Molecules in Southern
Molecular Clouds:
A Millimetre-wave Study
of Dense Cores

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PLEASE NOTE

The greatest amount of care has been taken while scanning this thesis,

and the best possible result has been obtained.
Abstract

This thesis presents an observational study of molecular abundances in the dense cores of 27 prominent molecular clouds in the southern galactic plane. The molecular abundances and physical conditions in dense condensations have been derived from millimetre-wavelength observations of molecular rotational transitions. The observations have been undertaken with the CSIRO Australia Telescope National Facility Mopra millimetre-wave telescope in Australia, and the Swedish-ESO Submillimetre Telescope (SEST) at the European Southern Observatory in Chile. Over 20 molecular rotational transitions have been observed in each of the 27 molecular clouds of the sample.

This thesis has produced a comprehensive data set of transition intensities and abundances for 10 different molecules in bright southern molecular clouds, and the general characteristics of emission from these molecules such as optical depth, excitation and relative abundances are discussed. Molecular hydrogen, the major constituent of molecular clouds, cannot generally be observed directly due to its lack of a permanent dipole moment, and its density must be inferred from observations of trace molecules such as carbon monoxide. This thesis includes a comparison of different methods of calculating molecular hydrogen column density from observations of carbon monoxide emission.

The observed line emission has been modeled using both optically thin LTE (local thermodynamic equilibrium) and statistical equilibrium LVG (i.e. utilising the Large Velocity Gradient approximation) models to ascertain the physical conditions and molecular abundances in these condensations. This thesis includes a comparison of the results from the two models and the range of conditions for which the models may be used with confidence is determined and discussed.

Developing the millimetre-wave operational methodology of the Mopra Telescope, in particular the intensity and atmospheric calibration, has formed a significant part of this PhD thesis, and a description of the capabilities of the Mopra telescope is included.

Both the analysis and the data collected provide an excellent starting point for further observational and theoretical studies of molecular clouds in the southern Milky Way utilising new instruments such as the millimeter-wave upgrade to the Australia Telescope Compact Array and the Atacama Large Millimetre Array (ALMA).
Acknowledgements

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Many others have assisted with this work. They include friends and colleagues from the UWS, ATNF, and friends from outside the world of academia. To all I give my very sincere thanks.
I dedicate this thesis to the Memory of my Father
He was a clever man who saw the beauty in academic pursuits.
He is sadly missed.
Statement of Originality

This thesis describes the work carried out in the Department of Physics, Faculty of Science and Technology, University of Western Sydney Nepean, Australia (1994 – 1997), in the Nepean Centre for Astronomy, University of Western Sydney Nepean (1998 – 2000) and the School of Engineering and Industrial Design, University of Western Sydney (2001).

This thesis was also undertaken through the Australian Commonwealth Scientific and Industrial Research Organisation (CSIRO) Australia Telescope National Facility (ATNF$^1$) through a ATNF Studentship.

Some of this work had been published in


All other work presented here is original unless otherwise noted in the text.

Maria Rose Hunt
Sydney, Australia

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Chapter 1

Introduction

1.1 Molecules in the Interstellar Medium

1.1.1 Why study Molecules in the Interstellar Medium?

Molecules are an advanced step in the chemical evolution of the universe, which having started with the creation of hydrogen and heavy hydrogen, helium and a trace of lithium in the big bang, continues to the point where complex reproducing, chemical systems are capable of sitting at word processors and pondering their own evolution.

Molecules provide us with an invaluable tool for studying the interstellar medium. Molecular-line radiation provides us with information on the densities, pressures, chemical composition, excitation, kinematics and dynamics of molecular clouds, the components of the interstellar medium in which stars and planets form. However, this is not limited to providing information associated with star formation. Molecular-line radiation is an important tool in the study of the kinematics and dynamics of both our own Galaxy and other galaxies, and the study of the chemical evolution of galaxies from early times in the universe to the present epoch. And this of course brings us back to this complex life form pondering her own evolution.

The study of interstellar molecules has yet another broad application that holds the promise of exciting science in years to come. The new field of bioastronomy deals with the evolution of pre-biotic molecules in the interstellar medium and early results suggest that without a reservoir of highly complex organic molecules in the pre-solar nebula that life on earth may never have got started (Bailey et al. 1998).

1.1.2 The Interstellar Medium

Radiofrequency spectral-line observations of the interstellar medium (ISM) began in the early 1950s with the detection of the 21-cm transition of neutral atomic hydrogen (Ewen & Purcell 1951; van de Hulst 1951), the main constituent of the diffuse, atomic interstellar medium. The hydrogen in molecular clouds is in the form of H₂, which does not produce any readily observable transitions in cool molecular gas. Consequently it was not until some years later, following the discovery of microwave and millimetre transitions of OH (Barrett, Meeks & Weinreb 1964), NH₃ (Cheung et al. 1969) and CO (Wilson, Jeffers & Penzias 1970), that radiofrequency spectroscopy became a valuable tool for investigating the dense interstellar medium. In 1955, Charles Townes (Townes 1957) had in fact predicted the presence of these trace molecules in dense interstellar gas. However, until the actual detection of NH₃, the
first interstellar molecule found with more than two atoms, it was generally felt that complex molecules could not exist in interstellar space. To date, more than 100 different molecules have been identified in the ISM (see e.g. Ohishi 1997) and most of these have been discovered since 1968. For reviews of the historical development of radio and millimetre-wave observations of interstellar molecules see e.g. Martin & Barrett (1978), Solomon (1984) and Rydbeck & Hjalmarson (1985).

The last thirty years have seen a revolution in our understanding of ISM. Molecular clouds are now known to be the largest gravitationally bound structures within galaxies. An inter-cloud medium has been found between these clouds, composed of several components in pressure equilibrium with each other, but not gravitationally bound. Table 1-1 gives a brief description of the components of the ISM (Brinks 1990; Knapp 1990; Rohlfs & Wilson 1996; Emerson 1996; Dyson & Williams 1997).

<table>
<thead>
<tr>
<th>Component of the ISM</th>
<th>Description</th>
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| Dense molecular gas  | Temperature = 5 to $\geq$600K  
(Molecular medium, including hot molecular cores)  
Density $= 10^2$ to $\geq 10^8$ cm$^{-3}$ |
| Cold dense atomic gas | Temperature = 10 to 100K  
(Cold neutral medium)  
Density $= 10$ to $10^3$ cm$^{-3}$ |
| Warm neutral medium  | Temperature $\sim 10^3$ to $\sim 5 \times 10^3$K  
Density $= 0.3$ cm$^{-3}$ |
| Warm diffuse ionized medium | Temperature $\sim 10^4$K  
Density $= 0.3$ cm$^{-3}$ |
| H II regions         | Temperature $\sim 5 \times 10^3$ to $\sim 2 \times 10^4$ K  
Density $\sim 10^3$ to $\geq 10^9$ cm$^{-3}$ |
| Hot ionized medium   | Temperature $\sim 10^6$K  
Density $< 10^2$ cm$^{-3}$ |

1.1.3 Interstellar Chemistry

Molecular clouds act as ‘molecular nurseries’. Hydrogen molecules are self-shielding; i.e. the H$_2$ in the outer layers of a cloud absorb any UV radiation incident on the cloud, shielding molecules in the interior from dissociation. In addition, UV radiation generated within a cloud will be absorbed by H$_2$. The outer regions are called photon-dominated regions (PDRs), and exhibit significant differences in chemistry to the dense interior regions of molecular clouds. It is with the latter that this thesis is concerned. Dust grains also act as efficient absorbers of UV radiation, providing additional protection for molecular gas against dissociation. Dust grains constitute around 1% (by mass of cloud mass) of molecular clouds (Solomon 1984) and consist
of solid silicates and graphite compounds. They are mainly produced in the atmospheres of previous generations of cool evolved stars, and returned to the ISM through stellar winds and outflows. Not all the dissociating radiation is absorbed in the outer layers of clouds.

Cosmic rays are sparsely distributed throughout the ISM, but they do penetrate to the denser sections of molecular clouds. Cosmic rays produce a low rate of ionization within molecular clouds, leading to the ion-molecule reactions that drive much interstellar chemistry.

There are three types of chemistry that are important in dense molecular clouds:

1. Ion-Molecule Reactions

This is the dominant reaction mechanism in the gas phase of cool, quiescent molecular clouds (see e.g. Prasad & Huntress 1980; Leung, Herbst & Huebner 1984). Both atoms and molecules are ionized by the cosmic rays that permeate molecular clouds. The ions then react with neutral atoms or molecules within the cloud to produce new molecules. There are generally several reactions involved in a reaction network before the final, stable product is reached. Ion-molecule reactions are not temperature dependent, unlike neutral-neutral reactions, and dominate at low temperatures. Molecules such as CO, CS, HCN, HC$_3$N, HCO$^+$ and HNC are among those for which the abundance in quiescent molecular gas is satisfactorily predicted by ion-molecule reactions.

2. Grain Surface Reactions

At low temperatures, atoms and molecules collide with, and stick to, dust grain surfaces, forming an ice mantle. Small atoms are very mobile on grain surfaces and will react quickly (generally within a day: Tielens & Whittet 1997) with a heavier atom or molecule that can be considered essentially immobile. The product molecules (except for H$_2$, which leaves the grain surface immediately after formation: Hollenbach & Salpeter 1971) will generally remain on the grain surface unless the temperature increases (Hasegawa, Herbst & Leung 1992). Grain surface chemistry favours simple saturated species owing to the presence of mobile H atoms on the dust grains (see e.g. Tielens & Whittet 1997 and references therein). Dust grain mantles are found to contain significant quantities of H$_2$O, CH$_3$OH, CO, CO$_2$, OCS and CH$_4$ (Whittet et al. 1996). These molecules are evaporated from grain surfaces if the grain mantles are heated by nearby star formation. Different molecules evaporate at different temperatures; CO evaporates at the low temperature of 17 K, whereas CH$_3$OH evaporates at 85 K. All molecules will have evaporated from the grain surface at temperatures above 90 K (Tielens & Whittet 1997).

3. Gas-Phase Neutral-Neutral Reactions

The rate coefficient for neutral-neutral reactions depends on temperature, suggesting that at the cold temperatures of molecular clouds two-body neutral-neutral reactions play a very small part. However, recent laboratory measurements suggest that some
neutral-neutral reactions proceed simply at the collisional rate between the species, if the activation energy is small (Smith 1997). As the collisional rate increases with density, neutral-neutral reactions are likely to play a part in molecular abundances in warm, dense regions of molecular clouds (Herbst & Leung 1986). It is not yet clear which astrophysically important species are involved in neutral-neutral reactions owing to the difficulty of laboratory experiments in which interstellar conditions must be simulated.

1.2 Dense Molecular Gas in the ISM

Molecular clouds can be divided into two general categories: dark clouds and Giant Molecular Clouds (GMCs). The typical properties of these objects are discussed in this section. Both dark clouds and GMCs contain star-forming regions and during the star formation process the molecular gas is further differentiated into distinct regions.

Dark Clouds:

Dark clouds were first identified on optical plates as dark patches of sky in which the starlight from background stars was absorbed (see, e.g., Zhou 1997). Small dense clouds with an approximately spherical shape (known as Bok globules) had been detected and it was suggested that they are gravitationally bound entities collapsing to form stars (Bok & Reilly 1947). In our Galaxy, most detected dark clouds are close to the Solar System (within ~1 kpc). Detection of more distant objects is impeded by irregular galactic absorption and star density. Dark clouds typically have significantly lower H$_2$ column densities than GMCs. They are cooler than GMCs with typical temperatures of about 10 K and form only low mass stars, as evidenced by the lack of associated optical and radiofrequency ionised hydrogen (HII regions). Such regions are only found in proximity to massive O or B stars, which have strong UV emission that ionises the surrounding cloud.

GMCs:

GMCs are massive molecular clouds that contain up to $10^6 M_\odot$ of gas. They contain sites of recent and ongoing massive star formation, often associated with HII regions. GMCs form both high-mass and low-mass stars. Masers, outflows, shocked gas and HII regions provide the signatures of current and recent massive star formation. H$_2$O masers occur in gas where both high-mass and low-mass stars are forming, and they are particularly associated with high-velocity outflows from young stellar objects. OH and CH$_3$OH masers are generally associated only with regions of high-mass star formation and arise in the envelopes of ultracompact HII regions (Menten 1997).

Spatial Structure of Molecular Clouds:

Molecular clouds are not homogeneous, but instead are appear to have a clumpy structure. They are thought to consist of dense clumps in macro-turbulent motion with respect to one another and separated by an interclump medium. The density of the interclump medium is found to be one or two orders of magnitude lower than the density of the clumps while the clump to interclump ratio is found to be smaller
within cold dark clouds than for giant molecular clouds (Stutzki & Gusten 1990). The implication of this clumpy cloud structure for molecular line observations is that within the beam of the telescope there will be regions of varying density and hence varying emission. The emission measured by the telescope will in fact be an average of the emission from both the clumps and the interclump medium contained within the telescope beam.

Clumpiness within molecular clouds and its effects on observed line profiles and intensities are discussed further in sections 4.5.2 and 5.1.2 of this thesis. Further details on this topic can be found in Park, Hong & Minh (1996) and Park & Hong (1995).

1.2.1 Molecules as Pointers to Gas Density and Temperature.

The presence and strength of a molecular emission line depends on both the abundance and the excitation of the molecule. Line formation is discussed in detail in Chapter 2; some of the consequences of the theories are summarised here.

The excitation of an interstellar molecule depends on a number of factors, including the permanent dipole moment of the molecule (see Chapter 2 for more detail). The density at which the emission from a transition becomes significant is known as the critical density (see chapter 2) and is proportional to the dipole moment squared of the transition. Appendix C lists the critical densities for the transitions observed in this study. Molecules with a high dipole moment, such as CS, are tracers of dense gas. The CS J=2-1 transition has a critical density of $2.2 \times 10^5$ cm$^{-3}$. CO on the other hand has a very low dipole moment, and is easily excited with a critical density of around 740 cm$^{-3}$ (for the J=1-0 transition), so CO (1-0) is an effective tracer of low-density gas.

The other factor that affects the presence of an emission line is the abundance of the molecule. In dense molecular clouds the CO abundance is high and CO emission can be detected in regions with densities less than 100 cm$^{-3}$ (Rohlfs & Wilson 1996), similar to the density above which molecular hydrogen becomes the dominant species over atomic hydrogen. Also, it is generally assumed that CO is coextensive with H$_2$ in interstellar gas as the formation and dissociation rates are similar under similar physical conditions (Polk et al. 1988). For these reasons, CO is widely accepted as a tracer of generally undetectable H$_2$ (see Chapter 4).

Other molecules such as CS, HCN, HCO$^+$ and HNC are also commonly present throughout molecular gas and spectral lines from these molecules are commonly used to investigate the density and temperature of the gas from which they arise. On the other hand, molecules such as CH$_3$OH and SiO are found in the gas phase only after the gas has been warmed or shocked by the star formation process and are pointers to the presence of recent star formation.
1.2.2 The Physical Stages of Star Formation

The formation of a single, isolated low-mass star is thought to be relatively well understood compared to the more complex process of star formation in clusters, and the formation of low mass (T Tauri-type) stars is adopted as being representative of the star-forming process. The molecular signatures of star formation will also be applicable to the more complex situation although their interpretation will be correspondingly more complex.

A good overview of the formation of low-mass stars in isolation (as occurs in the dark cloud TMC 1) is given by Shu (1997) and has been used as a basis for the description here.

The initial stage of star-formation is characterised by isothermal collapse. Initially, dense pockets of gas and dust contract quasistatically within the parent molecular cloud to form dense molecular cores after a few million years, with magnetic fields in the gas acting against gravitational collapse. During this phase the pockets rotate at roughly the same angular speed as the surrounding molecular envelope.

The second stage is characterised by the dynamical collapse of the dense core, after a critical mass-to-magnetic-flux ratio is reached. Gravitational collapse occurs from the inside out, with the largest infall velocities occurring at the smallest radii.

The third stage of star formation begins when deuterium burning in the developing protostar creates an outer convection zone, allowing the creation of a magnetosphere that gives rise to a stellar wind, causing outflow from the protostar. The outflow self-collimates into bipolar jets that break through the surrounding molecular envelope near the rotational poles. Outflows from YSOs occur at supersonic velocities (Snell, Loren & Plambeck 1980), and so a shock wave forms at the interface between the outflow and the surrounding cold dense molecular gas. Infall continues in the equatorial regions of the protostar. In this stage of star formation infall and outflow occur simultaneously, and the differing chemistry of the two regions can be used to differentiate between signatures of the two processes.

The fourth stage of star formation begins when the outflow widens and then reverses the infall over the entire angular extent of the star, eventually leading to the clearing of the debris of star formation from the vicinity of the newly formed star.

A dense molecular core collapses to form a rotating protostar and circumstellar disk, known as a young stellar object (YSO). YSOs continue to accrete matter from a surrounding infalling envelope within the parent molecular cloud. The envelope dominates the emission in the youngest systems while the disk and star become dominant in older systems (Blake 1997).

Massive stars are thought to form in clusters, so the situation will be much more complex. In the case of massive star formation, an HII region will be formed immediately surrounding the YSO, and signatures of massive star formation such as OH and CH3OH masers will be found. As the YSO and HII region warm up the
surrounding molecular cloud a hot molecular core is formed. Dense molecular gas heated by recent, nearby, massive O and B star formation is often referred to as a ‘hot core’. Hot cores are often associated with ultracompact HII regions and typically have radii < 0.1 pc, temperatures of 100-600K, hydrogen densities of \(10^5-10^8\) cm\(^3\), and masses of 10-1000 M \(_\odot\) (Ohishi 1997; Millar 1997).

### 1.2.3 Molecules as Tracers of Star Formation

The different stages of the star formation process involve widely different temperatures and densities and have been extensively studied. For instance, Brown, Charnley & Millar (1988) and Caselli, Hasegawa & Herbst (1993) have investigated the time dependence of molecular abundances in collapsing cores during the protostellar and pre-main sequence stages, while van Dishoeck & Blake (1998) have provided a comprehensive review of the chemical evolution of star-forming regions.

**Pre-collapse Stage**

The pre-collapse stage is dominated by gas-phase ion-molecule reactions, apart from the formation of \(\text{H}_2\), which occurs on grain surfaces, with the \(\text{H}_2\) quickly being returned to the gaseous phase after formation.

**Isothermal and Gravitational Collapse Phases**

The isothermal collapse phase of the process leads to an increase in density, which in turn leads to an increased rate of collision between molecules and dust grains. The molecules stick to the cold dust grain surface and are lost from the gaseous phase. In quiescent gas surrounding protostars molecular depletion factors of 25-50 are found for all molecules, including CO (Blake et al., 1995; Kelly, Macdonald & Millar 1996), as predicted by chemical models (see eg. Rawlings et al. 1992; Bergin & Langer, 1997). However, the gas-phase abundance of \(\text{HCO}^+\) is predicted to remain high (van Dishoeck & Blake 1998) so this ion may be a good tracer of gas in the initial collapse phase, and this has been confirmed observationally (Moriaty-Schieven et al. 1995; Ohashi et al. 1996).

The molecules trapped on the grain surfaces in the depleted gas become involved in grain surface chemistry, with some species not previously present in the gas phase such as \(\text{CH}_3\text{OH}\) and \(\text{H}_2\text{CO}\) being produced on the grain surfaces but remaining trapped while the temperature of the gas remains low. HNC on the other hand will be consumed in grain surface reactions (Charnley, Tielens & Millar 1992; Caselli, Hasegawa & Herbst 1993).

The observational detection of depleted gas is difficult due to the probably small spatial extent of the depleted gas. The depleted gas undergoing isothermal collapse will be surrounded by a ‘skin’ of quiescent molecular gas in which the abundances are normal (van Dishoeck & Blake 1998). An overlying layer in which the abundances are a factor of 10 to 100 higher than in the depleted gas may mask depletions deep inside the core (Mundy & McMullin 1997). However, evidence for infalling gas may be seen...
as self-absorption in the line profiles of CS, HCO$^+$ and H$_2$CO (Zhou et al. 1993; Choi et al. 1995; Gregersen et al. 1997).

The kinetic signature of the gravitational collapse phase can also be seen in asymmetric line profiles of optically thick molecules, with the red-shifted portion of the line wings being weaker than the blue-shifted portion due to self-absorption (Shu 1997). This effect arises for the following reasons. As previously stated, gravitational collapse is predicted to occur from the inside out, with the largest infall velocities occurring at the smallest radii. Higher density at smaller radii leads to higher collisional excitation of molecules in the central regions, so the bulk of the detected emission is likely to arise from these regions. The blue shifted emission travels only a small distance through emission at similar velocities, whereas the length of the path that the red shifted emission travels (through emission at similar velocities) will be longer, with a correspondingly greater likelihood that the emission will be absorbed within the gas. Self-absorption is possible only if the velocities of the emitting and absorbing gas are similar, due to Doppler shifting (see Chapter 2).

**Star-formation Phase**

As the YSO warms up the surrounding molecular cloud the ices on the grain mantles melt, returning the trapped molecules to the gas phase, altering the gas phase abundances in the warm gas. The gas phase chemistry changes at this point, due to both the increased temperatures and the different composition of the gas (see eg. Willacy, Rawlings & Williams 1994; Bergin, Langer & Goldsmith 1995). New, complex species such as HCOOCH$_3$ (Blake 1997) now form in the gas phase.

An outflow has a significant impact on the chemistry of the envelope surrounding the YSO. As it encounters dense, cold gas, it compresses and heats this gas, resulting in strong emission from the post-shocked gas (Blake 1997). Refractory molecules such as SiO are produced in the shocked gas due to sputtering and shattering of grains rather than from the more gentle process of evaporation, and are therefore particularly useful for tracing shocks. The molecule SiO is found to be enhanced in the region where the outflow interacts with the molecular envelope (Blake et al. 1994), while HCO$^+$ is destroyed in hot or shocked gas and so traces the infalling molecular envelope of quiescent molecular material (van Langevelde et al. 1994; Bachiller 1997). Molecules generally found to be enhanced in shock regions are SiO, CS, CH$_3$OH, H$_2$CO, HCN, SO, SO$_2$, H$_2$O and H$_2$CS. On the other hand, the ubiquitous molecules C$_2$H$_2$, N$_2$H$^+$ and HCO$^+$ are not generally found in shocked gas (Bachiller 1997). H$_2$O masers almost certainly originate in outflows as they require densities of $10^7$ to $10^9$ cm$^{-3}$ and temperatures of around 500 K to be excited.

1.2.4 Molecular Abundances in Cold Dense Gas

Cold dense gas is characterised by temperatures of around 10 K and densities of around $10^4$ cm$^{-3}$. Cold dense cores are in a pre-collapse phase and are dominated by gas-phase ion-molecule reactions. Molecules that form via ion-molecule reaction networks such as CO, CS, HCN, HNC, CN and HCO$^+$ are among the most abundant. The relative abundances of the molecules HCN and HNC provide a good pointer to
the presence or absence of star formation. In cold dense gas unaffected by star formation the relative abundance of the molecules HCN and HNC is predicted to be $\approx 1$ (Brown, Charnley & Millar 1988). Molecules that form primarily on dust grains such as CH$_2$OH remain frozen on grain surfaces.

Cold dense cores are rich in large, linear, unsaturated molecules such as HC$_{2n+1}$N and in carbenes such as C$_3$H$_2$, which are expected to be formed by gas phase chemistry at low temperatures driven by cosmic ray ionisation (see e.g. Millar et al. 1989; Millar & Herbst 1990; Herbst et al. 1994). Quiescent dark clouds such as TMC 1, which do not form massive stars, are found to be particularly rich in these molecules (Millar 1997).

1.2.5 Molecular Abundances in Hot Cores

At the temperatures present in hot cores the grain mantles will have evaporated (Tielens & Whittet 1997), so hot core gas should to a certain extent reflect the molecular abundances on grain mantles in the cold quiescent phase (Wahmsley 1989). For example, saturated species such as CH$_3$OH, H$_2$O, NH$_3$ and CH$_3$CH$_2$OH that form primarily on grain mantles will now be found in the gas phase (Ohishi 1997). The abundance ratio of HCN to HNC is also expected to differ after the evaporation of grain mantles takes place. HNC is believed to be converted to HCN on grain surfaces (Brown, Charnley & Millar 1988) so the HCN/HNC abundance ratio is expected to exceed unity in hot cores (c.f. HCN/HNC $\sim 1$ in cold dense gas).

Ion-molecule reactions become less important at high densities as cosmic ray ionisation is less efficient (Millar 1997), so the long carbon chain unsaturated molecules found in cold dense gas are not so readily formed. HC$_3$N is an exception as it is readily produced in warm gas (Millar, Macdonald & Gibb 1996). HCO$^+$ and N$_2$H$^+$ are also not generally found in warm cores as they are consumed in chemical reactions with CH$_3$OH and H$_2$O evaporated from grain mantles (Charnley, Tielens & Millar 1992).

The sulphur-bearing molecules CS, SO, OCS and SO$_2$ are readily formed in hot neutral gas from H$_2$S evaporated from grain mantles and are common in hot cores. OCS is also believed to form on grain mantles as well as being produced in the gaseous phase of the warm gas. CS is initially formed from S liberated by dissociation of H$_2$S, and is converted to SO in the environment of the hot core. SO is in turn converted to SO$_2$, suggesting that the relative abundances of CS, SO and SO$_2$ in hot cores may be indicative of the time elapsed since the evaporation of the grain mantles (Charnley 1996). SiO is formed in the gas phase from evaporated SiH$_4$ (MacKay 1995), although very large fractional abundances of SiO will be due to violent shock interaction rather than thermal liberation of icy mantles (Millar 1997).
1.2.6 Summary

Dense molecular cores are intimately associated with the star formation process. The evolution of a dense molecular core through the initial collapse, star formation phase and post-star formation evolution can be traced by differing chemistries. Table 1-2 is adapted from Table 1 of Mundy and McMullin (1997) and gives an overview of the chemistry associated with the dynamical evolution of dense molecular cores. The first two columns are taken from Mundy and McMullin while the remaining columns summarise the discussion of the previous section. It should be noted at this point that the actual process of star formation is likely to be more complex than the previous discussion of the chemical signatures of star formation may suggest, however the above (and Table 1-2) is adopted as a working hypothesis for the remained of the thesis.
<table>
<thead>
<tr>
<th>Dynamical Status</th>
<th>Chemical Status</th>
<th>Molecular Signatures</th>
<th>Other Features</th>
<th>Molecules not Generally Detected</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identifiable core</td>
<td>Normal abundances for molecules produced by ion-molecule reactions.</td>
<td>CO, CS, HCN, HNC, (HCO^+), (CN, C_2H_2, N_2H^+), (HC(NH_2))N</td>
<td>HCN/HNC &lt;1</td>
<td>Molecules formed primarily in shocked gas or on grain surfaces: (CH_3OH, OCS, NH_3, H_2CO, SiO, SO_2)</td>
</tr>
<tr>
<td>Contracting core</td>
<td>Weak depletions at centre, increasing with time.</td>
<td>As above, but with lower gas-phase abundances due to gas phase molecules sticking to grain surfaces, except for (HCO^+). The abundance of (HCO^+) relative to other molecules may increase.</td>
<td>As above</td>
<td>As above</td>
</tr>
<tr>
<td>Dynamical collapse</td>
<td>Strong depletions in centre, weak depletions throughout</td>
<td>As above</td>
<td>As above</td>
<td>As above</td>
</tr>
<tr>
<td>Stellar object forms</td>
<td>Maximum depletions</td>
<td>As above</td>
<td>As above</td>
<td>As above</td>
</tr>
<tr>
<td>Stellar wind starts</td>
<td>Shock enhancements begin.</td>
<td>Molecules produced or enhanced in shocked gas first begin to appear or have enhanced abundances: (SiO, CH_3OH, H_2CO, SO_2, H_2CS)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind and photon heating</td>
<td>Shock enhancements and grain mantle evaporation near star and spreading out with time.</td>
<td>Gas-phase abundances reflect grain-mantle abundances and chemistry during collapse phase. (CH_3OH, OCS, H_2O, HCN, CS, NH_2, and complex saturated molecules such as (CH_3CH_2CN and CH_3CH_2OH) appear or are enhanced.</td>
<td>HCN/HNC &gt;1 due to destruction of HNC on grain mantles</td>
<td>Abundance of CS/(SO) and SO/(SO_2) decreases with time.</td>
</tr>
<tr>
<td>Appearance of star</td>
<td>Evaporation of mantles throughout core.</td>
<td>Warm neutral chemistry leads to the production of molecules such as (CS, SO, OCS, SO_2, HCOOCH_3)</td>
<td>HCN/HNC &gt;1</td>
<td>Abundance of CS/(SO) and SO/(SO_2) decreases with time.</td>
</tr>
</tbody>
</table>
1.3 This Thesis: An Investigation of Molecules in Southern Dense Molecular Cores

The southern part of the galactic plane contains the innermost parts of the galaxy and many major dense molecular clouds and star-forming regions. Many of these molecular clouds are difficult to observe with Northern Hemisphere telescopes due to their southern declinations. Consequently molecular line emission, molecular abundances and physical conditions in these clouds have not been extensively investigated, particularly for those clouds at declinations south of $-30^\circ$.

The molecular abundances predicted for dense molecular clouds in various stages of star-formation discussed in Chapter 1 have been observationally tested largely in molecular clouds accessible from Northern Hemisphere telescopes. The aim of this thesis work is to produce a statistical database of molecular spectral-lines and molecular abundances in southern molecular clouds to see if these results hold generally.

This thesis consists of the following parts:

1. Observations at millimetre wavelengths of dense cores in southern sky molecular clouds.
2. The derivation of physical conditions and molecular abundances in the dense cores.
3. A comparison of the observational results and derived parameters with the theoretical predictions for core chemistry and evolution.

Molecular lines occur primarily at millimetre and submillimetre wavelengths. The commissioning of a millimetre wave receiver on the Mopra\(^1\) Radio Telescope in 1994 provided the opportunity to observe molecular transitions at 3-mm with high resolution, and Mopra has been used extensively to obtain the observations reported here. Complementary observations of 1-mm, 2-mm and 3-mm transitions have been obtained with the SEST\(^2\). A significant part of this project involved the use of SEST observations to provide an intensity calibration scheme for the Mopra Telescope. The intensity calibration scheme is described in Chapter 3.

A sample of 27 molecular clouds with declinations south of $-30^\circ$ was chosen for investigation. The Galactic centre molecular cloud G1.6-0.025 with a declination of $-27^\circ$ has also been included. This object has been subjected to additional studies not included in this thesis. The criteria for the selection are described in detail in Chapter 4; however, brief mention of the selection process is made here.

The molecular clouds were required to be bright so that a large number of molecules could be observed in a reasonable period of time, and show some evidence of complex chemistry. Previous molecular line surveys (Gardner & Whiteoak 1974; Whiteoak & Gardner 1978; Gardner & Whiteoak 1978; Batchelor et al. 1981; Dickinson et al.

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\(^1\) The 22-m ‘Mopra’ antenna of the Australia Telescope (operated by the Australia Telescope National Facility, CSIRO) is situated near Coonabarabran in New South Wales, Australia.

\(^2\) The Swedish-ESO Submillimetre Telescope (SEST) is situated at the European Southern Observatory at La Silla in Chile, about 600 km north of Santiago.
1982; Gardner & Whiteoak 1984; Peters et al. 1986) along the southern galactic plane were used to select a sample of 50 candidate molecular clouds with declinations south of -30 degrees. The Mopra telescope was then used to observe this initial sample, the final sample being selected from the Mopra observations as detailed in Chapter 4.; these observations were some of the first mm-wave observations obtained with this telescope.

Generally one position was chosen for investigation in each molecular cloud, towards the peak $^{13}$CO emission (see Chapter 4), and so these positions represent the dense cores in the molecular clouds.

Transitions of the molecules CO, CS, HCN, HNC, HCO$^+$, HC$_3$N, OCS, CH$_3$OH and SO and several of their isotopomers were observed in each molecular cloud. Table 4.2 lists the transitions of each molecule that were observed. CO was used as both a tracer of hydrogen column density and an indicator of cloud kinetic temperature. CS, HCN, HNC, HCO$^+$ and SO are among the most abundant molecules and are useful for investigating general properties of the molecular cloud such as velocity structure. As suggested in Table 1.2, their abundances relative to each other can provide an indication of the evolutionary state of a dense molecular core.

Chapter 2 sets the theoretical basis for the molecular abundances and physical conditions derived in Chapter 5. An LTE analysis has been used to calculate the abundances of these molecules, while observations of optically thin isotopomers have been used to account for optical depth effects. Although HC$_3$N is less abundant than the molecules listed in the previous paragraph, it is very sensitive to cloud temperature and density (Avery 1980) and has a number of transitions likely to be observable in the frequency ranges available on the Mopra Telescope and the SEST. Up to five transitions of HC$_3$N have been observed in each cloud, and these observations have been used for LVG modelling to obtain the HC$_3$N abundance and H$_2$ density of the dense cores. The abundance of HC$_3$N has also been calculated with an LTE rotation diagram analysis and compared with the results of the LVG analysis (section 5.3.5).

The molecules CH$_3$OH and OCS are formed primarily on grain surfaces and are expected to be present in the gas phase only after the onset of star formation. They also have several transitions in the range of frequencies observed and have been analysed by means of an LTE rotation diagram to find the abundance and excitation temperature. Several other molecules were observed in a limited number of sources as reported in the results. Both the observations and the derived parameters for each source are reported in Appendix A-1.

Chapter 6 discusses the results of A-1 for each source, and attempts to interpret both the observed and the derived parameters in terms of the physical and evolutionary state of the dense core. Chapter 6 concludes by examining the abundances from the perspective of the entire sample and attempts to draw conclusions from the similarities and differences between sources. Chapter 7 provides a brief summary of the findings of this study.
Chapter 2

Using Molecular Line Spectroscopy to Probe the Interstellar Medium

2.1 Introduction

A molecular spectral line can be described by line intensity, line width and frequency. To translate these parameters into information about the physical and chemical conditions within molecular clouds requires an understanding of the physical processes that lead to line formation.

This chapter examines the way in which the general emission and absorption properties of a gas influence the emission observed from a molecular cloud (section 2.2 Radiative Transfer), and how the intensity of the emission is related to the temperature of the emitting gas (section 2.3 Planck’s Law). These general properties are then related to spectral-line radiation (section 2.6) and to specific absorption and emission properties of molecules (section 2.8 Einstein Coefficients), allowing the calculation of temperatures, molecular abundances and densities in molecular clouds (section 2.10). The following discussion borrows heavily from Rohlfs & Wilson (1996) and Emerson (1996), however, the formulation is common to many texts on radio astronomy.

2.2 Radiative Transfer

The brightness of a molecular cloud, as measured at the telescope, can be related to the temperature and other physical properties of the cloud by considering how radiation is emitted and absorbed as it proceeds through the cloud and to the telescope.

The radiation, along the line of sight, which emerges from a molecular cloud, will be the sum of:

1. Radiation emitted from within the cloud that is not reabsorbed, and
2. Radiation from behind the cloud that passes through without being absorbed.

