (2011) show a jet-like outflow in the NE–SW direction on $40''$ scales. The same maps also indicate that there may be another outflow in the NW–SE direction on $10''$ scales. At $2.2 \mu\text{m}$, Tamura et al. (1991) observed an extended NE–SW bipolar signature using scattered light (about $20''$ in size) together with a cluster of point sources, among which NIRS 1 (corresponding to SMA3) and NIRS 3 (corresponding to SMA1) are proposed to be associated with the bipolar feature. From their $2 \mu\text{m}$ polarimetric observations, Simpson et al. (2009) further suggest that SMA1 (NIRS 3) may be the driving source of the NE–SW bipolar feature, while SMA3 (NIRS 1) may be the driving source of a smaller bipolar feature in the N–S direction (about $10''$ in size). The NE–SW bipolar feature can be seen in $\text{Br}\gamma$ emission on $\sim 20''$ scales, H_2 line emission on $\sim 30''$ scales and H_2O maser emission at subarcsecond scales with a position angle of about 67° , which traces shock activity from the jet or outflow originating from SMA1 (Howard et al. 1997; Miralles et al. 1997; Goddi et al. 2007). It is likely that the jet-like CO outflow in the NE–SW direction (Y. Wang et al. 2011) is correlated with the features seen at infrared and radio wavelengths. Based on this disk-outflow geometry, SMA1 is a promising target for the search for disk signatures. Interestingly, there is a velocity gradient roughly perpendicular to the NE–SW outflow observed in CH_3CN and HCOOCH_3 lines on $\sim 2''$ scales (Y. Wang et al. 2011), although the emission is barely resolved. Certainly, high angular resolution observations are required to further investigate the nature of the massive disk target SMA1.

In Sect. 5.2, we present our sub-arcsecond eSMA observations and data reduction. Observational results and data analysis are reported in Sect. 5.3, while discussions are presented in Sect. 5.4. We summarize our work in Sect. 5.5.

5.2 Observations

The expanded Submillimeter Array (eSMA) project (Bottinelli et al. 2008) combines the Submillimeter Array (SMA¹), the James Clerk Maxwell Telescope (JCMT²), and the Caltech Submillimeter Observatory (CSO³) telescope as a single interferometer, which aims to enhance the sensitivity of the most extended SMA configuration in the 345-GHz band (Bottinelli et al. 2008). As part of science verification, S255IR was observed on February 10, 2010 with the SMA (7 antennas) and the JCMT only, resulting in uv sampling ranging from 100 k λ (2'') to 700 k λ (0.3'') at 345 GHz. The phase center was $\alpha(2000) = 06^{\text{h}}12^{\text{m}}54^{\text{s}}.00$, $\delta(2000) = 17^{\circ}59'23''.0$. The total on-source time is about 4 hours. A single spectral setup to observe CO $J = 3 - 2$ at 345.796 GHz was adopted. With this setup, we were able to observe the continuum at 345 GHz as well as some molecular lines within the total 4-GHz bandwidth (334.2 – 336.2 GHz and 344.2 – 346.2 GHz; see Sect. 5.3). We adopted 128 channels to sample each spectral window, resulting in a velocity resolution of 0.7 km s⁻¹. The quasars 0532+075 (~ 0.4 Jy; 14° away) and 0750+125 (~ 1.0 Jy; 24° away) were observed every 15 minutes for gain calibration. 3C273 was observed for passband calibration. Pallas (1.0 Jy) was adopted as the flux reference. We estimate the absolute flux uncertainty to be about 20%.

Data reduction was conducted by using the MIR package (Scoville et al. 1993) adapted for the SMA, while imaging and analysis were performed in MIRIAD (Sault et al. 1995). The phases of the continuum visibilities were self-calibrated by selecting the brightest clean components as the model. We applied natural weighting to both continuum and line data for best sensitivity. Line identification was conducted with the aid of molecular spectroscopy databases of JPL⁴ (Pickett et al. 1998) and CDMS⁵ (Müller et al. 2005).

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²The James Clerk Maxwell Telescope is operated by the Joint Astronomy Centre on behalf of the Science and Technology Facilities Council of the United Kingdom, the National Research Council of Canada, and (until 31 March 2013) the Netherlands Organisation for Scientific Research.

³Caltech Submillimeter Observatory is operated by the California Institute of Technology under cooperative agreement with the National Science Foundation (AST-0838261).

⁴<http://spec.jpl.nasa.gov/>

⁵<http://www.astro.uni-koeln.de/cdms/>

5.3 Results and analysis

5.3.1 Continuum emission at 345 GHz

Figure 5.1 shows the images and vector-averaged visibilities of the continuum emission at 345 GHz. The target source S255IR–SMA1 is resolved by the eSMA. We derive the source size in the visibility domain by assuming a Gaussian geometry. The deconvolved source size for SMA1 is $0''.23 \times 0''.19$ ($\sim 370 \text{ AU} \times 300 \text{ AU}$ at $d = 1.6 \text{ kpc}$) with P.A. of -29° (Table 5.1). Although the aspect ratio (~ 0.8) is close to unity, the position angle implies that the continuum emission may trace a flattened structure roughly perpendicular to the large scale CO outflow with P.A. $\sim 65^\circ$ (Y. Wang et al. 2011). From the visibility modeling of the peak position of SMA1, we found an offset $\sim 0.08''$ to the south-east direction relative to the position derived from the SMA 1.3mm observations (Table 5.1; Y. Wang et al. 2011). The offset may be real, or due the phase error since the adopted phase calibrators are faint and no so close to the target (Sect. 5.2), or due to the self-calibration process.

The other mm-wave sources, SMA2 and SMA3 reported by Y. Wang et al. (2011), are not detected at the $1-\sigma$ level ($2.4 \text{ mJy beam}^{-1}$). SMA4 observed by Zinchenko et al. (2012) is outside our field of view. The non-detection of SMA2 and SMA3 is likely due to the spatial filtering of the eSMA observations. The array is not sensitive to structures larger than $2''$. From SMA observations of S255IR at 1.3 mm, Y. Wang et al. (2011) reported peak flux densities of SMA1, SMA2 and SMA3 of 95, 52 and 30 mJy beam^{-1} (beam size $\sim 2''$), respectively. Assuming all the sources have the same spectral index and source size, our detected peak flux density of 179 mJy of SMA1 at 345 GHz implies that the peak flux density of SMA2 and SMA3 at 345 GHz should be 98 and 57 mJy beam^{-1} , respectively, which should be detected with an S/N of at least 24. From the SMA 1.3 mm continuum image (Y. Wang et al. 2011), the emission toward SMA1 is compact and centrally peaked, while SMA2 is resolved with the $\sim 2''$ beam and less centrally peaked. The weaker and diffuse emission from SMA3 is likely from the common envelope of SMA1 and SMA2. Therefore, we suggest that the continuum emission of SMA2 and SMA3 at 345 GHz is likely resolved out by the eSMA.

5.3.1.1 H_2 mass and column density

From the measured 345-GHz continuum, we estimate the H_2 mass and H_2 column density toward S255IR–SMA1. Assuming optically thin emission, the H_2 column density at the emission peak can be estimated via

$$N(\text{H}_2) = \frac{I_\nu a}{2m_{\text{H}}\Omega_b\kappa_\nu B_\nu(T_{\text{d}})}, \quad (5.1)$$

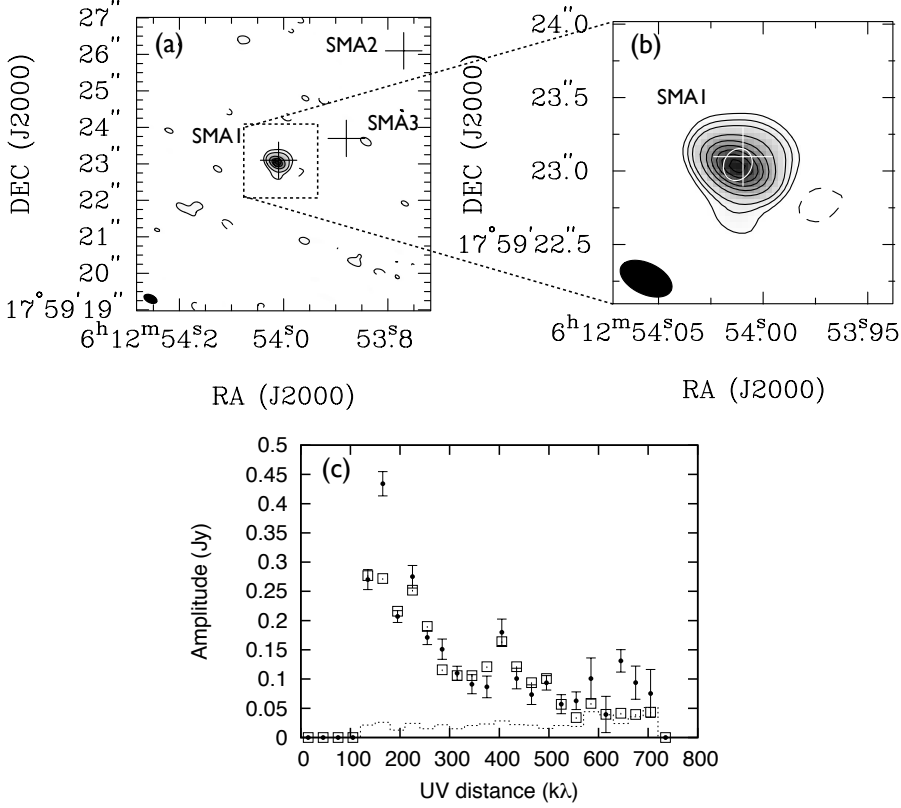


Figure 5.1 (a) Continuum image of S255IR at 345 GHz. Natural weighting is applied, resulting a clean beam size of $0.38'' \times 0.21''$, P.A. 65° (filled ellipse at bottom-left corner). Contour levels are -3, 3, 10, 30, 50, and 70σ with $1\text{-}\sigma$ noise level of 2.4 mJy beam^{-1} . The peak intensity is 179 mJy beam^{-1} . The positions of the continuum sources SMA1, SMA2 and SMA3 detected by Y. Wang et al. (2011) are marked as crosses. The sources SMA2 and SMA3 are not detected at $1\text{-}\sigma$ noise level. (b) Continuum image of S255IR–SMA1 at 345 GHz. Contour levels are -3, 3, 6, 10, 20, 30, 40, 50, 60 and 70σ with $1\text{-}\sigma$ noise level of 2.4 mJy beam^{-1} . The white cross is the peak position derived from the SMA observations at 1.3 mm. The white ellipse represents the source FWHM size derived from the visibility fit. The best-fit source FWHM size is $0.23''$ ($\sim 370\text{ AU}$) by $0.19''$ ($\sim 300\text{ AU}$) with P.A. -29° . (c) Vector-averaged visibilities of the continuum emission at 345 GHz. The observed data are shown as filled circles with error bars and the model fit with a Gaussian is shown as open squares. The dotted histogram represents the zero-intensity values.