From consideration of a generic molecular cloud (Figure 2.1), the intensity of the emergent radiation \( I_e \) in a particular direction will be the sum, along the path length \( x \), of the radiation emitted and absorbed in each interval \( dx \). \( I_0 \) is the intensity of the external radiation incident on the cloud.
Figure 2-1 Molecular cloud of depth $x$ along the line of sight. $I$ is the intensity of radiation and $\tau$ is the optical depth, along the line of sight.

The change in the intensity of radiation as it proceeds from one point in the molecular cloud to another will be given by

$$\frac{dI_\nu}{dx} = -\kappa_\nu I_\nu + \varepsilon_\nu$$

(2.1)

where: $\kappa_\nu$ = the fractional absorption of radiation over the interval $dx$ at frequency $\nu$
$\varepsilon_\nu$ = the intensity of the radiation emitted over the interval $dx$ at frequency $\nu$, and

$\nu$ = Energy (in a particular direction) per unit area, per unit time, per unit solid angle, per unit frequency

Equation (2.1) is the basic equation of radiative transfer.

It is useful to define a quantity, optical depth ($\tau$), which describes the absorption properties of the medium.

$$d\tau_\nu = -\kappa_\nu dx$$

(2.2)
2.3 Planck's Law

Under the conditions of full thermodynamic equilibrium (i.e. for a source radiating as a black body), the intensity of the emergent radiation at any frequency can also be described by Planck’s law, which is

\[ B_{\nu}(T) = I_{\nu} = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{kT}} - 1} \]  

(2.3)

where:
- \( B_{\nu}(T) \) = The source brightness function (intensity of radiation that will be emitted from a source in thermodynamic equilibrium at temperature \( T \)).
- \( h \) = Planck’s constant
- \( c \) = speed of light
- \( k \) = Boltzmann’s constant

2.3.1 Rayleigh-Jeans Approximation

At low frequencies the Planck curve is well approximated by the simpler Rayleigh-Jeans relationship

\[ B_{\nu}(T) = I_{\nu} = \frac{2\nu^2kT}{c^2} \]  

(2.4)

as can be seen from comparing (2.3) and (2.4). The Rayleigh-Jeans approximation holds if

\[ \frac{h\nu}{kT} \ll 1 \]

This will be generally be true at cm and mm wavelengths, although it may not be a good approximation for emission from cold clouds at mm and sub-mm wavelengths.

The Rayleigh-Jeans approximation can be used to define a source temperature, \( T_b \), as the temperature implied by the radiation received from the source. If the source fills the telescope beam, and is assumed to be in thermodynamic equilibrium, \( T_b \) is a physical temperature. \( T_b \) is used throughout radio astronomy whether or not the source is actually in thermodynamic equilibrium or the Rayleigh-Jeans approximation holds.

2.3.2 Local Thermodynamic Equilibrium (LTE)

Planck’s law and the Rayleigh-Jeans approximation are used extensively in deriving the equations needed to find temperatures, densities and molecular abundances in molecular clouds, usually with the unstated assumption that the source is in thermodynamic equilibrium. A molecular cloud is unlikely to be in full thermodynamic equilibrium: in reality a temperature variation across or throughout a cloud might be expected. However, we can define a local thermodynamic equilibrium
(LTE) that assumes that in a "local" volume of the molecular cloud all constituents of the gas are in thermodynamic equilibrium (i.e. thermalised) at the temperature $T$ implied by Planck's law. LTE in the interstellar medium can be a reasonable assumption as elastic collisions between the various constituents predominate, tending to share energy equally among the constituent particles of the molecular gas. Molecular hydrogen ($\text{H}_2$) is the major constituent of molecular clouds, forming about $90\%$ by number of the molecular gas. The extent to which any molecule will approach LTE with $\text{H}_2$ will depend on the abundance of the particular molecule with respect to $\text{H}_2$ and the density of $\text{H}_2$ molecules (because both determine the probability of collisions) as well as on intrinsic properties of the molecule itself.

2.4 Kirchoff's Law: Combining Planck's Law with the Equation of Radiative Transfer

In full thermodynamic equilibrium the net transfer of energy from point to point in a molecular cloud will be zero: as much radiation will be absorbed at any point as is emitted at that point.

i.e. \[
\frac{dI_\nu}{dx} = 0
\]

Substituting this into (2.1), the equation of radiative transfer gives

\[
I_\nu = B_\nu(T) = \frac{\varepsilon_\nu}{\kappa_\nu} = S
\]  \hspace{1cm} (2.5)

where: $B_\nu(T)$ = Planck function, and $S = $ source function.

Equation (2.5) is known as Kirchoff's Law and it will generally hold under conditions of LTE. The quantity $\varepsilon_\nu/\kappa_\nu$ is also known as the source function. The quantities $\kappa_\nu$ and $\varepsilon_\nu$ can be related to the physical properties of a medium so that determination of $I_\nu$ by observation can be used to determine these physical parameters.

2.5 Radiative Transfer in an Isothermal Medium

In an isothermal medium, with constant $\varepsilon$ and $\kappa$, the equation of radiative transfer (2.1) can be computed explicitly, after substitution of (2.2), as

\[
I_\nu(x) = I_\nu(0)e^{-\tau} + (B_\nu(T)) \left(1 - e^{-\tau}\right)
\]  \hspace{1cm} (2.6)

If there is no external radiation incident on the molecular cloud then (2.6) becomes

\[
I_\nu(x) = (B_\nu(T)) \left(1 - e^{-\tau}\right)
\]  \hspace{1cm} (2.7)
$I_r(x)$ is the intensity emergent from the molecular cloud and is the quantity observed at the telescope, while $B_v(T)$ is the Planck brightness distribution that describes the molecular cloud. If the Rayleigh-Jeans approximation is substituted for both $I_r(x)$ and $B_v(T)$ then (2.7) becomes

$$T_b = T_s \left(1 - e^{-\tau}\right) \quad (2.8)$$

where $T_b =$ Source brightness temperature observed by telescope (see section 3.5).

$T_s =$ Thermodynamic temperature of source.

If $\tau \gg 1$ then it can be seen from (2.8) that

$$T_b \approx T_s \quad (2.9)$$

On the other hand, if $\tau \ll 1$ (optically thin emission), then (2.8) becomes

$$T_b \approx T_s \tau \quad (2.10)$$

2.6 Spectral-Line Radiation

The preceding analysis is equally applicable to continuum and spectral line radiation. No mention has been made of the properties of individual molecules and their relationship to the emissivity and absorptivity of the emitting gas.

In the ISM spectral lines arise when a molecule or atom undergoes a transition from one energy state to another. Energy levels in atoms and molecules are quantized. A transition from one energy level to another involves the gain or loss of energy equal to the difference in energy state. The frequency of radiation emitted or absorbed in a transition is related to the energy difference between the upper and lower states by

$$E = h \nu \quad (2.11)$$

where:

- $E =$ the energy difference between energy states of molecule or atom,
- $h =$ Planck’s constant and
- $\nu =$ the frequency of emitted radiation.

Spectral line radiation occurs in addition to ‘continuum’ radiation and originates from different processes. The total emission at any frequency will simply be the sum of the continuum and spectral line emission at that frequency. The two components

---

1 Continuum radiation arises from many processes, including those that involve the deceleration of charged particles. The difference between the initial and final velocities of the particle is emitted as radiation. The radiation forms a continuum because the velocity difference forms a continuum (ignoring quantum effects). Bremsstrahlung, as emitted from HII regions is continuum radiation. Thermal continuum radiation is also emitted by dust grains within the molecular cloud.
are analysed separately by subtracting the continuum emission before analysis of the line emission.

In a high optical depth situation the brightness temperature of both the line and the continuum emission will approach the thermodynamic temperature of the molecular cloud, as in equation (2.9). Emission from a molecule that is optically thick gives the temperature of a molecular cloud but no information on optical depth (equation 2.9). On the other hand, emission from optically thin molecules gives information on the optical depth, if the temperature is known (equation 2.10). A common strategy in molecular line observations is to observe both an optically thick transition (such as CO) to determine the thermodynamic temperature of the molecule, and an optically thin transition of an isotopically substituted species (isotopomer) of the same molecule (such as $^{13}$CO) to ascertain optical depth.

2.6.1 Spectral-line profiles

A spectral-line profile contains information on the kinematics and temperature of the emitting molecular gas.

The radiation that forms a spectral line is not monochromatic but has a finite frequency range, which comes about in three different ways:

- Intrinsic (natural) line width due to the quantum mechanical uncertainty in the energy difference of the transition;
- Pressure (collisional) broadening which arises from the effect that colliding particles have on the energy difference of a transition, and
- Doppler shifting of radiation due to the motions of the emitting particles.

Doppler shifting dominates the width of spectral lines arising in molecular clouds over intrinsic and pressure broadening and has two distinct causes: thermal broadening and broadening due to large-scale motions of the molecular gas.

Thermal broadening results from the Maxwellian velocities of the particles in the gas and is dependent on temperature. The normalised line profile and the full-width at half-maximum (FWHM) of the spectral line due to thermal broadening can be derived from Maxwell’s equation and the Doppler shift and is found to be Gaussian in form. The Doppler width due to thermal motions is given by

\[
\Delta v_D = \frac{v_0}{c} \sqrt{\frac{2kT}{m}} \quad (2.12)
\]

where \( m \) is the mass of the molecule.

The relationship between Doppler width and full-width at half-maximum (FWHM) is given by (Emerson 1996)

\[
FWHM = 1.667\Delta v_D . \quad (2.13)
\]
Generally, the line widths observed in molecular clouds are greater than the line width that would be expected due to thermal broadening. The reasons for this have been discussed at length in the literature but the consensus seems to be that the line width observed in molecular clouds is indeed due to Doppler shifting, but it is Doppler shifting due to the gross motions of atoms and molecules within the gas. The motions can be due to infall, outflow, streaming motions, rotation or macro turbulence of the molecular gas.

2.6.2 Molecular Energy States

Molecules have intrinsic rotational, vibrational and electronic motions that combine to give differing energy states. The energy that any one molecule has will be a combination of its rotational, vibrational and electronic states. If a molecule absorbs a photon or gains energy from a collision it may move to a higher rotational energy level (in which case its angular momentum and hence speed of rotation will increase), or it may increase its internal vibrational energy, or the electrons in the molecule may move into higher energy configurations. In cool, dense, molecular gas, rotational transitions will be most important. Vibrational and electronic energy states are high-energy states, and in quiescent gas most molecules will be found in the ground vibrational and electronic state. Electronic states have the highest energy and will only be populated in hot and/or shocked gas. However, it should be possible to find vibrational or electronic transitions in absorption in the far infrared against a background of warm dust emission.

2.6.3 Defining Thermodynamic Temperature in Molecular Clouds

The different molecules that make up a molecular gas may have different thermodynamic temperatures. The thermodynamic temperature of H$_2$ (because it is the major constituent of molecular clouds) defines the kinetic temperature of the gas.

The temperature of any gas is defined by the velocity distribution of particles within the gas, which in a molecular cloud can be assumed to be Maxwellian due to the frequency of elastic collisions. If the gas is in LTE, then all molecules/particles will have the velocity distribution appropriate to the kinetic temperature of the gas. As the major constituent of molecular clouds, H$_2$ will have an energy level population described by the Boltzmann distribution,

\[
\frac{N_i}{N} = \frac{g_i}{U} e^{-\frac{E_i}{kT}}
\]  

(2.14)

where:

- $N_i$ = the number of particles in state $i$,
- $N$ = the total number of particles over all states,
- $E_i$ = the energy of level $i$,
- $g_i$ = statistical weight (number of degenerate states), and
- $U$ = is the partition function
The partition function is a sum over all energy states that normalizes the distribution (i.e., ensures that the sum of the terms \( N_i \) totals to \( N \)) and is given by

\[
U = \sum_i g_i e^{-\frac{E_i}{kT}}
\]  
(2.15)

The temperature implied by the Boltzmann distribution of \( H_2 \) will be the kinetic temperature of the gas. Any molecule for which the population distribution in the various energy levels is the same as for that of \( H_2 \) is by definition in LTE and determining the population of one energy level \( (N_i) \) allows the total population \( (N) \) to be determined.

The concept of temperature is more complicated when LTE is not present. Several specific definitions of temperature are used. If a molecule is not in LTE with \( H_2 \) the kinetic temperature of the gas will not describe the population of the energy levels for that molecule. Instead, there are two possibilities:

1) Another temperature, different to the kinetic temperature, may describe, in terms of the Boltzmann distribution, the population of all energy levels of the molecule in question. This temperature is generally termed the excitation temperature of the molecule. If the excitation temperature can be ascertained then determination of the population in one energy state \( (N_i) \) will still allow a determination of the total population \( (N) \) (i.e., the abundance of that molecule). The difficulty here, of course, is demonstrating that a single temperature describes the populations of all energy levels.

2) The distribution of the populations in the different energy levels cannot be described by the Boltzmann distribution. The number in each energy level can be used to define, in terms of equation (2.14), a temperature for that level, but the temperature for each level will be different. In this case, the temperature implied by (2.14) for any one level is referred to as the transition temperature of that level.

Different constituents of the gas in a molecular cloud may have different temperatures. For example CO is usually thermalized, whereas the CS population will often be sub-thermal; that is, the Boltzmann temperature that characterizes the energy level distribution of the CS population will be lower than the kinetic temperature of the gas.

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\(^2\) Appendix C discusses the calculation of partition functions and the values used in this work.
2.7 Energy Distribution in a Molecular Cloud

The gas in a molecular cloud is usually assumed to be in a steady state. This means that while, at the microscopic scale, energy is exchanged between individual particles and processes, the macroscopic parameters of the gas do not change.

2.7.1 Energy flow into and out of the molecular gas.

Energy enters the gas as either photons or particles. The photons may come from the microwave background radiation, nearby stars, or more exotic and energetic objects. Particles in the gas (molecules, atoms or ions) absorb the photons and move to higher energy states. This is radiative excitation. Dust grains in the cloud may be heated by the absorption of photons. Particles may enter the gas as outflows from nearby stars, or from the interaction of a supernova remnant with a molecular cloud. Energetic particles collide with molecules or dust grains leading to collisional excitation.

Energy usually leaves the gas as photons. A molecule in an excited state will spontaneously emit a photon: this is radiative de-excitation. The photon may escape from the gas or it may be absorbed elsewhere within the gas. Photons that escape from the gas remove energy from it. Photons absorbed elsewhere in the gas redistribute energy within the gas.

Energy is redistributed within the gas. A particle will lose or gain energy by interacting with other particles. Collisions, usually with hydrogen, which is the dominant constituent of the gas, redistribute energy throughout the gas. Most collisions are elastic, changing only the momentum of the interacting particles, however a molecule may change its vibrational or rotational energy state in a collision: collisional excitation and de-excitation. Photons emitted and then re-absorbed elsewhere within the gas also redistribute energy. Star formation within a cloud is particularly effective in redistributing energy via UV radiation, stellar winds and outflows etc.

2.7.2 Excitation and Rotational Temperatures within a Molecular Cloud

The excitation temperature of a component of a molecular cloud will generally be somewhere between the kinetic temperature and the temperature of the radiation field within the cloud (which will be the microwave background temperature of 2.7 K in the absence of nearby heat sources)\(^3\). Coupling between different components of the gas (i.e. how strongly they interact with one another) will lead to a sharing of energy between the components. The more strongly the different components interact, the closer their temperatures will approach one another and the closer the situation will be to LTE. As the density of a molecular cloud increases so too will the frequency of interaction between the various components, so a high-density situation will be more

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\(^3\) However, note that it is possible to have population inversions under specific excitation conditions, leading to a negative excitation temperature and maser emission.
likely an LTE situation. If the density is high, then collisional excitation will dominate and the excitation temperature of the constituents of the cloud will approach the temperature of the most common collision partner, H$_2$ (i.e. the kinetic temperature of the molecular cloud). On the other hand, if the gas density is low, the interaction with the radiation field in the molecular cloud will dominate and the excitation temperature will tend towards the radiation temperature.

2.8 Radiative Transfer in Terms of Molecular Properties

The equations of radiative transfer describe the observed brightness distribution (or brightness temperature) of a molecular cloud in terms of its excitation temperature, optical depth, emissivity ($\varepsilon_\nu$) and absorptivity ($\kappa_\nu$) (see section 2.2). The macroscopic quantities $\kappa_\nu$ and $\varepsilon_\nu$ can be related to the microscopic properties of the emitting molecule, and hence can link the observed brightness temperature to the excitation temperature and abundance of the molecule observed. The actual link is provided by the radiative transition probabilities.

2.8.1 Radiative Transition Probabilities: Einstein Coefficients

The probability that a molecule (or atom) will undergo a radiative transition is described by its Einstein coefficients:

- $A_{ji}$ is the probability (per second per unit volume) of a spontaneous radiative transition from energy level $j$ to energy level $i$.
- $B_{ji}$ is the probability of a stimulated transition between energy levels $j$ and $i$.
- $B_{ij}$ is the probability of photon absorption leading to a transition from $i$ to $j$.

These coefficients describe the probability of a photon being emitted by a molecule and subsequently escaping a molecular cloud without re-absorption. The coefficients are dependent on molecular properties and are related to each other: $B_{ji}$ and $B_{ij}$ can be expressed in terms of $A_{ji}$. The relationships are

$$g_i B_{ji} = g_j B_{ij} \quad (2.16)$$

and

$$A_{ji} = \frac{8\pi h \nu_i^3}{c^3} B_{ji} \quad (2.17)$$

where $g$ is the statistical weight of the energy state.

The emissivity and absorptivity of a constituent of the molecular gas can be expressed in terms of its Einstein coefficients as
\[ \kappa_\nu = \frac{\hbar \nu_0}{c} N_i B_{ij} \left( 1 - \frac{g_i N_j}{g_j N_i} \right) \varphi(\nu) \]  
\[ (2.18) \]

and

\[ \varepsilon_\nu = \frac{\hbar \nu_0}{4\pi} N_j A_{ji} \varphi(\nu), \]  
\[ (2.19) \]

where:
- \( N_i \) = the number in state \( i \)
- \( N_j \) = the number in state \( j \), and
- \( \varphi(\nu) \) = the normalized line profile function (i.e. the variation of intensity with frequency over the line, normalized to a total area of 1)

For a transition between energy states \( i \) and \( j \), the emission or absorption properties of a molecule within a molecular cloud are dependent on the number in both the upper and lower states of a transition. (It is assumed here that state \( i \) is lower than state \( j \).)

The distribution of the molecular population between all possible energy states will depend on many factors including the temperature and density of the molecular gas, the radiation field within the gas and the relative abundance of the molecule. For example, an increase in temperature moves the molecular population to higher energy levels, while an increase in density pushes the relative distribution among the various energy levels towards the Boltzmann distribution. Determining the energy level population distribution is crucial to using molecular emission to find molecular abundances and other properties of the molecular gas.

### 2.9 Determining Molecular Abundances

The equations of radiative transfer (2.1), the Einstein coefficients (2.16, 2.17) and the Boltzmann distribution (2.14) can be combined to link molecular properties with the rotation temperature and level populations for a particular transition.

In molecular-line astronomy it is usual to work in units of velocity rather than frequency and the equation for absorptivity in terms of the Einstein coefficients (2.18) can be transformed to units of velocity.

\[ \kappa_\nu = \hbar N_i B_{ij} \left( 1 - \frac{g_i N_j}{g_j N_i} \right) \varphi(\nu) \]  
\[ (2.20) \]

After substituting for \( B_{ij} \) using (2.16) and (2.17) and for \( N_j/N_i \) from (2.14), (2.20) becomes

\[ \kappa_\nu = \frac{c^3}{8\pi \nu_0^2} \frac{g_j}{g_i} N_i A_{ji} \left( 1 - e^{-\frac{\hbar \nu_0}{kT}} \right) \varphi(\nu) \]  
\[ (2.21) \]
The Einstein $A$ coefficient in cgs units in terms of molecular properties is

$$A_u = \frac{64\pi^4}{3\hbar c^3} (|\mu_u|^2)$$  \hspace{1cm} (2.22)

where $u$ and $l$ are the upper and lower levels respectively, $\mu$ is the mean electric dipole moment of the molecule, and $|\mu_u|$ is the dipole moment matrix for the transition.

Appendix C discusses the calculation of $|\mu_u|$ and $A_u$ for different types of molecules and lists the values for $A_u$ used in this work. In keeping with common practice in millimetre wave spectroscopy cgs units are used throughout. Due to differences in the definition of fundamental quantities, the equations, as well as the values of constants, will be different when expressed in SI (MKS) units.

Substituting (2.20) into the definition of optical depth (2.2) and integrating over both velocity and path length, $x$, through the gas gives

$$\int_{-\infty}^{\infty} \tau_v dv = \frac{c^3}{8\pi v_0^3} \frac{g_u}{g_l} A_u \left[ 1 - e^{-\frac{hv}{kT}} \right] \int_0^{\infty} N_l(x) dx$$  \hspace{1cm} (2.23)

The column density of the number in the lower energy state is defined as

$$N_l = \int_0^{\infty} N_l(x) dx.$$  \hspace{1cm} (2.24)

i.e. the total number of molecules along the line of sight in a cylinder which has a front surface area of 1 cm$^2$ and length (usually unknown) through the molecular cloud.

Equation (2.23) then becomes

$$N_l = \frac{8\pi v_0^3}{c^3} \frac{g_l}{g_u} A_u \left[ 1 - e^{-\frac{hv}{kT}} \right]^{-1} \int_{-\infty}^{\infty} \tau_v dv$$  \hspace{1cm} (2.25)

Equation (2.25) may also be derived for $N_u$, the column density of the upper level population of a transition. As long as $T$ is known, if the molecule observed is in LTE a knowledge of either $N_l$ or $N_u$ will suffice for determining the total population. $N_l$ can be found if the optical depth and excitation temperature of a transition are known. If LTE conditions can be assumed, then the Boltzmann distribution (2.14) can be used to determine the total column density of the molecule, which is the main quantity of interest in studying abundances.
2.10 Abundances under LTE and Non-LTE Conditions

If a Boltzmann distribution for the level populations can be assumed the processes that redistribute energy within the gas do not need to be considered explicitly. It is assumed that collisional excitation and de-excitation merely operate to bring about the Boltzmann distribution of the level populations. If this is not the case, then both collisional and radiative processes must be considered and the problem becomes considerably more complex.

The first step in calculating molecular abundances is to decide on the assumptions to be made with respect to LTE and optical depth. The assumptions can be derived from previous observations of the molecular cloud, knowledge of the usual conditions in molecular clouds for the observed molecule and/or observations of multiple transitions or isotopomers of the same molecule.

Five possible cases are described below, together with analytic methods that can be used in each case, and the information that these methods give.

1) \( \tau \) is \( \gg 1 \)

If \( \tau \) is \( \gg 1 \) then (2.9) can be used to estimate the excitation temperature of the transition. Abundances cannot be obtained from the measurement of an optically thick transition. However, an optically thick transition can be observed to obtain an excitation temperature that can then be adopted for an optically thin transition of the same molecule or one of its isotopomers. In this case the assumption is that LTE applies, or at least that all isotopomers of a molecule will be at the same excitation temperature. However, if there is a temperature gradient across the molecular cloud the estimated excitation temperature may apply only to the front of the cloud.

2) \( \tau \ll 1 \) and LTE conditions apply.

If \( h \nu \ll kT \) so that the Rayleigh Jeans approximation can be used, then (2.25) becomes

\[
N_i = \frac{8\pi v_i^2}{c^3} \frac{g_i}{g_s A_{wi}} \frac{1}{h} \left[ \frac{kT_{ex}}{h} \right] \int_{-\infty}^{\infty} v \, dv
\]  

(2.26)

If \( \tau \ll 1 \), then from (2.10) \( T_b = T_{ex} \tau \), and this can be substituted into (2.26) to give

\[
N_i = \frac{8\pi v_i^2}{c^3} \frac{g_i}{g_s A_{wi}} \frac{1}{h} \left[ \frac{k}{h} \right] \int_{-\infty}^{\infty} T_b \, dv
\]  

(2.27)

In observational terms this means that if almost all photons escape the gas then the observed emission will be proportional to the number of molecules in the column of gas within the telescope beam. For \( N_i \) to be the true column density the gas
must be spatially extended with respect to the telescope beam. Without a priori
knowledge it is always assumed that the gas uniformly fills the beam. If the spatial
extent of the gas is smaller than the beam the column density will be greater than
that given by (2.27).

Because LTE occurs, the value of \( N_l \) from (2.27) can be used in (2.14) to find the
total column density of the molecule.

If a number of transitions of the same molecule have been observed the equations
derived from (2.27) and (2.14) can be solved simultaneously to find a solution for
both \( N_{tot} \) and \( T_{ex} \), or a graphical method may be used: the rotation diagram
analysis (see section 2.10.3).

3) \( \tau << 1 \) and LTE conditions do not apply.

In this case, (2.27) can be used to find the level populations of the transition, but
(2.14) cannot be used to find the total column density of the molecule; instead, a
non-LTE analysis must be used (see case 5).

4) LTE conditions apply but \( \tau \) is not \( << 1 \).

In this case, some way is needed to estimate both the excitation temperature and
the optical depth of the transition. The excitation temperature \( (T_{ex}) \) can be
estimated by observing a transition that is known to be optically thick and using
equation (2.9). This excitation temperature can then be used to estimate optical
depth in optically thin transitions, provided LTE applies (or a single excitation
temperature describes the level populations). It is also possible to estimate optical
depth from molecular transitions with hyperfine structure using (2.26).

Once an estimate of the optical depth is found the approximation

\[
T \int_{-\infty}^{\infty} \tau(v)dv \approx \frac{\tau_0}{1 - e^{\tau_0}} \int_{-\infty}^{\infty} I_B(v)dv
\]  

(2.28)

can be substituted into (2.26) to give an equation similar to (2.27) that does not
require \( \tau << 1 \). According to Rohlfis & Wilson (1996), equation (2.28) is accurate
to 15% for \( \tau_0 < 2 \), but it always underestimates column density if \( \tau_0 > 1 \).

5) LTE conditions do not apply and \( \tau \) is not \( << 1 \).

If LTE does not hold, and the Boltzmann distribution does not describe the level
populations, equations of statistical equilibrium can be used. The assumption of
statistical equilibrium is that for each energy level, the rate of population departure
to all other levels will be equal to the rate of arrival from all other levels.

Assuming that the molecular gas is in a steady state (i.e. the macroscopic
properties are not changing) then the number of particles entering an energy level
(i) due to both radiative and collisional processes will be equal to the number
leaving that level by all processes. In mathematical terms this gives what is known as the rate equation.

$$\sum_j N_j (R_{ij} + C_{ij}) = \sum_j N_j (R_{ji} + C_{ji})$$  \hspace{1cm} (2.29)$$

where:
- $R_{ij}$ = rate of radiative processes that cause a transition from $i$ to $j$
- $C_{ij}$ = rate of collisional processes that cause a transition from $i$ to $j$
- $R_{ji}$ = rate of radiative processes that cause a transition from $j$ to $i$
- $C_{ji}$ = rate of collisional processes that cause a transition from $j$ to $i$.

The sum must include all levels $j$ for which a radiative or collisional transition with level $i$ is possible. The collisional rates for the transitions, $C_{ij}$ and $C_{ji}$, are complex to calculate or measure and are discussed further in section 2.10.1.

The radiative rates are (assuming that level $j$ is the upper level)

$$R_{ij} = B_j \langle U_{ij} \rangle$$  \hspace{1cm} (2.30)$$

and

$$R_{ji} = A_{ji} + B_j \langle U_{ij} \rangle$$  \hspace{1cm} (2.31)$$

$A$ and $B$ are the Einstein coefficients and $\langle U_{ij} \rangle$ is the average radiation field at the frequency of the transition $i$ to $j$.

The radiation field within the molecular cloud at a radius $r$ from the centre of the cloud can be described by

$$\langle U_{ij}(r) \rangle = (1 - \beta_{ij}(r))S_j + \beta B_j(v_g, T_{BB})$$  \hspace{1cm} (2.32)$$

where $\beta$ is the probability that a photon emitted at a radius $r$ will escape from the molecular cloud, $S_j$ is the source function (2.5) and $B_j$ is the 2.7 K microwave background radiation field.

In practice, solving the equations generated by (2.29) is difficult and can only be done with the use of a model that makes assumptions about radial variation of the radiation field within the molecular cloud, the geometry of the cloud and the background radiation temperature.

Modeling the form of radial variation of the radiation field is a complex problem and for optically thick transitions allowance must be made for photon trapping (photons emitted and then reabsorbed within the molecular cloud). The most widely used method of modeling the radiation field without making the assumption of LTE (and consequent assumption of Planck's Law) is the Large Velocity Gradient (LVG) approximation.
Qualitatively, the LVG approximation makes the assumption that there are large-scale systemic motions in a molecular cloud so that velocity is a function of distance from the centre. It is also assumed that the systematic velocity is much greater than any collisional or thermal line width. Under these conditions a photon emitted at one position in the cloud can only interact with molecules that are nearby. If a photon is not reabsorbed close to where it is emitted it will escape the molecular cloud. This simplification allows the probability that a photon emitted at a particular radial distance will escape the molecular cloud to be expressed in terms of optical depth as

$$\beta(r) = \frac{1 - e^{-3\tau_{ij}}}{3\tau_{ij}}$$

(2.33)

$\beta(r)$ is the probability that a photon emitted at a radius r will escape from the molecular cloud and $\tau_{ij}$ is the optical depth of the transition between levels $i$ and $j$. Equation (2.33) assumes a plane-parallel geometry.

The actual form of LVG approximation for the radiation field is dependent on the geometry assumed for the molecular cloud. The photon escape probability (2.33) and the average radiation field (2.32) can be substituted into the rate equations for the various energy levels (2.29). These can then be solved simultaneously to estimate the excitation temperatures and optical depths of transitions, or the abundance of the molecule under consideration, or the hydrogen density or kinetic temperature of the molecular cloud, if some of these of these quantities can be ascertained by other means. The LVG method is discussed quantitatively in Scoville and Solomon (1974), Goldreich & Kwan (1974) and Castor (1970).

2.10.1 Collisional Rates

The rate of collisional excitation or de-excitation between levels $i$ and $j$ is given by

$$C_{ij} = N \langle \sigma(v)v \rangle$$

(2.34)

where: $N =$ number density of colliding particles (primarily $H_2$)
$\sigma(v) =$ the collision cross section, which is velocity dependent, and
$v =$ the velocity of the colliding particles.

The term $\langle \sigma(v)v \rangle$ is average of the product $\sigma(v)v$ over the velocities of the colliding particles. The collisional rate will be proportional to the number density of collision partners, $H_2$ and $He$. Although $He$ is inert and does not take part in chemical reactions, it forms about 10% of the molecular gas and so is a likely collision partner. Collisional cross sections must be measured in a laboratory situation or calculated. However, for neutral collision partners the value of the cross section does not vary greatly, and $\sigma = 10^{-15}$ cm$^2$ can be used as a first approximation to calculate collision rates for different densities (Emerson 1996).
2.10.2 Excitation Temperature and Critical Density

The relationship between the collisional and radiative rates for a transition can be used to infer the H$_2$ density. As seen from (2.34) the collisional rate will be directly proportional to the number density of H$_2$. As the density of the molecular gas increases $T_{ex} \to T_k$. In a low density situation, $T_{ex} \to T_b$. If $T_{ex} = T_b$, the molecular line radiation will be in thermodynamic equilibrium with the radiation field and line radiation will not be distinguishable. For moderate densities $T_{ex}$ will be between $T_k$ and $T_b$.

The relationship between the collisional and radiative rates determines excitation temperature ($T_{cx}$) for a transition. If the radiative rate for a transition ($A_{ij}$) is small, radiative transitions will be less frequent, and collisional excitation will play a corresponding greater role, driving $T_{ex}$ towards $T_k$. The density at which the collisional and radiative rates for a transition are equal is known as the critical density, and in the optically thin case it is at this density that emission in a line becomes significant, leading to an observable line. If optical depth is high, then the density of gas required to excite a transition will be lower than the critical density because photons reabsorbed within the molecular cloud lead to more molecules being in the higher energy state than would otherwise be the case.

An estimate of the critical density ($n^*$) for a transition can be obtained by using $\sigma = 10^{-15}\text{ cm}^2$ and assuming an average velocity of colliding particles of $1\text{ km s}^{-1} = 10^5\text{ cm s}^{-1}$. Then

$$A_{ij} = C_{ij}$$
$$A_{ij} = n^*<\sigma v>$$
$$n^*(\text{cm}^{-3}) = A_{ij} (10^{10}\text{ cm}^{-3})$$

(2.35)

If $\tau \gg 1$, then $A_{ij}$ in (2.35) should be replaced by $A_{ij}/\tau$ (Rohlfs & Wilson 1996).

An observable transition hence sets a lower limit to the density in the molecular gas from which it arises. $A_{ij}$ is proportional to the dipole moment of the molecule, so observable emission from a molecule with a high dipole moment sets the lower limit for the density of the molecular cloud.

2.10.3 Rotation diagram analysis

The 'rotation diagram' method of analysis utilizes observations of multiple transitions of a molecule and can give a reliable estimate of both the excitation temperature and the molecular column density, provided the emission from all transitions is optically thin and the condition of LTE is satisfied. However, examination of the rotation diagram can support (or otherwise) the assumptions of LTE and optically thin emission.

If LTE is assumed, the level populations of a molecule will be given by the Boltzmann distribution (equation 2.14, repeated here).
\[
\frac{N_l}{N} = \frac{g_l}{g_u} \frac{e^{-\frac{E_l}{kT}}}{U} \quad (2.36)
\]

The number of molecules in the upper state per statistical weight will be

\[
\frac{N_u}{g_u} = \frac{N_{Tot}}{U} \frac{e^{-\frac{E_u}{kT}}}{U} \quad (2.37)
\]

where \(N_{Tot}\) is the column density of the molecule and the other symbols have the same meaning as in (2.14).

Taking the natural logarithm of both sides of (2.37) gives

\[
\ln \left( \frac{N_u}{g_u} \right) = \ln \left( \frac{N_{Tot}}{U} \right) - \left( \frac{E_u}{k} \right) \left( \frac{1}{T} \right). \quad (2.38)
\]

For a number of transitions, if the log of the column density in the upper state, per statistical weight, is plotted against the energy of the upper state above the ground state divided by \(k\), for a number of transitions, the result will be a straight line with slope \((1/T)\) and intercept \(\ln(N_{Tot}/U)\), provided that the energy levels are populated according to the Boltzmann distribution.

The column density of molecules in the upper energy level of a transition can be derived from observations of the transition, provided the emission is optically thin. Equation (2.27) gives the column density in the lower level for optically thin emission and by using the Boltzmann equation, and assuming that \(h\nu/kT \gg 1\), the column density of the upper level is given by

\[
N_u = \frac{8\pi k v_0^2}{hc^3} \int_{-\infty}^{\infty} T_b dv. \quad (2.39)
\]

For optically thin emission in LTE, the rotation diagram will give the kinetic temperature of the molecular cloud if all levels are thermalized, or the sub-thermal excitation temperature of the molecule if a single sub-thermal excitation temperature characterizes all level populations. For \(\tau < 2\) the correction factor given in (2.28) can be applied to the emission to partially compensate for optically thick emission.

A rotation diagram that cannot be fitted by a straight line may indicate that the assumptions of optically thin emission and/or a Boltzmann distribution of level populations are not correct. An excellent and detailed discussion of the use of a rotation diagram in analysing molecular line emission can be found in Goldsmith & Langer (1999), including using the rotation diagram as a diagnostic tool for optically thick emission or non-LTE situations. The following observations are drawn from this paper.
The total column density derived from a rotation diagram will have an uncertainty that is closely related to deviations from a Boltzmann distribution of the level populations. The presence of optically thick emission will in addition cause an underestimation in the total column density and an error in the excitation temperature determined from the rotation diagram.

A non-linear rotation diagram may also result from a molecular cloud that is smaller than the beam of the telescope used to observe it. If appropriate correction for changing beamwidth with frequency is not applied, the emission in a transition will be underestimated by the beam-filling factor (angular area of source relative to the angular area of the telescope beam broadened by the source). As the area of the telescope beam is inversely proportional to the frequency of observation each transition may have a different beam-filling factor.

2.11 Determining Physical Conditions and Molecular Abundances

Determining the physical conditions and molecular abundances in molecular clouds involves observing a number of different transitions and molecules to build up a picture of the molecular cloud being investigated. Molecular abundances can be determined from the equations and methods in section 2.10. An important part of this process is the estimation of excitation temperatures, optical depths and deviations from LTE so that the correct analysis method for the particular situation can be used.

2.11.1 Determining kinetic temperature and hydrogen column density from CO

The usual starting point for investigating a molecular cloud is CO because it is the most abundant molecule after H₂ and is believed to be a good tracer of H₂. Due to both its abundance and its low dipole moment it can be, for the lower rotational transitions at least, assumed to be in LTE. The $^{12}$CO isotopomer is invariably found to be optically thick, and hence gives the kinetic temperature of a molecular cloud. The optically thin isotopomers ($^{13}$CO, C$^{18}$O, C$^{17}$O) can then be used together with the kinetic temperature derived from $^{12}$CO to find the molecular abundance of the optically thin species.

From this point, empirical formulae can be used to find the $^{12}$CO and H₂ abundance. The abundance of $^{12}$CO can be estimated from knowledge of the $^{12}$C:$^{13}$C and $^{16}$O:$^{18}$O isotopic ratios. The H₂ column density can be estimated from empirical relationships between $^{12}$CO emission and H₂ column density (see e.g. Wolfire et al. 1993, Kwitter & Leung, 1985, Taylor et al. 1993), and between $^{13}$CO and C$^{18}$O column densities and H₂ column density (Lada et al. 1994). These methods of analysis are discussed in detail in Chapter 4.
2.11.2 Determining excitation temperatures and optical depths for molecules other than CO

LTE cannot as readily be assumed for other molecules. Molecules with higher intrinsic dipole moments are likely to have sub-thermal excitation temperatures, and may not even have a level population with a Boltzmann distribution.

Ideally, the use of a statistical equilibrium analysis together with the observation of many transitions can be used to find the rotation temperature and optical depth for any transition, together with the total molecular abundance, if factors such as the kinetic temperature and H₂ density are known by other means. However, the procedure is complex and simpler LTE methods are used where the LTE approach can be justified. An additional uncertainty in the LVG approach is the required assumption of a value for the velocity gradient across the molecular cloud.

The rotation diagram method of analysis using multiple transitions of a molecule can be used to find the excitation temperature and column density. It assumes that the emission is optically thin; however as pointed out already, examination of the rotation diagram can test the assumption of LTE.

Observations of both an optically thick transition and an optically thin transition of an isotopomer can be used in a similar fashion to that for CO (see section 2.8) to estimate the excitation temperature, optical depth and abundance of the both species. However, this method does not give any information on deviations from LTE.

If only one or two transitions of a molecule have been observed, then the determination of the excitation temperature involves using an educated guess as to what the excitation temperature may be on the basis of other information. If excitation temperatures from other molecular species are available these may be used together with consideration of chemical and physical properties of the molecule being observed, particularly for molecules that have similar structure and excitation. A more detailed discussion of these matters follows in Chapter 4.
Chapter 3

Equipment and Calibration

3.1 Introduction

Chapter 2 concentrates on the theory needed to determine molecular cloud properties from observations of molecular spectral lines. A critical quantity observed by the telescope is the source brightness distribution within a specific frequency range, defined in equation (2.7), and usually expressed as a source brightness temperature as in equation (2.8). Ideally, the source brightness temperature obtained from observations and used in the equations of chapter 2 should be independent of the equipment used to obtain the information.

The current chapter describes the way in which the signals obtained at the radio telescope must be corrected to produce a telescope-independent brightness temperature, and the extent to which this has been possible in the observations described in this thesis. The telescopes used to make the observations are described in section 3.2; characteristics of the signals received directly at the telescope are described in section 3.3, and observing strategies are discussed in section 3.4. The calibration of millimetre-wave observations is described in sections 3.5 and 3.6, and the specific calibration for the Mopra telescope is described in section 3.8. The accuracy of the Mopra calibration is examined in section 3.9 and section 3.10.

3.2 Telescopes Used for Observations

3.2.1 The Mopra Radio Telescope

The 22-m 'Mopra' antenna of the Australia Telescope (operated by the Australia Telescope National Facility, CSIRO) is situated near Coonabarabran in New South Wales, Australia. The telescope is at latitude 31° south and has an elevation of 850 metres above sea level. In 1994 the telescope was fitted with a millimetre-wave receiver allowing it to operate at frequencies between 85 and 116 GHz. The antenna has a 'shaped' parabolic surface area to increase its forward gain and until 1999 it had a solid reflecting surface extending over a diameter of only 15 metres. Thus at millimetre wavelengths the reflecting surface had an effective diameter of 15 m, resulting in a half-power-beam-width that varied from 47 arcsec to 35 arcsec across the range 85 – 116 GHz.

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1 Resulting from funding contributions from the University of New South Wales, the solid surface was extended over the full diameter in 1999, extending the millimetre-wave collecting area to 22-metres.
The Mopra mm-wave receiving system includes a cryogenically cooled SIS (Superconductor Insulator Superconductor) amplifier that can be tuned to either single or double side-band mode. For single sideband operation, the response of the unwanted sideband can be decreased to at least 10 dB below the other sideband response using a calibration signal injected into both sidebands. A polarization splitter is used to separate the incoming signal into two channels that can be tuned separately, allowing the observation of two frequencies simultaneously. The ‘backend’ is a digital autocorrelator, providing two simultaneous outputs with available bands, with widths ranging from 4 to 64 MHz, which can be split into a maximum of 4096 channels.

Both the antenna and the digital correlator have features in common to those used in the Australia Telescope Compact Array, and further details can be found in the Special Edition of the Journal for Electrical and Electronic Engineering, Australia, Vol 12, N° 2 (1992).

3.2.2 The SEST

The Swedish-ESO Submillimetre Telescope\(^2\) (SEST) is situated at the European Southern Observatory at La Silla in Chile, about 600 km north of Santiago. The SEST has a Cassegrain design and a parabolic collecting surface with a diameter of 15 metres, giving a half power beam width ranging from 57 arcsec at 86 GHz to 15 arcsec at 346 GHz.

The SEST is fitted with three SIS receivers that collectively cover the frequencies 78 – 117 GHz, 128 – 170 GHz, 215 – 270 GHz and 320 – 363 GHz. A polarization splitter allows the observation of two different frequencies simultaneously, although the combinations of frequencies are limited to 3-mm and 2-mm, or 3-mm and 1.6-mm.

Three Acousto-Optical Spectrometers (AOS) provide backends to the receivers. The high resolution AOS has a maximum band of width 86 MHz, which can be divided into up to 2000 channels.

For more instrumentation details see Booth et al. (1989) or The SEST Handbook (1997).

3.3 Signal Received by a Single Dish Radio Telescope

A radio telescope with a parabolic collecting area measures the power per unit area over the observing bandwidth, per unit solid angle incident from a particular direction. The response of this antenna to the incident power is directional and can be described by the normalized power pattern, or beam pattern of the telescope. Figure 3.1 is reproduced from Rohlfis & Wilson (1996) and shows a typical beam for a parabolic antenna. The beam is divided into the main lobe, side lobes and stray pattern, with the stray pattern being a combination of the far side lobes.

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\(^2\) The SEST is operated jointly by the Swedish Natural Science Research Council and the European Southern Observatory.
3.3.1 Signal Received at the Telescope

The signal received directly by the single dish telescope will not be the source brightness distribution. The power received by the telescope will include contributions from all lobes of the beam, over $4\pi$ steradians (often termed the full beam). However, the signal that is wanted is normally only that from the main beam pointed towards the object under observation. Ideally, the power pattern of the antenna should be such that the main beam receives all the power and the side lobes are suppressed, but in practice this is not possible. Any interpretation of the power received by the antenna must correct for the 'efficiency' of the main beam (i.e. the power in the main beam relative to the total power in all lobes). Complexities arise when the target object is extended and contributes power through some of the side lobes, or when the side lobes pick up power from other sources of radio emission.

In addition, at millimetre wavelengths the signal from the source will be attenuated as it passes through the Earth's atmosphere, providing an additional level of complication to the calibration of millimetre observations.

![Figure 3-1 Antenna beam-pattern showing the main beam, and near (forward) and far side lobes. The weaker far side lobes have been combined to form the stray pattern (reproduced from Rohlfs & Wilson 1996).](image-url)
3.3.2 Antenna Temperature

The power received by a radio telescope can be calibrated in units of antenna temperature \( T_A \), which is consistent with the source temperature \( T_b \) defined by the Rayleigh-Jeans approximation (2.8). The relationship between the power received at the telescope and antenna temperature is given by Nyquist's theorem.

\[
W = kT_A
\]  
(3.1)

Where: \( W \) = power received by telescope  
\( k \) = Boltzmann's constant  
\( T_A \) = antenna temperature.

The antenna temperature is the temperature that a resistor would have if it were putting out the same amount of power per unit frequency as that received by the telescope.

3.4 Observing Strategies

When the telescope is pointed at the source, the observed signal contains contributions from the Earth's atmosphere, the ground and the electronics of the receiving system. In particular, the gain of the receiver will vary with frequency, giving a spectral baseline across the bandwidth that is markedly uneven. These contributions generally overwhelm the signal from the source and must be removed. There are several strategies for doing this.

3.4.1 Position Switching

In position-switching mode the telescope is moved between the position of the source and a nearby off-source reference position free from the object or other objects. Comparing the source observation and the reference observation removes background and sky contributions. Best results are obtained if the source and reference positions are close in the sky, and if the time interval between the two observations is small. In this situation the sky and background contributions will be similar. Position switching has been the only observing mode currently available with the Mopra Telescope.

3.4.2 Beam Switching

Beam switching is in principle the same as position switching. However, rather than moving the telescope, a rotating focal-plane 'chopper mirror' (in the case of the SEST a nutating subreflector in a Cassegrain system), switches the beam between the source position and a reference position several arcminutes away, generally in azimuth. The SEST beam chopper rotates with a frequency of 6 Hz, so that the source and the reference positions are observed almost simultaneously. However, the path of the telescope beam is
different for the two positions, resulting in a poor spectral baseline in the difference spectrum. To overcome this a dual observing mode is adopted in which different spectra are obtained with the source successively in each beam. Averaging the two difference spectra gives a very flat spectral baseline. The disadvantage of beam switching is that the maximum beam throw for the SEST is 11 arcmin and the method is not suitable for observing extended sources or complex regions such as the centre of the Galaxy.

3.4.3 Frequency Switching

In frequency switching mode for spectral line observations the telescope remains pointed at the target. Pairs of spectra are obtained with observing frequencies offset from each other. Differenting and dividing one spectrum by another yields a positive and a negative feature and the spectrum can be manipulated to provide an appropriate average of the two features. Frequency switching is very useful for observing extended sources, as long as the line is significantly narrower than the observing bandwidth. The disadvantage of frequency switching is that the gain of the receiver varies with frequency and the final baseline obtained by this method may be complicated and difficult to remove from the spectrum.

3.5 Intensity Calibration of Millimetre Wave Telescopes

Calibration is the process of recovering the true source brightness distribution from the observed signal. The aim of calibration is to place the observed signal onto a telescope-independent measurement scale, so that telescopes with similar angular resolution will give the same measurement for a given source.

3.5.1 Some Definitions

Some symbols and terms used in the discussion of calibration are defined below. These terms generally follow the notation and analysis of Rohlfs & Wilson (1996), although some (e.g. $T_A$, $T_A'$) are defined in a more specific way, according to their usage in this thesis.

Telescope Beam

Figure 3.1 shows a typical antenna power pattern. The power pattern can be divided into the main beam (see figure 3.1), the forward beam (which includes the main beam and forward facing side lobes), the inner side lobes (forward facing side lobes) and the back lobes (far side lobes).

Forward Beam Efficiency ($F_{\text{eff}}$)

The fraction of power in the forward beam of the antenna (main beam and forward facing side lobes).
**Main Beam Efficiency ($B_{eff}$)**

The fraction of power in the main beam.

**Beam Filling Factor ($f_{BEAM}$)**

The relative area of the main beam filled by the source. $f_{BEAM}$ has a maximum value of one for a source that fills or is larger than the beam. A beam-filling factor of less than one can result from a source of angular extent less than the main beam, from a clumpy structure within a source that is apparently extended, or from both these effects.

**Back-Scattered Radiation**

Radiation entering the receiver from directions away from the antenna’s forward beam.

**Source Brightness Temperature ($T_b$)**

Temperature of a blackbody which would give the same power per unit area, per unit frequency, per unit solid angle as the observed source, as defined by the Rayleigh-Jeans relationship. This brightness temperature is a property of the source only, and is independent of the telescope.

**Antenna Temperature ($T_A$)**

Power detected by a telescope expressed in terms of an equivalent blackbody temperature. $T_A$ is not corrected for aperture efficiency, ohmic losses, electronic noise, far side lobe contributions (back scattered radiation) or atmospheric attenuation of signal.

**Calibrated Antenna Temperature ($T_A'$)**

Antenna temperature corrected for atmospheric attenuation, backscattered radiation and noise added by telescope electronics (e.g. receiver temperature).

**Corrected Antenna Temperature ($T_A^*$)**

Calibrated antenna temperature ($T_A'$) which has also been corrected for the forward beam efficiency ($F_{eff}$) of the telescope. $T_A^*$ will be the true source brightness temperature of a very extended source that fills the forward beam of the telescope (main beam and forward side lobes).

**Main Beam Brightness Temperature ($T_{MB}$)**

Calibrated antenna temperature after correction for the main-beam efficiency ($B_{eff}$) of the telescope. $T_{MB}$ will be the true source brightness temperature of a source that just fills the main beam. $T_{MB}$ and $T_A^*$ are related by

$$T_{MB} = (T_A^*)(F_{eff})/(B_{eff}) \quad (3.2)$$
**Primary Calibrator**

Source of radio emission for which the brightness temperature \( T_b \) and angular extent is known. Observation of such a source allows calculation of antenna efficiency parameters. The bright, extended molecular clouds M 17SW and Orion KL were used as primary calibrators for the Mopra observations (see Table 4.1 for positions). These can be considered homogeneous across the telescope main-beam at mm wavelengths for both the SEST and Mopra. These molecular clouds are used to monitor the absolute calibration of the SEST (The SEST Handbook 1997).

**Secondary Calibrator**

A source which can be observed repeatedly and is used for the relative calibration of observations. For this thesis, any source for which repeated observations were available, including the primary calibrators, was used to check the internal consistency of the calibrated Mopra observations.

### 3.6 Correcting Observations via the “Chopper Wheel” Method

The method used to correct both the SEST and Mopra observations for atmospheric attenuation is known as the “chopper wheel” method. This method is used on-line at the SEST; however, the Mopra radio telescope did not have on-line intensity calibration at mm-wavelengths and the data had to be calibrated after collection.

The “chopper wheel” method corrects for atmospheric attenuation and antenna efficiency.

#### 3.6.1 Background

The Earth’s atmosphere is only partially transparent at millimetre wavelengths. Water vapour and oxygen molecules in the atmosphere both emit and absorb radiation at these wavelengths. Emission is seen as increased noise in a spectral line observation, whereas the absorption causes an attenuation of the spectral-line intensity; both depend on the mass of oxygen and water vapour between the telescope and the source. Two main atmospheric components, oxygen and water vapour, contribute independently (Kutner 1978). The oxygen content is fairly stable and the attenuation due to this component will be relatively constant at any particular elevation. On the other hand, the mass of water vapour in the atmosphere can vary significantly on time scales of a few minutes, and under such conditions observations must be corrected for attenuation at similar intervals.

A technique historically called the ‘chopper-wheel’ method can correct for optical depth fluctuations on short time scales. It is based on the insertion of an ambient temperature source into the antenna beam. First suggested by Penzias and Burrus (1973), it is now the method most commonly used to calibrate spectral line data at millimetre wavelengths. Comprehensive treatments of this method can be found in Kutner and Ulich (1981) and Rohlfs and Wilson (1996). For the calibration of mm-wave observations obtained with
the Mopra antenna, we have developed a technique based on this method, as discussed in the following sections.

3.6.2 Overview of Method

The method is based on alternate observations of a ‘blackbody’ source at ambient temperature (inserted directly in front of the receiver system), and of empty sky at a similar elevation to the object being observed. The temperature difference between these two observations is then used to correct the data. This method corrects antenna temperature measured at the telescope ($T_A$) for atmospheric attenuation. The calibrated signal (commonly termed $T_A'$) is that which would be measured above the Earth’s atmosphere by a lossless antenna.

Two further corrections are necessary to obtain absolute temperatures independent of the telescope used. Correcting $T_A'$ for the main beam efficiency of the telescope will give the main-beam brightness temperature $T_{MB}$; this is the quantity commonly given in the literature. To obtain the source brightness temperature $T_b$, a further correction is required based on the relative angular sizes of object and telescope beam. $T_b$ is the actual brightness temperature of the source and is independent of the telescope. The determination of true source brightness temperature is imperative if observations made with different beam sizes or from different telescopes are to be compared.

3.6.3 The Theory

We start by formulating a model for the atmospheric attenuation. We assume a plane, stratified atmosphere and derive the equations below. A signal suffers an exponential attenuation on its passage through the atmosphere. The optical depth at an angle $z$ from the zenith will be the product of the zenith opacity ($\tau_0$) and $\sec(z)$.

If $T_{sou}$ is the source temperature that would be observed above the Earth’s atmosphere (i.e. equivalent to $T_A$), $T_{amb}$ is the ambient atmospheric temperature, $T_{rec}$ is the receiver temperature, and $\tau_0 \sec(z)$ is the optical depth of the atmosphere along the line of sight to the source, then the signal received at the telescope when looking at the source will be:

$$T_{sig} = T_{rec} + T_{sou}e^{-\tau_0 \sec(z)} + T_{amb}(1 - e^{-\tau_0 \sec(z)})$$

(3.3)

and the signal received at the telescope when looking at empty sky at the same zenith angle will be:

$$T_{ref} = T_{rec} + T_{amb}(1 - e^{-\tau_0 \sec(z)})$$

(3.4)

Subtracting (3.4) from (3.3) leaves only the exponentially attenuated source temperature:
\[ \Delta T = T_{\text{sig}} - T_{\text{ref}} = T_{\text{sou}} e^{-\tau_0 \sec(z)} \]  

Now if a ("blackbody") source at ambient temperature is used to provide a calibration signal at zenith angle \( z \), then

(a) the receiver output when the calibration source is placed in front of the receiver is:

\[ P_{\text{BB}} = GT_{\text{rec}} \pm GT_{\text{amb}}, \]  

where \( G \) is a gain factor related to the receiver.

(b) the receiver output when the calibrator is removed is:

\[ P_{\text{ref}} = GT_{\text{rec}} \pm GT_{\text{amb}}(1 - e^{-\tau_0 \sec(z)}) \]  

The calibration signal is then given by the output difference:

\[ P_{\text{cal}} = P_{\text{BB}} - P_{\text{ref}} = GT_{\text{amb}} e^{-\tau_0 \sec(z)} \]  

Dividing \( \Delta T \) (3.5) by the calibration signal (3.8) gives:

\[ \frac{\Delta T}{P_{\text{cal}}} = \frac{T_{\text{sou}}}{GT_{\text{amb}}} \]  

Multiplying (3.9) by the ambient temperature and the constant \( G \) gives us \( T_{\text{sou}} \), which is \( T_A' \).

This is the standard "chopper wheel" method for the calibration of mm-wave data. However, there are some differences in the way this method must be applied to data collected with the Mopra telescope (see section 3.8.2).

3.7 What Calibration is Required?

3.7.1 Mopra Data

Unlike the situation for other mm-wave telescopes, the antenna temperatures obtained from the Mopra telescope were not automatically calibrated for atmospheric absorption at the time of observation, and this calibration was undertaken later. The Mopra intensities were also on an arbitrary "Mopra" antenna temperature scale, which had to be related to an absolute brightness temperature scale. For sources that are extended, and homogeneous across the telescope forward-beam, these two steps will give the source brightness temperature.
The calibration used to correct the observations for atmospheric attenuation is described in the following sections. The corrected observations were then placed onto the SEST antenna temperature scale using the clouds M 17 SW and Orion KL as primary calibrators. These are both extended molecular clouds that have been observed extensively with the SEST for intensity calibration at the frequencies of prominent molecular line transitions.

3.7.2 SEST Data

The antenna temperatures from SEST have been corrected for atmospheric attenuation and the forward beam efficiency of the telescope (i.e. they are on the $T_A^*$ scale), and the SEST antenna temperature scale is well determined by regular absolute calibration. For an extended, homogeneous cloud that just fills the main-beam, $T_A^*$ will give the true cloud brightness temperature (after a simple correction is made for the SEST main-beam efficiency).

3.7.3 SEST and Mopra Data

For small-diameter clouds (or clouds with small-scale structure) a correction must be made for the size of the source compared to the size of the telescope beam (see ‘beam-filling factor’ section 3.5.1). The complex structure and irregular shape of many molecular clouds makes an exact determination of the beam-filling factor difficult and in work of this type the assumption is often made that this factor is always one; i.e. that all clouds are extended, homogeneous, and fill the main beam of the telescope (Rohlfs & Wilson 1996).

3.8 Calibrating the Data

Calibration of the Mopra data has formed a major part of this thesis. As already stated, the Mopra radio telescope did not have on-line intensity calibration at mm-wavelengths, and the observed intensities are on an arbitrary scale that must be calibrated using observations from another telescope. In this case the SEST has been used, not only because the SEST scale is well determined, but also because SEST molecular line observations are included in this thesis study.

Figure 3.2 outlines the procedure used to calibrate both the Mopra and the SEST observations.

3.8.1 A Note on Using the SEST to Calibrate Mopra Observations

The primary calibrators were used to put the observed arbitrary Mopra antenna temperatures ($T_A$) on to the SEST $T_A^*$ scale. The two telescopes have the same aperture
and similar beam sizes (although the shaped-parabolic nature of the Mopra reflecting surface has resulted in smaller beam sizes for the Mopra telescope). The impact of the different beam sizes is that the two telescopes will measure intensities for small-diameter clouds due to slightly different beam dilutions. For extended molecular clouds such as M 17 SW and Orion the observed intensities will be the same, allowing the calibration of Mopra to the SEST scale.

![Diagram of Mopra Observations]

**Mopra Observations**

Observation of source sample interspersed with observation of primary and secondary calibrators.

\[ T_A \]

Correct for atmospheric attenuation.

\[ T_A' \ (\text{Mopra scale}) \]

Use Primary calibrators to place Mopra observations on SEST scale.

\[ T_A^* \ (\text{SEST scale}) \]

Correct for SEST beam efficiency. \( (T_{MB} \) is the quantity reported in Chapter 4)

\[ T_{MB} \]

Use secondary calibrators to calculate uncertainties

**SEST Observations**

\[ T_A^* \ (\text{SEST scale}) \]

*Figure 3-2 Flow chart describing the steps necessary to calibrate Mopra and SEST observations to produce the final source brightness temperatures.*

3.8.2 Applying the ‘Chopper Wheel’ Method to Mopra Observations.

Conventionally, the calibration process is carried out automatically as part of the observing routine, and the calibration signal is measured in the same units as are used for the source being observed. In such a system, \( T_A' \) is obtained by merely scaling the observed temperature by the effective ambient temperature divided by the calibration temperature. However, for spectral line observations at Mopra, the line and calibration intensities are obtained with different programs and the calibration is more complex.
At Mopra, the ‘gated’ total power (GTP) output of the receiving system can be used to derive the calibration signal. The blackbody calibration source is a ‘paddle’ that can be moved in front of the receiver input. In the following discussion, \( P_{BB} \) is the GTP when the receiver is looking at the paddle, \( P_{ref} \) is the GTP when the telescope is looking at empty sky (i.e. when the paddle is withdrawn).

The Mopra spectral-line observing program did not difference the signals at the on and off-source positions as in (3.5), but in fact produced a quotient (\( Q_T \)) of the intensities which was scaled by a factor \( K \) defined by input parameters in the program and by the receiver temperature:

\[
Q_T = K \left( \frac{\text{sig} \cdot \text{ref}}{\text{sig} \cdot \text{ref}} \right) T_{\text{ref}}
\]  

(3.10)

We define a calibration factor \( F_{cal} \) as:

\[
F_{cal} = \frac{P_{ref}}{P_{BB} \cdot P_{ref}} = \frac{P_{ref}}{P_{cal}}
\]

(3.11)

which for Mopra is equivalent to the GTP output divided by the difference in GTP output for the blackbody inserted and then removed.

After substituting the equations (3.6) and (3.7) into (3.11) and multiplying by (3.10) we get the final result:

\[
(Q_T)(F_{cal}) = (T_{\text{ref}})(K T_{\text{ref}})/T_{\text{amb}}
\]

which can be written as

\[
(Q_T)(F_{cal}) = CT_A^\prime
\]

(3.12)

The final result is merely \( T_A^\prime \) multiplied by a constant \( C \) that is proportional to \( K(T_{\text{ref}}/T_{\text{amb}}) \), (in practice, both of these temperatures can be regarded as being constant with time for a selected observing frequency). We have determined the scaling factor \( C \) by comparing the Mopra calibrated antenna temperatures with corresponding values for \( T_A^* \) obtained from the SEST.

By applying the factor \( F_{cal} \) and the constant \( C \) (obtained from the comparison of SEST and Mopra observations M 17SW and Orion KL) to the data collected from Mopra we can correct the observations for atmospheric attenuation and place the Mopra values on the SEST \( T_A^* \) scale.
In addition, both SEST and Mopra values of $T_A^*$ need to be corrected for the SEST main beam efficiency using equation (3.2) to recover $T_{MB}$.

### 3.9 Comparison of Mopra and SEST Observations for Calibrator Sources

In the following discussion:

- $Q_T$ refers to the raw Mopra data (before atmospheric calibration is applied);
- $T_A'$ refers to Mopra data after the atmospheric calibration is applied (i.e. $T_A' = Q_T(F_{cal})$);
- $T_A^*$ is used for Mopra data which has been put onto the SEST $T_A^*$ scale by multiplying $T_A'$ by the factor C in (3.12). $T_A^*$ is also the form in which data from the SEST is obtained;
- $T_{MB}$ refers to SEST or Mopra data that has been corrected for main-beam efficiency.

For the comparison of SEST and Mopra results we observed molecular lines with frequencies between 86 and 115 GHz in the Orion and M 17SW molecular clouds. Both clouds are extended relative to the beams of both telescopes. The observations were collected during the various observing runs described in Chapter 4. Where possible at Mopra, multiple observations of the calibration sources were made at each frequency, in a variety of weather conditions, which included periods of heavy cloud cover.

The Mopra observations were corrected for atmospheric attenuation in the manner already described, whereas the more conventional method was used at SEST, using equations (3.3) to (3.9) directly. Figure 3.3 shows the percentage difference of each individual observation (% residual) of a primary calibrator from the mean for all observations of that calibrator at that frequency, plotted against integrated brightness temperature. Figure 3.3(a) shows the data before calibration i.e. $Q_T$ from equation (3.10). The root-mean-square (rms) of the values is 17.4% ($n = 43$). Figure 3.3(b) shows the results after calibration i.e. $T_A'$ (on an arbitrary Mopra scale). The rms is 7.2% ($n = 43$). The calibrated data show significantly less spread around the mean value, with the majority of calibrated observations being within 10% of the mean.

---

3 This correction is necessary if the source is less than a few arcminutes in size, as are all sources in our sample. For very extended sources, e.g. the Moon (30 arcminutes), the main beam efficiency correction is not used as all of the forward beam including the main side lobes will be filled by the source. In this case the more appropriate correction is for the forward beam efficiency of the telescope rather than the usual larger correction for the main beam efficiency. Values on the $T_A^*$ scale already include correction for the forward beam efficiency.
Figure 3.3 Percentage difference of each individual observation of a calibrator from the mean for all observations of that calibrator at that frequency (% residual), plotted against corrected integrated brightness temperature ($T_A'$) (a) Raw observations, before calibration ($Q_r$) (b) Data after calibration ($T_A'$). The scatter in the data points is substantially reduced.

Figure 3.4(a) shows the uncalibrated Mopra peak antenna temperatures ($Q_r$) plotted against SEST corrected antenna temperatures ($T_A^*$) for spectral-line observations of both the M 17SW and Orion KL molecular clouds at all frequencies ($r^2 = 0.87$). Figure 3.4(b) shows the same data set after calibration; the calibrated antenna temperatures on the Mopra scale ($T_A'$) are the plotted against $T_A^*$ from SEST. There is a reduced scatter about the straight line of best fit compared with the uncalibrated observations, and this results in a significantly higher correlation coefficient. The equation for the line of best fit is ($T_A^* - SEST = 1.62(T_A' - \text{Mopra}) - 1.1$ and the correlation coefficient is $r^2 = 0.99$. The regression constant, $1.62 \pm 0.06$, is the calibration factor defined in equation (3.12). The calibration factor is not 1 due to uncalibrated factors within the receiver and correlator system.
These results show that despite the indirect approach to calibration that must be used, it has been still possible to produce an effective antenna temperature scale for the Mopra Telescope. The scaling factor $C = 1.62 \pm 0.06$ to put the Mopra observations on to the SEST brightness temperature scale is obtained from Figure 3.4(b). The calibration scheme used here corrects for atmospheric attenuation and for arbitrary scaling factors in the data collection system, and the correction is vital for the data to be meaningful.

Figure 3-4. Comparison of SEST and Mopra data before and after calibration of Mopra data. (a) SEST corrected antenna temperature ($T_A^*$) plotted with Mopra antenna temperature before calibration ($Q_T$). The correlation coefficient is $r^2 = 0.87$. (b) SEST corrected antenna temperature ($T_A^*$) plotted with corrected peak antenna temperature from Mopra ($T_A'$) for the same data after calibration. The correlation coefficient is $r^2 = 0.99$.

3.10 Calibrating the Observations and Calculating Uncertainties

The observations from the Mopra telescope were calibrated using the outlined method to put them on to the SEST $T_A^*$ scale using the factor determined from Figure 3.4(b), $C = 1.62 \pm 0.06$. Observations from both Mopra and the SEST telescope were then corrected for the SEST beam efficiency using equation (3.2) resulting in a data set given in terms of $T_{MB}$. The results reported in Chapter 4 are in terms of $T_{MB}$. 
3.10.1 Assigning Uncertainties to the Data

Uncertainties in the Mopra data were calculated using repeated Mopra observations of several molecular clouds. This was done after the calibration from $Q_T$ (Mopra scale) to $T_{MB}$ (SEST scale). The sample of repeated observations is given in Table 3.1 together with the transitions observed and the number of observations for each transition. This sample provides a check on the internal consistency of the Mopra calibration.

The normalised-difference of each observation from the mean for that source (in terms of brightness temperature integrated over the line profile), at that frequency, is shown in Figure 3.5. The observations are plotted against integrated main-beam brightness temperature ($\int T_{MB}(v)dv$) from calibrated Mopra observations.

There is a strong temperature dependent component to the uncertainties, and the maximum uncertainty envelope can be clearly seen in figure 3.5. There also appears to be a temperature independent component to the uncertainties of about $5-10\%$.

To quantify this relationship the uncertainty was assumed to consist of two independent components: a constant temperature-independent component and a temperature dependent component. The total uncertainty in any particular observation will be the sum, in quadrature, of the constant temperature-independent uncertainty and the temperature-dependent uncertainty.

The sum of the two uncertainties can be represented by

$$\frac{\delta \int T_{MB} dv}{\int T_{MB} dv} = \left[ \left( \frac{A}{T_A'} \right)^2 + B^2 \right]^{1/2}$$  \hspace{1cm} (3.13)

where

- $A$ is a constant that describes the data envelope at low $\int T_{MB} dv$,
- $B$ is a constant % error that describes the uncertainties at high $\int T_{MB} dv$, and
- $T_{MB}$ is the calibrated Mopra main-beam brightness temperature.

The constants $A$ and $B$ are calculated by separating the data, arbitrarily at $T_{MB} = 5$ K, into a high temperature and a low temperature sample.

The low-temperature sample has an average of $0.00 \pm 0.04$ ($\sigma = 0.168$, $n = 20$) and the high-temperature sample has an average of $0.00 \pm 0.01$ ($\sigma = 0.083$, $n = 57$).
Figure 3-5 Normalised-residuals for repeated spectral-line observations, after calibration, plotted against integrated main-beam brightness temperature.

There is a correction necessary before the above standard deviations are substituted into (3.13). The sample of repeated observations contains many transitions for which there are only two observations. Using the residuals for pairs of observations requires a slightly different handling than if \( n > 2 \). In this case, the constants \( A \) and \( B \) need to be multiplied by \( \sqrt{2} \) before being substituted into equation (3.13) (Then, \( A = 0.168 \times \sqrt{2} = 0.238 \) K km s\(^{-3} \), \( B = 8.3\% \times \sqrt{2} = 0.118 \)).

Equation (3.13) now becomes

\[
\frac{\delta \int T_{MB} \, dv}{\int T_{MB} \, dv} = \left[ \frac{0.238}{T_{A'}} \right]^2 + 0.118^2 \right]^{\frac{1}{2}} \tag{3.14}
\]

Equation (3.14) has been used throughout this thesis to calculate the relative uncertainty in data collected with the Mopra telescope. Figure 3.6 shows equation (3.14) plotted together with the data from Figure 3.5 for integrated main-beam brightness temperatures < 20 K km s\(^{-1} \). The uncertainties calculated using (3.14) describe an envelope that agrees well with the actual relative uncertainties.
Figure 3.6 Relative uncertainties computed from equation (3.13) compared with actual values of relative uncertainties for calibrated Mopra data, plotted with integrated main-beam brightness temperature. The diamonds show the predicted values, while the crosses show the values obtained from repeated measurements.