Table 5.1. Physical properties of the 345 GHz continuum in S255IR

Component	RA(J2000) (h m s)	Dec(J2000) (° ' ")	θ_{maj}^a (")	θ_{min}^a (")	P.A. ^a (°)	I_ν^b (mJy beam ⁻¹)	S_ν^c (Jy)	$N(\text{H}_2)^b$ ($\times 10^{24}$ cm ⁻²)	$M(\text{H}_2)^c$ ($M_\odot$)	$n(\text{H}_2)^c$ ($\times 10^9$ cm ⁻³)
SMA1 ^{d,e}	06 12 54.01	17 59 23.1	0.23	0.19	-29	179	0.30	2.5	0.36	3.4
SMA2 ^e	06 12 53.77	17 59 26.1	...	...	...	< 2.4	...	< 0.03	...	...
SMA3 ^e	06 12 53.88	17 59 23.7	...	...	...	< 2.4	...	< 0.03	...	...

Note. — ^aGaussian FWHM size and position angle. ^bPeak intensity and beam-averaged H_2 column density assuming $T_{\text{dust}} = 140$ K. $1-\sigma$ upper limit is given for SMA2 and SMA3. We note that our dataset is not sensitive to scales greater than $\sim 2''$ (100 k λ). The emission from SMA2 and SMA3 is likely filtered out. ^cIntegrated flux density, H_2 mass and H_2 volume density. We assume $T_{\text{dust}} = 140$ K. The values are calculated assuming a distance of 1.6 kpc. If the distance is not 1.6 kpc, $M(\text{H}_2)$ and $n(\text{H}_2)$ are scaled as $0.36(d/1.6 \text{ kpc})^2 M_\odot$ and $3.4(d/1.6 \text{ kpc})^{-1} \text{ cm}^{-3}$, respectively. ^dThe peak position derived from the visibility fit is RA(J2000) = 06^h12^m54^s.012, Dec(J2000) = 17°59'23".05. ^eThe listed positions are adopted from Y. Wang et al. (2011).

where I_ν is the peak flux density, a is the gas-to-dust ratio (100), Ω_b is the beam solid angle, m_H is the mass of atomic hydrogen, κ_ν is the dust opacity per unit mass and $B_\nu(T_d)$ is the Planck function at dust temperature T_d (Hildebrand 1983). We apply the interpolated value of $\kappa_\nu(870\mu\text{m}) \approx 2.1 \text{ cm}^2 \text{ g}^{-1}$ as suggested by Ossenkopf & Henning (1994) for gas densities of $10^6 - 10^8 \text{ cm}^{-3}$ and coagulated dust particles with thin ice mantles. The dust temperature is assumed to be 140 K (see excitation analysis, Sect. 5.3.2.2). The H_2 mass is estimated from the total flux density derived from the visibility fit (Table 5.1) via

$$M(\text{H}_2) = \frac{S_\nu d^2 a}{\kappa_\nu B_\nu(T_d)}, \quad (5.2)$$

where S_ν is the total flux density of dust emission and d (1.6 kpc) is the distance to the source (Hildebrand 1983). Assuming a spherical source with 330 AU in diameter (geometric mean of the decomposed size), the H_2 number density is also derived. The calculations of N_{H_2} and M_{H_2} are not corrected for any contribution of free-free emission at 345 GHz. The VLA measurement of free-free emission at 15 GHz is 3.1 mJy (Ojha et al. 2011). The extrapolated optically thin free-free emission at 345 GHz is 2.3 mJy, which is only 0.8% of the total flux density at 345 GHz. Therefore, the free-free emission at 345 GHz can be ignored. We summarized these results in Table 5.1. Toward S255IR–SMA1, we find that the beam-averaged H_2 column density is $\sim 2.5 \times 10^{24} \text{ cm}^{-2}$. The H_2 mass is $0.36 M_\odot$. This is only a few percent of the stellar mass expected for an early B-type star. A high H_2 number density of $\sim 3.4 \times 10^9 \text{ cm}^{-3}$ is derived. If the assumed dust temperature has an uncertainty of a factor of 2, the derived quantities have a factor of 2 in uncertainty. We expect that a significant amount of the continuum flux is missing due to the limited short spacing data of the eSMA, therefore the derived quantities should be treated as lower limits. It is because of this spatial filtering that we can study the dense environment of S255IR down to few hundred AU scales for the first time without the contamination from structures at thousand AU scales.

5.3.2 Molecular line emission

The 4-GHz bandwidth of the eSMA allows us to observe several molecular lines including simple molecules (CO, SO, SO_2 , H^{13}CN and HCCCN) as well as hot-core molecules (HCOOH , CH_3OH and NH_2CHO). All of our detected species and transitions are summarized in Table 5.2.

5.3.2.1 Molecular images and spectra

In Fig. 5.2, we present the molecular gas distributions of S255IR–SMA1 and the individual spectra taken at the continuum peak position. We do not image

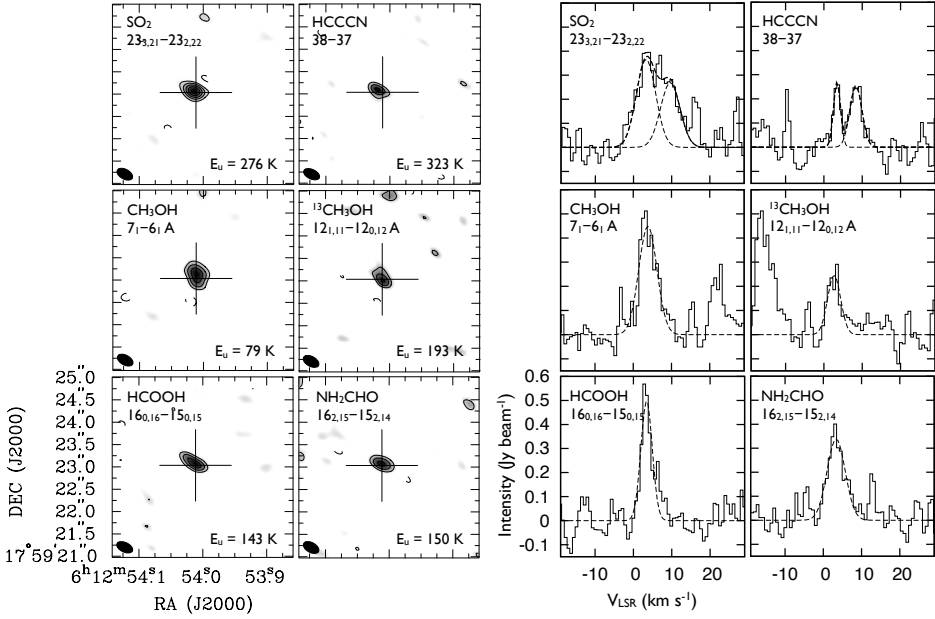


Figure 5.2 (Left) Sample zero moment maps of molecular species toward S255IR–SMA1. The cross represents the peak position of the continuum emission derived from our data. The typical angular resolution is $0''.38 \times 0''.22$, P.A. 63° . The contour levels are $-3, 3, 5, 7, \dots \sigma$ for all the molecules except ¹³CH₃OH that the contours are $-3, 3, 4, 5, \dots \sigma$. The $1\text{-}\sigma$ noise levels for SO₂, HCCCN, CH₃OH, ¹³CH₃OH, HCOOH and NH₂CHO are 0.40, 0.28, 0.34, 0.22, 0.25 and 0.28 Jy beam⁻¹ km s⁻¹, respectively. (Right) The beam averaged spectra taken at the position of the continuum peak. The species are identical to the maps shown in the left panels. The dashed lines represent the Gaussian fit of the spectra. The fitting results are summarized in Table 5.2.

the CO $J = 3 - 2$ emission due to the missing flux (expected $> 90\%$; Sect. 5.2). SO $8_8 - 7_7$ is blended with CH₃OH at 344.312 GHz and H¹³CN $J = 4 - 3$ is blended with SO₂ at 345.338 GHz. Therefore, we do not show their images in Fig. 5.2. For the other species, we found that the emission is compact and near the position of the continuum peak: CH₃OH $7_1 - 6_1 A$ is resolved, and SO₂ $23_{3,21} - 23_{2,22}$ is barely resolved. Other species are unresolved. Our results suggest that S255IR–SMA1 contains active hot-core chemistry because we detect compact emission from complex organic molecules which are also observed by Y. Wang et al. (2011) and Zinchenko et al. (2012).

Table 5.2. Detected molecular lines in S255IR–SMA1

Molecule	Frequency (MHz)	Transition	E_u^a (K)	V_{LSR}^b (km s ⁻¹)	ΔV^c (km s ⁻¹)	$\int I_\nu dV^d$ (Jy beam ⁻¹ km s ⁻¹)	Note
1st velocity component							
CO	345795.990	3–2	33	...	...	...	Not imaged.
SO	344310.612	8 ₈ –7 ₇	87	3.8 (fixed)	8.9 ± 1.3	2.35 ± 0.44	b ^c :CH ₃ OH(344312)
H ¹³ CN	345339.760	4–3	41	~ 3.4	~ 4.9	...	b ^c :SO ₂ (345338)
SO ₂	334673.352	8 _{2,6} –7 _{1,7}	43	5.7 ± 0.8	13.3 ± 1.8	2.86 ± 0.33	single line fit, 2σ detection
	336089.226	23 _{3,21} –23 _{2,22}	276	3.3 ± 0.4	6.0 (fixed)	2.33 ± 0.21	
	345338.539	13 _{2,12} –12 _{1,11}	93	~ 3.4	~ 4.9	...	b ^c :H ¹³ CN(345339)
HCCCN	345609.010	38–37	323	3.4 ± 0.2	2.1 ± 0.5	0.61 ± 0.13	
HCOOH	334265.827	15 _{2,14} –14 _{2,13}	142	2.8 ± 0.2	3.5 ± 0.7	1.89 ± 0.14	
	345030.596	16 _{0,16} –15 _{0,15}	143	3.4 ± 0.1	3.5 ± 0.3	1.86 ± 0.15	
CH ₃ OH	334426.571	3 ₀ –2 ₁ E , $v_t = 1$	314	4.6 ± 0.6	6.6 ± 1.5	0.82 ± 0.16	
	335133.570	2 ₂ –3 ₁ A	45	3.6 ± 0.2	3.1 ± 0.4	1.36 ± 0.14	
	335582.017	7 ₁ –6 ₁ A	79	3.8 ± 0.2	5.6 ± 0.5	2.67 ± 0.22	
	344312.267	10 ₋₂ –11 ₋₃ E , $v_t = 1$	492	3.8 (fixed)	4.9 (fixed)	1.69 ± 0.30	b ^c :SO(344310)
	344443.433	19 ₁ –18 ₂ A	451	4.0 ± 0.2	3.7 ± 0.4	1.53 ± 0.14	
	345903.916	16 ₁ –15 ₂ A	333	2.7 ± 0.3	5.0 ± 0.7	2.42 ± 0.31	
	345919.260	18 ₋₃ –17 ₋₄ E	459	4.0 ± 0.5	5.3 ± 1.1	2.13 ± 0.38	
¹³ CH ₃ OH	335560.207	12 _{1,11} –12 _{0,12} A	193	2.7 ± 0.3	4.0 ± 0.6	1.05 ± 0.15	
NH ₂ CHO	336136.877	16 _{2,15} –15 _{2,14}	150	3.4 ± 0.4	5.6 ± 1.0	2.02 ± 0.30	
	345182.618	17 _{0,17} –16 _{0,16}	152	3.7 ± 0.2	3.7 ± 0.4	2.09 ± 0.19	
	345326.689	16 _{1,15} –15 _{1,14}	145	3.3 ± 0.4	5.3 ± 0.9	2.52 ± 0.43	partially b ^c :SO ₂ (345338)

Table 5.2 (cont'd)

Molecule	Frequency (MHz)	Transition	E_u^a (K)	V_{LSR}^b (km s ⁻¹)	ΔV^c (km s ⁻¹)	$\int I_\nu dV^d$ (Jy beam ⁻¹ km s ⁻¹)	Note
2nd velocity component							
SO	344310.612	8 ₈₋₇ 7	87	10.6 ± 0.2	3.3 ± 0.4	1.26 ± 0.18	
H ¹³ CN	345339.760	4-3	41	~ 8.7	~ 4.2	...	b ^e :SO ₂ (345338)
SO ₂	336089.226	23 _{3,21} -23 _{2,22}	276	9.6 ± 0.5	6.0 (fixed)	1.72 ± 0.21	
	345338.539	13 _{2,12} -12 _{1,11}	93	~ 8.7	~ 4.2	...	b ^e :H ¹³ CN(345339)
HCCCN	345609.010	38-37	323	8.3 ± 0.3	3.7 ± 0.7	1.01 ± 0.17	

Note. — ^aUpper level energy. ^bLine center velocity. The formal fitting errors are given, however, the channel resolution is ~ 0.7 km s⁻¹. ^cFWHM line width. The formal fitting errors are given, however, the channel resolution is ~ 0.7 km s⁻¹. ^dIntegrated line intensity. The formal fitting errors are given. The absolute flux error (~ 20%) is not considered. ^eLine blending.

Although spatially the distributions of the molecules presented in Fig. 5.2 (Left) are similar, in the velocity domain these species show significant differences (Fig. 5.2, Right). To quantify the line profiles, we applied Gaussian line profile fits to all the imaged molecules and transitions. The results are summarized in Table 5.2. For simple molecules such as SO_2 and HCCCN , the lines appear wider than the hot-core molecules (e.g., CH_3OH , HCOOH and NH_2CHO). A significant difference in LSR velocity also exists between these two groups of molecules. The $\text{HCCCN } J = 38 - 37$ spectrum shows that the line profile may be double-peaked. The double-peaked line profile can be seen much more clearly in the $\text{SO } 8_8 - 7_7$ and the $\text{H}^{13}\text{CN } J = 4 - 3$ spectra although these two line profiles are contaminated by other molecules (Fig. 5.3). We suggest that the double-peaked line profile is likely real since the depth of the dip is significantly greater than the noise level. We assume that the double-peaked profile is a combination of two different velocity components. To fit the SO line profile, we assumed that the LSR velocity of $\text{CH}_3\text{OH } 10_{-2} - 11_{-3} \text{ Ev}_t = 1$ is fixed to the mean value (3.8 km s^{-1}) derived from other isolated CH_3OH lines. To fit the blended $\text{H}^{13}\text{CN}/\text{SO}_2$ line profile, only one set of double-peaked profile is used since the difference of the rest frequencies of the two lines is small ($\sim 1 \text{ km s}^{-1}$).

Our eSMA data show that there are two velocity components around S255IR–SMA1: a “blue-shifted” one at mean LSR velocity of 3.6 km s^{-1} and a “red-shifted” one at mean LSR velocity of 9.2 km s^{-1} . These two components are different in chemical point of view. The “blue-shifted” component contains both simple molecules and hot-core molecules, while the “red-shifted” component only shows the emission from simple molecules. Y. Wang et al. (2011) reported that the LSR velocity of $^{13}\text{CO } J = 2 - 1$ from the IRAM 30m telescope (7.7 km s^{-1}) is different from the velocity measured by the SMA based on CH_3CN (5.2 km s^{-1}). From NH_3 observations, Zinchenko et al. (2012) reported a LSR velocity of 4.4 km s^{-1} . Combining all the observational results, we suggest that the hot-core species are concentrated in a compact and dense region while the simple molecules are widely distributed (and observed in both velocity components). The nature of the difference in LSR velocities of the two groups, however, is not clear. The $\text{C}^{18}\text{O } 2-1$ velocity map presented by Y. Wang et al. (2011) shows a clear velocity gradient from SMA1 ($V_{\text{LSR}} \sim 5 \text{ km s}^{-1}$) to SMA2 ($V_{\text{LSR}} \sim 9 \text{ km s}^{-1}$) and this velocity gradient can be modeled as Keplerian rotation. Likely, $\text{C}^{18}\text{O } 2-1$ traces the common envelope of the binary SMA1 and SMA2, which has a higher mean LSR velocity. In this case, the widely distributed simple molecules are more affected by the interaction of SMA1 and SMA2, while the compact hot-core molecules are less affected by SMA2 and therefore can represent the true systemic velocity of S255IR–SMA1.

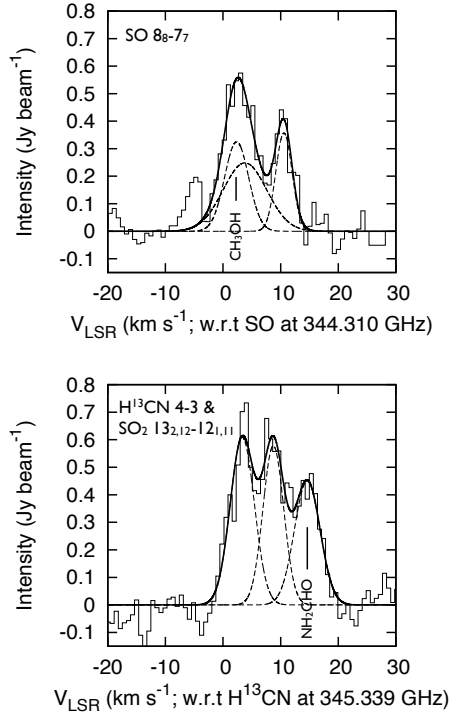


Figure 5.3 Blended line profiles of SO $8_8 - 7_7$ and $\text{H}^{13}\text{CN } J = 4 - 3$ plus $\text{SO}_2 \ 13_{2,12} - 12_{1,11}$. The dashed lines represent the Gaussian fit of individual components, while the solid lines are the synthetic spectra.

5.3.2.2 Excitation analysis

The detected seven transitions of CH_3OH allow us to perform excitation analysis toward S255IR–SMA1. We adopted the “population diagram” method described by Goldsmith & Langer (1999). The observed intensity of a given transition of CH_3OH can be transformed to the upper state column density per upper state statistical weight in logarithmic scale via

$$\ln\left(\frac{N_u^{\text{obs}}}{g_u}\right) = \ln\left(\frac{2.04 \times 10^{20}}{\theta_a \theta_b} \frac{W}{g_I g_K \nu_0^3 S \mu_0^2}\right) \text{ cm}^{-2}, \quad (5.3)$$

where θ_a and θ_b are the major and minor axes of the clean beam in arcsec, respectively, W is the integrated intensity in $\text{Jy beam}^{-1} \text{ km s}^{-1}$, g_I and g_K are the spin and projected rotational degeneracies, respectively, ν_0 is the rest frequency in GHz, S is the line strength and μ_0 is the dipole moment of the transition in Debye. Assuming that the level populations of CH_3OH follow a Boltzmann distribution at a single excitation temperature T_{ex} , the left hand side of Eq. 5.3 can

be modeled as

$$\ln\left(\frac{N_{\text{u}}^{\text{model}}}{g_{\text{u}}}\right) = \ln\left(\frac{N_{\text{tot}}}{Q}\right) - \frac{E_{\text{u}}}{kT_{\text{ex}}} - \ln C_{\tau} + \ln f, \quad (5.4)$$

where N_{tot} is the total column density, Q is the partition function, E_{u} is the upper state energy, k is the Boltzmann constant, C_{τ} ($= \tau/1 - e^{-\tau}$) is the correction term of line opacity, and f is the beam filling factor (≤ 1). The line center opacity assuming a Gaussian line profile is

$$\tau = \frac{c^3}{8\pi\nu_0^3} \frac{A_{\text{ul}}}{\Delta V} \frac{g_{\text{u}} N_{\text{tot}}}{Q} e^{-E_{\text{u}}/kT_{\text{ex}}} (e^{h\nu_0/T_{\text{ex}}} - 1), \quad (5.5)$$