Calculating the uncertainties in this empirical way takes into account all sources of error and was felt to be the best way, given that there are several sources of uncertainty in the data and none are individually well determined a priori.

Similar plots were produced for the fractional residuals against gated total power (a measure of cloud cover and atmospheric humidity), zenith angle and frequency. No systematic relationship above the 5% level was found. This suggests that the calibration procedure was fairly successful in removing attenuation due to the atmosphere and other zenith-dependent variations. Any relationship at the 5% level would have been included in the empirical uncertainty analysis.
Table 3-1 Repeated Observations of Molecular clouds in Sample.

<table>
<thead>
<tr>
<th>Molecular Cloud</th>
<th>Transition</th>
<th>No of Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>311.6+0.3</td>
<td>CS (2-1)</td>
<td>2</td>
</tr>
<tr>
<td>327.3-0.5</td>
<td>HC$_{18}$O$^+$ (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>327.3-0.5</td>
<td>OCS (7-6)</td>
<td>2</td>
</tr>
<tr>
<td>331.5-0.1</td>
<td>HC$_3$N (10-9)</td>
<td>2</td>
</tr>
<tr>
<td>351.6-1.3</td>
<td>HNC (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>G1.6</td>
<td>OCS (9-8)</td>
<td>2</td>
</tr>
<tr>
<td>M 17SW</td>
<td>CO (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>M 17SW</td>
<td>$^{13}$CO (1-0)</td>
<td>3</td>
</tr>
<tr>
<td>M 17SW</td>
<td>C$_{18}$O (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>M 17SW</td>
<td>CS (2-1)</td>
<td>2</td>
</tr>
<tr>
<td>M 17SW</td>
<td>HC$_3$N (12-11)</td>
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</tr>
<tr>
<td>M 17SW</td>
<td>HC$_3$N (10-9)</td>
<td>4</td>
</tr>
<tr>
<td>M 17SW</td>
<td>HCN (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>M 17SW</td>
<td>HCO$^+$ (1-0)</td>
<td>2</td>
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<td>2</td>
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<td>HC$_{18}$O$^+$ (1-0)</td>
<td>2</td>
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<td>NGC 6334 (H)</td>
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</tr>
<tr>
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<td>HC$_{18}$O$^+$ (1-0)</td>
<td>2</td>
</tr>
<tr>
<td>NGC 6334 (N)</td>
<td>OCS (7-6)</td>
<td>2</td>
</tr>
<tr>
<td>NGC 6334 (S)</td>
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</tr>
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<td>Orion KL</td>
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<tr>
<td>Orion KL</td>
<td>CS (2-1)</td>
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</tr>
<tr>
<td>Orion KL</td>
<td>HC$_3$N (10-9)</td>
<td>4</td>
</tr>
<tr>
<td>Orion KL</td>
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<td>Orion KL</td>
<td>OCS (7-6)</td>
<td>3</td>
</tr>
<tr>
<td>Orion KL</td>
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</tr>
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</tr>
<tr>
<td>RCW 92</td>
<td>OCS (7-6)</td>
<td>2</td>
</tr>
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</table>

3.11 Comparing Mopra and SEST Spectral-line Observations for Molecular Clouds other than the Primary Calibrators

As well as observations of calibrator clouds, there was some overlap in molecular lines observed with Mopra and the SEST. As a further check on the calibration the integrated main-beam brightness temperatures from these overlap observations were compared with one another. Table 3.2 lists the clouds, molecules and transitions observed with both telescopes. Figure 3.7 shows Mopra integrated main-beam brightness temperatures plotted against the corresponding SEST values. Error bars are shown on each point. The line of equality is drawn on the plot. Clearly there are a significant number of values that
fall above the line. The most likely cause is that some of the clouds are of small diameter (or have small-scale structure) and the SEST value of $T_{MB}$ will be underestimated relative to the Mopra value due to the larger SEST beam at the same frequency (the Mopra beam-width was 0.8 that of that for the SEST). Thus, Mopra would yield a higher antenna temperature for a small diameter source and this must be reflected in the figure.

Figure 3-7 Mopra integrated main-beam brightness temperatures plotted against corresponding SEST values for the transitions listed in Table 3.2. The line of equality has been added to the plot.
Table 3-2 Molecular Clouds and transitions observed with both the Mopra Telescope and the SEST.

<table>
<thead>
<tr>
<th>Source</th>
<th>Molecule</th>
<th>Transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>268.4-0.8</td>
<td>HC$_3$N</td>
<td>10 - 9</td>
</tr>
<tr>
<td>268.4-0.8</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>311.6+0.3</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>326.7+0.6</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>327.3-0.5</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>331.5-0.1</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>333.0-0.6</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
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</tr>
<tr>
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<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>345.5+0.3</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>351.6-1.3</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
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<td>CS</td>
<td>2 - 1</td>
</tr>
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<td>NGC 6334(CO)</td>
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<td>2 - 1</td>
</tr>
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<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>NGC 6334(N1)</td>
<td>HC$_3$N</td>
<td>10 - 9</td>
</tr>
<tr>
<td>NGC 6334(N)</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>NGC 6334(N)</td>
<td>HC$_3$N</td>
<td>10 - 9</td>
</tr>
<tr>
<td>NGC 6334(S)</td>
<td>OCS</td>
<td>8 - 7</td>
</tr>
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<td>NGC 6334(S)</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
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</tr>
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<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>345.5+1.5</td>
<td>OCS</td>
<td>8 - 7</td>
</tr>
<tr>
<td>265.1+1.5</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
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<td>Lupus</td>
<td>CS</td>
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</tr>
<tr>
<td>348.7-1.0</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>322.2+0.6</td>
<td>CS</td>
<td>2 - 1</td>
</tr>
<tr>
<td>RCW 92</td>
<td>OCS</td>
<td>8 - 7</td>
</tr>
</tbody>
</table>
Chapter 4

Observations and Results

4.1 Introduction

The observations were undertaken in several stages. A large sample of sources was initially identified and then observed with the aim of selecting a more manageable sample for detailed study. The selection of both the initial and final source samples is described in section 4.2 while the observations of the final sample are described in section 4.3. The results for the final sample are given from section 4.4 onwards.

4.2 Selection of Target Sources

The aim was to select about twenty-five bright southern molecular clouds for the final study. They were required to be bright so that a large number of molecules could be observed in a reasonable period of time, and show some evidence of complex chemistry. One or more positions (usually close to the \(^{13}\)CO J=1-0 emission peak) would be selected in each source as the target position for the observations. The sizable sample of southern molecular clouds would provide a database of high-resolution observations of molecular rotational transitions that could be used to study physical conditions and chemistry. The molecular clouds OMC-1 and M 17, which have previously been studied extensively, were added to the final sample for calibration and comparison purposes.

Because of the way in which the sources were selected, the sample is of course biased towards objects where the molecular abundances and excitation are high. In particular, it may not include those clouds in the final stages of collapse, where all molecules (including possibly CO) are predicted to be severely depleted (see e.g. Brown et al. 1998).

4.2.1 Source Selection

The molecular clouds in the final sample were selected in a two-step process. Firstly, previous molecular line surveys (Gardner & Whiteoak 1974; Whiteoak & Gardner 1978; Gardner & Whiteoak 1978; Batchelor et al. 1981; Dickinson et al. 1982; Gardner & Whiteoak 1984; Peters et al. 1986) along the southern galactic plane provided a sample of 50 candidate molecular clouds with declinations south of \(-30\) degrees. The second step in the selection involved using the Mopra telescope to observe this initial sample; this included some of the first mm-wave observations obtained with this telescope.
4.2.2 Observations of the Initial Sample

The initial cloud sample was observed in the 3-mm rotational transitions of CS, HCN and HCO\(^+\) (with frequencies of 98.0, 88.6 and 89.2 GHz respectively) as part of the commissioning of a new receiving system between 1994 September and 1994 November. These transitions were used because they are bright and widespread, and most importantly they were within the limited range of frequencies available during the receiver test period. A 64-MHz bandwidth divided into 1024 channels was used in each case, giving a velocity resolution of about 0.2 km s\(^{-1}\) per channel. The average beam size of the telescope for these frequencies was about 44 arcsec. These initial observations were used to locate the emission peaks for each molecule and to select 25 of the brighter clouds for further study. An effort was made to include some objects that showed unusual intensity ratios for the three transitions, and also several dark clouds. The observations were made before a comprehensive pointing model for the telescope was available. Although the positional calibration was checked by regular observations of 86-GHz SiO maser positions, it was still uncertain by up to 20 arcsec. Therefore, the positions for the molecular emission peaks were used only as a guide for further investigation. The observations of these transitions were repeated at a later time after the formulation of a better positional calibration and intensity calibration scheme (see chapter 3 for details).

4.2.3 Selecting the Final Sample

The 25 galactic molecular clouds, two calibration clouds, and positions selected for the final study are given in Table 4.1. The positions were selected from Mopra observations of the \(^{13}\)CO J=1-0 transition at 110 GHz in 1995 September. The beam size of Mopra at this frequency is 37 arcsec, and the clouds were mapped over an area of several arcmin\(^2\), at half-beam intervals, to determine both the position of the peak and the angular size of the \(^{13}\)CO 1-0 emission. The velocity resolution was 0.17 km s\(^{-1}\) per channel. The receiver temperature was 112 K (single-sideband mode). The selected positions are believed to be within 20 arcsec of the \(^{13}\)CO 1-0 emission peak in each cloud (or condensation within a cloud if multiple positions have been selected).

At this point, a word on the positional calibration of Mopra is appropriate. During late 1994 and mid-1995 an accurate positional calibration model for Mopra was being formulated. The pointing during the \(^{13}\)CO 1-0 mapping was generally 10 – 15 arcsec but discrepancies of up to 20 arcsec or so were sometimes found. For all observations after 1995 September the pointing was better than 15 arcsec. The \(^{13}\)CO observations towards the selected positions were repeated in 1996 May, and have the same positional accuracy as the observations of other transitions. Thus, the \(^{13}\)CO maps were used only for selecting the observational positions and determining source size.
4.3 Observations of the final sample

The positions listed in Table 4.1 were observed in molecular rotational transitions at 3-mm and 2-mm using both the Mopra Telescope and the SEST. The observations were collected between 1994 September and 2000 March. Table 4.2 lists the transitions and frequencies observed, the date of the observations, and the telescope used for data collection. In all cases the observations were carried out with a 64 MHz bandwidth divided into 1024 channels. During the time of these observations both the Mopra and SEST telescopes were equipped with dual polarization SIS receivers. Details specific to each telescope are given below.

<table>
<thead>
<tr>
<th>Table 4-1 Galactic molecular clouds and positions selected for final sample.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orion M.C.</td>
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<tr>
<td>HH46 D.C.</td>
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<td>G265.1+1.5</td>
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</tr>
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</tr>
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Table 4.2 (continued)

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<th>Date Observed</th>
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<td>85.13910</td>
<td>Mopra</td>
<td>1996 September</td>
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</table>

4.3.1 Observations of Molecular Transitions with the Mopra Telescope

Molecular transitions between 85 and 116 GHz were obtained with the Mopra Telescope towards the positions listed in Table 4.1; Table 4.2 lists the observed transitions. The observations were collected between 1995 October and 1996 September. The SIS receiving system provided single-sideband receiver temperatures that varied between 85 and 130 K. The observations were obtained in position-switching mode with a positional difference of 30 arcmin between on-source and off-source positions, except for extended sources such as dark clouds where a position difference of 60 arcmin was used. At the observing frequencies the reflecting surface of the antenna had an effective diameter of 15 m, with a shaped non-parabolic surface yielding a half-power beamwidth decreasing from 47 arcsec to 35 arcsec. As pointed out previously, periodic observations of SiO masers with well-established positions provided a pointing accuracy better than 15 arcsec. As for earlier observations, the spectra were obtained with a combination of 1024 correlator channels and 64 MHz bandwidth; this provided a velocity resolution varying between 0.44 and 0.32 km s\(^{-1}\) after Hanning smoothing, for the above frequency range. The observing cycle consisted of pairs of on-source/off-source observations. Intensity calibration was carried out in a manual two-step process, described in detail in Chapter 3. The observed intensities were corrected for atmospheric attenuation using observations of an ambient temperature load (commonly called the chopper wheel method). They were then transformed to a corrected antenna temperature \(T_A^*\) scale by comparing the results for the sources Orion KL and M17 SW with standard values given for spectra obtained with the SEST.

In March and September 2000, observations of the \(^{13}\)CS 2-1, \(^{13}\)CN 1-0, \(^{13}\)C\(^{1}\)N 1-0 and \(^{13}\)CO\(^{+}\) 1-0 transitions were collected with Mopra. Although the receiver and correlator configuration was unchanged, the antenna had been resurfaced in 1999 to extend the solid reflecting surface from 15 to 22 metres. This resulted in a smaller giving a half-power beamwidth ranging from 35 arcsec to 38 arcsec at the observing frequencies. The observations were calibrated as above.
4.3.2 Observations with the SEST

The SEST was used in 1999 June to observe transitions as listed in Table 4.2. The positions listed in Table 4.1 were observed. The observing frequencies ranged from 84 to 147 GHz. The half-power beamwidths ranged from 59 arcsec at 85 GHz to 35 arcsec at 147 GHz. SIS receivers operating at 3-mm and 2-mm were used in single side-band mode and typical system temperature ranges were 170 – 250 K at 3-mm and 230 – 400 K at 2-mm. The observations were generally obtained in dual beam switching mode with a throw of 11 arcmin between the on-source and reference positions, except for observations of extended clouds where line emission may be present in the reference position. In the latter case the observations were collected in frequency-switching mode with a throw in frequency of 4 MHz. Periodic observations of SiO masers with well-established positions provided focus checks and a pointing accuracy believed to be better than 5 arcsec. The spectra were obtained with a digital correlator; a combination of 1000 correlator channels and 42 MHz bandwidth provided a velocity resolution varying between 0.30 and 0.17 km s\(^{-1}\) after Hanning smoothing. The data were calibrated using the standard chopper wheel method (Chapter 3). The corrected antenna temperature, \(T_A^*\), was converted to a main-beam brightness temperature, \(T_{MB}\), using a main beam efficiency, \(B_{eff}\), varying from 0.75 to 0.66 between 85 GHz and 147 GHz (Booth et al. 1989, SEST Observers Handbook). Chapter 3 gives a detailed description of terms and procedures.

4.4 Data Reduction

The spectra obtained with the Mopra Telescope and the SEST were reduced using the CLASS (Continuum and Line Analysis Single-dish Software) software package of the GILDAS working group\(^1\). The procedure for each spectrum was as follows:

1) Hanning smoothing was applied to the spectrum to increase the signal to noise ratio. If the signal to noise ratio was still poor a more drastic "boxcar" smoothing function was applied to the spectrum, averaging 3 – 5 adjacent channels.

2) A polynomial fit was made to the baseline of the spectrum, excluding channels that contained line emission, and this fit was then subtracted from the spectrum, leaving line emission only.

3) One or more Gaussian curves were fitted to each line. The assumption was that spectral line emission has a Gaussian shape and that more complicated spectral profiles are the resultant of more than one Gaussian line profile, probably emitted from/absorbed by sub-components within the molecular gas. Except in cases where it is obvious that there is more than one physical component in the emission (e.g. Orion KL or G1.6-0.025) no physical significance is claimed for

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\(^1\) The GILDAS working group is a collaborative project of the Observatoire de Grenoble and the Institut de Radio Astronomie Millimétrique (IRAM).
Gaussian sub-components – they are merely a means to determining the total emission in a spectral profile.

4) For Mopra spectra, the peak and integrated intensity of the Gaussian components were then corrected for atmospheric attenuation and placed on the SEST $T_A^*$ scale (see Chapter 3).

5) All the observations, at this stage on the SEST $T_A^*$ scale, were put onto the main-beam brightness scale, $T_{MB}$. This is the true brightness temperature if the source just fills the main beam of the telescope (once again, see Chapter 3 for details). Brightness temperatures were not estimated because cloud sizes are required, and in most cases, accurate size determination would require observations at significantly higher resolution than any reported here. However, the main-beam brightness temperatures can be corrected in the future when cloud dimensions are available.

4.5 Results

The results are presented in Appendix A. All data for each molecular cloud position (including derived parameters such as abundances) are collected in Appendix A, in Tables A-1 to A-31 (a), (b), (c), (d) and (e).

4.5.1 Spectral Line Intensities and Profiles

Table (a) for each molecular cloud lists the observed molecular transitions and the results of the spectral analyses. Where more than one component was required to fit a line profile the results of the Gaussian deconvolution are given. No physical interpretation is claimed for multiple fitted Gaussian components unless there is other supporting evidence. Columns 3, 4, 5 and 6 give the line centre, full-width at half maximum, peak and integrated main-beam brightness temperatures respectively for each fitted component. The observing frequency for HCN was centred on the $J=2-1$ hyperfine component, and the velocities quoted for the $F=1-1$ and $F=0-1$ hyperfine transitions have not been corrected for this. This is because the hyperfine components are blended in many cases, so all fitted lines were left uncorrected for consistency.

Columns 7 and 8 respectively give the total integrated main-beam brightness temperature summed for all components fitted to a line, and its associated uncertainty. The form of the uncertainty for Mopra brightness temperatures has been discussed in detail in Chapter 3. The uncertainties in the data obtained with the Mopra Telescope were found to have a temperature-dependent and a temperature-independent component that can be described by equation (3.14). This relationship accounts for all sources of uncertainty including those arising from the calibration and from the Gaussian fitting procedure.
The calibration uncertainties for SEST data are assumed to be 10% at 3mm and 15% at 2mm (SEST Observers Manual, Heikkinen 1998). The total uncertainty quoted for SEST data in column 8 is the sum, in quadrature, of the uncertainty provided by the CLASS Gaussian fitting routine (GAUSS) and the calibration uncertainty. The values are very close to those calculated for Mopra data of the same integrated brightness temperature.

The upper limits quoted in Column 7 have been calculated using $\sqrt{2}$ times the rms noise in the spectrum multiplied by the average FWHM velocity width for those transitions detected at that position. This is lower than the 3-sigma value often used but is consistent with the integrated brightness temperatures of the weakest transitions detected in these observations.

Figures B-1 to B-31 (a) and (b) of Appendix B show selected spectra for each position observed. Figures (a) show spectra of CO, $^{13}$CO, C$^{18}$O, HCN and HCO$^+$, while Figures (b) show other selected transitions.

The CO spectra often show emission features covering a significantly wider range of velocities than found for other molecules. Self-absorption is evident in about a third of the CO spectra, and can also be seen in some spectra of $^{13}$CO and C$^{18}$O. Self-absorption is also evident in some cases in transitions of CS, HCN, HCO$^+$ and SO, but not generally in transitions of OCS, HC$_3$N and CH$_3$OH, implying that these latter transitions are more likely to be optically thin. The physical interpretation/s of self-absorption are discussed in section 4.5.2. In addition to the presence of self-absorption, the spectra, particularly those of $^{12}$CO, often show a complex emission/velocity structure that cannot be fitted by a single Gaussian curve. As expected, emission from the dark clouds in the sample (HH 46, the Coal Sack dark cloud, the Chameleon dark cloud, and the Corona Australis dark cloud) is distinguished by narrow line widths compared to other clouds in the sample.

High velocity wings are seen in the spectra of a number of molecular clouds (see e.g spectra of CO, CS, HCN and SO observed towards the positions NGC 6334(CO) and NGC 6334 (N)) suggesting that outflows (presumably from YSOs) are present.

Quantitative analyses of the spectra are presented in Chapters 5 and 6.

4.5.2 Self-absorption

As already mentioned, many of the molecular clouds in the sample exhibit self-absorbed line profiles in optically thick transitions. For a cloud with a radial excitation gradient and a hotter core, the effect arises because the optical depth in the line centre will increase more rapidly than that in the line wings. As the optical depth grows, the gas providing the emission near the line centre will be localized closer to the cloud surface, and the brightness temperature at the line center will have the temperature of the cooler surface gas. One the other hand, the line wings will have a lower optical depth and will be representative of the higher temperature deeper into the molecular cloud. Thus, the line profile becomes self-reversed.
In reality, the picture is somewhat more complex than this. Temperature gradients almost certainly exist across many molecular clouds, and as the most commonly observed lines tend to be optically thick in dense molecular clouds, self-absorbed line profiles should be more common than are found. Two main factors (not mutually exclusive) have been invoked to explain this. Firstly a velocity gradient perpendicular to the line-of-site is often observed. If emission is not reabsorbed close to where it occurs, Doppler shifting of the emitted frequency will prevent its re-absorption at another position within the molecular cloud, where the gas will have a different velocity. In this scenario self-reversal of line profiles requires either infall or outflow along the line-of-site to match the velocities in an outer layer of a cloud with velocities in the centre. The second explanation for the absence of self-reversed line profiles is that giant molecular clouds have a clumpy structure and the dense clumps can be in turbulent motion with respect to one another. The emergent line profile is the sum of the emission from many clumps, leading to a broadened line profile. The motion of the clumps with respect to one another prevents the absorption of the emission from one clump by another. In this situation infall or outflow again need to be invoked to explain a self-reversed line profile.

Self-absorption leads to difficulties in determining the kinetic temperature of a molecular cloud from the peak temperature of the \(^{12}\text{CO}\) emission profile. If the self-absorption occurs at velocities close to the line centre, the peak of the self-absorbed line will give only a lower limit to the kinetic temperature. If it is well displaced from the line centre and narrow, then the profile peak may still yield an accurate kinetic temperature. However, it is usually difficult to determine the proximity of the self-absorption to the line centre on the basis of a single spectrum and observations of an optically thin isotopomer may be necessary to settle the issue.

An associated problem is the differentiation of a self-absorbed profile from a profile composed of several components at different velocities. Once again, observation of optically thin isotopes, possibly in conjunction with mapping techniques, are usually required.

4.5.3 Isotopomer Intensity Ratios

It was stated in Chapter 1 that CO is generally believed to have a high optical depth in dense molecular clouds. Is the assumption that CO is optically thick valid? This can be tested by examining the intensity of the \(^{12}\text{CO}\) emission compared to that of \(^{13}\text{CO}\). Although the terrestrial ratio of \(^{12}\text{C}:^{13}\text{C}\) is 89, the molecular abundance of \(^{12}\text{CO}:^{13}\text{CO}\) in nearby molecular clouds is found to be around 50, and significant variations in this ratio have been found in individual molecular clouds. It is also likely that the ratio \(^{12}\text{CO}:^{13}\text{CO}\) varies with galactocentric distance. Langer and Penzias (1990) have found a value of 57 for molecular clouds at solar system distances from the galactic centre, with values ranging from 25 near the centre of the Galaxy to 70 at a distance of 12 kpc. Figure 5.1 shows the integrated \(^{12}\text{CO}\) J=1-0 emission plotted with integrated \(^{13}\text{CO}\) J=1-0 emission for molecular clouds in this sample. The average ratio from the data is \(3.1 \pm 0.2\) (\(\sigma_n\)).
with values ranging from 1.7 to 5.1. This average ratio is far lower than any of the $^{12}\text{CO}:^{13}\text{CO}$ ratios quoted above so the $^{12}\text{CO}$ can reasonably be assumed to be optically thick. The data point lying far above the line of best fit is from Orion KL, with a ratio of 10; this point has not been included in the average. Orion KL is known to have an anomalous $^{12}\text{CO}$ to $^{13}\text{CO}$ emission ratio (Langer & Penzias 1990), and it is possible that in this molecular cloud the $^{12}\text{CO}$ has a particularly high optical depth.

![Graph showing integrated $^{12}\text{CO}$ emission compared with integrated $^{13}\text{CO}$ emission.](image)

**Figure 4-1 Integrated $^{12}\text{CO}$ emission compared with integrated $^{13}\text{CO}$ emission.**

Table 4-3 lists the emission intensity ratios for $^{12}\text{C}$:$^{13}\text{C}$ isotopomers of CO, CS, HCN, HNC and HCO$, as well as the sample standard deviation ($\sigma_{n-1}$), the minimum and maximum values of the ratio, and the number of molecular clouds for which the ratio has been calculated. Table 4-4 list the same values for the ratio of $^{13}\text{C}$:$^{18}\text{O}$ isotopomers.

As stated above, the mean ratio for the intensity of $^{12}\text{CO}$ emission (hereafter I$^{12}$) to emission from $^{13}\text{CO}$ (hereafter I$^{13}$) is $3.1 \pm 0.2$ for this sample of southern molecular clouds. This is very close to the value for I$^{12}$:I$^{13}$ of $3.0 \pm 0.9$ found for a sample of northern Galactic-plane GMCs between $l = 34^\circ$ and $l = 51^\circ$ (Polk et al. 1988) suggesting that there is no systematic difference in this ratio between the northern and southern galactic plane. Doty & Neufeld (1997) have modelled I$^{12}$:I$^{13}$ for the dense quiescent star-forming cores of molecular clouds, assuming an approximately Solar System ratio for
$^{12}$CO:$^{13}$CO abundance of 100:1. They have predicted an $I^{12}$:$I^{13}$ ratio of between 2 and 6, which is again consistent with the findings of this study.

The mean ratio of $I^{13}$ to emission from C$^{18}$O (hereafter I$^{18}$) is 6.9 ± 0.4. This is somewhat higher than the value for this ratio of 5 that would be expected for optically thin emission if Solar System ratios for atomic $^{12}$C:$^{13}$C and $^{16}$O:$^{18}$O were assumed. The values for $I^{13}$:$I^{18}$ for individual clouds range from 2.5 to 15.2, so in some molecular clouds the ratio is far higher than expected from Solar System values. The ratio I$^{12}$:$I^{18}$ found in this study is 25 ± 3, with a range of 4.2 to 98. Doty & Neufeld (1997), assuming Solar System ratios predicted that I$^{12}$:$I^{18}$ should be between 5 and 20, assuming that $^{12}$CO and C$^{18}$O were coextensive. A possible reason for the high ratios found in this study is that the emission from $^{12}$CO and $^{13}$CO arises from a larger volume of gas than does emission from C$^{18}$O. This suggestion is supported by the average line-widths for $^{12}$CO and C$^{18}$O emission for the sample. The average line-width for $^{12}$CO is 8.7 km s$^{-1}$, while the average line-width for C$^{18}$O is 4.1 km s$^{-1}$, suggesting that $^{12}$CO emission arises from a larger volume of the gas (assuming that line-width is proportional to radius, as if will be if there is a large velocity gradient across the molecular cloud). The average line-width of $^{13}$CO is 5.3 km s$^{-1}$, similar to that for C$^{18}$O, suggesting that the C$^{18}$O and $^{13}$CO emission arise from a similar volume of gas. If this is the case, then the optical depth of the $^{12}$CO emission is even higher than that implied by the emission ratios in Table 4-3. The critical densities (Appendix C, Table C-2) for $^{13}$CO and C$^{18}$O are lower than that for $^{12}$CO, implying that the difference in volume of the emitting gas is due to a lower abundance of the rarer isotopomers in outer regions of the molecular cloud rather than to varying excitation conditions. The values of $I^{13}$:$I^{18}$ suggest that the C$^{18}$O emission arises from a smaller volume of gas than the $^{13}$CO emission, and the relative average line widths (4.1 km s$^{-1}$ for C$^{18}$O, 5.3 km s$^{-1}$ for $^{13}$CO) provide some support for this assertion. It is possible that self-shielding (from dissociating UV radiation both within and incident on the molecular cloud) in the more abundant isotopomers accounts for their apparently wider distribution within the molecular gas (Langer & Penzias 1990).

<table>
<thead>
<tr>
<th>CO/$^{13}$CO</th>
<th>CS/$^{13}$CS</th>
<th>HCN/ $^{13}$CN</th>
<th>HNC/ $^{15}$N</th>
<th>HCO$^{+}$/ $^{13}$CO$^{+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>3.6</td>
<td>12.0</td>
<td>7.8</td>
<td>11.9</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>1.9</td>
<td>5.7</td>
<td>5.4</td>
<td>5.6</td>
</tr>
<tr>
<td>Minimum</td>
<td>1.7</td>
<td>6.1</td>
<td>0.9</td>
<td>2.7</td>
</tr>
<tr>
<td>Maximum</td>
<td>10.0</td>
<td>30.2</td>
<td>25.1</td>
<td>21.7</td>
</tr>
<tr>
<td>Number of Observations</td>
<td>33</td>
<td>19</td>
<td>25</td>
<td>20</td>
</tr>
</tbody>
</table>
Table 4-4 Emission Intensity Ratios for $^{13}$C:$^{18}$O Isotopomers of CO and HCO$^+$. 

<table>
<thead>
<tr>
<th></th>
<th>$^{13}$CO/$^{18}$O</th>
<th>HCO$^+$/HC$^{18}$O$^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.9</td>
<td>15.3</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>2.6</td>
<td>13.7</td>
</tr>
<tr>
<td>Minimum</td>
<td>2.5</td>
<td>6.3</td>
</tr>
<tr>
<td>Maximum</td>
<td>15.2</td>
<td>60.0</td>
</tr>
<tr>
<td>Number of Observations</td>
<td>33</td>
<td>15</td>
</tr>
</tbody>
</table>

The average ratio of emission from $^{13}$CO$^+$ to that from HC$^{18}$O$^+$ is 15.3 ± 3.5 (Table 4-4). Once again, this is far higher than would be expected from optically thin emission from both isotopomers if Solar System ratios of atomic $^{12}$C:$^{13}$C and $^{16}$O:$^{18}$O apply. The high ratio suggests that the HC$^{18}$O$^+$ emission may arise from a smaller volume of gas than the H$^{13}$CO$^+$ emission, once again probably due to self-shielding in the more abundant isotopomer (H$^{12}$CO$^+$). The higher ratio for emission from H$^{13}$CO$^+$:HC$^{18}$O$^+$ compared with that from $^{13}$CO:C$^{18}$O may also support this suggestion. HC$^{18}$O$^+$ can be expected to be far less abundant than C$^{18}$O, and consequently full self-shielding from dissociating UV radiation will occur at a significantly smaller cloud radius. On the other hand, the high ratio may be due to chemical fractionation effects. Chemical fractionation (the preference for a molecule consisting of one isotope over another in a chemical reaction) can lead to different isotope ratios in the molecular products of a reaction with respect to the reactants. More complex products have a higher ratio of the lighter to the heavier isotope (e.g. a higher $^{16}$O:$^{18}$O ratio) (Engel & Macko 1998), so HC$^{18}$O$^+$ may be less abundant with respect to its $^{13}$C isotopomer than C$^{18}$O.

The average emission ratios of the $^{12}$C to $^{13}$C isotopomers of CS, HCN, HNC and HCO$^+$ (Table 4-3) suggest that the $^{12}$C isotopomer of these molecules is generally optically thick in dense molecular clouds, although less so than $^{12}$CO. A surprising result is that the minimum value for the emission ratio HCN:H$^{12}$CN is 0.9, and the minimum value for HCO$^+$:HC$^{13}$O$^+$ is 0.3. Both these low values occur in the same molecular cloud, the Chameleon dark cloud. No other molecular clouds have values less than unity for these ratios. In fact, all ratios for emission from $^{12}$C isotopomers to $^{13}$C isotopomers in the Chameleon dark cloud are low compared to other molecular clouds. The reason for this is not clear, but one possibility is diffuse gas along the line of sight (that may or may not be associated with the molecular cloud) containing an overabundance of the $^{13}$C isotopomers with respect to the $^{13}$C isotopomers, due to self-shielding in the more common isotopomer. It is also possible that the Chameleon dark cloud has a low elemental ratio of $^{12}$C:$^{13}$C. Further observations of the Chameleon dark cloud will be required to clarify the situation.
4.6 Summary

Transitions of 10 different molecules and several of their isotopomers have been observed in a sample of 26 southern molecular clouds. The observational results are as follows:

1. The CO spectra often show a significantly wider range of velocities than found for other molecules.

2. Self-absorption is present in about a third of the CO profiles, and in some profiles of $^{13}\text{CO}$, $^{18}\text{O}$, CS, HCN, HCO$^+$ and SO.

3. Self-absorption is not generally observed in transitions of OCS, HC$_3$N and CH$_3$OH, suggesting that these transitions are optically thin in most molecular clouds of the sample, or that these transitions only exist in the higher-excitation, inner parts of the clouds.

4. CO is optically thick in all molecular clouds of the sample. The average emission ratio for $^{12}\text{CO}:{^{13}\text{CO}}$ is $3.1 \pm 0.2$, very close to values found in surveys of northern hemisphere molecular clouds, and predicted by models.

5. The average emission ratio for $^{13}\text{CO}:^{18}\text{O}$ is $6.9 \pm 0.4$, higher than would be expected for optically thin emission if Solar System ratios for $^{13}\text{C}:{^{18}\text{O}}$ were assumed. This may be because $^{18}\text{O}$ occupies a smaller volume of gas than does $^{13}\text{CO}$, due to self-shielding of $^{13}\text{CO}$.

6. The average emission ratio of $^{13}\text{HCO}^+:^{18}\text{O}^+$ is $15.3 \pm 3.5$, also higher than would be expected for optically thin emission if Solar System ratios for $^{13}\text{C}:{^{18}\text{O}}$ were assumed. Self-shielding in $^{13}\text{HCO}^+$ is a possible explanation, however chemical fractionation effects may also be responsible for the high ratio.

7. CS, HCN, HNC and HCO$^+$ are generally found to be optically thick for the molecular clouds of the sample.

8. The Chameleion molecular cloud has $^{12}\text{C}:{^{13}\text{C}}$ isotopomer ratios of less than unity for HCN and HCO$^+$, and has low $^{12}\text{C}:{^{13}\text{C}}$ isotopomer ratios for all molecules. Further observations will be required to clarify the reasons for this situation.
Chapter 5

Physical Conditions and Molecular Abundances of Dense Cores

Tables A-1(b) to A-31(b) in Appendix A quote several molecular cloud parameters derived from the results of Chapter 4. Kinetic temperature ($T_{\text{kin}}$), H$_2$ column density (N(H$_2$)) and H$_2$ volume density ($n$(H$_2$)) have been calculated using the transitions of CO and its isotopically substituted species, and their derivation is discussed in this chapter. The central velocity quoted is an average velocity for all transitions with $T_{MB} > 5$ K, excluding the $^{12}$CO 1-0 transition (which has high optical depth or may be affected by self-absorption) and transitions where hyperfine components are blended. The error quoted is the standard error in the mean. The width is the average value for emission from all molecules with $T_{MB} > 8$ K, excluding $^{12}$CO and any blended transitions. A higher brightness temperature cutoff for width was used because for $T_{MB} \leq 8$ K line width tended to be overestimated as an artifact of noise in the spectrum.

5.1 Calculation of Kinetic Temperature and $H_2$ Density

5.1.1 Kinetic Temperature

As noted in Chapter 2, the kinetic temperature of a molecular cloud is the thermodynamic temperature of the major constituents of the gas: molecular hydrogen and atomic helium. Collisions between constituents in the molecular gas will be frequent enough that the velocity distribution can be assumed to be Maxwellian.