where c is the speed of light, A_{ul} the Einstein-A coefficient, ΔV is the FWHM line width, and h is the Planck constant. For a given set of T_{ex} , N_{tot} and f , the left hand side of Eq. 5.4 can be calculated and compared with the left hand side of Eq. 5.3. We perform χ^2 minimization to search for a best-fit model. In Fig. 5.4, we plot the logarithm of the column densities from our data (Eq. 5.3) versus E_{u} (Eq. 5.4) as the red circles. The best-fit model is overplotted as the blue crosses. From this simple analysis, we found that all the CH₃OH transitions have opacities close or greater than unity. The excitation temperature is 140 ± 20 K. The beam averaged column density is $2.0 \pm 0.5 \times 10^{18} \text{ cm}^{-2}$. The beam filling factor is 0.55 ± 0.10 , indicating either a single compact structure in the beam or a clumpy structure filling the beam. Since CH₃OH is resolved (Fig. 5.2), the later interpretation is favored. We further estimate the fractional abundance of CH₃OH toward S255IR–SMA1 by taking the ratio of CH₃OH column density and H₂ column density derived from continuum emission (Sect. 5.3.1.2). We find that $X[\text{CH}_3\text{OH}]$ is about 8×10^{-7} . In this estimate, we assume the derived H₂ column density is totally associated with the hot-core component ($V_{\text{LSR}} \sim 4 \text{ km s}^{-1}$). Therefore, the derived CH₃OH fractional abundance should be treated as a lower limit, and may be twice as high, assuming equal contributions from both velocity components. The high CH₃OH fractional abundance implies an active hot-core chemistry (e.g., Garrod et al. 2008). For other molecules, we estimate the total column densities and fractional abundances with the assumptions of optically thin emission, a single excitation temperature at 140 K and beam filling factor unity via Eq. 5.4. If the assumed excitation temperature has a factor of 2 in uncertainty, the derived column density has a factor of ~ 2 in uncertainty. The optically thin assumption may not be valid if the peak intensity for a given molecule is similar to the one of CH₃OH. For a consistency check, we estimate the line center opacities of the observed lines via Eq. 5.5. We find that all observed lines do have moderate opacities (0.2–0.5) except CH₃OH which is optically thick (≥ 1). Therefore, the derived molecular column densities are underestimated by 10%–30%. Results are summarized in Table 5.3.

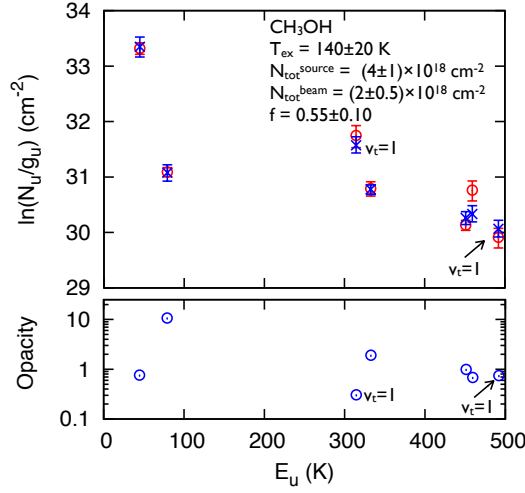


Figure 5.4 Population diagram analysis of the CH₃OH transitions. The red color represents the observed data, while the blue color represents the best-fit model. The estimated line center opacities are also shown in the bottom panel. See Sect. 5.3.2.2 for details.

Table 5.3. Molecular column density and fractional abundance

Molecule	N (cm^{-2})	τ_0^a	X	Note
SO	5.4×10^{15}	0.3	2.2×10^{-9}	
SO ₂	7.1×10^{16}	0.4	2.8×10^{-8}	
HCCCN	4.3×10^{14}	0.2	1.7×10^{-10}	
HCOOH	3.3×10^{16}	0.5	1.3×10^{-8}	
CH ₃ OH	2.0×10^{18}	≥ 1	8.0×10^{-7}	derived from PD
NH ₂ CHO	1.7×10^{15}	0.4	6.7×10^{-10}	

Note. — We assume an excitation temperature of 140 K in the estimation. The derived column density and fractional abundance should be treated as lower limits since non-negligible opacities are present. We only report the values for the blue-shifted component and we assume that the adopted H₂ column density ($2.5 \times 10^{24} \text{ cm}^{-2}$) refers to the blue-shifted component only. ^aEstimated line center opacity.

From the population diagram analysis outlined above, we found that the excitation temperature toward S255IR–SMA1 is about 140 K. The high H_2 volume density ($3 \times 10^9 \text{ cm}^{-3}$) derived from the continuum emission (Sect. 5.3.1.2) implies that collisions may dominate the excitation of CH_3OH and hence the derived excitation temperature may be a good approximation of the true kinetic temperature of the source. To further investigate this issue, we adopted the non-LTE code RADEX in the large velocity gradient (LVG) regime (van der Tak et al. 2007) to model the observed CH_3OH lines. Limited by the collisional rate coefficients (Rabli & Flower 2010; Schöier et al. 2005), we only included the four *A*-type transitions in the calculations (Table 5.2). The free parameters in RADEX are kinetic temperature, H_2 volume density and CH_3OH column density. We fix a mean FWHM line width of 3.8 km s^{-1} in the calculations. Additionally, the beam filling factor is also taken into account for comparing with the observations. To find the excitation conditions, we performed χ^2 minimization in the 4-dimensional parameter space. The χ^2 distributions near the global minimum along each parameter axis are shown in Fig. 5.5. We found that the derived H_2 number density ($\geq 10^9 \text{ cm}^{-3}$) is quite high and is comparable to the one estimated from the continuum emission. At such a high H_2 density, the level populations are likely thermalized (c.f., the critical density of CH_3OH is about $10^6\text{--}10^7 \text{ cm}^{-3}$). The derived kinetic temperature is similar to the excitation temperature obtained from the population diagram analysis. In addition, the derived CH_3OH column density and beam filling factor are similar to the solution derived from the population diagram analysis as well. We conclude that the level populations of CH_3OH are dominated by collisions with H_2 in S255IR–SMA1. A gas density of at least 10^9 cm^{-3} is present in a clumpy environment with a kinetic temperature of 140 K.

5.3.2.3 Kinematics

In Fig. 5.6, we show the gas kinematics traced by SO_2 , HCOOH and CH_3OH . We observed velocity gradients roughly in the north-south direction, which is approximately perpendicular to the large scale jet-like CO outflow observed by Y. Wang et al. (2011). A similar velocity gradient in the north-south direction is also seen in CH_3CN and HCOOCH_3 lines at about $2''$ resolution (Y. Wang et al. 2011). Our sub-arcsecond resolution eSMA observations allow us to further obtain the kinematic information down to scales of few hundred AU. A clear velocity gradient traced by CH_3OH is seen, suggesting a rotating structure. In Fig. 5.7, we show the position-velocity (PV) maps of SO_2 , HCOOH and CH_3OH . The PV cut is centered at the continuum peak position with P.A. 155° . The emission morphology in the PV maps does not follow Keplerian rotation. Rather, the signature is more like a linear velocity gradient. This observed gradient can be the result of two different motions: rigid-body rotation, or Keplerian-like rota-

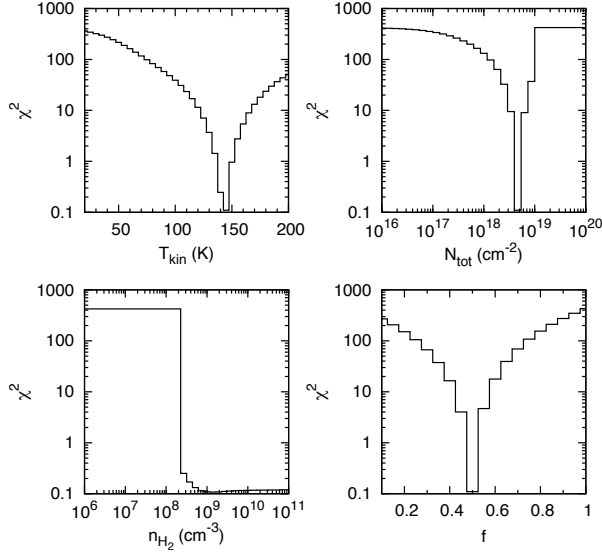


Figure 5.5 Excitation analysis of CH_3OH lines with the non-LTE code RADEX. The χ^2 distributions near the global minimum along each parameter axis are shown.

tion plus strong turbulence which smears out the “butterfly” signature of a pure Keplerian rotation. In addition, the observed spectra from the hot-core molecules (Fig. 5.2) are all single-peaked, not double-peaked as usually seen from a Keplerian rotating structure. We estimated the magnitude of the linear velocity gradient to be $0.8 - 2.3 \text{ km s}^{-1}$ per 100 AU, or $1.3 - 3.8 \text{ km s}^{-1}$ at a radius 165 AU (the geometric mean radius from continuum emission). From the spatial distribution of the CO outflow (Y. Wang et al. 2011) and water masers (Goddi et al. 2007), the rotating structure is not likely face-on. Assuming an disk inclined by 45° , the Keplerian rotation speed at radius 165 AU is about 4.6 km s^{-1} for a stellar mass of $8 M_\odot$. The observed velocity gradients imply that the stellar mass is only $0.6 - 5.5 M_\odot$ if the rotation is Keplerian. From this analysis, we suggest that pure Keplerian rotation for a luminous massive source ($2 \times 10^4 L_\odot$) does not fit our data. The observed rotating structure may have sub-Keplerian rotation and turbulence, or rigid-body rotation. Sensitive observations at at least $0.03''$ resolution may be helpful to resolve the kinematics.

We further study the kinematics traced by CH_3OH by adopting a toy model with the radiative transfer code RATRAN (Hogerheijde & van der Tak 2000). Due to the low S/N ratio of CH_3OH data, we only focus on the morphology of PV map and the line profile and perform a qualitative study. We assume a sphere with a diameter of 330 AU. The gas density and kinetic temperature profiles are cho-

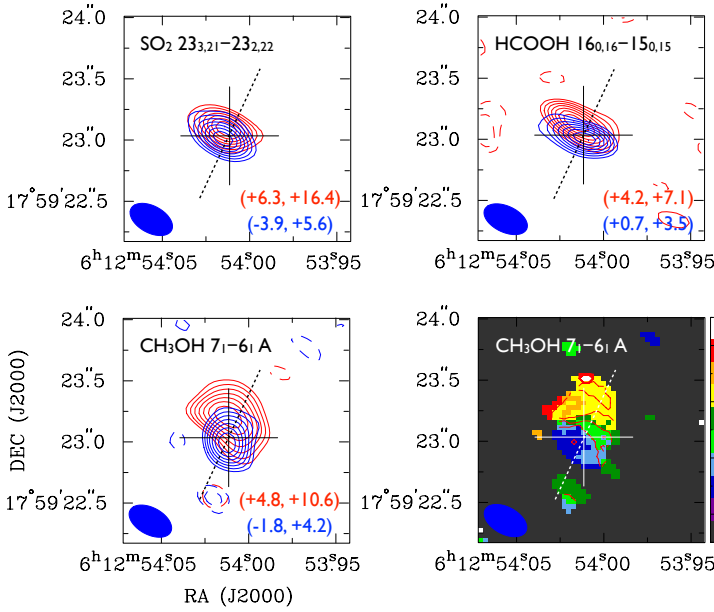


Figure 5.6 Kinematics of S255IR–SMA1 traced by SO₂ 23_{3,21}–23_{2,22}, HCOOH 16_{0,16}–15_{0,15} and CH₃OH 7₁–6₁ A. Maps with blue and red contours are the the zero moment maps integrated over different velocity ranges as indicated on the plots. The first moment map of CH₃OH 7₁–6₁ A is plotted in color scale. The cross and the ellipse in each map represent the peak position of the continuum emission and the clean beam size, respectively. The dotted line represents the position-velocity cut at P.A. 155°.

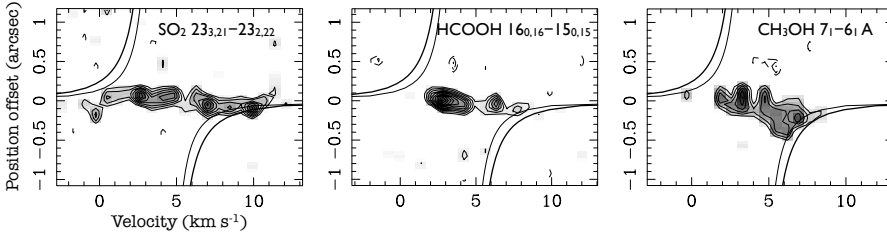


Figure 5.7 Position-velocity maps taken at the continuum peak with P.A. 155°. The curves represent the projected (45°) Keplerian rotation velocities of a star with 14 $M_{\odot}$ (thick) and a star with 8 $M_{\odot}$ (thin). None of the observed position-velocity maps fits the Keplerian rotation.

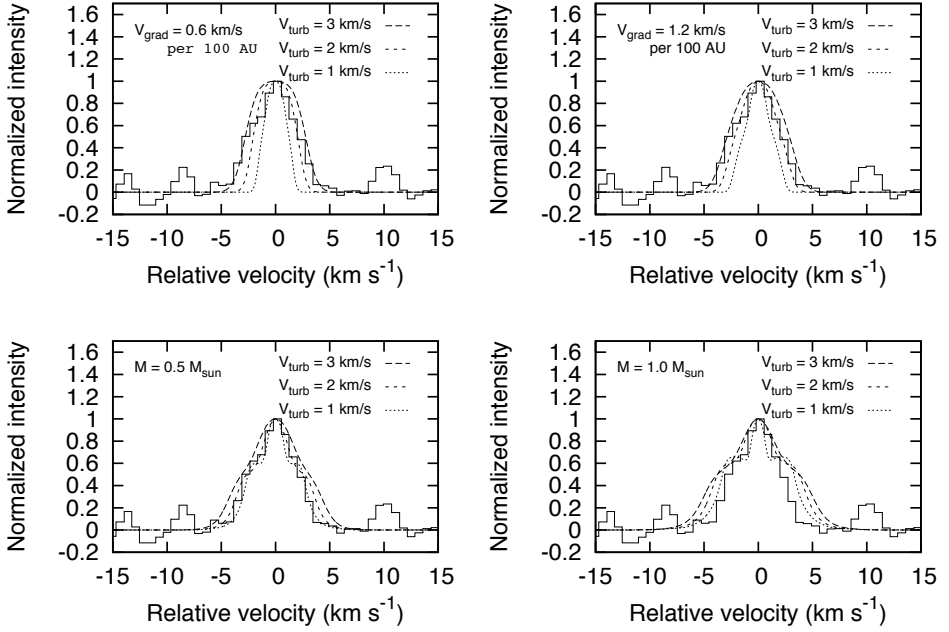


Figure 5.8 Toy models of kinematics. The upper panels are the rigid-body rotation models, while the bottom panels are the Keplerian models.

sen as $n(r) = 1.7 \times 10^9 (r/165\text{AU})^{-1.5} \text{ cm}^{-3}$ and $T(r) = 103 (r/165\text{AU})^{-0.4} \text{ K}$, respectively. The reference density is chosen such that the mean density is matched to the derived value from our 345-GHz continuum. The reference temperature is selected such that the mass-weighted temperature equals the kinetic temperature derived from the excitation analysis. Since the observed CH₃OH lines are optically thick, the fractional abundance of the test molecule is chosen to make the model line optically thick as well. We consider two different kinematics: Keplerian rotation and rigid-body rotation, in which stellar mass and the strength of the linear velocity gradient are the respective free parameters. In addition, the strength of turbulent FWHM line width is set as free parameter. We do not perform any parameter optimization, but rather focus on the general trend.

In Fig. 5.8, the rigid-body rotation models are shown in the upper panels, while the Keplerian models are presented in the bottom panels. The observed CH₃OH spectrum (averaged over a $0.8'' \times 0.8''$ region) is shown in solid lines. The observed CH₃OH line profile is single-peaked, rather than double-peaked. This fact sets a strong constraint on the stellar mass in the Keplerian models. As we demonstrate in Fig. 5.8 (bottom-right), a stellar mass of $1 M_{\odot}$ generates too wide a line profile even if the turbulent line width is small. If we reduce the stellar mass to $0.5 M_{\odot}$, the observed line profile can be modeled well with

turbulent FWHM line widths of $1\text{--}2 \text{ km s}^{-1}$. Based on our simple Keplerian toy models, we suggest that the observed rotating structure traced by CH_3OH is not in Keplerian rotation around a star of the expected mass of $\geq 8 M_\odot$. The rotation may be strongly sub-Keplerian. In the rigid-body rotation models, we found that the line profiles are more sensitive to the adopted turbulent line width. Our results suggest that it is possible to model the kinematics traced by CH_3OH as rigid-body rotation with a typical turbulent line width of $2\text{--}3 \text{ km s}^{-1}$. Based on our toy models, we cannot distinguish these two different kinematics in our data. Turbulence is important in shaping the line profiles.

5.4 Discussion

5.4.1 Luminosity, stellar mass, and accretion rate

The observed total luminosity ($L_{\text{total}} \sim 2 \times 10^4 L_\odot$ at 1.6 kpc; Minier et al. 2005) sets an upper limit of the stellar mass of S255IR–SMA1 of about $16 M_\odot$ by comparing with the luminosities of main-sequence stars (Mottram et al. 2011, and reference therein). The detection of an ultracompact HII region toward S255IR–SMA1 (Snell & Bally 1986) implies that the central powering source is more massive than about $8 M_\odot$ which sets a lower limit of the stellar mass of S255IR–SMA1. This mass range ($8 < M_\star/M_\odot < 16$) suggests that S255IR–SMA1 is forming an early B-type star.

The 345-GHz continuum image allows us to estimate the core mass and H_2 volume density of S255IR–SMA1, which are $0.36 M_\odot$ and $3.4 \times 10^9 \text{ cm}^{-3}$, respectively (Sect. 5.3.1.2). Within the possible range of central stellar masses, the free-fall timescale,

$$t_{\text{ff}} = \sqrt{\frac{3\pi}{32G\bar{\rho}}}, \quad (5.6)$$

where G is the gravitational constant and $\bar{\rho} = \frac{M_\star + M_{\text{core}}}{4/3\pi R_{\text{core}}^3}$ is the mean density of the core, is found to be 100 to 150 yrs for stellar mass between 8 and $16 M_\odot$. We adopted $R_{\text{core}} = 165 \text{ AU}$ as the geometric mean of the radii derived from the visibility fit (Table 5.1.) On 330 AU scales around S255IR–SMA1, we find that the free-fall accretion rate ($\dot{M} = M_{\text{core}}/t_{\text{ff}}$) is about $2\text{--}4 \times 10^{-3} M_\odot \text{ yr}^{-1}$, which set an upper limit of accretion rate if gas moves in slower than free fall. This derived high accretion rate implies a stellar accretion luminosity,

$$L_{\text{acc}} = \frac{GM_\star\dot{M}}{R_\star} \quad (5.7)$$

of about $1\text{--}3 \times 10^5 L_\odot$, where $R_\star$ is the stellar radius. In the above calculations, we adopted the main-sequence properties of stars at different stellar masses based on (Mottram et al. 2011, and reference therein). In Fig. 5.9, we plot the

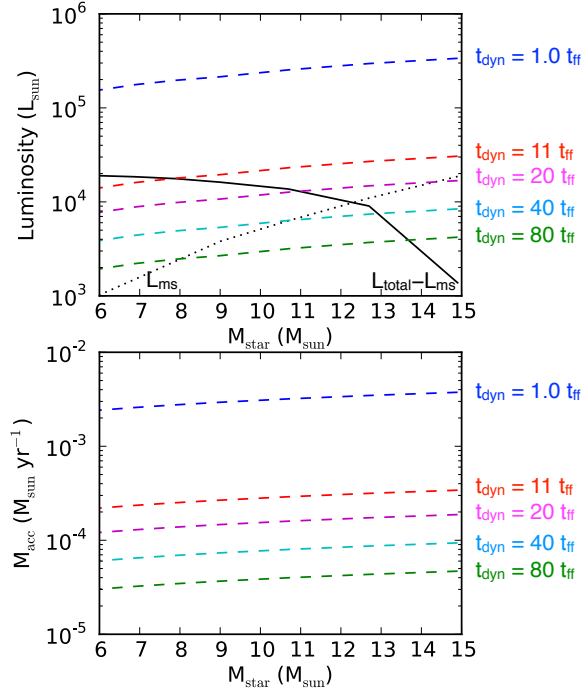


Figure 5.9 (Upper) Luminosity versus stellar mass. The main-sequence stellar luminosities taken from Mottram et al. (2011, and reference therein) are plotted in black dotted line, while the differences of the observed total luminosity and the main sequence luminosity are plotted in black solid line. The observed total luminosity sets an upper limit of the stellar mass to be about $20 M_{\odot}$. The other dashed lines in different colors denote the accretion luminosities for different dynamical time scales. (Bottom) Accretion rate versus stellar mass plot. The dashed lines in different colors represent the derived accretion rates at different dynamic time scales.

luminosity and accretion rate versus stellar mass in the 8 to $16 M_{\odot}$ range. We found that the derived stellar accretion luminosities exceed the observed total luminosity ($\sim 2 \times 10^4 L_{\odot}$), which implies that the central star does not obtain its mass via spherical free-fall accretion in one free-fall time.