Emission from the J=1-0 transition of CO (and its isotopically substituted species $^{13}$CO and C$^{18}$O) has been used to determine the kinetic temperature and $H_2$ density of the molecular clouds in the sample.

In deriving the molecular cloud temperatures from the brightness temperatures of Appendix A, equation (2.7) has been used with the Rayleigh-Jeans approximation substituted for $L$, but with Planck's law substituted for $B_\nu(T)$. A further correction has been made for the brightness distribution of the universal microwave background so that the equation becomes

$$T_B = \frac{h \nu}{k} \left( \frac{1}{e^{\frac{h \nu}{kT}} - 1} - \frac{1}{e^{\frac{h \nu}{kT_{\text{ex}}}} - 1} \right) \left(1 - e^{-\tau}\right) \quad (5.1)$$

where $T_B$ is the peak $^{12}$CO J=1-0 observed brightness temperature, $T_{\text{ex}}$ is assumed to be the kinetic temperature of the molecular cloud and $\tau$ is assumed to be $\gg 1$. 


Three assumptions have been made in equation 5.1:

1) CO\(^1\) is in LTE with the other components of the gas (mostly molecular hydrogen and atomic helium) so that the excitation temperature of CO is the same as the kinetic temperature;
2) That CO is optically thick, and
3) That the CO emission region fills the telescope beam.

As demonstrated in chapter 4, the ratio of the \(^{12}\text{CO}\) to \(^{13}\text{CO}\) emission is consistent with \(^{12}\text{CO}\) being optically thick for all clouds in the sample. Main-beam brightness temperatures have been used in the calculation of source kinetic temperatures on the basis that \(^{13}\text{CO}\) J=1-0 mapping shows the CO emission to be extended with respect to the telescope beam for all molecular clouds in the sample.

\[5.1.2 \text{Calculation of } H_2 \text{ Column Density (N(H}_2)\]

Although \(H_2\) is the major constituent of molecular clouds, its lack of a permanent dipole moment means it is not generally observable, due to a lack of low energy rotational transitions. The higher-energy quadrupolar rotational transitions are found at infrared wavelengths and are very weak except in hot or shocked gas. Because of this, the \(H_2\) density must be inferred from observations of trace molecules; the ubiquitous and easily excited CO is usually used as a tracer. Methods for converting observed CO intensities and column densities to \(H_2\) column densities have been investigated extensively (see e.g. Wolfire et. al. 1993, Kutner & Leung, 1985, Taylor et al. 1993). However, the best factor to use in converting a measured CO column density to an assumed \(H_2\) column density remains uncertain. A variation of more than 400\% is found to be present in various determinations of the conversion factor from studies of individual clouds (Rohlfis & Wilson 1996). The molecule CS has also been investigated as a possible tracer of hydrogen column density (Lada et al. 1994).

The \(H_2\) column densities given in Appendix A result from the comparison of values calculated in 4 different ways. This approach was used as none of the methods, which use the J=1-0 transitions of CO (and its isotopically substituted species) and the J=1-0 transition of CS, have any obvious advantage over the other, and all are imprecise. However, the methods using \(^{12}\text{CO}\), \(^{13}\text{CO}\) and \(^{18}\text{O}\) intensities were found to be better than the method using the CS transitions and the average of these three values has provided the listed \(H_2\) column densities. The uncertainties given are the standard error in the mean. The four methods together with their applicability and limitations are described below.

**Method 1. Direct conversion of the observed \(^{12}\text{CO}\) J=1-0 integrated brightness temperature to \(H_2\) column density.** Empirically it has been found that in dense molecular clouds within our Galaxy there is a constant ratio between \(^{12}\text{CO}\) J=1-0 integrated brightness temperature (hereafter I(\(^{12}\text{CO}\))) and \(H_2\) column density (Rohlfis & Wilson 1996). There has been much discussion in the literature as to the theoretical

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\(^1\)If no atomic number is specified the isotopomer is that of the most common isotopes of the constituent elements: e.g. CO is \(^{12}\text{C}^{16}\text{O}\)
basis for this somewhat surprising finding (given that the $^{12}$CO J=1-0 transition is optically thick). One possibility is that a nearly constant fraction of the cooling from a molecular cloud occurs via emission from the CO J=1-0 transition, and both the heating and the cooling of a molecular gas are proportional to the number density of H$_2$ (Taylor et al. 1993). Another suggestion is that molecular clouds have a clumpy structure, being composed of dense clumps separated by a thinner inter-clump medium. The optically thick CO emission then arises mainly from the surfaces of the clumps contained within the telescope beam. The surface area of the clumps will be proportional to the mass contained in the clumps, so $\Sigma^{13}$CO is proportional to H$_2$ column density. Models of giant molecular clouds with a clumped structure have been used to investigate CO emission (Wolfire et al. 1993) and the $^{12}$CO J=1-0 to H$_2$ ratio has been found to be constant to within a factor of 3 over a wide range of temperatures and metallicities. The conversion factor used here is $2.3 \times 10^{20}$ (Rohlfs & Wilson 1996), although conversion factors from $1-4 \times 10^{20}$ have been used in the literature, giving

$$N(H_2) = 2.3 \times 10^{20} \int T_{MB} dv$$

(5.2)

where N(H$_2$) is the H$_2$ column density (cm$^{-2}$) and $\int T_{MB} dv$ is the integrated $^{12}$CO J=1-0 brightness temperature (K km s$^{-1}$).

Methods 2 and 3. The column densities of $^{13}$CO (hereafter $N(^{13}$CO)) and C$^{18}$O (hereafter $N$(C$^{18}$O)) have been found to be directly proportional to H$_2$ column density over a moderate range of H$_2$ densities. The relationships used here are (Rohlfs & Wilson 1996)

$$N(H_2) = 4.4 \times 10^6 \text{N(C}^{18}\text{O}_{\text{LTE}} \quad \text{for } N(H_2) < 1.5 \times 10^{22} \text{ cm}^{-2} \quad (5.3)$$

$$N(H_2) = 4.6 \times 10^5 \text{N(^{13}CO}_{\text{LTE}} \quad \text{for } N(H_2) < 5 \times 10^{22} \text{ cm}^{-2} \quad (5.4)$$

These relationships were derived by comparing CO abundances with infrared determinations of $A_v$, the visual extinction due to dust (Lada et al. 1994). The subscript LTE refers to the fact that the CO abundances were derived from an LTE analysis. Assuming a constant ratio of dust to H$_2$ column density Rohlfs and Wilson assumed that 1 magnitude of visual extinction is equivalent to an N(H$_2$) column density of $10^{21}$cm$^{-2}$ to convert the results of Lada et al. (1994). A constant gas-to-dust mass ratio is assumed because metals (such as C and Si that form dust) have a constant abundance of about 1% in the ISM (Rohlfs & Wilson 1996). In addition, the ratio of dust to gas in molecular clouds has been found to have a constant value of about 1% (Solomon 1984). A scatter of between 2 and 5 is found in the correlations of (5.3) and (5.4) towards individual positions, and the scatter increases with increasing visual extinction. The upper limits to the H$_2$ column densities given for (5.3) and (5.4) are the densities at which the scatter in the correlation increases markedly. For N($^{13}$CO) a scatter of 5 is found above N(H$_2$) = $5 \times 10^{22}$ cm$^{-2}$, whereas for N(C$^{18}$O) the scatter remains close to 2 for densities greater than $1.5 \times 10^{22}$ cm$^{-2}$. An additional uncertainty may be introduced into these relationships due to variations in isotopic abundance ratios between individual molecular clouds (section 4.5.3).
The calculated H$_2$ column densities listed in Appendix A range from $3.9 \times 10^{21}$ to $2.1 \times 10^{23}$ cm$^{-2}$, with an average value of $(8.1 \pm 0.1) \times 10^{22}$ cm$^{-2}$. Although many of the clouds in the sample have somewhat larger column densities than the density range specified by (5.3) and (5.4) the scatter should not a priori be larger than that of method 1.

Method 4. A correlation between CS column density (hereafter N(CS)) and H$_2$ column density has been determined by Lada et al. (1994) in the same way as for the CO isotopomers. Using the conversion factor between $A_v$ and H$_2$ column density given previously, the relationship is

$$N(\text{H}_2) = 2.2 \times 10^9 \text{N(CS_{LTE})} \quad \text{for } N(\text{H}_2) < 5 \times 10^{22} \text{ cm}^{-2}$$

(5.5)

As before, the subscript LTE refers to N(CS) values obtained from an LTE analysis.

5.1.3 Comparison of Methods for determining N(H$_2$)

Equations (5.2) to (5.5) were used to calculate N(H$_2$) at each position. The values obtained by the different methods are compared in Figure 5-1. Each plot (except for 5-1(c)) gives the ratio of the H$_2$ column density obtained by one particular method to that obtained from $I(^{12}\text{CO})$, plotted against the H$_2$ column density derived from $I(^{12}\text{CO})$ (method 1). $I(^{12}\text{CO})$ was chosen as the reference for H$_2$ column density because this conversion factor has been studied extensively for Galactic clouds, and is determined to within a factor of $\sim 4$, and will yield N(H$_2$) to this accuracy provided the $^{12}\text{CO}$ emission is optically thick. It has been established already that the $^{12}\text{CO}$ optical depths are high for the sample under consideration. The median ratios for N(H$_2$) derived by each method together with the values of the 1$^{st}$ and 3$^{rd}$ quartiles are given in Table 5-1.

<table>
<thead>
<tr>
<th>Methods</th>
<th>Median ratio of N(H$_2$)</th>
<th>1$^{st}$ Quartile</th>
<th>3$^{rd}$ Quartile</th>
</tr>
</thead>
<tbody>
<tr>
<td>N($^{13}\text{CO}$): $I(^{12}\text{CO})$</td>
<td>1.5</td>
<td>0.8</td>
<td>2.0</td>
</tr>
<tr>
<td>N($^{16}\text{O}$): $I(^{12}\text{CO})$</td>
<td>1.7</td>
<td>0.7</td>
<td>2.3</td>
</tr>
<tr>
<td>N($^{18}\text{O}$): $N(^{13}\text{CO})$</td>
<td>1.0</td>
<td>0.8</td>
<td>1.2</td>
</tr>
<tr>
<td>N(CS$_{LTE}$): $I(^{12}\text{CO})$</td>
<td>1.7</td>
<td>1.2</td>
<td>2.7</td>
</tr>
<tr>
<td>N($^{13}$CS): $I(^{12}\text{CO})$</td>
<td>16.8</td>
<td>10.0</td>
<td>32.8</td>
</tr>
</tbody>
</table>
Figure 5-1 Ratio of $N(\text{H}_2)$ derived from various transitions to $N(\text{H}_2)$ derived from $^{13}\text{CO}$ plotted against $N(\text{H}_2)$ derived from $^{13}\text{CO}$. For the sake of brevity the labeling of the graphs has been abbreviated so that e.g. $N(\text{H}_2)$ derived from $^{13}\text{CO}$ is labelled as $N(^{13}\text{CO})$. See text for further discussion.
For the sake of brevity the labels on the axes of the graphs have been abbreviated so that e.g. the ratio of N(H$_2$) derived from N($^{15}$CO) to N(H$_2$) derived from I($^{12}$CO) is labelled as N($^{15}$CO)/I($^{12}$CO). Figure 5-1(a) shows the variation of the ratio of N(H$_2$) derived from N($^{13}$CO) to that derived from I($^{12}$CO). As listed in Table 5.1, the median ratio of H$_2$ density from N($^{13}$CO) to that from I($^{12}$CO) is 1.5 (with 1st and 3rd quartiles of 0.8 and 2.0 respectively), showing that N($^{13}$CO) tends to overestimate H$_2$ density with respect to values obtained from I($^{12}$CO). Given that both methods compared here are stated to have scatters of 4 to 5 the agreement is very good. There is no significant increase in scatter at higher N(H$_2$). This is surprising given that Lada et al. found a scatter of up to 5 for the ratio between N($^{13}$CO) and N(H$_2$) for A$_v$ values of 5 to 30 (N(H$_2$) = 1.5 x 10$^{22}$ to 3 x 10$^{22}$ cm$^{-2}$), and is especially surprising given that we have N(H$_2$) greater than 10$^{23}$ cm$^{-2}$ (equivalent to A$_v$ = 100) in our sample. The difference between our results and those of Lada et al. may be because we have observed the cores of dense molecular clouds whereas Lada et al. derived the relationship (5.4) from observations towards different positions in the dark cloud IC 5146. Unlike giant molecular clouds, dark clouds do not have a clumped structure. The inter-clump medium of GMCs allows emission from clumps in the interior of a cloud to contribute to the emergent line profile and hence N($^{13}$CO) column density may be a better indicator of H$_2$ column density than I($^{12}$CO) in GMCs. Whatever the reason, the result for our sample of 30 dense southern molecular clouds suggests that equation (5.4) can validly be used to estimate H$_2$ density in GMCs over the range 10$^{21}$ to 10$^{23}$ cm$^{-2}$.

Figure 5-1(b) shows the variation of the ratio of N(H$_2$) derived from N(C$^{18}$O) to that derived from I($^{12}$CO). The median ratio of H$_2$ density from N(C$^{18}$O) to that from I($^{12}$CO) (Table 5-1) is 1.7 (with 1st and 3rd quartiles of 0.7 and 2.3 respectively), showing that N(C$^{18}$O) also tends to overestimate H$_2$ density with respect to values obtained from I($^{12}$CO). The somewhat larger scatter in this ratio compared to that for N($^{13}$CO)/I($^{12}$CO) probably results from poorer signal to noise in the weaker C$^{18}$O J=1-0 transition.

Densities obtained from N($^{13}$CO) and N(C$^{18}$O) are compared in Figure 5-1(c), which shows N(C$^{18}$O)/N($^{13}$CO) plotted against N($^{13}$CO). The results obtained from these methods agree closely, with a median of 1.0 (with 1st and 3rd quartiles of 0.8 and 1.2 respectively), except at densities close to 10$^{21}$ cm$^{-2}$, which are dark clouds in the sample. The increased scatter in these two points is apparent in 5.1(b) and (c) but not in 5.1(a) suggesting it is due to the C$^{18}$O emission. Once again poor signal to noise is a likely explanation.

Figure 5-1(d) and (e) show the results obtained from method 4 (i.e. for transitions of CS). Figure 5-1(d) shows the ratio of H$_2$ column density (derived from an LTE analysis) of N($^{12}$CS$_{LTE}$) to I($^{12}$CO), plotted with N(H$_2$) derived from I($^{12}$CO). The median ratio of 1.7 (with 1st and 3rd quartiles of 1.2 and 2.7 respectively) for N($^{12}$CS$_{LTE}$) I($^{12}$CO) is close to the ratios of N($^{13}$CO) and N(C$^{18}$O) to I($^{12}$CO). However, column densities derived using an LTE analysis are only valid if the emission is optically thin. The CS J=2-1 transition is often optically thick in dense molecular clouds. Comparison of $^{13}$CS emission with $^{12}$CS emission for the molecular clouds of the sample shows that in most cases the CS J=2-1 transition is optically
thick, with a mean ratio of $T_{MB}(^{12}\text{CS})/T_{MB}(^{13}\text{CS})$ of 11.7 and range 5 to 29 for the 20 positions for which observations of both isotopomers are available (c.f. 40 – 80 for the abundance ratio of $^{12}\text{C}/^{13}\text{C}$ in molecular clouds of the galactic disk). In view of this, H$_2$ column densities derived using LTE values for N(CS) should be at least a factor of 5 lower than those derived using isotopomers of CO.

An alternative way of calculating N(CS) was used to avoid the problems posed by high optical depth. An LTE analysis of the $^{13}\text{CS}$ emission provided N($^{13}\text{CS}$), which was in turn used to estimate N($^{12}\text{CS}$) assuming an abundance ratio of 50 for $^{12}\text{C}/^{13}\text{C}$. N(H$_2$) was then found using (5.5) and Figure 5-1(e) shows the ratio of N(H$_2$) obtained in this way to N(H$_2$) from $^{12}\text{CO}$. The median is 16.8, much higher than when CO is used. The uncertainty in the appropriate $^{12}\text{C}/^{13}\text{C}$ notwithstanding, N($^{12}\text{CS}$) estimated from N($^{13}\text{CS}$) should be a better estimation than that derived from an LTE analysis of $^{12}\text{CS}$, so (5.5) is not a good predictor of N(H$_2$) although in the clouds within the sample LTE-derived values are in reasonable agreement with N(H$_2$) from other methods. The most likely explanation for the disparity is that the CS observations of Lada et al. in IC 5146 used to derive (5.5) had a similar optical depth to many of the molecular clouds in this sample. If this is the case then there is an inherent assumption in this equation of a particular optical depth (i.e. equation (5.5) is really a relationship between the excitation temperature rather than the column density of CS and N(H$_2$)).

Methods 1, 2 and 3 provide determinations of H$_2$ column density that utilize three independently measured quantities (integrated emission of $^{12}\text{CO}$, $^{12}\text{CO}$ and C$^{18}$O) and give values that agree to within a factor of 3 over a total column density range of two orders of magnitude. The average value of the three has been adopted as the H$_2$ column density. In particular, methods 2 and 3 (N($^{13}\text{CO}$) and N(C$^{18}$O)) give very consistent results, and the ratio between N(H$_2$) derived from these column densities is very close to unity. However, despite the consistency, the accuracy of all three determinations as a measure of N(H$_2$) depends on the accuracy of the relationships (5.2) to (5.5).

The H$_2$ column density has been estimated as carefully as possible because the abundances of trace species in molecular clouds are traditionally reported as a ratio with respect to this quantity, and uncertainties would therefore be reflected in the final abundance determinations.
5.2 Calculation of Hydrogen Spatial Densities

The hydrogen spatial densities given in Tables A-1(b) to A-31(b) have been obtained by a very simple model which assumes that the diameter of a molecular cloud will be directly proportional to line width of the $^{12}$CO emission and inversely proportional to any large velocity gradient through the cloud. The justification for this is that the width of an emergent line profile is believed to be due to a summation of the emission from individual clumps within a molecular cloud, all of which are in motion with respect to one another. The emission from individual clumps will have a (narrow) line width that results from thermal broadening within each clump and Doppler shifting of the emission from each clump with respect to the gross turbulent motion of the clump leads to a far broader emergent line profile. Many clumps in turbulent motion will presumably occupy a larger area of space and lead to a large FWHM of the spectral line. The FWHM needs to be divided by the velocity gradient across the cloud to account for differences in the turbulent velocities in individual molecular clouds. Unless there are grounds for assuming a different value, the velocity gradient across the molecular clouds of the sample is assumed to have a typical value of 1 km s$^{-1}$ pc$^{-1}$. These assumptions result in the relationship

$$n(H_2) = \frac{N(H_2) \left( \frac{dv}{dr} \right)}{3.08 \times 10^{18} \text{ FWHM}}$$

(5.6)

where $n(H_2)$ = spatial density in cm$^{-3}$

$N(H_2)$ = column density in cm$^{-2}$

$dv/dr$ = velocity gradient in km s$^{-1}$ pc$^{-1}$

FWHM is velocity width of the $^{12}$CO line in units of km s$^{-1}$,

and the constant $3.08 \times 10^{18}$ is the number of cm in a pc.

The values of $n(H_2)$ in Tables A-1(b) to A-31(b) are meant only as an approximation and are listed for comparison to other indicators of $n(H_2)$ only. They are stated without uncertainties.

It should be stressed that this is a very simple model, and will only be a first order approximation to H$_2$ spatial density. In addition to the assumptions stated above, it is assumed that the H$_2$ column density, $N(H_2)$, is not affected by beam dilution effects. $N(H_2)$ as calculated here is in fact a lower limit, so the H$_2$ spatial densities quoted here are at best lower limits, if the assumption regarding velocity gradient is met.

5.3 Abundance of Molecules other than CO

Molecular abundances for molecules other than CO were calculated in a variety of ways, depending on the number of observed transitions.

1) The abundance of molecules for which only one transition was observed were calculated assuming LTE and that $\tau \ll 1$ (see section 2.10(case 2)). Equation (2.27) was used to calculate the column density of molecules in the upper level of the transition, and then the Boltzmann distribution (2.14) was used find the total molecular column density ($N_{\text{col}}$ in Tables A-1(c) – A-31(c)). The values for the Einstein-A coefficients and partition functions used in the above equations are
listed in Appendix C. The excitation temperature to be used in \( (2.27) \) was unknown and had to be assumed. An estimate to the excitation temperature can be derived by considering properties of both the molecule and the molecular cloud, but it remains a large source of uncertainty in the calculation of molecular abundances (see section 5.3.1). In addition, if less than 3 transitions are observed no information is available to support or contradict the assumptions of LTE and \( \tau \ll 1 \) (deviations from these conditions can sometimes be diagnosed from a rotation diagram). Generally, transitions of rarer (and therefore optically thin) isotopomers have also been observed and the abundance was calculated from these transitions. This method gives information on the optical depth of the most common isotopomer (assuming that the isotope abundance ratios are known).

2) The abundance of a molecule for which three or more transitions were observed was calculated using a rotation diagram (see section 2.10.3). This method also relies on the assumptions that the molecular gas is in LTE and that \( \tau \ll 1 \). However, at least some information about the appropriateness of these assumptions is available from the data distribution in the rotation diagram (see below). The rotation diagram gives the total molecular column density \( N_{\text{tot}} \) in Tables A-1(c) – A-31(c)) and the excitation temperature of the molecule.

3) For H\(_2\)N\(_3\), in addition to application of the rotation diagram method, the abundance was also calculated using an LVG model utilising code kindly supplied by Dr Peter Schilke of the Max-Planck-Institut für Radioastronomie, Bonn, Germany. The LVG code does not assume either LTE or \( \tau \ll 1 \), although it does assume a constant velocity gradient with radius, and that the hydrogen number density and kinetic temperature are constant throughout the molecular gas. In particular, this model is not suitable for molecular clouds with two distinct density components, e.g. a core-halo type situation.

5.3.1 Excitation Temperatures for Abundance Calculations from One Transition

As stated in the previous section, calculating molecular abundances from a single transition is a very uncertain process. The actual excitation temperature that should be adopted for equation \( (2.14) \) could range in principle between the microwave background radiation temperature of 2.7 K and the kinetic temperature of the molecular cloud. The excitation temperature may even be higher than the kinetic temperature if a molecule is sampling only the warmest gas in a molecular cloud, or negative if the level populations are inverted as in masers.

Several pieces of information were taken into account in estimating the appropriate excitation temperatures for the abundance calculations reported in tables A-1(c) to A-31(c):

1) Knowledge of the likely relationship of molecular excitation temperatures between one molecule and another and kinetic temperatures in molecular clouds obtained from prior studies of molecular clouds (see e.g. Blake et al. 1987).
2) Use of the relationship (Scoville and Solomon 1974)

\[ T_{lu} \propto (\alpha n_m C_{ul})^{k/3} T_k \]  

where \( T_{lu} \) is the transition temperature (excitation temperature for the transition from the lower level \( l \) to upper level \( u \), \( n_m \) is the hydrogen density, \( C_{ul} \) is the downward rate for a collisional transition, \( T_k \) is the kinetic temperature of the molecular cloud, and

\[ \alpha = g_u C^3/(8\pi v^3 dv/dz) \]  

where \( g_u \) is the statistical weight ratio of the upper and lower levels of the transition.

Equation 5.7 and the results of prior observations were used only to place molecules into ‘groups’ likely to have similar excitation temperatures as both the hydrogen density (needed to find \( C_{ul} \)) and the individual molecular densities are unknowns.

On the basis of equation (5.7) and the observations reported in Blake et al. (1987), the groups of molecules assumed to have similar excitation temperatures were:

1. CO, \(^{13}\)CO and \(^{18}\)O
2. HC\(_3\)N and OCS
3. CH\(_2\)OH, C\(_2\)H and SO
4. CS, HCN, HCO\(^+\) and HNC.

3) The final step was to then assign an excitation temperature to a ‘group’ of molecules for each molecular cloud on the basis of molecules for which the excitation temperature could be calculated from a rotation diagram (HC\(_3\)N, OCS, CH\(_2\)OH) or for which the optical depth was believed to be high (CO, CS). Isotopomers were always assumed to have the same excitation temperature as the most common isotopomer (e.g. \(^{13}\)CO and \(^{18}\)O were assumed to have the same excitation temperature as \(^{12}\)CO).

### 5.3.2 Results of Abundance Calculations

The results of abundance calculations for each molecular cloud, based on optically thin LTE models, are presented in the (c) tables of Appendix A. The first column lists the molecule, the second column the excitation temperature (excitation temperatures in brackets are assumed excitation temperatures), the third column the column density of the molecule and the fourth column gives the relative abundance (molecular column density divided by hydrogen column density).

The following notes give information specific to the abundance calculations for each molecule. The method for assuming excitation temperatures was discussed in section 5.3.1, the rotation diagram results are discussed in section 5.3.3 and the LVG calculations are discussed and compared to LTE models in section 5.3.4 and 5.3.5. The results and implications of the calculations for individual sources are discussed in Chapter 6.
As

The column densities of $^{13}$CO and C$^{18}$O were calculated using equation (2.27), assuming that both these isotopomers are optically thin and that they have the same excitation temperature as that for $^{12}$CO.

$HC_3N$, $OCS$ and $CH_3OH$

Generally more than three transitions of these molecules were observed over frequencies ranging from 85 to 150 GHz, and a rotation diagram analysis was used to determine molecular column density and excitation temperature. The rotation diagrams are shown in figures A-1(a) – A-31(a). The least-squares fit to the data is shown on the diagrams. When only two transitions were detected the rotation diagram method was still used to gain an estimate of the molecular column density and excitation temperature. However, these diagrams are not shown. In addition, molecular abundances of $HC_3N$ were calculated using an LVG model. The results of the LVG models for each molecular cloud are presented in tables A-1(e) – A-31(e) and figures A-1(b) – A-31(b). Details of the LVG calculations and a comparison of LTE and LVG models are presented in section 5.3.4.

$CS$

The $^{12}$CS $J=2-1$, $^{13}$CS $J=2-1$ and $^{12}$CS $J=3-2$ transitions were observed. The $^{12}$CS $J=2-1$ transition was assumed to be optically thick and was used to determine an upper limit to the CS excitation temperature using an equation similar to that used for CO (5.1). The assumption is made that the CS population may be sub-thermal with respect to the kinetic temperature but that one excitation temperature will characterise all transitions, and if $\tau >> 1$ the brightness temperature of the $^{12}$CS transition will approach the excitation temperature of CS. The $^{13}$CS $J=2-1$ was assumed to be optically thin and used to calculate the molecular column density, with the assumption that $^{12}$CS and $^{13}$CS should have the same excitation temperature. The abundances and excitation temperatures presented in the tables are those obtained by this method.

$HCN$, $HNC$ and $HCO^+$

These molecules were observed in both the $^{12}$C and $^{13}$C isotopomers, while HCO$^+$ was also observed in the $^{18}$O isotopomer. The excitation temperature for these molecules was assumed to be the same as that for CS, and the molecular abundance was calculated from the $^{13}$C isotopomer.

$C_2H$ and $SO$

The only information available for these molecules was the observation of a single transition in the most common isotopomer. The excitation temperature for SO and C$_2$H was assumed to be the same as the excitation temperature for CH$_3$OH (see section 5.3.1).

5.3.3 Abundances from Rotation Diagrams

Table 5.2 gives the correlation coefficients for least squares fits to the rotation diagrams for $HC_3N$, OCS and CH$_3$OH in each source (fig. A-1(b) – A-31(b)). The correlation coefficients range from 0.66 to 1.00, so in all cases there is a statistically significant correlation between ln[N$_v$/g$_v$] and E$_v$/k. However, visual inspection of the
rotation diagrams shows that only some have the straight-line relationship expected for optically thin emission under LTE conditions. A fairly simple criterion has been chosen to separate rotation curves that are consistent with optically thin LTE emission (for a particular molecule and molecular cloud) from those that are not. Only rotation data that can be fitted with a straight line that includes all data points (within the limits of error bars) are considered to be consistent with optically thin emission in LTE (although there could be other reasons for the non-linearity, such as beam dilution). Correlation coefficients in table 5.2 for data that do not meet this criterion are marked with an asterisk. As an example, the rotation diagrams for the molecular cloud 268.4-0.8 (fig. A-4(b)) were classified as good fits while those for 333.0-0.6 (fig. A-17(b)) were considered poor fits.

In line with this separation, all correlation coefficients of 0.88 and above give a linear fit that includes all data points within error bars (n = 25). All correlation coefficients of 0.77 or less do not give a linear fit that includes all data points (n = 13), while coefficients between 0.78 and 0.87 may fall in either category (n = 7 for good fits; n = 14 for poor fits).

The shape of the rotation diagram curve (including its linearity) can give information about physical conditions in the gas from which the emission arises. Goldsmith and Langer (1999) (hereafter GL) have investigated the rotation diagram as a tool for analysing molecular line emission and their results may be summarised as follows. (Figures 5-2(a) - (c) and 5-3(a) and (b) are reproduced from GL.)

**Linear Molecules**

1) *Optically thin emission in LTE:* A straight-line rotation diagram will be obtained with the slope of the line being equal to 1/T_{ex}, and the value of the ordinate extrapolated to zero (y-intercept) yielding N_{tot} as described in section 2.10.3 (see also fig 5-2(a)).

2) *Optically thin emission not in LTE:* A straight line may still be obtained due to quasi-thermalisation of most transitions at a single excitation temperature considerably lower than the kinetic temperature (fig 5.2(b)). The accuracy of N_{tot} derived in this manner will depend on how well the quasi-thermalisation describes all transition temperatures.

3) *High optical depth:* The effects of high optical depth are similar in both LTE and non-LTE situations (figures 5-2(a) and (c)). Erroneously high or low T_{ex} may be found if only a limited number of transitions are observed, and the relationship may well appear to be linear. The y-intercept and hence N_{tot} will also be affected by the apparently linear relationship, with N_{tot} likely to be underestimated by a factor of the optical depth (τ). For the dense molecular cores observed in this study τ is likely to be greatest for the λ = 3 mm transitions (GL).

4) *Beam dilution effects (due to clumpiness or small source diameter)* should not change the general shape of the rotation curve (or therefore the derived excitation temperature) but will cause N_{tot} to be underestimated (GL).
However, if an appropriate correction for changing telescope beamwidth with frequency is not applied, the emission in a transition may be underestimated by the beam-filling factor and this will possibly affect the shape of the rotation diagram (see 2.10.3).

Non-linear Molecules

Figures 5-3(a) and (b) show the results obtained by GL for models for CH$_3$OH emission. 5-3(a) shows the effect of increasing optical depth on LTE excitation, while 5-3(b) shows the effects of non-LTE excitation on a rotation diagram. Both figures suggest that either high optical depth or non-LTE conditions will lead to a considerable scatter from a straight-line relationship for transitions from different k-ladders.

Table 5-2. Correlation coefficients for least squares fits to rotation diagrams for HC$_3$N, OCS and CH$_3$OH

<table>
<thead>
<tr>
<th>Source</th>
<th>HC$_3$N</th>
<th>OCS</th>
<th>CH$_3$OH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orion KL</td>
<td>-</td>
<td>0.99</td>
<td>0.88</td>
</tr>
<tr>
<td>268.4-0.8</td>
<td>0.99</td>
<td>-</td>
<td>0.89</td>
</tr>
<tr>
<td>Cha 4</td>
<td>0.80</td>
<td>-</td>
<td>0.88</td>
</tr>
<tr>
<td>RCW 57(E)</td>
<td>0.66*</td>
<td>-</td>
<td>0.93</td>
</tr>
<tr>
<td>RCW 57(W)</td>
<td>0.95</td>
<td>-</td>
<td>0.80</td>
</tr>
<tr>
<td>CS 1</td>
<td>-</td>
<td>-</td>
<td>0.51</td>
</tr>
<tr>
<td>RCW 65</td>
<td>0.87*</td>
<td>-</td>
<td>0.81</td>
</tr>
<tr>
<td>305.4+0.2</td>
<td>0.91</td>
<td>0.78</td>
<td>0.67</td>
</tr>
<tr>
<td>311.6+0.3</td>
<td>0.98</td>
<td>-</td>
<td>0.61</td>
</tr>
<tr>
<td>RCW 92</td>
<td>0.90</td>
<td>0.78*</td>
<td>0.85</td>
</tr>
<tr>
<td>Lup 4</td>
<td>1.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>326.7+0.6</td>
<td>0.86*</td>
<td>-</td>
<td>0.85</td>
</tr>
<tr>
<td>327.3-0.5</td>
<td>0.83*</td>
<td>0.75*</td>
<td>0.56</td>
</tr>
<tr>
<td>331.5-0.1</td>
<td>-</td>
<td>-</td>
<td>0.88</td>
</tr>
<tr>
<td>333.0-0.8</td>
<td>0.73*</td>
<td>-</td>
<td>0.76</td>
</tr>
<tr>
<td>333.4-0.4</td>
<td>-</td>
<td>0.95</td>
<td>0.95</td>
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<td>-</td>
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<td>0.84</td>
</tr>
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<td>0.86*</td>
<td>0.77</td>
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<td>0.99</td>
<td>-</td>
</tr>
<tr>
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<td>R Cr A</td>
<td>-</td>
<td>-</td>
<td>0.70</td>
</tr>
</tbody>
</table>

Notes:
* least squares fit is not a straight line fit to all data within error bars.
Fig. 2.—Population diagrams for HC₃N. The H₂ density of 10⁶ cm⁻³ ensures that all transitions are thermalized, so the LTE applies. At the kinetic temperature of 22 K, a = hE/kT = 0.01. The curves correspond to different fractional abundances per unit velocity gradient as indicated by the symbols shown in the lower left. The maximum optical depth for X = 10⁻¹¹ is 377, which occurs for the J = 10 → 9 transition. The corresponding optical depth of the 1 → 0 transition is 10, and for the 18 → 17 transition is 130. The optical depths scale directly with the fractional abundance.

Fig. 6.—Population diagrams for HC₃N levels up to 70 K above ground state (including J = 0 to J = 18). The fractional abundance HC₃N per unit velocity gradient is chosen to make all transitions optically thin for all hydrogen densities considered, which vary from 10⁶ cm⁻³ to 10⁷ cm⁻³ as indicated by the symbols shown at lower left of figure. In hydrogen densities s(H₂) ≥ 10⁷ cm⁻³, all transitions are thermalized so the population diagram curves are straight lines characteristic of the kinetic temperature of 22 K. For lower densities, a variety of effects are seen, including quasi thermalization at a temperature considerably less than the kinetic temperature.

Fig. 7.—Effect of finite optical depth on sub thermally excited HC₃N. The curves are for different molecular fractional abundances. A velocity of 1 km s⁻¹ pc⁻¹ has been used to form the population diagram. The maximum values of the optical depth for collisional excitation are in the region 2 ≤ Jᵣ ≤ 2, while for LTE, the optical depth is much more widely distributed and peaks at Jᵣ = 11.