In order to solve the above “luminosity problem”, we suggest that the dynamic age (t_{dyn}) of the source must be greater than one free-fall time. This will reduce the accretion rate and hence the accretion luminosity. We assume that the observed total luminosity can be simplified to the sum of the main-sequence luminosity and the accretion luminosity ($L_{\text{total}} = L_{\text{ms}} + L_{\text{acc}}$). In the top panel of Fig. 5.9, we plot the difference between the observed total luminosity and the main-sequence luminosity ($L_{\text{total}} - L_{\text{ms}}$) in black. The accretion luminosities

with different dynamic timescales (11, 20, 40 and 80 free-fall times) are over-plotted as color dashed lines. From this analysis, we suggest that the dynamic time scale of the source must be at least 11 free-fall time (about 1400 yrs) in order to match the minimum stellar mass of $8 M_{\odot}$. The real dynamic timescale of the source requires a better estimate of the central stellar mass. In the bottom panel of Fig. 5.9 we also present the modified accretion rates at different dynamic ages. We note that the modified accretion rates are a few times 10^{-5} to a few times $10^{-4} M_{\odot} \text{ yr}^{-1}$, which are typical values (Keto 2003) for massive star formation.

The derived minimum dynamic time scale (about 1400 yrs) implies that S255IR–SMA1 may be a very young forming early B-type star. Since S255IR–SMA1 cannot undergo free-fall collapse, we alternatively suggest that a disk may have been formed in order to help regulate the mass transport from the inner envelope to the star. Indeed, the velocity gradient seen in CH_3OH (Fig. 5.6) supports this idea. CH_3OH traces a rotating structure perpendicular to the optical jets (Howard et al. 1997; Miralles et al. 1997) and the alignment of water maser spots (Goddi et al. 2007). The non-unity beam filling factor derived from CH_3OH excitation analysis implies the rotating structure is likely clumpy, perhaps due to fragmentation. It is unclear what supports the observed rotating structure around SMA1 against collapse. As we demonstrate in Sect. 5.3.2.3, turbulence does play a role in shaping the line profile of a rotating structure. The non-Keplerian rotation may be due to the presence of a magnetic field (e.g., Seifried et al. 2011). To summarize, we propose that S255IR–SMA1 is a forming early B-type star surrounded by a rotating structure seen in CH_3OH . We suggest that the rotating structure is part of the inner envelope which covers both infalling and rotating gas components. There might be a true Keplerian disk close to the star with a size much less than 330 AU, which requires at least $0.03''$ resolution observations to properly resolve the kinematics.

5.4.2 Hot-core molecules in S255IR–SMA1: tracing forming massive star

It has been suggested that the hot core phase, during which complex organic molecules such CH_3OH , CH_3CN , HCOOCH_3 , etc. can be observed, is one of the early stages of massive star formation (Zinnecker & Yorke 2007). Our eSMA observations toward S255IR–SMA1 show that hot core molecules trace massive star formation activity. We find two velocity components along the line of sight of S255IR–SMA1, of which only one component shows emission from hot core species. The derived high CH_3OH fractional abundance in the gas phase ($\sim 10^{-6}$) is an indication that the source has been heated recently. As a comparison, the gas-phase CH_3OH fractional abundance in dark clouds is a few times 10^{-8} (Ohishi et al. 1992). By comparing the derived fractional abundances of hot

core molecules with the gas-grain warm-up chemical models proposed by Garrod et al. (2008), we found that the chemical timescales are about $3 - 4 \times 10^4$, $1 - 2 \times 10^5$, and 7×10^5 yrs, depending on the warm-up speeds of star-forming core (respectively for models F, M, and S; Garrod et al. 2008). Based on the timescale estimated from the luminosity analysis presented in Sect. 5.4.1, we suggest that the heat up process in S255IR–SMA1 may be relatively fast (model F). However, the implied chemical timescale (few 10^4 yrs) from our data is about an order of magnitude greater than the minimum timescale derived from our luminosity analysis. We suggest that this is still in good agreement if we consider all the uncertainties of both approaches. Nevertheless, the presence of rich hot-core molecules toward S255IR–SMA1 suggests that the dynamic age of S255IR–SMA1 is only $\sim 10^{3-4}$ yrs.

5.5 Summary

We summarize our findings toward S255IR–SMA1 based on the subarcsecond resolution eSMA observations in the following:

- (1) The continuum emission at 345 GHz toward S255IR–SMA1 is elongated in a direction roughly perpendicular to the NE-SW outflow, indicative of a disk-like structure.
- (2) The inferred H_2 column density, mass, and volume density are $2.5 \times 10^{24} \text{ cm}^{-2}$, $0.36 M_\odot$, and $3.4 \times 10^9 \text{ cm}^{-3}$, respectively. Our eSMA observations probe the innermost densest part of S255IR–SMA1.
- (3) From the molecular line observations, two velocity components are identified, with one at $V_{\text{LSR}} \sim 4 \text{ km s}^{-1}$ tracing the massive star formation activities of S255IR–SMA1, judging from the presence of hot-core molecules. The component at $V_{\text{LSR}} \sim 9 \text{ km s}^{-1}$ may trace the common envelope of the binary system covering SMA1 and SMA2.
- (4) Excitation analysis of CH_3OH lines suggests a mean temperature of 140 K and a mean volume density of 10^9 cm^{-3} for the inner dense parts of S255IR–SMA1.
- (5) CH_3OH line shows a velocity gradient roughly perpendicular to the reported jet/outflow in the NE-SW direction. However, the PV map cannot be explained by pure-Keplerian rotation for the expected stellar mass of an early B-type star. It is likely that the observed structure is the inner part of the star-forming core undergoing infall and rotation. High-angular resolution observations at at least $0.03''$ in optically thin lines are required to reveal if there is a true Keplerian disk associated with S255IR–SMA1.

- (6) The accretion rate is estimated to be a few times 10^{-5} to a few times $10^{-4} M_{\odot} \text{ yr}^{-1}$. The dynamical age of S255IR–SMA1 is likely small (10^{3-4} yrs) based on the luminosity analysis in Sect. 5.4.1 and from the comparison of the derived CH_3OH abundance with chemical models.

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Nederlandse samenvatting

Sterren zijn de “atomen” van ons universum. Wat betreft massa worden ze ingedeeld in lichte sterren ($M \sim 0,05\text{--}2 M_{\odot}$), middelzware sterren ($M \sim 2 M_{\odot}\text{--}8 M_{\odot}$) en — het hoofdthema van deze dissertatie — zware sterren ($M \geq 8 M_{\odot}$). De massa van deze laatste klasse overschrijdt per definitie de Chandrasekharlimiet ($\sim 1,4 M_{\odot}$). Die overschrijding heeft als gevolg dat de dood van de ster, die gepaard gaat met een catastrofale ineenstorting van de kern van de ster, resulteert in een neutronenster ($M \sim 8 M_{\odot}\text{--}25 M_{\odot}$) of in een zwart gat ($> 25 M_{\odot}$). Anders dan lichte sterren, die de meest voorkomende klasse vormen, zijn zware sterren naar verhouding zeldzaam. In een sterpopulatie komt de meeste massa voor de rekening van de lichte sterren, terwijl de meeste lichtkracht van de zware sterren afkomstig is. De zeldzame zware sterren zijn er dus toe in staat om de gehele evolutie van het Interstellair Medium (ISM) van sterrenstelsels aan te drijven.

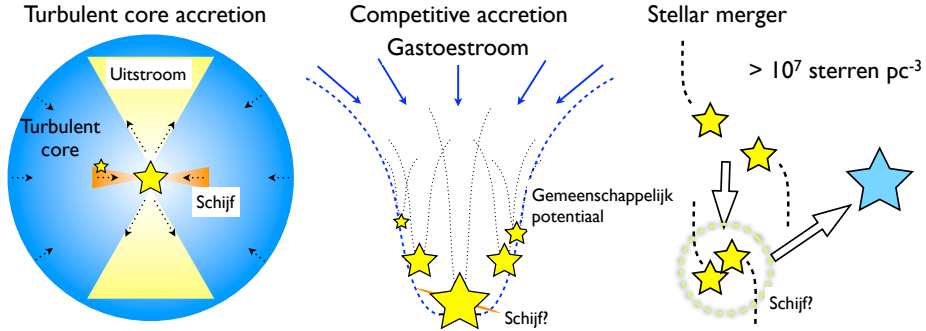
Zware sterren vormen ondanks hun zeldzaamheid de belangrijkste bron voor de synthese van atomen tot aan ijzer (tijdens de hoofdreeksfase van hun leven) en zwaardere elementen (tijdens de supernovafase). Deze verrijking van het ISM is op kosmische tijdschaal een erg kort proces omdat het leven van een ster doorgaans maar enkele miljoenen jaren duurt. In deze korte tijd scheiden de zware sterren grote hoeveelheden materiaal af aan het ISM door middel van intense en omvangrijke uitstroom, dissociatieve UV-straling, krachtige sterrenwind, uitzetting van HII-gebieden en supernova-explosies. Deze vormen een bron van turbulentie in het ISM van sterrenstelsels en men vermoedt dat dit een belangrijk mechanisme is voor de regulering van het ontstaan van sterren en de evolutie van sterrenstelsels.

Vergeleken met onze kennis van de vorming van lichte sterren staat ons begrip van de vorming en vroege evolutie van zware sterren nog in de kinderschoenen. De vorming van lichte sterren vindt plaats in condensaties met hoge dichtheid (omvang: $0,03\text{--}0,2$ pc, dichtheid: $10^{4\text{--}5} \text{ cm}^{-3}$) die zijn ingebed in donkere moleculaire wolken. De temperatuur van een prestellare kern bereikt vlak voor de algehele ineenstorting een lokaal minimum van ~ 10 K. Op het moment van gravitationele ineenstorting wordt de kern van binnenuit verhit en dit brengt reacties op hoge temperatuur op gang die gepaard gaan met een rijk emissiespectrum van complexe organische moleculen. Dankzij het behoud van

het impulsmoment van de ineenslopende kern ontstaan er circumstellaire schijven in Keplerrotatie. In dit stadium wordt op grote schaal massa overgedragen van de wolk naar de schijf en daarna van de schijf naar de ster. Op hetzelfde moment wordt het overschot aan impulsmoment afgestoten door middel van bipolaire uitstroom. Dit is het stadium waarin het grootste gedeelte van de uiteindelijke ster massa wordt gevormd (tijdsduur van de voornaamste accretie: $\sim$ enkele honderdduizenden jaren). In een later, minder ingebed stadium met weinig massaoverdracht van een eventueel overgebleven omhulsel op de schijf, bevindt de ster zich, omgeven door een protoplanetaire schijf, boven de hoofdreeks en genereert nog altijd een zwakke bipolaire uitstroom. Later houdt de bipolaire uitstroom op en trekt de pre-hoofdreeksster langzaam samen richting de hoofdreeks. De tijdschaal waarop de overgang van een lichte voorhoofdreeksster tot hoofdreeksster zich via samentrekking afspeelt is ongeveer 10 miljoen jaar. De totale tijd die nodig is om een volwassen planetenstelsel, zoals ons Zonnestelsel, te vormen, gerekend van het begin van de samentrekking van de prestellaire kern, is meer dan 10 miljoen jaar. De vorming van een lichte ster duurt ongeveer 0,1 % van het totale leven van de ster.

De onduidelijkheden rond de vorming van zware sterren komen voort uit het feit dat ze niet alleen zeldzaam zijn maar ook erg snel evolueren, namelijk in honderdduizend jaar of anders gezegd een paar procent van hun totale levensduur van een paar miljoen jaar, en omdat ze dan nog altijd sterk zijn ingebed. Er is met name geen goed gedefinieerde pre-hoofdreeksfase voor zware sterren. Een duidelijk verschil tussen de vorming van lichte en zware sterren is dat zware sterren intense en dissociatieve UV-straling genereren, wat leidt tot stralingsdruk die voldoende is om accretie te stoppen en HII-gebieden te genereren. Dit is het welbekende “probleem van de stralingsdruk” voor de vorming van zware sterren. Simulaties van massa-instroom in de aanwezigheid van een schijf doen vermoeden dat het stralingsprobleem niet zo groot is, aangezien de schijf in het evenaarsvlak rond de zich vormende zware ster de stellaire straling helpt ombuigen in de richting van de polen waardoor accretie rond de evenaar mogelijk wordt. Dit is het zogeheten “flashlight-effect”. De gaten die worden gecreëerd door bipolaire uitstroom dragen bij aan het flashlight-effect. Straling hoeft niet altijd een destructief effect te hebben, omdat zware sterren kunnen worden gevormd door straling gedreven Rayleigh-Taylor-instabiliteiten. Ook kan het stralingsprobleem worden opgelost door toevoeging van een hoge accretiesnelheid, in de orde van 10^{-3} tot $10^{-4} M_{\odot} \text{ jr}^{-1}$, genoeg om de naar binnen gerichte beweging vast te houden. Merk op dat in het geval van zware sterren die door accretie worden gevormd, de noodzaak van een hoge accretiesnelheid volgt uit de korte levensduur.

Ons begrip van de vorming van zware sterren blijft niet alleen achter vanwege theoretische problemen, maar ook vanwege observationele beperkingen. Gebieden waar de vorming van zware sterren zich voltrekt, bevinden zich door-



Figuur 1: Modellen van de vorming van zware sterren.

gaans op een paar kpc van de zon, zodat men waarnemingen met hoge spatiële resolutie moet uitvoeren. Naast de afstand is er het probleem dat de kernen waarin zware sterren zich vormen sterk zijn ingebed, waardoor slechts de golflengtes van het centimeter-, millimeter-, submillimeter en mid- en ver-infrarooddomein kunnen doordringen. Verder wordt het selecteren van het object bemoeilijkt door de snelle evolutie van de kernen waarin zware sterren zich vormen. Door de mengeling van massa uitstroom en de hoge kolomdichtheden van materiaal waar sterren uit voortkomen is de interpretatie van observationele data niet eenvoudig.

De vorming van zware sterren gaat volgens één van twee zeer verschillende scenario's: accretie of samensmelting. In het laatste model wordt het stralingsprobleem ontweken met directe botsing van stellaire componenten in clusters met hoge dichtheid. Het eerste model kan verder worden opgedeeld in twee verschillende accretiemechanismen: *turbulent core accretion* en *competitive accretion*. Deze drie verschillende concepten van de vorming van zware sterren staan in Fig. 1 schematisch samengevat.

Het model van de turbulent core accretion (ook wel het model van de monolithische ineenstorting) correspondeert met de vorming van geïsoleerde lichte sterren zoals hierboven beschreven, maar met aangepaste turbulentie en accretiesnelheid. De turbulentie is sterk genoeg om fragmentatie van de kern te voorkomen voordat vorming van de zware ster zich verder voltrekt. De hoge accretiesnelheden (10^{-3} tot $10^{-4} M_{\odot} \text{ jr}^{-1}$) kunnen de accretie in gang houden in een omgeving met sterke stralingsdruk. Accretie kan via een schijf verlopen en dat draagt bij aan het ombuigen van de straling in de richting van de polen. De uiteindelijke massa van de ster is gecorreleerd aan de beginmassa van de kern waarin de zware ster zich vormt. Met andere woorden, accretie is een lokaal fenomeen. Het algehele plaatje van de vorming van zware sterren komt overeen met dat van de lichte ster (namelijk, een ineenstortende kern met de vorming van een schijf en uitstroom).

Competitive accretion is gebaseerd op de fysica van de zwaartekracht en de observatie dat zware sterren zich doorgaans vormen in een geclusterde omgeving. De oorspronkelijke wolk waaruit de ster zich vormt (een schaal van pc) valt uiteen tot de thermische Jeans-massa ($\sim 1 M_{\odot}$). In gebieden met een hogere (proto)stellaire dichtheid kan Bondi-Hoyle-accretie verdere *runaway growth* mogelijk maken. Bondi-Hoyle-accretie is het accretieproces dat een sferisch object doormaakt dat door het interstellaire medium beweegt, of de getijdeaccretie veroorzaakt door het gezamenlijke gravitatiepotentiaal van sterrenclusters. De relatief zware sterren (nog niet noodzakelijkerwijs $> 8 M_{\odot}$) die zich aan de onderkant van het gezamenlijke gravitationele potentiaal bevinden hebben de grootste kans om zwaardere sterren te worden ($> 8 M_{\odot}$). Accretie gebeurt globaal op de schaal van wolken tot aan de schaal van kernen (dat wil zeggen, de massa van een bepaalde zware ster kan van elk willekeurig gedeelte van de moederwolk afkomstig zijn en hangt af van de manier waarop het samenklonterende materiaal wordt verdeeld over de zwaarste clusterleden).

Het indrukwekkendste mechanisme van de vorming van zware sterren is samensmelting van lichte protosterren of hoofdreekssterren in het centrum van clusters met hoge dichtheid, namelijk met stellaire dichtheden van meer dan $\sim 10^7 \text{ pc}^{-3}$. Dit samenkloningsscenario is een extreem krachtig proces waarbij circumstellaire schijven worden vernietigd, uitstroom wordt verstoord en mogelijk sterren worden uitgeworpen.

In de drie belangrijkste theorieën over de vorming van zware sterren zijn schijven en uitstroom essentiële onderdelen, maar op verschillende manieren. De structuren hebben volgens het model van de turbulent core accretion een lange levensduur maar in de andere twee modellen zijn ze van korte duur en wordt hun evolutie onderbroken. Het veel voorkomen van omvangrijke bipolaire uitstromen die te zien zijn nabij de kernen waarin zware sterren zich vormen is een sterk teken dat bij de vorming van zware sterren het schijfaccretieproces loopt zoals beschreven door het model van de turbulent core accretion. Het is daarom interessant om de kernen waarin zware sterren zich vormen op kleine schaal (een schaal van $\leq 0,1 \text{ pc}$) te bestuderen met waarneming met hoge spatiële resolutie en in te zoomen op de bewegingen van het gas, zoals turbulentie, samenkloning, uitstroom en met name rotatie. Verder dient gezien de aanwezigheid van schijven de mogelijkheid van planeetvorming rond zware sterren zich aan.

Waarnemingen op de schaal van de millimeter- en de submillimetergolflengtes zijn van belang op het gebied van stervorming. Koud en heet stof kunnen op deze golflengtes worden gedetecteerd door het meten van de warmtestraling. Fysische condities, zoals de temperatuur, de dichtheid, kinematica en de chemische condities, zoals de vraag welke elementen veel voorkomen en hoe ze verdeeld zijn, kunnen worden onderzocht aan de hand van rotatie-overgangen van interstellaire moleculen. Door de komst van faciliteiten om metingen te verrichten met millimeter- en submillimeterinterferometrie zoals de Submillimeter

Array (SMA), de Combined Array for Millimeter Astronomy (CARMA) en de Plateau de Bure Interferometer (PdBI), is het nu mogelijk om de fysische en chemische condities van de kernen waarin zware sterren zich vormen in detail te bestuderen. Interferometrische waarnemingen zijn met name bruikbaar in de jacht naar zware schijven aangezien gebieden van zich vormende zware sterren zich doorgaans op een paar kpc van de zon bevinden en de omvang van de zware schijven slechts een paar 1000 AU of minder is, wat overeenkomt met $\sim 1''$ of minder. In deze dissertatie gebruiken wij zowel waarnemingen met individuele antennes als (sub)millimeter interferometrische waarnemingen om op individuele basis en op verschillende schalen de gaskinematica in de kernen waarin zware sterren zich vormen te bestuderen. Om de informatie over de kinematica uit de waargenomen lijnprofielen te achterhalen gebruiken we een stralingsoverdracht-code als middel om lijnprofielen te modelleren met samenklontering, rotatie en turbulentie en dit te vergelijken met de waarnemingen.