Figure 5-2. Population diagrams for models of HC₃N emission (a linear molecule) in molecular clouds reproduced (including captions) from Goldsmith & Langer (1999). (a) (Fig. 2 of GL) shows emission in LTE for a range of HC₃N column densities, demonstrating the effect of optical depth. (b) (Fig. 6 of GL) shows optically thin HC₃N emission for a range of H₂ densities, demonstrating the possibility of quasi-thermalization at Tₑ < T_k. (c) shows the effect of high optical depth on sub-thermally excited HC₃N.
Figure 5.3. Population diagrams for models of CH$_3$OH emission (a non-linear molecule) in molecular clouds reproduced (including captions) from Goldsmith 
& Langer (1999). (a) (Fig. 5 of GL) shows emission in LTE for a range of 
CH$_3$OH column densities, demonstrating the effect of optical depth. (b) (Fig. 8 of 
GL) shows optically thin CH$_3$OH emission for a range of H$_2$ densities.

5.3.4 General Comments on the Rotation Diagrams of A-1(a) – A-31(a)

HC$_3$N

As shown in table 5.2, good fits are obtained for just over half the rotation diagrams. 
In the absence of undetected optical depth effects due to a limited number of 
transitions being observed these rotation curves should give good estimates of $T_{ex}$ and 
$N_{tot}$. Of the 11 rotation curves where the fit was classed as poor, IRAS 16562, NGC 
6334(N1) and RCW 122 have a curve shape that may be attributable to high optical
depth effects. In the remaining 8 cases, the poorer fit is due to scatter in the diagram and the reasons for this are unclear. Excitation far from LTE or a complex molecular cloud temperature and density structure are possible explanations. Calibration problems are an unlikely source of error given that less than half the rotation diagrams are affected, and that all data were treated in the same way.

Simple beam dilution effects have been ruled out as a cause of the scatter. The data were corrected for a range of source sizes less than the beam sizes of the observations, with no improvement in the scatter. This is as expected from the results of GL. The HC$_3$N rotation diagrams are discussed further in the next section, together with the results of LVG models for HC$_3$N emission.

**OCS**

Two thirds of the OCS rotation diagrams are well fitted by a straight line using the criterion of all data points lying on the least-squares line of best fit within the error bars. OCS is primarily excited/formed in the warmest gas and the emission may therefore arise from a denser, more homogeneous region than emission from HC$_3$N, so that OCS emission is more likely to be thermalised.

**CH$_3$OH**

In contrast to OCS, only one third of the CH$_3$OH rotation diagrams have a good fit to a straight line. This is consistent with the increased scatter expected for non-LTE excitation and/or high optical depth effects, and suggests that only a third of the molecular clouds in the sample satisfy the requirements of LTE and optically thin emission, in this molecule at least.

### 5.3.4 Abundance of HC$_3$N from LVG Models

LVG abundances for HC$_3$N were calculated by comparing observed line intensities to the line intensities predicted by LVG models. Theoretical line intensities were generated for LVG models of varying $T_{\text{kin}}$, $N_{\text{mol}}/(dv/dr)$ (where $dv/dr$ is the velocity gradient) and $n$(H$_2$) (see Chapter 2, section 2.10). The column density of hydrogen, $N$(H$_2$), was an assumed input parameter. The theoretical line intensities were compared with the observed line intensities to ascertain which combinations of $T_{\text{kin}}$, $N_{\text{mol}}/(dv/dr)$ and $n$(H$_2$) were consistent with the observed values, within errors. Only detected transitions of HC$_3$N were used in the modeling; upper limits to transitions were not considered; treating upper limits as measured values invariably led to very poor fits to the models.

The consistency of the different LVG models was determined using the method described by Lampton, Margon & Bowyer (1976). The parameter, $\chi^2$, was used to quantify the variation between predicted and observed line intensities:

$$\chi^2 = \sum_{i=1}^{N} \frac{(O_i - C_i)^2}{\sigma_i^2}$$

5(9)
where $O_i$ is the observed brightness temperature of a transition, $C_i$ is the predicted value of the transition, $\sigma_i$ is the expected variance in the observed value (uncertainty), and $N$ is the number of transitions observed.

For any group of LVG models (i.e. for all models pertaining to an individual source) the minimum $\chi^2$ is first found, and then models which have $\chi^2 = \chi^2_{\text{min}} + \Delta\chi^2$ are classified as being acceptable fits to the observed data. For three free parameters ($T_{\text{kin}}$, $N_{\text{mol}}/(\text{dv}/\text{dr})$ and $n(H_2)$), the appropriate value of $\Delta\chi^2$ to use is 3.5 (Lampton, Margon & Bowyer 1976). This value gives a confidence of 0.68 (or 1σ) that the correct model will be included in the set of acceptable solutions.

The discussion of the previous paragraph assumes that at least some solutions are consistent with the observed values. This assumption can be tested by examining the value of the reduced $\chi^2_{\text{min}}$, which is defined as

$$\chi^2_{\text{red}} = \chi^2 / (N - p) \quad (5.10)$$

where $N$ is the number of transitions observed and $p$ is the number of free parameters.

If the observed and predicted values agree to within the measurement errors then $\chi^2_{\text{red}}$ should be close to 1. If $\chi^2_{\text{red}} > 1$ then it suggests that either none of the tested models are a good fit to the data, or that the observational errors have been underestimated.

It is important to note that there is a statistical uncertainty associated with the observational measurements. Although $\chi^2_{\text{min}}$ is stated in the results, any of the values with $\Delta\chi^2 < 3.5$ are likely, to the 0.68 confidence level, and so it is the range of plausible values that is important.

Tables A-1(e) – A.31 (e) summarise the results of the LVG modelling. In the first column $T_{\text{kin}}$ at $\chi^2_{\text{min}}$ is quoted and in the second column the range for which $\Delta\chi^2 < 3.5$ is given. Likewise, columns 3 and 4 specify $N(\text{HC}_3\text{N})/(\text{dv}/\text{dr})$ and columns 6 and 7 specify $n(H_2)$. Column 5 gives the relative abundance of $N(\text{HC}_3\text{N})/(\text{dv}/\text{dr})$ with respect to $N(H_2)$ for $\chi^2_{\text{min}}$.

Graphical summaries of the results of LVG modeling are shown in figures A-1 (b) – A-31 (b). The left-hand figure shows a grey-scale plot of $\chi^2$ as a function of the log of the molecular hydrogen density (log[$n(H_2)$]) and the log of the HC$_3$N column density per unit velocity gradient (log[$N($HC$_3$N)/($\text{dv}/\text{dr}$)], for the kinetic temperature ($T_{\text{kin}}$) at $\chi^2_{\text{min}}$. The right-hand figure shows a grey-scale plot of $\chi^2$ as a function of log[$n(H_2)$] and $T_{\text{kin}}$ for log[$N($HC$_3$N)/($\text{dv}/\text{dr}$)] at $\chi^2_{\text{min}}$. The position of $\chi^2_{\text{min}}$ is marked with an X in each figure, while the solid line shows the boundary for plausible values at the 0.68 confidence level. The grey-scale contours are for $\Delta\chi^2 = 3.5$ (1σ), 6.25 (2σ), 11.3 (3σ), 25, 50, 75 and 100.
Four or five transitions of HC$_3$N were observed for most molecular clouds in the sample. However, in some cases as few as two transitions were observed. In cases where less than four transitions were observed $\chi^2_{\text{red}}$ has no meaning. It should be noted in these cases that $\chi^2_{\text{min}}$ tends to be $<< 1$, but this just reflects the fact that if few transitions are available it is easier to find a scenario that matches the observations (i.e. the model is underdetermined by the data). In cases where only two transitions were observed, very little constraint is placed upon the values of the free parameters, as can be seen from figures A-1 (b) – A-31 (b), particularly for $T_{\text{kin}}$ and $n$(H$_2$). The molecular cloud RCW 36 (figure A-3 (b)) is a good example. Only two transitions of HC$_3$N were detected and no constraints on $T_{\text{kin}}$ and $n$(H$_2$) can be placed for the values of these parameters investigated by the LVG models, and only an upper limit can be placed on N(HC$_3$N)/(dv/dr). The limits on the axes in each figure show the parameter space that was investigated for each molecular cloud.

Inspection of figures A-1 (b) – A-31 (b) show that N(HC$_3$N)/(dv/dr) is generally well constrained by LVG modeling, while $T_{\text{kin}}$ and $n$(H$_2$) are less well constrained.

5.3.5 Comparison of LTE and LVG models.

Tables A-1(d) to A-31(d) give the transition temperatures obtained from LVG modeling of HC$_3$N emission for the transitions observed in each molecular cloud. These can be compared to the transition temperatures implied by the rotation diagrams (figures A-1(a) to A-31(a)), and therefore provide a check on the LTE rotation diagram analyses.

Table 5.3 summarises the molecular cloud parameters derived from LVG and LTE models of HC$_3$N emission. The second column lists $T_{\text{kin}}$ derived from LVG modelling of HC$_3$N while the third column lists $T_{\text{kin}}$ derived from the $^{12}$CO peak brightness temperature. N(HC$_3$N) and $T_{\text{ex}}$ are derived from LVG modelling and from LTE rotation diagrams. The parameter $T_{\text{ex}}$, derived from LVG modeling, is given for each transition detected in the molecular cloud. The average of $T_{\text{ex}}$ for the 10-9, 11-10 and 12-11 transitions is given in the column headed Mean $T_{\text{ex}}$. The average of the three lower energy transitions has been calculated for comparison to $T_{\text{ex}}$ derived from the rotation diagrams as the higher 15-14 and 16-15 transitions are frequently sub-thermal (i.e. have $T_{\text{ex}}$ significantly lower than the lower energy transitions). The final two columns in table 5-3 give $T_{\text{ex}}$ derived from a LTE rotation diagram analysis and the correlation coefficient ($r^2$) for the linear fit to the rotation diagram respectively.
Table 5-3. A comparison of molecular cloud parameters derived from LVG and LTE models of HC$_3$N emission. $T_{\text{kin}}$ is derived from LVG modelling and from $^{12}$CO; N(HC$_3$N) and $T_{\text{ex}}$ are derived from LVG modelling and from LTE rotation diagrams. $T_{\text{ex}}$ derived from LVG modelling is given for each transition detected in the molecular cloud. The mean $T_{\text{ex}}$ is the average of the 10-9, 11-10 and 12-11 transitions. The correlation coefficient refers to the fit to the rotation diagram.

<table>
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<tr>
<th>Molecular Cloud</th>
<th>$T_{\text{kin}}$ (LVG)</th>
<th>$T_{\text{kin}}$ (CO)</th>
<th>N(HC$_3$N) (LVG)</th>
<th>N(HC$_3$N) (LTE)</th>
<th>$T_{\text{ex}}$(LVG) (10-9)</th>
<th>$T_{\text{ex}}$(LVG) (11-10)</th>
<th>$T_{\text{ex}}$(LVG) (12-11)</th>
<th>$T_{\text{ex}}$(LVG) (15-14)</th>
<th>$T_{\text{ex}}$(LVG) (16-15)</th>
<th>Mean $T_{\text{ex}}$ (10-9, 11-10, 12-11) (LVG)</th>
<th>Mean $T_{\text{ex}}$ (10-9, 11-10, 12-11) (LTE)</th>
<th>$r^2$</th>
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</table>
Figure 5-4. Log of the HC$_3$N column density derived from an LTE rotation diagram analysis plotted with the log of the HC$_3$N column density derived from LVG modelling. The least squares line of best fit is shown.

Figure 5-4 shows the log of the HC$_3$N column density derived from an LTE rotation diagram analysis plotted with the log of the HC$_3$N column density derived from LVG modelling. Figure 5-4 includes data from all molecular clouds in the sample, including those where only two transitions of HC$_3$N were detected/observed. The line of best fit is shown on the graph ($r^2 = 0.7$). The median value of $N$(HC$_3$N)$_{LTE}/N$(HC$_3$N)$_{LVG}$ is 1.3, with 1$^{st}$ quartile of 0.7 and 3$^{rd}$ quartile of 1.9. The interesting conclusion from this comparison is that, for the dense cores of the sample, the two models give values for $N$(HC$_3$N) that agree to within a factor of about two. This suggests that the abundances derived from an LTE rotation diagram analysis for HC$_3$N emission from dense cores can be considered accurate to within a factor of two, despite the wide range of $T_{\text{kin}}$ and $T_{\text{ex}}$ derived from LVG models for each molecular cloud. A likely corollary of this result is that HC$_3$N emission is generally optically thin in dense molecular cores, and this suggestion is supported by the fact that the characteristic rotation diagram curve expected for optically thick emission from linear molecules was seen in only three cases (section 5.3.4).

The correlation between $T_{\text{ex}}$ and $T_{\text{kin}}$ derived from LTE models and those derived from LVG models is not so strong.
The ratio $T_{\text{kin}}(\text{CO})/T_{\text{kin}}(\text{LVG})$ has a median of 0.8, a 1st quartile of 0.5 and a 3rd quartile of 1.5. This suggests that generally the peak brightness temperature of CO underestimates $T_{\text{kin}}$ derived from LVG modelling of the HC$_3$N emission by about 20%. This result is plausible in that the peak CO brightness temperature gives $T_{\text{kin}}$ in the outer regions of a dense molecular cloud (due to its high optical depth), while the HC$_3$N emission, which is likely to be optically thin (see previous paragraph), originates deeper within the cloud. In several cases $T_{\text{kin}}$ from an LVG analysis is far higher than the factor of 1.5 of the 3rd quartile of the data and it may be that in these cases the HC$_3$N emission samples dense gas surrounding protostars. However, it is important to bear in mind that the LVG modelling assumes a homogeneous cloud temperature structure, so the high $T_{\text{kin}}$ from LVG modelling compared to peak brightness temperature of CO may be an artifact of a complex molecular cloud temperature gradient. The significance of a high $T_{\text{kin}}$ derived from LVG modelling in any particular molecular cloud is considered in the context of other observations of the cloud in Chapter 6.

The ratio $T_{\text{ex}}(\text{LTE})/T_{\text{ex}}(\text{LVG})$ has a median of 0.9, a 1st quartile of 0.5 and a 3rd quartile of 1.4. $T_{\text{ex}}(\text{LVG})$ is the average of the 10-9, 11-10 and 12-11 transitions of HC$_3$N. The excitation temperatures derived from the LTE and LVG models generally agree to within a factor of two; however once again several molecular clouds have $T_{\text{ex}}$ derived from LVG models far in excess of a factor of 1.4 of the $T_{\text{ex}}$ derived from LTE models. These molecular clouds are RCW 65, 305.4-0.2, 333.0-0.6, IRAS 16562, NGC 6334(S) and NGC 6334(N1). Of these, for IRAS 16562 and NGC 6334(N1), the discrepancy may be accounted for by high optical depth of the transitions of HC$_3$N (see section 5.3.4). For the remaining molecular clouds, excitation conditions far from LTE must be considered as a likely explanation.

In view of the fact that if kinetic temperature is low only a few lower energy levels of HC$_3$N are populated significantly, it might be better to use the LVG modeling only to ascertain the abundance of HC$_3$N and the H$_2$ spatial density, rather than having 3 free parameters. $T_{\text{kin}}$ can be determined from the $^{12}$CO intensity (with the caveat that a uniform cloud temperature is assumed), in which case, with $T_{\text{kin}}$ specified a much tighter constraint can be placed on H$_2$ spatial density. Alternatively, although the information is not available from the observations presented here, if an independent measurement of n(H$_2$) were available, then the LVG modeling could be used to find $T_{\text{kin}}$.

5.4 Summary

The observations reported in Chapter 4 have been used to calculate kinetic temperature, hydrogen column density and molecular abundances for each position in the sample. The following points should be noted:

1. H$_2$ column densities were calculated from three independently measured quantities (integrated emission of $^{12}$CO, $^{13}$CO and C$^{18}$O) and give values that agree to within a factor of 3 over a total H$_2$ column density range of two orders of magnitude.
2. Abundances were calculated for HC$_3$N, OCS and CH$_3$OH using LTE rotation diagrams. Linear fits (which imply that this method should give a good estimation of the total molecular abundance) were found for about half the HC$_3$N, about two thirds of the OCS and for about one third of the CH$_3$OH diagrams.

3. In addition, abundances for HC$_3$N were calculated using LVG models. For the dense cores of the sample, both LTE rotation diagrams and LVG models generally give results that agree to within a factor of 2, despite the fact that only half the HC$_3$N rotation diagrams were considered well fitted by a straight line.
Chapter 6

Properties of Southern Sky Dense Molecular Clouds

In this chapter, the molecular clouds of the sample are discussed in terms of the observational results reported in Chapter 4 and the physical properties and molecular abundances derived in Chapter 5. In section 6.1 some general information about the molecular clouds of the sample is given, while in section 6.2 comments are made on individual molecular clouds observed in this study. Section 6.3 discusses the overall properties of the sample.

6.1 General Information

6.1.1 Previous Observations

As mentioned already, all the selected molecular clouds associated with HII regions have previously been considered in surveys of the molecules H$_2$CO and HCO$^+$ (Whiteoak & Gardner 1974; Batchelor, McCulloch & Whiteoak 1981; Gardner & Whiteoak 1984) and in continuum and hydrogen recombination-line surveys (Caswell & Haynes 1987b; Whiteoak & Gardner 1974; Goss and Shaver 1972; Wilson et al. 1970). Most clouds have been observed in the 12-GHz transition of methanol (Peng & Whiteoak 1992) and in the 24-GHz transitions of ammonia (Scalise et al. 1981; Peters et al. 1986). In addition, the clouds are within the area of surveys of 1665-MHz OH and 22-GHz H$_2$O maser emission covering the galactic plane from longitude 233° to 2° (through 360°) (Caswell et al. 1974; Caswell & Haynes 1987; Caswell 1998). H$_2$O maser emission is generally associated with shocked gas in outflows, and may occur in expanding disk shells surrounding young massive stars (Genzel & Downes 1977, Reid & Moran 1981). The sources with RCW designations are optical H II regions that were investigated in H-$\alpha$ by Rogers, Campbell & Whiteoak (1960); because they are visible at optical wavelengths, they are relatively close to the Sun (i.e. within about 2 kpc). The previous observations mentioned in this section were obtained with beam sizes that varied by several arcminutes, and so may not be directly comparable with each other and with the observations reported here.

6.1.2 Distances

The adopted distances of the molecular clouds associated with HII regions are from Caswell and Haynes (1987a) unless otherwise stated. Caswell and Haynes (hereafter CH) based their distance calculations on hydrogen recombination-line velocities, using a model for galactic rotation with the Sun located 10 kpc from the galactic centre and rotating about the Galactic Centre with a velocity of 250 km s$^{-1}$. (The adopted distances scale linearly with the assumed distance to the galactic center, so for an assumed galactic center distance of 8.5 kpc, the distances quoted in this thesis should be scaled by 0.85.) For sources located inside the solar circle there may be an
ambiguity in the distance determination, with two distances being possible for an observed velocity. In this case it is necessary to decide on the more likely distance on the basis of other information, such as the presence or otherwise of an optical counterpart, or the velocity of molecular clouds absorbing the HII regions along the line of sight.

The distances to dark clouds are given together with references in the comments on individual sources.

6.1.3 Selected Molecules.

The majority of the molecules observed are expected to be detected in any dense molecular cloud, although the intensities and the ratios of different transitions will vary between individual clouds. These would include molecules such as CO, CS, HCN, HC3N and HCO+ that are already formed in the gas phase of quiescent molecular clouds. Exceptions to this may be the molecules OCS and CH3OH, which form but then remain on dust grains during the quiescent phase. It is only after the gas is heated by nearby star formation and shock processes that these molecules evaporate from the grain surfaces and then become detectable by their rotational transitions. For this reason, the detection of CH3OH and OCS is a good pointer to star formation.

It should be noted that in many of the 12CO spectra presented in Figures B-1 to B-31 show unrelated emission components along the line-of-sight (e.g. Figure B-18(a) for G 333.6-0.2). However these components are ignored unless they are believed to be associated with the molecular cloud.

6.1.4 Molecular Abundances.

Tables 6-1 to 6-3 summarise the relative molecular abundances for the molecular clouds of the sample. Table 6-1 gives the molecular abundances relative to hydrogen in each of the listed molecular clouds; Table 6-2 summarises the statistical properties of the molecular emission for all clouds in the sample; Table 6-3 gives the relative molecular abundance for each molecular cloud normalized to the median abundances given in Table 6-2. i.e. Table 6-3 gives the factor by which the molecular abundances are greater than or less than the median abundance. This table provides a useful summary for comparing abundances both within a molecular cloud and between molecular clouds.

The uncertainties in the molecular abundance determinations are not clear, due to uncertainties in T_ex, optical depth, and the applicability of LTE (see Chapter 5 for discussion). However, as stated in section 5.4, both LTE rotation diagrams and LVG models for HC3N generally give results that agree to within a factor of 2. Given that the entire data set has been treated in a consistent manner it is likely that the comparative abundances within the data set are generally accurate to a factor of 2.

The consistency of the abundances obtained in this study with those obtained in other studies has been examined by comparing the abundances for Orion KL to those
obtained by Blake et al. (1987) towards the same position. Table 6-4 gives the abundances derived for Orion KL, and also abundances derived towards this position by Blake et al. (1987) for the extended ridge and the hot core (see section 6.2 for details of the deconvolution). It should be noted that in this study the emission has not been deconvolved into different velocity components (again see section 6.2), and this should be taken into account when comparing the values in Table 6-4. The fifth column gives the average molecular abundances derived by Blake et al., while the sixth column compares these values with the abundances obtained in this study. Simply taking the average of the emission for the two components listed by Blake et al. does not produce the same result as convolving the spectra for the extended ridge and hot core and then calculating abundances; however it is useful for comparison purposes. Note that Orion KL has been an intensity calibration source for this study. Nevertheless, it is still useful to note the consistency of the abundance calculations even if the intensity measurements are not truly independent (Although our calibration was carried out against SEST observations, whereas Blake et al. obtained spectra at the Caltech Owens Valley Radio Observatory (Sutton et al. 1985)).

Notwithstanding the previous comments, the molecular abundances derived in this study compare well with those of Blake et al. For all molecules other than CS and HCN the values are different by a factor of less than 2. If the CS and HCN values are compared to the values obtained by Blake et al. for the extended ridge, ignoring the hot core, then these values compare quite closely with those obtained in this study, so it is likely that the spectra for these molecules are dominated by extended ridge emission. It is reasonable to conclude from Table 6-4 that the abundance values in this study are accurate to a factor of 2 to 3 for comparison with externally obtained data.

Hence Tables 6-1 to 6-3 are used to compare molecular abundances between different molecules and molecular clouds. It is assumed to be of significance if the abundance variations are greater than a factor of 2 to 3.

The molecular abundance ratios for HCN/HNC and SO/CS are thought to be useful as pointers to recent star formation (see section 1.2.6 and Table 1-2). These ratios are tabulated for each molecular cloud in Table 6-5.

It should be mentioned at this stage that the HCN, HNC and SO column densities were obtained by the measurement of only one transition, assuming both LTE conditions and optically thin emission (see section 5.3 this thesis). The ratio of emission from the $^{12}\text{C}$ to $^{13}\text{C}$ isotopomer of both HCN and HNC is far less than the solar system value of 90:1, or even the ISM average of 45:1 for most molecular clouds (see Table 4-3), so the assumption of optically thin emission is not generally met. No isotopomers of SO were measured, so no information regarding the optical depth of this molecule is available. The HCN and HNC abundance ratios given in Table 6-5 should be considered in light of this. However, given that the optical depths implied by both HCN and HNC compared to their $^{13}\text{C}$ isotopomers are similar, the ratios of the HCN and HNC abundances may well be significant.
Table 6-1 Molecular abundances (relative to H$_2$ column density).

<table>
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<tr>
<th></th>
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<td>n.d.</td>
<td>0.6</td>
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<td>0.1</td>
<td>0.02</td>
<td>n.d.</td>
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<td>n.d.</td>
<td>0.5</td>
<td>0.09</td>
<td>0.8</td>
<td>0.6</td>
<td>0.2</td>
<td>n.d.</td>
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<td>268.4-0.8</td>
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<td>2.9</td>
<td>0.4</td>
<td>4.5</td>
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<td>0.4</td>
<td>0.8</td>
<td>2.0</td>
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<td>0.2</td>
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<td>1.0</td>
<td>n.d.</td>
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<td>2.4</td>
<td>1.4</td>
<td>0.09</td>
<td>1.2</td>
<td>0.7</td>
<td>0.1</td>
<td>n.d.</td>
<td>2.2</td>
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<td>2.7</td>
<td>0.2</td>
<td>0.9</td>
<td>1.4</td>
<td>0.1</td>
<td>0.2</td>
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<td>1.0</td>
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<td>1.0</td>
<td>0.2</td>
<td>n.d.</td>
<td>0.4</td>
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<td>0.2</td>
<td>1.9</td>
<td>1.4</td>
<td>0.10</td>
<td>n.d.</td>
<td>0.2</td>
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<td>0.6</td>
<td>0.2</td>
<td>0.9</td>
<td>0.9</td>
<td>0.2</td>
<td>n.d.</td>
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<td>0.2</td>
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<td>0.7</td>
<td>0.5</td>
<td>0.4</td>
<td>0.5</td>
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<td>n.d.</td>
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<td>0.5</td>
<td>1.3</td>
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<td>2.9</td>
<td>n.d.</td>
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<td>0.4</td>
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<td>5.3</td>
<td>2.9</td>
<td>0.09</td>
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<td>1.4</td>
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<td>8.2</td>
<td>0.6</td>
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<td>5.1</td>
<td>2.0</td>
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<td>9.7</td>
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<tr>
<td>NGC 6334(N)</td>
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<td>5.3</td>
<td>0.1</td>
<td>1.4</td>
<td>0.5</td>
<td>0.3</td>
<td>0.3</td>
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<td>0.3</td>
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<td>348.7-1.0</td>
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<td>0.2</td>
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<td>1.7</td>
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<tr>
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<td>0.2</td>
<td>0.9</td>
<td>1.2</td>
<td>0.7</td>
<td>0.4</td>
<td>1.0</td>
</tr>
<tr>
<td>1.6-0.025(SO)</td>
<td>X</td>
<td>*</td>
<td>2.9</td>
<td>0.8</td>
<td>1.6</td>
<td>1.4</td>
<td>1.4</td>
<td>7.8</td>
<td>1.0</td>
</tr>
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<td>1.6-0.025(155)</td>
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<td>*</td>
<td>3.2</td>
<td>0.6</td>
<td>3.5</td>
<td>0.9</td>
<td>0.4</td>
<td>4.8</td>
<td>0.6</td>
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<tr>
<td>R Cr A</td>
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<td>0.4</td>
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</tr>
<tr>
<td>tOrion KL</td>
<td>X</td>
<td>320</td>
<td>3.1</td>
<td>1.4</td>
<td>8.9</td>
<td>2.3</td>
<td>0.7</td>
<td>12</td>
<td>28</td>
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</tbody>
</table>

Notes: X means not observed; n.d. means not detected in this molecular cloud.
* The abundance of CH$_3$OH in G1.6-0.025 was not calculated due to blending of multiple transitions.
† Calibrator source

Table 6-2 Statistical properties of the relative abundances for the entire sample.

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<td>0.3</td>
<td>3.3</td>
<td>2.1</td>
<td>0.9</td>
<td>2.8</td>
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<tr>
<td>Median</td>
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<td>5.2</td>
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<td>2.0</td>
<td>1.4</td>
<td>0.6</td>
<td>0.4</td>
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<tr>
<td>S.D</td>
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<td>6.2</td>
<td>3.7</td>
<td>0.4</td>
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<tr>
<td>Max</td>
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<td>320</td>
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<td>6.3</td>
<td>2.9</td>
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</table>
Table 6-3 Relative abundances normalized to the median abundance for each molecule.

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<td>n.d.</td>
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<td>1.0</td>
<td>0.2</td>
<td>0.5</td>
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<td>0.1</td>
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<td>n.d.</td>
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<td>n.d.</td>
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<td>4.5</td>
<td>4.4</td>
<td>0.6</td>
<td>1.4</td>
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<td>345.5+0.3</td>
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</tr>
<tr>
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<td>3.8</td>
<td>5.5</td>
<td>3.6</td>
<td>3.2</td>
<td>5.3</td>
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<td>NGC 6334(CO)</td>
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<td>1.0</td>
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<td>0.9</td>
<td>0.7</td>
<td>0.4</td>
<td>0.4</td>
<td>0.7</td>
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<td>4.0</td>
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<td>1.3</td>
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<td>n.d.</td>
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<td>0.9</td>
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<td>0.8</td>
<td>1.0</td>
<td>2.3</td>
<td>18.3</td>
<td>1.0</td>
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<td>1.6-0.025(155)</td>
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<td>2.7</td>
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<td>0.6</td>
<td>11.2</td>
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<td>R Cr A</td>
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<td>9.4</td>
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<td>1.7</td>
<td>2.9</td>
<td>2.6</td>
<td>1.8</td>
<td>1.1</td>
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<td>1.2</td>
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Notes:  
X means not observed;  
n.d. means not detected in this molecular cloud.  
* The abundance of CH$_3$OH in G1.6-0.025 was not calculated due to blending of multiple transitions.  
‡ Calibrator source  
‡‡ C$_2$H was not included in this table, as it was not observed in about 1/3 of the sample.
Table 6-4 Molecular abundances (relative to H2) for Orion KL.

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<th>[N(X)/N(H2)]</th>
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<td></td>
<td>This Study</td>
<td>Extended Ridge (Blake et al. 1987)</td>
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<tr>
<td>CO</td>
<td>1.1E-04(^a)</td>
<td>5.0E-05</td>
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<td>CH(_3)OH</td>
<td>3.2E-07</td>
<td>1.2E-07(^b)</td>
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<tr>
<td>CS</td>
<td>3.1E-09</td>
<td>2.5E-09</td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>1.4E-09</td>
<td>1.3E-10</td>
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<tr>
<td>HCN</td>
<td>8.9E-09</td>
<td>5.0E-09</td>
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<tr>
<td>HCO(^+)</td>
<td>2.3E-09</td>
<td>2.3E-09</td>
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<tr>
<td>HNC</td>
<td>7.3E-10</td>
<td>5.3E-10</td>
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<tr>
<td>OCS</td>
<td>1.2E-08</td>
<td>3.3E-09</td>
</tr>
<tr>
<td>SO</td>
<td>2.8E-08</td>
<td>-</td>
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</tbody>
</table>

\(^a\) Calculated from \(^12\)CO abundance assuming \(^12\)C: \(^13\)C = 60.
\(^b\) Johansson et al. 1984.

Table 6-5 Molecular abundance ratios for HCN/HNC and SO/CS.

<table>
<thead>
<tr>
<th>Molecular Cloud</th>
<th>Abundance Ratio</th>
<th>Molecular Cloud</th>
<th>Abundance Ratio</th>
</tr>
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<td></td>
<td>HCN/HNC</td>
<td>SO/CS</td>
<td>HCN/HNC</td>
</tr>
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<td>HH 46 D.C.</td>
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<td>3.5</td>
<td>333.4-0.4</td>
</tr>
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<td>265.1+1.5</td>
<td>2.7</td>
<td>2.5</td>
<td>333.6-0.2</td>
</tr>
<tr>
<td>266.4-0.8</td>
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<td>0.7</td>
<td>345.5+1.5</td>
</tr>
<tr>
<td>Cham D.C.</td>
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<td>3.6</td>
<td>345.5+0.3</td>
</tr>
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<td>1.6</td>
<td>NGC 6334(S)</td>
</tr>
<tr>
<td>291.3-0.7 (W)</td>
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<td>0.5</td>
<td>NGC 6334(CO)</td>
</tr>
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<td>Coalsack D.C.</td>
<td>0.8</td>
<td>1.4</td>
<td>NGC 6334(N)</td>
</tr>
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<td>8.6</td>
<td>0.1</td>
<td>NGC 6334(N1)</td>
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<td>305.4+0.2</td>
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<td>0.1</td>
<td>348.7-1.0</td>
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<td>311.6+0.3</td>
<td>4.2</td>
<td>1.0</td>
<td>351.6-1.3</td>
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<td>322.2+0.6</td>
<td>3.5</td>
<td>0.2</td>
<td>353.4-0.4</td>
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<td>Lupus D.C.</td>
<td>0.4</td>
<td>1.3</td>
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<tr>
<td>326.7+0.6</td>
<td>2.9</td>
<td>0.2</td>
<td>1.6-0.025(155)</td>
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<td>R Cr A</td>
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<td>M 17</td>
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<td>3.7</td>
<td>0.05</td>
<td>Orion KL</td>
</tr>
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</table>

Median Ratio | 3.7 | 0.3 |
6.2 Comments on Individual Molecular Clouds

The discussions on individual molecular clouds make frequent reference to a number of sections and tables of this thesis. For convenience, these are summarised here.

Chapter 1: Section 1.2.6. and Table 1-2.
Summary of the molecular abundances and abundance ratios expected at different stages of star-formation.

Table 6-1.
Summary of the relative molecular abundances for the molecular clouds of this sample.

Table 6-2.
The average and median relative abundances for all molecular clouds in the sample.

Table 6-3.
Summary of the relative molecular abundances in each molecular cloud divided by the median abundances of Table 6-2.

Table 6-5.
Molecular abundance ratios for HCN/HNC and SO/CS, which can be used as pointers to the presence of star formation.

Appendix A.
Tables A-1 to A-31 contain the results of the observations and the derived physical parameters and abundances. Tables (a) contain the Gaussian parameters of the observed emission, Tables (b) contain derived physical parameters such as $T_{\text{kin}}$ and $N_2$ column density, Tables (c) contain the results of LVG modelling of HC$_3$N, Tables (d) contain the LTE molecular abundances and excitation temperatures and Tables (e) contain the predicted LVG excitation temperatures for each observed transition.

Appendix B.
Figures B-1 to B-31 (a) and (b) contain selected spectra towards the observed positions.

Orion KL

The Orion molecular cloud has been included because it is used for intensity calibration (see Chapter 3) and for comparing these results with those of other studies.

Orion KL is an extremely complex active star forming region and is one of the most extensively studied GMCs in the Galaxy (see e.g Ungerechts et al. 1997; Blake et al. 1987). The position chosen in this study is in the sub-condensation OMC-1, towards
the Kleinmann-Low nebula (Orion-KL). The SiO position in the cloud is observed regularly by the SEST for its intensity calibration. Orion-KL lies behind the Great Nebula in Orion, M 42, about 1' NW of the Trapezium cluster and contains young massive stars with associated outflows. It is close to the Sun, at a distance of around 450 pc, and can be observed with very high spatial resolution. There are three distinct regions in Orion-KL that are not resolved by the Mopra beam but are distinguished by their velocity signatures. Many studies of Orion-KL deconvolve the molecular line spectra into the three components with very different physical and chemical structure (see e.g. Blake et al. 1987): an extended ridge, a plateau associated with outflows, and a hot core.

The line profiles obtained with Mopra are in good agreement with those observed with the SEST, and two components are well defined in many spectra: a broad component with FWHM of around 25 km s\(^{-1}\) and a narrow component with FWHM of around 4 km s\(^{-1}\). These components roughly correspond to the plateau and ridge areas of the source respectively. The spectra of OCS and CH\(_3\)OH have a narrower line width for the broad component (8-15 km s\(^{-1}\)) that could perhaps be consistent with the hot core source. However Blake et al. have ascribed these features to the plateau on the basis of their central velocity of 6-7 km s\(^{-1}\). There are other striking features about the emission from Orion KL, including the strong emission from many molecules and the very wide SO and HCN line profiles.

The derived physical parameters and abundances are presented in Tables A-1(b) to (e). Analyzing the assumed components of ridge and plateau together gives \(T_{\text{kin}} = 69\) K and \(N(\text{H}_2) = 1.5 \times 10^{23}\) cm\(^{-2}\) (Table A-1(b)). The results compare favourably with the values of \(T_{\text{kin}} = 55-60\) K and \(N(\text{H}_2) = 3 \times 10^{23}\) cm\(^{-2}\) for the ridge emission found by Blake et al, providing that the ridge emission dominates the determination of \(T_{\text{kin}}\) using \(^{12}\)CO.

The varying kinetic and excitation temperatures listed in Tables A-1(b) to (e) deserve some comment. The \(T_{\text{kin}}\) of 69 K given in Table A-1(b) is derived from the peak temperature of \(^{12}\)CO. The emission in Table A-1(a) was classified as belonging to a velocity component at either 4 or 25 km s\(^{-1}\) and these separate components were used for the LVG line modelling (Table A-1(c)). LVG modelling suggests a \(T_{\text{kin}}\) of 75 K for the 25 km s\(^{-1}\) emission component and \(T_{\text{kin}}\) of 15 K for the 4 km s\(^{-1}\) component; however, the latter \(T_{\text{kin}}\) is probably too low for any component of Orion KL (c.f. Blake et al. 1987) so the narrow component of the simple deconvolution probably does not have any physical significance. The broader component is probably dominated by the ridge emission, given the agreement between \(T_{\text{kin}}\) from the LVG modelling and \(T_{\text{kin}}\) from CO. In addition, only 2 transitions of HC\(_3\)N were observed, rendering the LVG modelling additionally uncertain (see section 5.3.4).

The abundances for the optically thin LTE models (Table A-1(d)) have been calculated using the integrated emission for the entire spectrum. The abundance calculations are generally in good agreement with those of Blake et al. (see section 6.1.4).

The calculated excitation temperatures are in reasonable agreement with those either calculated or assumed by Blake et al. (1987). \(T_{\text{ex}}\) for CH\(_3\)OH (132 K), calculated from
a rotation diagram in this study, compares well with 146 K in Blake et al. The T_{ex} for CS (20 K) agrees well with the value of 20 K assumed by Blake et al. The T_{ex} calculated from rotation diagrams for OCS (32 K) and HC_3N (19 K) are about a third of the values assumed by Blake et al. (100 K for OCS and 60 K for HC_3N); however the values of Blake et al. are assumed values, not calculated values.

The low values for OCS and HC_3N are surprising, given that many other molecular clouds in this sample have T_{ex} close to T_{kin} for these molecules. The low values of T_{ex} may be an artifact of analyzing the spectrum without deconvolution into velocity components. T_{ex} for HC_3N obtained from the rotation diagram is close to the LVG value of 15 K obtained for the emission component at 4 km s^{-1}. However, with only two transitions of HC_3N observed in Orion KL, no real significance can be assigned to this result.

Menten et al. (1988) have observed the four 97 GHz transitions of CH_3OH with the 30-m telescope of the Instituto de Radioastronomica Millimétrica (IRAM) towards the same position as this transition was observed with Mopra. A source size of 25" (the size of the IRAM beam at 97 GHz) was assumed for the IRAM observations. Figure 6-1 shows the spectra from the two different telescopes and Table 6-6 compares the integrated emission. The emission for Mopra is given as measured with the Mopra beam of 46", and after correction for the larger beam. Menten et al. estimate their calibration uncertainties to be on the order of 20% and those of Mopra are close to 12% for these values of \int T_{MB} dv. Given these constraints, the agreement between the two sets of observations is good, although it is not clear why there is a systematic \approx1.5 km s^{-1} offset in the velocity scale.

<table>
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<th>Transition</th>
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<th>IRAM</th>
</tr>
</thead>
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<td></td>
<td></td>
<td>Mopra</td>
<td>IRAM</td>
</tr>
<tr>
<td></td>
<td>Centre</td>
<td>\int T_{MB} dv (46&quot;)</td>
<td>\int T_{MB} dv (25&quot;)</td>
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<td>K km s^{-1}</td>
<td>K km s^{-1}</td>
<td>km s^{-1}</td>
</tr>
<tr>
<td>2\nu-1, E</td>
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<td>14.7</td>
<td>64.5</td>
</tr>
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<td>2\nu-1, E</td>
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<td>18.24</td>
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</table>
Figure 6-1 Comparison of Mopra and IRAM (Menten et al. 1988) spectra of the 97 GHz transitions of CH$_3$OH. (a) shows the Mopra spectrum, while (b) shows the IRAM spectrum.

**HH 46 Dark Cloud**

The HH 46 Dark Cloud is a Bok globule which is also known as ESO 210-6A. It is quiescent despite being near the Herbig-Haro optical jet HH46/47, a highly collimated bipolar outflow seen at optical wavelengths (Dopita et al. 1982) with an associated molecular outflow (Olberg et al. 1992). The outflow appears to be driven by the heavily obscured infrared source IRAS 08242-5050, which Dopita et al. found to be a very luminous T Tauri star.
The position observed in this study is \( \sim 3 \) arcmin south of IRAS 08242-5050, and \( \sim 2 \) arcmin south of any obvious molecular outflow associated with HH46/47. On this basis, given that there is no evidence for star formation occurring other than that given above, the observed position should contain quiescent gas not yet affected by the star formation process.

The kinetic temperature derived from \(^{12}\text{CO}\) is 17.7 \( \pm \) 2.1 K (Table B-2(b)), similar to that found by Olberg et al. for \(^{12}\text{CO}\) (15 \( \pm \) 1 K) and by Kuiper et al. (1987) for NH\(_3\) (17 \( \pm \) 2 K), for gas towards IRAS 08242-5050.

The spectra in Figures B-1(a) and (b) are consistent with the presence of quiescent gas. There is no evidence for high velocity wings (as seen in spectra towards the molecular outflow) and the profiles are consistently narrow (\( \sim 1 \) km s\(^{-1}\)). No emission is found from either OCS or CH\(_3\)OH, the molecules which should be found in gas warmed by recent star formation. On the other hand, the high molecular abundance ratio of SO/CS and the high ratio of HCN/HNC (see Table 6-5) are more in keeping with those expected from warm gas after the formation of a stellar object (see Chapter 1, Table 1-2 and section 1.2.6). HH 46 was the only molecular cloud of the sample in which HC\(_3\)N was not detected in any transition, although this molecular cloud has a low abundance (compared to the median for all clouds in the sample: Table 6-3) for all molecules other than SO. In fact SO is more abundant than any of the other molecules in Table 6-1, except for C\(_2\)H.

One possible scenario to explain the abundances determined in HH 46 is that a protostar has recently formed within the Bok globule and has begun to warm the surrounding gas, with outflows still being at a very early stage. The low abundances of HNC, HC\(_3\)N and CS are consistent with the presence of molecular depletions in an envelope of infalling gas, although no self-absorption is seen in the HCO\(^+\) profile, and HCO\(^+\) also has a very low abundance c.f. the median abundance for the sample (Table 6-2). HCO\(^+\) is predicted to be depleted to a lesser extent than other molecules in cold infalling gas. The high abundance of HCN and SO may due to contributions from warm dense gas close to the protostar. The spatial extent of any outflow would not be great enough to allow detection of CH\(_3\)OH or OCS with a single dish telescope, due to beam dilution effects. Another possibility is that the observed position is sampling quiescent gas with low abundances of all molecules, although the high abundance of SO is not consistent with this.

Further investigation of HH 46 is required. Higher spatial resolution observations are required to separately investigate any infalling envelope, hot core or nascent outflow, if indeed these features exist. Single dish telescope observations of SO\(_2\) should also be undertaken, as SO\(_2\) forms from SO in warm gas.

There is one more feature of the emission in HH 46 worth noting. The hyperfine transitions of HCN 1-0 have intensity ratios different from the LTE ratios of 5:3:1 for F=2-1; F=1-1; F=0-1 (figure B-1(a)). The ratios in this case are 7.5:3.0:2.5, so it is possible that some non-LTE excitation effects are occurring within the molecular gas. This could account for an apparently high HCN abundance, especially as the lower
energy transitions of linear molecules can act as weak masers under the right conditions (Avery 1980).

\textit{G265.1+1.5 (RCW 36)}

The H\textalpha-emission region RCW 36 is part of a thermal radio continuum source associated with the dense, elongated molecular cloud G265.1+1.5. The complex is located at around 700–900 pc from the solar system (Liseau et al. 1992). This cloud is part of a complex of clouds known as the Vela molecular ridge (Yamaguchi et al. 1999). The molecular cloud shows many signs of active star formation. The position chosen for study is the radio continuum peak. Infrared radiation near this position is associated with dust with a temperature of 44 K and is thought to be heated by one or two deeply embedded O type stars (Verma et al. 1994). The observed position is within 15 arcsec of the bright infrared source IRAS 08576-4334, believed to pinpoint a newly formed massive star (Yamaguchi et al. 1999; Lenz 1991) and H$_2$O maser emission (Braz & Scalise 1982). Another far infrared peak is located 1 arcmin south of the observed position. Both Whiteoak & Gardner (1977) and Verma et al. note that the molecular cloud is clumpy on arcminute scales.

The spectra towards G265.1+1.5 (Figures B-2(a) and (b)) are complex, with high optical depth transitions showing two or three velocity components, whereas transitions with lower optical depth tend to show only one. This is almost certainly due to self-absorption by cooler foreground gas. A possibility that two or three distinct clouds exist but only one is detected in the less abundant molecules can be discounted fairly easily by inspection. Where more than one velocity component is present the peaks are generally found evenly distributed either side of the velocity found for single peaks. The average velocity of the emission for molecules with multiple components ($6.3 \pm 0.5$ km s\(^{-1}\)) is close to the average velocity of the peak emission where only one component is present ($7.0 \pm 0.2$ km s\(^{-1}\)). Thus the velocity of the single components should correspond to the peaks seen in optically thick species if the self-absorption were not present. Self-absorption is seen in transitions of CS, HCN, HNC, $^{12}$CO, $^{13}$CO, C$_2$H and HCO$^+$. Despite the narrow line widths, the hyperfine components of HCN seem to be blended, and are affected by self-absorption, so no comment can be made on the hyperfine intensity ratios. It is also possible that there are two velocity components present in the HCN profile, rather than self-absorption. The $^{12}$CO and $^{13}$CO profiles show some evidence for blue-shifted line-wings, although the significance of these is not clear.

G265.1+1.5 is clearly a complex molecular cloud and is being observed and mapped in detail in observations not associated with this thesis. These further observations show that the self-absorption is widespread in the extended cloud and affects many optically thick molecules. The relationship between the cooler molecular gas and the warmer cores is not yet clear and requires further investigation. It is possible that G265.1+1.5 consists of a number of hot cores deeply embedded in the cool, parent molecular cloud, which is causing the self-absorption. It is also possible however that the absorbing gas may not be associated with G265.1+1.5 and may in fact be cool foreground molecular gas. Observing time on the SEST has been requested to observe
transitions of CN, C$_2$H, C$_2$H$_2$ and N$_2$H$^+$, which are likely to be found primarily in a low-density envelope (van Dishoeck et al. 1995).

The lines of many transitions (e.g. OCS and CH$_3$OH) are surprisingly weak for a cloud with active star formation. As listed in Table 6-3, most molecules have a relative abundance less than half that of the median for the entire sample. The average line width of 2.1 km s$^{-1}$ (Table A-3(b)) is also low, and is closer to the characteristic line widths of dark clouds than to that for GMCs. The ratio of HCN/HNC of 2.7 is within a factor of about three of unity and given the factor of 2 uncertainty assumed in the abundance determinations for comparisons within the sample (section 6.1.4) is probably consistent with quiescent gas (c.f. HCN/HNC ~ 1 for quiescent gas: section 1.2.6). The SO/CS ratio of 2.5 is however significantly greater than the median value for the entire sample of 0.3 (Table 6-5), and this is consistent with warm gas after the onset of star formation.

$T_{\text{kin}}$ derived from both CO (25 K) and the LVG modelling of HC$_3$N (30 K) are in good agreement (Tables A-3(b) and (c)). $T_{\text{ex}}$ for HC$_3$N derived from the rotation diagram (Table A-3(c)) is close to $T_{\text{kin}}$, and is consistent with the $T_{\text{ex}}$ predicted for individual transitions from LVG modelling (Table A-3(e)). As is the case with many other molecular clouds in the sample, the $T_{\text{ex}}$ for the lower energy rotational transitions (10-9, 11-10, 12-11) are similar and close to $T_{\text{kin}}$, whereas those for the higher transitions (15-14, 16-15) are sub-thermal. $T_{\text{ex}}$ for CS (derived in this case from a CS rotation diagram) is decidedly sub-thermal, and this is also a general result for all molecular clouds in the sample.

**G268.4-0.8**

G268.4-0.8 is a dense molecular cloud associated with a radio H II region at a distance of 1.8 kpc (CH). The H II region does not have an optical counterpart (CH), which at this distance suggests that it is behind or embedded in dense molecular gas. No masers have been detected in this molecular cloud.

The results of these observations are in Table A-4(a) and accompanying spectra are shown in figure B-3(a) and (b). Fairly strong emission is found for most molecules (Table 6-3), including CH$_3$OH and OCS, suggesting the presence of recent star formation. Self-absorption is seen in the CO and HCO$^+$ spectra only. Self-absorption in HCO$^+$ has been suggested to arise from infalling gas accreting onto a protostar or YSO (see e.g. Chapter 1; van Langevelde, Dishoeck & Blake 1994), so it may be that there is current star formation in G268.4-0.8, with outflows still being at an early stage. This is supported by the lack of maser activity or significant wings on the spectral-line profiles, although there is some evidence for blue-shifted emission on the HCO$^+$ line profile (consistent with infall) and red-shifted emission on the $^{12}$CO line profile (consistent with outflow). The ratio of HCN/HNC of 10.7 is $>>$ 1, and the SO/CS ratio of 0.7 is higher than the median, consistent with the idea that star formation is occurring.
The hyperfine transitions of HCN 1-0 are clearly separated, and the intensity ratios are close to the LTE ratios of 5:3:1 for F=2-1: F=1-1: F=0-1 (figure B-3(a)), suggesting that LTE conditions apply in the molecular gas, and that HCN has low optical depth. Further support for this supposition is provided by the linearity of the rotation diagrams (figure A-4(b)) and the close agreement between $T_{\text{ex}}$ for HC$_3$N from the rotation diagram (29 K) and the LVG modelling (30 K), and for the predicted values for $T_{\text{ex}}$ for the individual transitions (Table A-4(e)).

**Chameleon Dark Cloud.**

The observed position is a condensation in the Chameleon I dark cloud (Wagner Corradi, Franco & Knude 1998). At a distance of 160 pc (Whittet et al. 1999) Cha I is one of the closest star-forming regions to the Sun. It contains many young stellar objects, as well as detected HH objects and a bipolar outflow (Oasa et al. 1999).

The results are in Table A-5(a), with representative spectra in figures B-4(a) and (b). The $^{12}$CO 1-0 transition is self-absorbed. Transitions of both OCS (weak) and CH$_3$OH (strong) are detected in this molecular cloud, and the $^{12}$CO, $^{13}$CO and HC$^+$ spectra show evidence of high velocity wings suggestive of outflows. These features are consistent with a region that is actively forming stars.

The line-widths are narrow (0.7 km s$^{-1}$), consistent with a dark cloud, despite the presence of star formation. The hyperfine transitions of HCN 1-0 have intensity ratios different from the LTE ratios (figure B-4(a)). The ratios in this case are 4.6:3.0:2.9, in contrast to the ratios expected for LTE of 5:3:1. Non-LTE excitation must be considered as a possible cause. High optical depth effects are unlikely; if this were the cause for the non-LTE ratios it would seem reasonable that the strongest component would be the most affected. $T_{\text{kin}}$ from CO (14 K) and from LVG modelling of HC$_3$N (15 K) is in good agreement, as are the predicted $T_{\text{ex}}$ for the individual transitions. However, $T_{\text{ex}}$ from the rotation diagram is far higher (27 K vs ~13 K from LVG) and it may be that despite the apparently linear fit the transitions of HC$_3$N are optically thick.

The HCN/HNC and SO/CS ratios are both high, consistent with what is expected in warm gas after the onset of star formation.

**G291.3-0.7 (RCW 57)**

G291.3-0.7 is associated with the bright H$\alpha$ region RCW 57 (also known as NGC 3576). It is a located at a distance of 3.6 kpc (CH). It contains several embedded infrared sources at least one of which is thought to be a protostar (Ghosh et al. 1989), and maser emission from H$_2$O and CH$_3$OH (Knowles & Bachelor 1978; Caswell et al. 1995), suggesting that an outflow is present. A compact H II region is detected within 2 arcmin of the observed positions (Walsh et al. 1997). Two positions have been observed in this molecular cloud, labeled (E) and (W). G291.3-0.7(W) is at the peak of the $^{13}$CO emission and is about 15 arcsec southwest of the discrete infrared source RCW57/IRS 3 (Frogel & Persson 1974), in a region of heavy optical
obscuration. G291.3-0.7(E) is about 2 arcmin east and 1 arcmin north of the $^{13}$CO peak and was observed for comparison purposes.

The line profiles towards G291.3-0.7(E) are particularly complex, with triple peaked profiles in CS and HNC. The original reason for selecting this position was the appearance of the line profiles, and the possibility that these may be due to outflows or other complex dynamics. However, the generally lower abundances of most molecules compared to the (W) position and the non-detection of OCS would seem to rule out this possibility. Instead, self-absorption is seen in SO at a similar velocity to the middle emission peak in CS and HNC, suggesting that there may be overlying gas with a lower $T_{\text{ex}}$ for SO and a higher $T_{\text{ex}}$ for CS and HNC. This seems unlikely, and mapping would be needed to clarify the situation.

The spectra towards G291.3-0.7(W) are not as obviously complex, however the CO and $^{13}$CO profiles do show some evidence for self-absorption, while the HCN, CO and $^{13}$CO profiles have red shifted line-wings. Weak OCS was detected towards (W) but not towards (E). Both positions have average or below average molecular abundances compared to the median (Table 6-3), but have similar abundances to each other. LVG modelling suggests that $T_{\text{kin}}$ is similar at both positions, although the HC$_3$N abundance towards (E) is less than half that towards (W). The $T_{\text{ex}}$ for the individual transitions towards (E) are consistent with $T_{\text{ex}}$ for the rotation diagram, however for (W) the rotation diagram gives a much lower temperature, so it is possible that it is affected by high optical depth in the transitions of HC$_3$N, consistent with the higher HC$_3$N abundance towards this position. Despite the discrepancy in $T_{\text{ex}}$, the rotation diagram and the LVG modelling give the same value for the HC$_3$N abundance.

The HCN/HCN abundances are high towards both positions, consistent with the presence of warm gas, although this is not reflected by the SO/CS ratio which is close to the median for (W) and higher for (E).

The presence of CH$_3$OH and OCS emission as well as H$_2$O maser emission and evidence for outflow in the line profiles suggest that current star formation is occurring in this molecular cloud.

**Coalsack Dark Cloud**

The Coalsack is a dense dark cloud located at a distance of around 180 pc from the solar system (Franco 1989). Corradi, Franco & Knude (1998) have suggested that the Coalsack and Chameleon dark clouds may be condensations embedded in the same extended interstellar structure. The Coalsack appears to be in a quiescent phase, without an embedded stellar population (Nyman, Bronfman & Thaddeus 1991). Despite this, there are some signs of star formation present in these observations, including red shifted line wings in CO, HCO$^+$, CS and HCN, and the detection of CH$_3$OH and OCS emission. The lines are generally narrow (average 1 km s$^{-1}$) and characteristic of a dark cloud despite the star formation. Only the 10-9 transition of HC$_3$N was detected so LVG modelling was not undertaken.
Table 6-3 shows that the abundances in the Coalsack are generally low compared to the median, with the exception of CH$_3$OH and OCS. It is possible that the Coalsack consists mostly of cold, dense depleted gas, consistent with a core that has recently collapsed to form a protostar, with some evaporation of grain mantles having taken place close to the protostar, hence the presence of OCS and CH$_3$OH. The HCN/HNC ratio is close to 1, consistent with quiescent gas, although the SO/CS ratio of 1.4 is significantly above the median of 0.3.

$G301.0+1.2$ (RCW 65)

The molecular cloud $G301.0+1.2$ is associated with the H$_e$ region RCW 65 and is located at a distance of approximately 5.1 kpc from the Sun (CH). OH and CH$_3$OH maser emission is detected towards this position (Caswell et al. 1995; Caswell 1998). It is close to an ultracompact H II region (Walsh et al. 1997) suggesting that a massive star has recently formed. Ultracompact H II regions are small, ionized bubbles around or near to embedded massive O or B stars.

Table 6-3 shows that the molecular abundances are generally within a factor of 2 of the median abundances for the entire sample. The HCN/HNC ratio is $> 1$, although the SO/CS ratio is low compared to the median. The $T_{\text{kin}}$ from CO is 34 K, although the $T_{\text{kin}}$ from HC$_3$N is considerably higher at 100 K, which may be evidence for a hot molecular core associated with the ultracompact H II region. Both the individual $T_{\text{ex}}$ from the LVG modelling and the shape of the rotation diagram suggest that the HC$_3$N emission is not in LTE, explaining the large discrepancy between $T_{\text{ex}}$ from the rotation diagram and that from LVG modelling. CH$_3$OH emission has been detected, but not OCS. The rotation diagram for CH$_3$OH also suggests the presence of non-LTE excitation, with the higher energy 5(-1)-4(0)E transition lying far above the line of best fit (see section 5.3.3). This is the only transition of CH$_3$OH detected in this molecular cloud for which there is a change of k-ladder. It is likely in the presence of non-LTE excitation that transitions involving a change of k-ladder will have a different $T_{\text{ex}}$ to those that do not (see e.g. Menten et al. 1986). The 2-1 transition of CH$_3$OH is surprisingly weak, for reasons that are not clear.

The status of on-going star-formation in this molecular cloud is not clear, and it may be that the CH$_3$OH is present as a result of recent star-formation. The molecular abundances in this cloud may be in the hot core phase, after outflows from the star formation have ceased. The lack of the H$_2$O maser emission or any signature of outflow on line profiles is consistent with this, although it is not possible to draw any conclusions without further observations.

Further observations of complex molecules expected to form in the gas-phase of a hot core such as SO$_2$ and HCOOCH$_3$ may help to clarify the situation, although OCS is also expected to form in a hot core, and it is very weak in this molecular cloud.
G305.4+0.2

G305.4+0.2 is a molecular cloud and associated HII region without an optical counterpart. The distance of the complex is ambiguous, with possible locations being 3.2 or 8.3 kpc from the solar system. CH favour the latter distance on the basis of HI absorption measurements, and this is supported by the results of 6-cm H2CO absorption towards this position (Whiteoak, private communication). The cloud shows many signs of active star formation including OH and CH3OH maser emission, which has been detected at positions within 5 arcmin of the observed position (Walsh et al. 1997, Moorwood & Salinari 1981). H2O maser emission is also present (Knowles & Bachelor 1978).

The results of Table 4.1(e) show two main components at velocities of -34 and -38 km s\(^{-1}\). These components are present in most spectra, including the species expected to be optically thin such as H\(^{13}\)CO\(^+\), and so are not likely to be due to self-absorption. The similarity of the velocities to 6.7-GHz CH3OH maser emission (detected at velocities of -34, -36 and -39 km s\(^{-1}\)) adds further weight to the presence of two components. Several spectra (e.g. CO, HNC, HC3N) show evidence of high velocity wings suggestive of an outflow, consistent with the idea that active star formation is occurring in this cloud. The presence of H2O maser emission supports the idea that outflow is present, as does the detection of CH3OH and OCS (although the OCS emission is weak).

As mentioned previously the LVG modelling was undertaken for a variety of assumed source sizes for molecular clouds where good agreement between the rotation diagram results and those of the LVG models were not obtained. In general no improvement to the agreement was obtained. However, G305.4+0.2 is one of the few molecular clouds where an apparent improvement in agreement between the rotation diagram T\(_{\text{ex}}\) and the individual T\(_{\text{ex}}\) from LVG modelling was obtained by assuming a small diameter. The results for the LVG modelling assuming both an extended cloud and a cloud diameter of 60 arcsec are presented in Tables A-10 (c) and (e). Although the two models give different results, the HC3N abundances are similar, and despite the better agreement between T\(_{\text{kin}}\) and T\(_{\text{ex}}\) for the smaller assumed diameter, the individual T\(_{\text{ex}}\) obtained assuming an extended cloud are qualitatively consistent with the shape of the rotation diagram (e.g. the 10-9 and 11-10 transitions have a higher T\(_{\text{ex}}\) on the rotation diagram). The rotation diagram for CH3OH is also consistent with the presence of non-LTE excitation. The presence of emission peaks at two velocities may be due to there being two dense star-forming cores superimposed on the line of sight through the molecular cloud, which may also explain the apparently non-LTE excitation, but further observations are needed to clarify the situation.

Table 6-3 shows that the molecular abundances are generally within a factor of 2 of the median for the entire sample, although the abundance of HNC and SO are only 0.2 of the median. The HCN/HNC ratio of 14.6 is the largest in the sample, however the SO/CS ratio is below the median at 0.1. The HCN/HNC abundance ratio is calculated from the abundances of the \(^{13}\)C isotopomers. That calculated from the 12C isotopomers (believed to be optically thick) is also high at ~8.
This molecular cloud contains an H II region (without optical counterpart) located at a distance of 6.6 kpc (CH). No maser emission has been detected towards this position, although it is associated with an ultracompact H II region (velocity \(-58 \text{ km s}^{-1}\)) (Walsh et al. 1997) suggesting that a massive star has recently formed. Previous H$_2$CO absorption measurements (Whiteoak & Gardner 1974) along the line of sight show velocity components at two velocities: \(-54\) and \(-49 \text{ km s}^{-1}\), close to the velocities of the two components seen in many spectra of Figures B-10(a) and (b) at \(-56\) and \(-49 \text{ km s}^{-1}\). The spectra with only one velocity component (HC$_3$N, CS) are centred on the \(-56 \text{ km s}^{-1}\) component (close to the velocity of the ultracompact H II region), as are the 3-1 and 5-4 transitions of CH$_3$OH. However, the 2-1 transitions of CH$_3$OH appear to be centred on the \(-49 \text{ km s}^{-1}\) component. It is not clear why this difference in velocity occurs, and whether there are contributions from both velocity components in the transitions of CH$_3$OH. It seems likely that the profiles are the result of two real velocity components rather than self-absorption, although, in addition, the $^{12}$CO line profile is self-absorbed, as is probably the CS emission, which shows 3 velocity components on the line profiles. Only 1 (weak) transition of OCS was detected in this molecular cloud.

The $T_{\text{kin}}$ from CO is very low for a star-forming core at 10.7 K, although this result is almost certainly affected by self-absorption. Added evidence for this comes from the LVG modelling of HC$_3$N, which gives $T_{\text{kin}}$ of 20 K and 35 K for an assumed cloud size that is extended and 60 arcsec respectively. In this case, the smaller cloud size does seem to give a result in good agreement with the results from the HC$_3$N rotation diagram.

Table 6-3 shows that in general, the abundances in G311.6+0.3 are lower than the median abundances for the entire sample. Given that this molecular cloud seems to be of small angular extent, the apparently low molecular abundances may be due to beam dilution effects, which may also be causing an erroneously low $T_{\text{kin}}$ from $^{12}$CO. The HCN/HNC ratio is greater than unity, as expected for warm gas, and the SO/CS ratio of 1 is larger than the median. There is no clear evidence for line-wings, except in the $^{13}$CO spectrum, which seems to have a red-shifted line wing.

The status of on-going star-formation in this molecular cloud is not clear, and it may be that the CH$_3$OH is present as a result of previous star-formation, as evidenced by the presence of the ultracompact H II region, that has however passed the outflow stage. The molecular abundances in this cloud may be in the process of returning from a hot-core chemistry to a quiescent chemistry, a process that is generally complete after about $10^4$ years (section 1.2.6; Table 1-2; Charnley et al. 1992; Caselli et al. 1993). The lack of maser emission also suggests that current star formation is not occurring.

Further observations of complex molecules expected to form in the gas-phase of a hot core such as SO$_2$ and HCOOCH$_3$ may help to clarify the situation, although OCS is also expected to form in a hot core, and it is very weak in this molecular cloud.
**G322.2+0.6 (RCW 92)**

The G322.2+0.6 molecular cloud contains the optical H\(_\alpha\) region RCW 92. Formaldehyde absorption measurements (Whiteoak & Gardner 1974) show velocity components at \(-54.1\) km s\(^{-1}\) and \(-40.2\) km s\(^{-1}\). The distance to RCW 92 is believed to be 3.6 kpc (CH). OH maser emission is detected towards this position (Caswell & Haynes 1987c).

The spectra (Figure B-11(a) and (b)) of CO, CS, HCN, HNC and HC\(_3\)N have blueshifted line wings that may be consistent with either infall or outflow. However, infall is perhaps not so likely as HCO\(^+\) does not show either line wings or self-absorption, as would be expected if this were the case (see Table 1-2; section 1.2.6). On the other hand, the H\(_2\)O maser emission consistent with an outflow is also not detected. Both OCS and CH\(_3\)OH are detected in this molecular cloud, suggesting the presence of recent star-formation. Both the peak temperature of CO and the LVG modelling of HC\(_3\)N suggest the presence of warm gas, although T\(_{\text{kin}}\) from HC\(_3\)N is higher (50 K) than that from CO (33 K). It may be that HC\(_3\)N is tracing warmer gas than CO. The T\(_{\text{ex}}\) from the rotation diagram is low (19 K) and may be affected by optical depth effects or non-LTE excitation. It is not clear which of these effects is the cause, as the LVG modelling suggests that the three lower-energy HC\(_3\)N transitions should be close to thermalised at a T\(_{\text{ex}}\) of about 45 K, with the 15-14 transition having about half this T\(_{\text{ex}}\). This is not really consistent with the shape of the rotation diagram curve.

Table 6-3 shows that the molecular abundances are consistent with the median values for the entire sample. The HCN/HNC ratio is greater than 1, consistent with warm gas, while the SO/CS ratio is close to the median for the entire sample at 0.2. The presence of the line wings and the OCS suggests that there has been recent star formation in this molecular cloud.

**Lupus Dark Cloud**

The Lupus molecular cloud is a nearby active low-mass star-forming region, which is at a distance of around 140 pc and possibly part of Gould's belt (Rizzo, Morras & Arnal 1998). The position observed here is in the sub-cloud Lupus 1 and is within 1 arcmin of the infrared source IRAS 15398-3359. High-velocity wings have been observed in \(^{13}\)CO towards IRAS 15398-3359, suggesting that it may be a recently formed protostar (Tachihara et al. 1996).

The average line width in Lupus is 0.7 km s\(^{-1}\) (Table A-13-(b)), consistent with emission from a cold, dark cloud. The spectra of figures B-12(a) and (b) show some evidence for blue-shifted line-wings in profiles of CO, although not in HCO\(^+\). There is however self-absorption seen in HNC, and given the lack of self-absorption in other line profiles this may be a signature of infall, which is more usually seen in HCO\(^+\) (section 1.2.6). Lupus has a particularly high relative density of HNC (Table 6-3) (a factor of 4.7 times the median for the entire sample) and this molecule probably has a high optical depth. Self-absorption is predicted to be a signature of infall in molecules with high optical depth (see section 1.2). Most other molecules have low or average abundances relative to the median, except for HC\(_3\)N (a factor of 3.3 times the
median), which is sometimes found to have a high abundance in quiescent dark clouds
(see section 1.2). No CH$_3$OH or OCS have been detected, so if star-formation is
occurring it is at an early stage. T$_{\text{kin}}$ and T$_{\text{ex}}$ from CO and HC$_3$N (both LVG and LTE
rotation diagram) all agree well, suggesting that LTE conditions apply within the gas.
The hyperfine components of HCN are not in the expected LTE ratios, being close to
equality rather than 5:3:1 for F=2-1: F=1-1: F=0-1 (figure B-12(a)), as expected for
high optical depth, with the strongest F=2-1 component being most strongly absorbed.

On the balance it seems likely that star-formation is occurring near this position in
Lupus, but at an early stage.

\textbf{G326.7+0.6}

The molecular cloud G326.7+0.6 contains a radio HII region and is associated with
the optical nebula RCW 95 (CH). It is at a distance of 3.1 kpc (CH). Maser emission
of CH$_3$OH (Schutte et al. 1993), OH (Caswell 1998) and H$_2$O (Kauffmann et al. 1977)
is present towards this position, as well as an ultracompact H II region (Walsh et al.
1997), suggesting that star formation is on-going.

The CO spectra show emission at around $-21$ km s$^{-1}$ in addition to the main emission
at $-40$ km s$^{-1}$. H$_2$CO absorption measurements towards this position also show
emission at $-21$ km s$^{-1}$, but it is not seen in other spectra presented here and is
believed to be an independent foreground cloud. The average line width is broad at 6
km s$^{-1}$, and consequently the hyperfine transitions of HCN are blended (Figure B-
13(a)), as are the CH$_3$OH (2-1) transitions (figure B-13(b)). The $^{13}$CO spectrum shows
evidence for both blue and red-shifted line wings, while HCO$^+$ and HNC have red-
shifted line wings. Interestingly, blue-shifted but not red-shifted line-wings are found
in both transitions of CS and in HC$_3$N (10-9). As HNC and HCO$^+$ are likely to be
more abundant in quiescent gas, the red-shifted emission may represent bulk motion
in the quiescent gas, although it is not consistent with infall (section 1.2.3). Outflows
and/or streaming motions seem to be present in this molecular cloud. The non-
detection of OCS is surprising given the H$_2$O maser emission and line-profile
evidence for outflows.

Both the LVG modelling and the HC$_3$N rotation diagram suggest that the HC$_3$N is
sub-thermally excited, giving T$_{\text{ex}}$ of 11.3 K from the rotation diagram, and consistent
values of T$_{\text{ex}}$ for the individual transitions from the LVG modelling. The T$_{\text{kin}}$ on the
other hand is higher, at 26 K from CO and 40 K from LVG modelling of HC$_3$N. The
molecular abundances in Table 6-3 are within a factor of 2 of the median for all
clouds in the sample.