In hoofdstuk 2 laten wij waarnemingen zien, die gedaan zijn met de James Clerk Maxwell Telescope (JCMT), gericht op 17 kernen waarin zware sterren zich vormen in lijnen C^{17}O , C^{34}S en CH_3CN nabij 345 GHz. Het doel is om vast te stellen of deze lijnen, zoals gesuggereerd in de literatuur over interferometrische observaties, inderdaad robuuste tracers van schijven zijn. We vergelijken deze spectrale waarnemingen met generieke stralingsoverdrachtmodellen waaronder samenklontering, rotatie en turbulentie, om een idee te krijgen van de oorsprong van de waargenomen lijnbreedte. We stellen vast dat met C^{17}O 3–2 turbulentie op de schaal van enkele tienduizenden AU het best is na te trekken, terwijl C^{34}S vooral geschikt is voor turbulentie voor de schaal van enkele duizenden AU. CH_3CN 18–17-lijnen zijn de beste tracers voor schijven op de schaal van 1000 AU of minder, in vergelijking met de twee andere transitieën. Gedetailleerdere stralingsoverdrachtmodellering van individuele bronnen is noodzakelijk om de bijdrage van instroom, turbulentie en rotatie te onderscheiden.

In hoofdstuk 3 presenteren wij interferometrische waarnemingen gedaan met de Submillimeter Array (SMA) op 354 GHz gericht op W3 IRS5, een proto-Trapezium. Met de continuüm en lijngegevens op $1''$ – $3''$ -resolutie kunnen we de structuur, kinematica en chemie bestuderen op de schaal van 2000–6000 AU. De continuümwaarnemingen vertonen vijf emissiepieken; twee daarvan zijn zich vormende zware sterren en drie daarvan zijn ofwel sterloze kernen of kernen waarin lichte sterren zich vormen met de potentie om in de toekomst zware sterren te worden. We zien dat de kinematica in de clusteromgeving van W3 IRS5 erg complex is. We stellen op basis van deze dataset voor dat de proto-Trapeziumcluster W3 IRS5 een ideale testcase vormt om onderscheid te kunnen maken tussen modellen van de vorming van zware sterren. Het is ofwel zo dat de accretie van zware sterren lokaal plaatsvindt vanuit de lokale kernen, in welk geval de kleine massa's van de kernen betekenen dat W3 IRS5 in het eindstadium (~ 1000 jr) van instroom en accretie zit; ofwel is het zo dat de accretie

van de sterren nog steeds plaatsvindt vanuit de globale ineenstorting van een zware, clustervormende kern. Er zijn betrouwbare waarnemingen van instroom van grote tot kleine schaal nodig om deze vraag te kunnen beantwoorden.

In hoofdstuk 4 tonen wij de interferometrische observaties met een resolutie van minder dan $1''$, gedaan met de Plateau de Bure Interferometer (PdBI) in de 1,3 mm- en 3 mm-banden gericht op de zich vormende ster van het late O-type AFGL 2591–VLA3. Vanuit een stralingsoverdrachtmodel van de lijnprofielen van HDO en H_2^{18}O stellen wij voor dat er een gelaagde schijfachtige structuur is die een sub-Kepler rotatie en radiële expansie rond AFGL 2591 VLA3 ondergaat. De sub-Kepler beweging zou het gevolg kunnen zijn van magnetische afremming in de schijf, terwijl de expansie een reflectie zou kunnen zijn van uitstroom of van een schijfwind. Uit onze waarnemingen valt op te maken dat late O-type sterren gevormd zouden kunnen worden volgens het model van de turbulent core accretion.

In hoofdstuk 5 presenteren wij de interferometrische observaties met een resolutie van een sub-boogseconde, gedaan met de uitgebreide Submillimeter Array (SMA) op 345 GHz in zowel de moleculaire lijnen als het stofcontinuum en gericht op de vroege B-type ster S255IR–SMA1. Het 345-GHz-continuum van SMA1 is voor het eerst opgelost met een resolutie van $\sim 0,3''$ (500 AU). We stellen vast dat de vorming van zware sterren gemarkeerd wordt door de aanwezigheid van de emissie van complexe moleculen in het hete centrum. Bovendien is er een schijfachtige structuur gevonden in de CH_3OH -lijnen waarin duidelijk een snelheidsgradiënt zichtbaar is loodrecht op grootschalige uitstromen. Uit een vergelijking van stralingsoverdrachtmodellen blijkt dat de waargenomen snelheidsgradiënt niet kan worden gekarakteriseerd als een Kepler rotatie bij de verwachte stellaire massa. Lichtkrachtanalyse toont aan dat S255IR–SMA1 een jonge (10^3 – 10^4 jr), zich vormende vroege B-type ster is met een hoge accretiesnelheid ($\sim 10^{-4} \text{ M}_\odot \text{ jr}^{-1}$). Onze waarnemingen bieden ook bewijs dat in overeenstemming is met het scenario van de turbulent core accretion als model van de vorming van vroege B-type sterren.

Met de belangrijkste conclusies die we hierboven hebben beschreven op zak zullen we onze jacht naar zware schijven voortzetten met behulp van de Atacama Large Millimeter/submillimeter Array (ALMA). De superieure gevoeligheid en de resolutie op sub-boogseconde schaal maakt ALMA het geschiktste instrument voor dit onderzoek. De jacht naar zware schijven kan met ALMA met een factor 10 tot 100 versneld worden in vergelijking met de huidige (sub)millimeter-interferometers. Gevoelige lijnwaarnemingen zijn essentieel voor gedetailleerde stralingsoverdrachtmodellering. Waarnemingen met grote bandbreedte zijn eveneens zeer geschikt voor het op uniforme wijze selecteren van goede schijftracers. ALMA kan antwoord bieden op de hamvraag van deze dissertatie: hoe worden zware sterren gevormd?

Curriculum vitae

I was born on the 29th of October 1981 in Taipei City, Taiwan which is a fast evolving small country in eastern Asia. Everything from my childhood is so different nowadays. The society changed completely from a closed one to an open one, especially after the declaration of the end of martial law in 1987.

In my childhood, the compulsory education was only up to junior high school and any higher education beyond that required entrance exams. It was a competitive era. To my surprise, since I never participated in the simulated exams, I passed the threshold to enter the best senior high school in northern Taiwan, Chien-Kuo high school. This opened up my great interest in natural science. Especially, I met many self-motivated good friends in high school, who inspired me a lot and encouraged me to move forward. I have really good memories of that period, perhaps the best ones so far in my life.

During my high school period, I was frequently thinking about what I would do for my future life. I did not find the answer at that moment, but what I was sure about was to be an engineer or a scientist. Again, entering the next stage, the university education, required another entrance exam, which was even tougher since the competitors came from the whole country. I finally decided to study mechanical engineering or civil engineering at university, but unfortunately I did not make it. This was a turning point in my early life.

As an university freshman in the year of 2000, I majored in geology at National Taiwan University (NTU) in Taipei City, Taiwan. This was a completely different field from what I planned to study for four years, although it is still an interesting and important topic to me nowadays, especially in the geologically young place, Taiwan. During the first year of my university life, I realized what I was really interested in was not only how to make things work together, but why things work individually. I migrated to the Department of Physics in my second year of university.

The first contact in Astronomy and Astrophysics happened in my fourth (last) year of university life in 2004. I joined the summer program organized by the Institute of Astronomy and Astrophysics, Academia Sinica (ASIAA), in Taipei, Taiwan. I worked on Submillimeter Array (SMA) observations of comets under the supervisions of Prof. Yi-Jehng Kuan (National Taiwan Normal University, ASIAA) and Dr. Sheng-Yuan Liu (ASIAA), who inspired me a lot. I started

my SMA study of the Orion hot molecular core during my master from 2004 to 2007 in the Institute of Astrophysics in NTU with Prof. Yi-Jehng Kuan and Dr. Sheng-Yuan Liu. I joined the SMA science verification campaign of 690 GHz observations in 2005. During this time I did learn a lot about (sub)millimeter interferometric observations. This set up my basis and momentum for pursuing a doctoral degree in Astronomy.

After finishing a short period of military service in 2007, I worked at ASIAA as a research assistant with Prof. Yi-Jehng Kuan and Dr. Sheng-Yuan Liu. In 2009, I moved to Leiden to start my PhD study on massive star formation on interferometric scales, with Dr. Michiel Hogerheijde (Leiden) and Prof. dr. Floris van der Tak (Groningen). My promotor is Prof. dr. Ewine van Dishoeck (Leiden, MPE).

During the past four years, I attended three big conferences: “Great Barriers in High Mass Star Formation” in 2010 in Townsville, Australia, “IAUS 280: The Molecular Universe” in 2011, in Toledo, Spain, and “Protostars & Planets” in 2013 in Heidelberg, Germany. I also attended several workshops regarding ALMA and star formation in Leiden, Amsterdam, and Garching. In 2013, I attended the 68th Dutch Astronomy Conference in Lommel, Belgium. I had three observing trips in the past four years: two visits to the JCMT on Mauna Kea, Hawaii, and one trip to the CARMA array in California.

My next stop will be in ASIAA in my home country Taiwan as a postdoctoral researcher with Dr. Sheng-Yuan Liu to work on ALMA observations of massive star-forming regions. Part of my time will be devoted to the ALMA regional center based in ASIAA.

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Finally, my long journey in Leiden has come to an end after four years. I feel very, very lucky to be able to study and live abroad, especially in the historical and beautiful town, Leiden. It was one of the little dreams in my life and now it has been fulfilled. There are so many people who helped me to finish this voyage, without whom I could not make it.

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I feel so glad to be able to join the big astrochemistry and star formation group in Leiden in the past four years. I thank all my Leiden colleagues for interesting discussions during group meetings and other moments, especially to Pamela Klaassen (thank you for your scientific and non-scientific suggestions!), Joe Mottram, Remo Tilanus (thanks for taking care of me in Hawaii!), Attila Juhász, Mihkel Kama, Tim van Kempen, Geoffrey Mathews, Magnus Persson, Markus Schmalzl, Catherine Walsh, Daniel Harsono, Daniel Szomoru (thanks! my officemate), Edith Fayolle, Karoliina Isokoski, Demerese Salter, Kalle Torstensson, Emanuele Di Gloria, Silvia Verdolini, Maria Drozdovskaya, Xiaohu Li, Nienke van der Marel (thank you so much for translating the Dutch summary), Umut Yildiz, and Irene San José García (our discussions were enjoyable).

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