The physical state and kinematics of this molecular cloud are obviously complex, and
it may be that there are several cloud components at slightly different velocities, with
different physical conditions. Observations of complex molecules expected to form in
the gas-phase of a hot core, such as SO$_2$ and HCOOCH$_3$, as well as mapping of
molecules that trace quiescent gas and/or low-density envelopes such as C$_2$H$_2$, C$_2$H,
N$_2$H$^+$ and HCO$^+$, may help to clarify the situation.
The molecular cloud G327.3-0.5 contains a radio HII region (CH). It has an ambiguous distance determination with the nearer distance of 3.4 kpc being favoured by CH on the basis of HI absorption measurements. Both OH and H$_2$O maser emission are detected towards this position (Caswell 1998; Caswell et al. 1974). This molecular cloud has been observed by Bergman (1992) who found that it consists of 2 dense cores separated by 60 arcsec. One core is warm ($T_{\text{kin}} \sim 30$ K) whereas the other is warm ($T_{\text{kin}} \sim 150$ K).

The average line is broad (5 km s$^{-1}$) and the hyperfine transitions of HCN are blended. There is evidence for blue-shifted line-wings in the line profiles of HC$_3$N, HNC and CS, but the HCO$^+$ profile shows no evidence for infall in quiescent gas. The presence of H$_2$O maser emission is consistent with the line-wings being due to outflow. The HCN/HNC ratio is larger than the median, while SO/CS is less. CH$_3$OH and OCS emission are present, but the abundances of these molecules are a factor of only 0.2 and 0.5 times the median for the entire sample.

The $T_{\text{kin}}$ derived from CO and LVG modelling are close (41 and 45 K respectively), and the HC$_3$N rotation diagram $T_{\text{ex}}$, and the individual transition $T_{\text{ex}}$ are consistent with each other and with $T_{\text{kin}}$. It is likely that the bulk of the molecular gas towards this position is similar to the cooler gas found by Bergman (1992).

The presence of line-wings and H$_2$O maser emission suggests that current star formation is occurring in this molecular cloud. This molecular cloud is a good candidate for investigation at high resolution with the Compact Array of the Australia Telescope (ATCA) at millimetre-wavelengths.

The molecular cloud G331.5-0.1 is associated with a radio HII region without optical counterpart. It has an ambiguous distance determination with the nearer distance of 6.5 kpc being favoured by CH on the basis of HI absorption measurements.

The position observed in these observations is located within one arcmin of an OH/H$_2$O maser complex (Knowles, Caswell & Goss 1976; Knowles & Batchelor 1978) and a young infrared protostar (Moorwood & Salinari 1981). H$_2$O maser emission is found over the velocity range 80 – 100 km s$^{-1}$, with the maser at –95.9 km s$^{-1}$ undergoing a significant outburst during the years 1981 and 1982 (Sestokas Filho & Scalise Jr. 1991). An ultracompact H II region is present (Walsh et al. 1997).

The CO profiles (Figure B-15(a)) show emission over the range of velocities –105 to –45 km s$^{-1}$. (Emission in the ranges –70 to –45 km s$^{-1}$ is seen only in CO, and is therefore assumed to be in the line-of-sight and not associated with G331.5-0.1). Emission between –105 and –80 km s$^{-1}$ is present as 2 components at –101 and –89 km s$^{-1}$, with the –89 km s$^{-1}$ component being present in all detected molecules. The –101 km s$^{-1}$ component is prominent in CO, HCO$^+$ and HNC only, suggesting that this is quiescent gas. No evidence for outflows is seen in the line profiles, and only weak CH$_3$OH and
OCS emission are present. This is surprising given the presence of OH and H$_2$O maser emission.

Table 6-3 shows that G331.5-0.1 is under-abundant in all molecules relative to the median abundances for the entire sample. The HNC/HCN abundance ratio is $\approx 1$, and SO was not detected in this molecular cloud. Only 2 transitions of HC$_3$N and 1 transition of OCS were detected, and the abundances seem more consistent with quiescent or depleted gas than gas in a region actively forming stars. The low $T_{\text{kin}}$ from LVG modelling and $T_{\text{ex}}$ from the HC$_3$N rotation diagram may arise because only 2 transitions of HC$_3$N were detected, and these temperature anomalies are probably not significant.

This molecular cloud has surprisingly low molecular abundances given the signs of active and current star formation such as H$_2$O masers and ultracompact H II regions.

G333.0-0.6

The molecular cloud G333.0-0.6 is associated with a radio H II region with a possible optical counterpart and most likely located at a distance of 3.8 kpc (CH). OH and CH$_3$OH maser emission are present near to this position (Caswell 1998; Caswell et al. 1995). An ultracompact H II region is also present (Walsh et al. 1997).

Blue-shifted line wings are seen in almost all the spectra of Figures B-16(a) and (b), the main exception being CH$_3$OH. The interpretation of this is not clear. It is possible that the presence of blue-shifted emission rather than red-shifted emission is tracing infall (section 1.2.3), and CH$_3$OH does not show obvious line wings because it is present only in the warm, dense gas nearest to the protostar or YSO. The lack of red shifted line-wings, H$_2$O maser emission and the weak OCS emission is perhaps consistent with a relatively young protostar or YSO, where outflow has not yet had a chance to impact on the surrounding molecular cloud. Table 6-3 shows that most molecules are within a factor of 2 of the median abundances in the entire sample, and CH$_3$OH and OCS emission are a factor of 0.5 and 0.7 of the median. The HCN/HNC abundance ratio is 3.7, consistent with warm gas where grain surface evaporation has commenced, although the SO/CS abundance ratio is low (0.05), which would be consistent with quiescent gas or the early stages of star formation.

The results of LVG modelling of HC$_3$N, and the HC$_3$N and CH$_3$OH rotation diagrams suggest that this molecular cloud does not have LTE excitation. The LVG $T_{\text{kin}}$ (200 K) and $T_{\text{ex}}$ suggest that the HC$_3$N may be tracing very warm gas, while $T_{\text{kin}}$ from CO is only 32 K (Table A-17(b)), suggesting that the outer regions of the cloud are considerably cooler. The decidedly non-linear rotation diagrams may arise because of the presence of a strong temperature gradient across the molecular cloud, which in turn may make the LVG modelling unreliable.

It is possible that this molecular cloud is undergoing collapse and that a YSO is in the process of forming at the observed position, with outflow still at too early a stage to
affect the surrounding gas. However, only one position in this molecular cloud has been investigated, so without further investigation the above comments are very speculative. Observations at higher resolution with the ATCA at millimeter-wavelengths are needed to investigate the plausibility of this scenario.

\textit{G333.4-0.4}

The molecular cloud G333.4-0.4 is associated with a radio H II region without optical counterpart (CH). It has an ambiguous distance determination and may be located at 3.8 or 14.0 kpc (CH). No maser emission is detected towards this position.

The spectra (Figures B-17(a) and (b)) show both red and blue-shifted line wings in CO. The red-shifted emission is not present in the line profiles of other molecules, however, blue-shifted line wings are seen in HNC and HCO\(^+\), with HCO\(^+\) also seeming to be self-absorbed. This is consistent with the presence of quiescent infalling gas, although another possibility is that there is dense quiescent gas at a slightly lower velocity than the main emission, which is seen in HCO\(^+\) and HNC (the molecules expected to be abundant in quiescent gas) and the ubiquitous CO. The average line-widths are broad (6 km s\(^{-1}\)) so the hyperfine components of HCN and the CH\(_3\)OH (2-1) transitions are blended.

\(T_{\text{kin}}\) from CO is 34 K, however \(T_{\text{kin}}\) from both LVG modelling of HC\(_3\)N and \(T_{\text{ex}}\) from the HC\(_3\)N rotation diagram is considerably lower (12 – 15 K). As only 2 transitions of HC\(_3\)N were observed in this source these results may be unreliable, although the CH\(_3\)OH and OCS rotation diagrams also suggests a low \(T_{\text{ex}}\) (7 K and 9 K respectively). It is possible that the bulk of the emission traces cool gas where many molecules are sub-thermally excited, although sub-thermal excitation is usually found in lower-density gas (see section 5.3.3) and the results of LVG modelling (\(n(\text{H}_2) \sim 10^{10} \text{m}^3\)) and the linearity of the rotation diagrams suggest that the cool gas is dense.

Interestingly, the abundances listed in Table 6-3 are almost all a factor of 0.5 below the median for the entire sample, and it may be that G333.4-0.4 is a molecular cloud in the process of collapsing, with most of the gas in the telescope beam being cool, dense, depleted gas. The blue-shifted wings in the line profiles of HNC and HCO\(^+\) and the self-absorption of HCO\(^+\) are certainly consistent with this idea. The lack of maser emission is certainly consistent with star formation being in an early stage. Although CH\(_3\)OH and OCS emission are present, these are relatively weak, and may arise from a small area of denser, warmer gas close to the protostar. The HCN/HNC abundance ratio is > 1, more consistent with warm, post-star formation gas, although the SO/CS ratio is low (0.1), as expected if star formation is not very advanced.

The observations presented here are consistent with G333.4-0.4 being a molecular cloud in the process of collapsing to form a protostar, however observations at higher resolution are needed to investigate this scenario further.
G333.6-0.2

The molecular cloud G333.6-0.2 is associated with a radio H II region without optical counterpart (CH). It has an ambiguous distance determination with the nearer distance of 3.5 kpc being favoured by CH on the basis of H I absorption measurements. G333.6-0.2 is a bright infrared source (Becklin et al. 1973) and is thought to be located on the front surface of a dense molecular cloud (Hyland et al. 1980). This scenario is supported by Fujiyoshi et al. (1998), who conclude that a cluster of O and B stars have recently formed in this molecular cloud. The detection of vibrationally excited molecular hydrogen (Storey 1983) and high rotational transitions of CO suggest the presence of hot shocked gas, at a temperature of between 200 and 800 K (Storey et al. 1989). Both OH and H2O maser emission have been detected towards this position. (Caswell 1998; Caswell 1974).

The CO spectra (Figure B-18(a)) show emission at a wide range of velocities, although only the main components appear on the spectra of other molecules (Figures B-18(a) and (b)), and only these main components are considered to be part of G333.6-0.2. Both blue-shifted and red-shifted line wings are seen in the CO, 13CO and HNC line profiles. Blue-shifted line wings are seen in the line profiles of HCO+ and HNC, while red-shifted line emission is seen in CS, HNC and HC3N.

One possible interpretation is that infall and outflow are occurring simultaneously in this molecular cloud, with accretion continuing, with a YSO or YSOs having recently formed. If a cluster of O and B stars is forming or has recently formed (Fujiyoshi et al. 1998), then the differing stages of stellar evolution within the cluster (and within the telescope beam) may explain the simultaneous signatures of both outflow and infall. The presence of H2O maser emission supports the presence of an outflow, although the lack of CH3OH and OCS emission is then surprising. Presumably this is because the YSOs have not yet had time to warm up a large area of the surrounding gas. On the other hand G333.4-0.4, which seems to be in an even earlier stage, does have detected CH3OH and OCS emission. The explanation for this discrepancy is not clear, but beam dilution effects (i.e. if G333.6-0.2 is more compact than G333.4-0.4) or different cloud chemistries leading to lower abundances of CH3OH and OCS in G333.6-0.2 are possible explanations.

The possibility that emission from G333.6-0.2 arises primarily from an area of small angular extent (with respect to the telescope beam) is strengthened by the results of LVG modelling. LVG modelling for HC3N assuming an extended source size yielded T_{kin} of 30 K, close to T_{kin} of 23 K from CO, but the individual T_{ex} for the transitions of HC3N and the H2 density suggest that all transitions should be thermalised, and therefore the rotation diagram for HC3N should give a good linear fit. Figure A-19(b) clearly shows that this is not the case, and the best correspondence between the individual T_{ex} and the results of the rotation diagram are found if an angular extent of 60 arcsec is assumed.

If a source size of 60 arcsec is assumed, T_{kin} from HC3N (95 K) is considerable higher than T_{kin} from CO (23 K), but this is consistent with the presence of strong IR emission and vibrationally excited H2 emission. The assumption is that there is a temperature gradient across the cloud, with T_{kin} from CO representing T_{kin} in the outer
areas of the molecular cloud, and $T_{\text{kin}}$ from LVG modelling representing $T_{\text{kin}}$ in the interior.

It is plausible that G333.6-0.2 is a molecular cloud with early YSOs, with both infall and outfall occurring simultaneously. Accretion is still occurring, as evidenced by blue-shifted line wings in HNC and HCO$^+$, while the signature of outflow is seen in red-shifted emission in line profiles of HNC, CS and HC$_3$N. The $T_{\text{kin}}$ of 95 K from LVG modelling of HC$_3$N is supportive of the presence of YSOs, while $T_{\text{kin}}$ from CO of 23 K suggests that the external regions of the molecular cloud contain quiescent gas, consistent with the recent formation of the YSOs.

Observations at higher resolution are needed to investigate the presence of several high-mass YSOs and their relative evolutionary states.

$G345.5+1.5$ (IRAS 16562-3959)

The molecular cloud surrounding the IRAS point source 16562-3959 was added to this sample of molecular clouds due to the strong emission lines found in many molecular transitions. No radio continuum emission (as expected from an H II region) is found towards this position, suggesting that if a star has formed it is of lower mass than an O or early B type star. In addition, no maser emission is detected.

The average line width of 4 km s$^{-1}$ is consistent with a GMC rather than a dark cloud, despite the lack of H II emission. There is some evidence for line wings in CO and HCO$^+$, and both OCS and CH$_3$OH are detected, so either recent or current star formation is likely. The molecular emission traced by HC$_3$N is warm, with $T_{\text{ex}}$ of 105 K from LVG modelling. This is very different to $T_{\text{ex}}$ from the rotation diagram (18 K), however the $T_{\text{ex}}$ for the individual transitions suggests that the gas is not in LTE. Also, the shape of the HC$_3$N rotation diagram suggests that it may be affected by high optical depth (see section 5.3.3), in which case CH$_3$OH and OCS may be similarly affected. The scatter of the points about the line of best fit in the CH$_3$OH rotation diagram is consistent with high optical depth, although non-LTE excitation may also be the cause (see section 5.3.3). A higher $T_{\text{ex}}$ than that calculated from the rotation diagram is likely for CH$_3$OH as the higher energy 2$_{1-1}$ E transition (at 28 cm$^{-1}$ above the ground state) is detected in this molecular cloud (c.f. 7-20 cm$^{-1}$ for the other CH$_3$OH(2-1) transitions).

Table 6-3 shows that the molecular abundances for most molecules are significantly above the median values for the entire sample, except for OCS. In fact, the molecular abundances in this molecular cloud are comparable with those in Orion KL, apart from the very much higher abundances of CH$_3$OH and OCS found in Orion KL. The lack of maser activity, obvious line wings and the relatively weak OCS would be consistent with a source in the earlier stages of star formation, before outflow has made a large impact on the abundances in the quiescent gas, but after the evaporation of icy grain mantles. Both the HCN/HNC and SO/CS abundance ratios (3.7 and 0.1 respectively) are consistent with this scenario.
This molecular cloud is a good candidate for searching for complex molecular species, and such observations would also help to pin down the exact state of star-formation.

G345.5+0.3

The molecular cloud G345.5+0.3 is associated with a radio HII region without optical counterpart. It has an ambiguous distance determination with the distance being either 2.5 or 16.9 kpc (CH). Maser emission from OH, CH$_3$OH and H$_2$O has been detected towards this position (Caswell 1998; Caswell et al. 1995; Caswell, Vaile & Forster 1995; Forster & Caswell 1989), as well as an ultracompact H II region (Walsh et al. 1997).

The spectra of CO, CS and HCO$^+$ (Figures B-20(a) and (b)) show some evidence for red-shifted line wings, and both CH$_3$OH and OCS are detected, suggesting that star formation is on-going in this molecular cloud. Somewhat surprisingly, the C$^{18}$O profile appears to be self-absorbed, but self-absorption is not seen on other line profiles. A comparison of the two velocity peaks in the C$^{18}$O line profile with the peak emission for other molecules suggests that the red-shifted peak is in fact a line-wing, probably tracing outflow.

The rotation diagrams (Figure A-21(b)) are all non-linear, suggesting that non-LTE excitation is present. Despite this, the molecular abundance from LVG modelling of HC$_3$N is in agreement with that of the rotation diagram. The kinetic temperature from LVG modelling is 50 K, higher than the CO temperature of 23 K, however the HC$_3$N may be tracing warm dense gas. It should also be noted that the lower limit to the LVG $T_{\text{kin}}$ is 25 K, which is consistent with that from CO. The abundance ratio of HCN/HNC is $> 1$, while the SO/CS ratio is low at 0.2.

Active star formation is occurring in this molecular cloud. The strong red-shifted line wing in the C$^{18}$O profile probably represents outflow, although mapping of the emission from this molecule would be needed to confirm this.

NGC 6334

NGC 6334 is a prominent H II region/molecular cloud complex with an angular extent on the sky of about 45 arcmin (Dickel, Dickel & Wilson 1977). It is at a distance of 1.7 kpc (Neckel 1978). There are many signs of active star formation in this molecular cloud, including masers, outflows and infrared sources. Four positions were observed in this complex, with positions as listed in Table 4-1. In each case, the position is towards a $^{13}$CO peak.
NGC 6334(S)

This position is located around 2 arcmin south of the Far-IR continuum concentration NGC 6334-V (McBreen et al. 1979) and is in the direction of a 1.6-GHz continuum peak (Brooks & Whiteoak 2001). Maser emission of CH$_3$OH (Caswell 1995), OH (Caswell 1998) and H$_2$O (Forster & Caswell 1989) is present within the antenna beam of these observations, as well as an ultracompact H II region (Walsh et al. 1997).

The spectra of Figures B-21(a) and (b) reveal both red and blue-shifted line wings in CO and HCO$^+$, with the blue-shifted emission being stronger. Blue-shifted line wings are seen in the line profiles of CS, HC$_3$N, HNC and SO. This could be consistent with the presence of infall, although the presence of strong OCS and CH$_3$OH and maser emission are more consistent with a YSO having already formed (as suggested by the presence of an ultracompact H II region), so the blue-shifted emission could be due to outflow directed towards the observer.

Table 6-3 shows that the molecular abundances are significantly above the median values for the entire sample, including both CH$_3$OH and OCS. The HCN/HNC abundance is high (5.5), consistent with star formation having already taken place, although the SO/CS ratio is close to the median (0.4).

LVG modelling of HC$_3$N emission suggests a $T_{\text{kin}}$ of 90 K, higher than the $T_{\text{kin}}$ from CO of 29 K, or $T_{\text{ex}}$ from HC$_3$N of 28 K. The individual $T_{\text{ex}}$ from the LVG modelling are consistent with what is seen on the rotation diagram, although the diagram itself is well fitted by a straight line, and $T_{\text{ex}}$ from the diagram is close to $T_{\text{kin}}$. In this case the apparently linear fit to the rotation diagram is probably spurious, and the abundance derived from the rotation diagram is a factor of 2 greater than that from the LVG modelling. The rotation diagrams from CH$_3$OH and OCS are also consistent with non-LTE excitation. The CH$_3$OH rotation diagram gives a low excitation temperature that is likely to be spurious, in view of the detection of the high energy CH$_3$OH 2$_1$-1$_1$ E transition towards this position.

NGC 6334(S) seems to be a hot core where star formation is on-going, as suggested by the ultracompact H II region and maser emission. It has high molecular abundances should be a good choice for the investigation of complex hot core chemistry and searching for complex species.

NGC 6334(CO)

This position is at the peak for CO emission. OH maser emission is detected within the beam of the observations (Caswell 1998).

The spectra of Figures B-22(a) and (b) show blue-shifted line-wings in CO and HCO$^+$ that may be consistent with the presence of infall, or may represent outflow towards the line of sight.
The molecular abundances of Table 6-3 are generally within a factor of 2 of the median for the entire sample. The HCN/HNC abundance ratio is > 1, however the SO/CS ratio is low, more characteristic of quiescent gas. CH$_3$OH and OCS are both detected towards this position, suggesting that star formation has occurred.

LVG modelling of HC$_3$N towards this position gives a surprisingly low $T_{\text{kin}}$ (15 K), which seems unlikely given that $T_{\text{kin}}$ from CO and $T_{\text{ex}}$ from the HC$_3$N rotation diagram are significantly higher (43 K and 37 K respectively). However, only 3 transitions of HC$_3$N were observed in this molecular cloud, and plausible values for $T_{\text{kin}}$ (i.e. where $\chi^2 > 3.5$) include all $T_{\text{kin}} > 15$ K. The $T_{\text{ex}}$ for CH$_3$OH of 9 K from the rotation diagram also seems too low, and is surprising given the good linear fit, although the higher-energy CH$_3$OH 2$_1$-1$_1$ E transition was not detected, suggesting a low $T_{\text{ex}}$.

The status of star formation towards this position is not clear. The lack of continuum emission and H$_2$O maser emission together with the presence of blue-shifted line wings may be consistent with the presence of a very young YSO, where infall is still occurring and outflow has not had sufficient time to impact significantly on the surrounding molecular gas. The low SO/CS abundance ratio is consistent with this scenario. However, further observations, including mapping of the molecules showing blue-shifted line wings, are needed to clarify the situation. High-resolution observations with the ATCA at millimeter wavelengths have the potential to find infall if it is occurring.

**NGC 6334(N)**

This position is located around 30 arcsec south-east of a 1.6-GHz continuum peak (Brooks & Whiteoak 2001). Maser emission of CH$_3$OH (Caswell 1995), OH (Caswell 1998) and H$_2$O (Forster & Caswell 1989) is present within the beam, as well as an ultracompact H II region (Walsh et al. 1997).

The spectra of Figure B-23(a) and (b) show a variety of features, including red-shifted line wings in CO, CS, HCO$^+$, SO and HNC. The spectra of $^{13}$CO, C$^{18}$O and HC$_3$N appear to be self-absorbed, but in fact the more negative velocity peak is at the same velocity as for other molecules. This suggests that the more positive velocity peak seen in $^{13}$CO, C$^{18}$O and HC$_3$N is in fact associated with the red-shifted line emission, and probably traces outflow. The prominence of this red-shifted peak in HC$_3$N should be noted, suggesting that HC$_3$N is enhanced in the gas from which the emission arises. Both the HC$_3$N LVG modelling and the HC$_3$N rotation diagram give a surprisingly low $T_{\text{ex}}$ and $T_{\text{kin}}$, however they are consistent with one another (20 K and 18 K respectively), and may be due to the unusual HC$_3$N profile. The HC$_3$N rotation diagram may show some evidence for high optical depth (see section 5.3.3), however the molecular abundances from the rotation diagram and the LVG modelling are close. It is possible that HC$_3$N is tracing a cool dense condensation along the line of sight, although the reasons for the line profiles and the low $T_{\text{ex}}$ clearly need further investigation. The low value of $T_{\text{ex}}$ from the CH$_3$OH rotation diagram seems spurious given that the higher-energy CH$_3$OH 2$_1$-1$_1$ E transition is detected towards this
position. The OCS emission seems to be tracing warm gas \((T_{\text{ex}} = 30 \text{ K})\), consistent with \(T_{\text{kin}}\) from CO of 41 K.

The molecular abundances towards NGC 6334(N) (Table 6-3) are generally significantly lower than the median for the entire sample, and this may be consistent with the presence of a cool, dense condensation along the line of sight. The HCN/HNC abundance ratio is >1, although the SO/CS ratio is low (0.1), arguing for the presence of cool gas unaffected by star formation.

NGC 6334(N) would be a good candidate for investigation with the ATCA at millimeter wavelengths, as it is possible that there are at least 2 very different condensations along the line of sight: One that is actively forming stars, giving rise to the maser emission and other signs of star formation, and one that is composed of cool, dense depleted gas, perhaps in the process of collapsing to form a protostar. The apparently enhanced red-shifter HC$_3$N emission should also be investigated.

**NGC 6334(N1)**

This position is located around 2 arcmin north of a 1.6-GHz continuum peak (Brooks & Whiteoak 2001), and is about 1 arcmin north east of NGC 6334(N). There is no maser emission detected coincident with this position.

The CO and CS spectra (Figures B-24(a) and (b)) show evidence of self-absorption, while the line profiles of HC$_3$N C$^{18}$O and HCO$^+$ may show evidence for blue-shifted line wings. This may be evidence for infall, although the strong CH$_3$OH and OCS emission detected towards this position would seem to argue against this.

The detection of the higher-energy CH$_3$OH $2_1$-$1_1$ E transition suggests the presence of a hot core. LVG modelling of HC$_3$N supports this, giving \(T_{\text{kin}}\) of 65 K. The individual \(T_{\text{ex}}\) are not consistent with the appearance of the HC$_3$N rotation diagram, although the rotation curve appears to be affected by optical depth effects (see section 5.3.3), and the rotation diagram gives an HC$_3$N abundance a factor of 2 greater than LVG modelling. \(T_{\text{kin}}\) from CO is 35 K, although this will indicate \(T_{\text{kin}}\) in the outer regions of the molecular gas. The CH$_3$OH rotation diagram gives a low \(T_{\text{ex}}\) of 12 K, and this seems unlikely given the detection of the CH$_3$OH $2_1$-$1_1$ E transition. OCS gives \(T_{\text{ex}}\) that seems consistent with \(T_{\text{kin}}\) from CO, although the three rotation diagrams show the effects of either non-LTE excitation or optical depth effects, with the OCS diagram being the closest to a good linear fit.

Table 6-3 shows that the molecular abundances are significantly higher than the median for the entire sample, although not to the same extent as NGC 6334(S). The HCN/HNC abundance ratio is >1, although the SO/CS ratio is low at 0.1.

It seems likely that current star formation is occurring at this position, although it may perhaps be in an early stage, as evidenced by the lack of maser emission and prominent line wings. However, a hot core seems to be present (suggested by the presence of the CH$_3$OH $2_1$-$1_1$ E transition) and the high \(T_{\text{kin}}\) from HC$_3$N modelling,
and this position would be worth investigating with high resolution and in the emission of complex molecules.

**NGC 6334 (General Comments)**

The molecular abundances towards the 4 observed positions show a variety of features, and are likely to be in different stages of star formation. There is the potential to investigate these regions at high resolution and in complex molecules usually found in hot cores, to estimate an age for each position since the onset of star formation. One puzzling aspect of the positions is that they all have abundance ratios of SO/CS less than the median for the entire sample, despite the different $T_{\text{kin}}$ and physical conditions. This low ratio may be a general feature of NGC 6334, due to initial elemental abundances in the molecular cloud, or it may be that all four positions are in the earlier rather than the later stages of star formation. These 4 cores could be used to investigate the CS:SO:SO$_2$ abundance ratios and the abundances of complex molecules formed in warm neutral gas to test chemical evolution theories (see Section 1.2.6 and Table 1-2).

**G348.7-1.0 (RCW 122)**

The molecular cloud associated with the H-α region RCW 122 is an active star-forming region located at a distance of 2.1 kpc (CH). The observed position in the current observations is within an arcminute of the far infrared point source IRAS 17167-3854, for which a dust temperature of 60 K is estimated from far-infrared measurements (Ghosh et al. 1989). Maser emission from OH, CH$_3$OH and H$_2$O has been detected towards this position (Caswell 1998; Caswell et al. 1995; Forster & Caswell 1989), as well as an ultracompact H II region (Walsh et al. 1997).

The spectra of CO, HCO$^+$ and HC$_3$N show some evidence for blue-shifted line wings, while the line profile of HNC may have both blue and red-shifted wings. The different central velocity for the CS (3-2) emission is spurious, due to an incorrect observing parameter and should be ignored.

The HC$_3$N rotation diagram has a shape that is consistent with high optical depth, and this may account for the difference between the rotation diagram $T_{\text{ex}}$ and that from LVG modelling, although the $T_{\text{kin}}$ from LVG modelling seems too low at 15 K (c.f. 38 K from CO). Despite the discrepancy in $T_{\text{kin}}$ and $T_{\text{ex}}$, the rotation diagram and the LVG modelling give similar estimates of the HC$_3$N abundance.

The molecular abundances are generally higher than the median for the entire sample (Table 6-3), and the presence of CH$_3$OH, OCS and maser emission is consistent with current star formation. However, although the HCN/HNC abundance ratio is $> 1$, the SO/CS ratio is low (0.1).

The observations are consistent with the presence of on-going star formation in this molecular cloud.
G351.6-1.3

G351.6-1.3 is a radio HII region that is not associated with an optical counterpart (CH). It has an ambiguous distance determination and may be located at 2.7 or 17.1 kpc. The high galactic latitude suggests the nearer distance, as at the far distance this source would be well below the Galactic plane. The H II region has a small diameter with a FWHP diameter of 6 arcsec at a frequency of 3-cm (Broderick & Brown 1974), and is coincident with a strong 10 μm compact infrared source (Frogel & Persson 1974). However, no maser emission or ultracompact H II regions have been detected towards this position.

Self-absorption is seen in the spectra of $^{13}$CO and C$^{18}$O, although as in the case of NGC 6334(N) the velocities of the peaks suggest that the second component is due to enhanced emission in the line wings. Blue-shifted line wings are prominent in CO, CS, HNC, SO and possibly present in HCO$^+$. No OCS and only weak CH$_3$OH emission are detected in this molecular cloud. It is possible that G351.6-1.3 is in an early stage of star formation, with infall being dominant.

The $T_{\text{kin}}$ from LVG modelling of HC$_3$N and from CO are in fairly good agreement at 40 K and 31 K respectively. However, the individual $T_{\text{ex}}$ and the $T_{\text{ex}}$ from the rotation diagram for HC$_3$N do not agree very well, and the abundances from both methods differ by a factor of more than 2.

The abundances in this molecular cloud are significantly less than the median for the entire sample, and this may be consistent with depleted gas in an early stage of star formation. The HCN/HNC abundance ratio is $> 1$, while the SO/CS ratio is a factor of 8 greater than the median. This appears to contradict other findings, being more consistent with star formation already having taken place.

G353.4-0.4

G353.4-0.4 is a radio HII region that is not associated with an optical counterpart (CH). It has an ambiguous distance determination and may be located at 3.8 or 16.0 kpc. Maser emission from OH and CH$_3$OH has been detected towards this position (Caswell 1998; Caswell, Vaile & Forster 1995; Norris et al. 1987), but not from H$_2$O. An ultracompact H II region is also present towards this position (Walsh et al. 1997).

The spectra of CO, HCO$^+$, CS, and HNC are self-absorbed towards this position. Both red and blue-shifted line wings are seen in the line profiles of CO and $^{13}$CO, while a red-shifted line wing is present in SO. The peak velocity of the self-absorption is close to the peak velocity for molecules that show only single peaks such as HC$_3$N, confirming that the “dips” are due to self-absorption.

The $T_{\text{kin}}$ from CO (25 K) is higher than from LVG modelling of HC$_3$N (15 K), although the values obtained for $T_{\text{ex}}$ from both LVG modelling and the rotation diagram are in good agreement. It may be that the HC$_3$N emission contains a strong component arising in the cool dense envelope or overlying gas that is causing the self-absorption, but further observations, including mapping of transitions (such as CN,
C$_2$H, C$_3$H$_2$ and N$_2$H$^+$) that are likely to be found primarily in a low-density envelope, would be required to investigate this possibility.

Table 6-3 shows that the molecular abundances in G353.4-0.4 are close to the median for the entire sample. CH$_3$OH and OCS are present, consistent with this being an active star-forming region. The HCN/HNC abundance ratio is close to 1, although the SO/CS ratio is higher at 1.9 than the median for the entire sample.

Current star formation is likely to be occurring in this molecular cloud. The structure and kinematics seem to be complex and investigation of the self-absorption and the HC$_3$N emission at high resolution should be undertaken.

**G1.6-0.025**

G1.6-0.025 is a warm, dense and apparently quiescent Galactic Centre cloud that shows evidence for a very complex kinematic structure and chemistry. Lacking in H II or infra-red regions, the cloud was first detected as a prominent 5-GHz H$_2$CO absorption feature (Whiteoak & Gardner 1979). NH$_3$ observations by Gardner et al. (1985) revealed a clumpy cloud with an average LSR velocity of about 50 km s$^{-1}$ and a kinetic temperature exceeding 50 K. In addition, a high-velocity component at 160 km s$^{-1}$ has been detected towards one of the clumps (Gardner & Boes 1987). Type I CH$_3$OH maser emission has been detected (Haschick & Baan 1993), but no OH or H$_2$O masers have been found. CH$_3$OH emission in this molecular cloud gives rise to a 12-GHz 2$_0$-3$_1$E transition in absorption, representing the best example of rare population 'anti-inversion' for this transition (Whiteoak & Peng 1989; Peng & Whiteoak 1993). Type I CH$_3$OH masers arise in high-velocity outflows and cloud-cloud collisions (Menten 1997), unlike Type II CH$_3$OH masers which are more directly associated with YSOs. Sobolev (1996) has suggested that a collision has occurred between the main cloud and another cloudlet with a relative velocity of 100 km s$^{-1}$, resulting in high kinetic temperatures and shock waves that create the CH$_3$OH masers.

Emission at near both 50 km s$^{-1}$ and 155 km s$^{-1}$ is detected in all molecules (Tables A-29(a) and (f)).

**G1.6-0.025 (Emission near 50 km s$^{-1}$)**

Emission at this velocity is strongly self-absorbed in most transitions (Table A-29(a), Figures B-29). The presence of only one peak on the profiles of emission thought to be optically thin (C$^{13}$S, HN$^{13}$C, H$^{15}$CO$^+$) confirms that the double peaked profiles are due to self-absorption. Emission from CH$_3$OH, SiO and OCS is detected, although given the lack of other signatures of star-formation (H II regions, infrared emission, OH, H$_2$O or Type II CH$_3$OH masers) it may be that these molecules (in particular SiO which traces shocked gas) are present due to shocked gas from a cloud-cloud collision rather than from current star formation. Strong SiO emission is found in both the (2-1) and (3-2) transitions. The OCS abundance ratio is particularly high at a factor of 18.3
higher than the median for all clouds in the sample, second only to Orion KL, which has an OCS abundance ratio compared to the median of factor 30.4.

The CH$_3$OH abundance has not been calculated in this molecular cloud due to the presence of both self-absorption and blending of the hyperfine components in CH$_3$OH line profiles; no sensible deconvolution could be effected. However, the CH$_3$OH emission is bright, and CH$_3$OH is certainly abundant, as shown by the presence of the 3$_1$-4$_0$ A$^+$ transition in absorption. The presence of this transition in absorption is consistent with Type I maser activity (Cragg et al. 1992), which in addition to other conditions requires a high abundance of CH$_3$OH. G1.6-0.025 is the only molecular cloud in the entire sample to have this transition in absorption, and this finding is consistent with the presence of the 12-GHz 2$_0$-3$_1$E transition of CH$_3$OH in absorption (Whiteoak & Peng 1989; Peng & Whiteoak 1993).

Apart from OCS (and possibly CH$_3$OH), the molecular abundances (Table 6-3) are close to the median values for all molecular clouds in the sample (in contrast to those for Orion KL). This may be another indication that the high OCS, CH$_3$OH and SiO abundances result from shocked emission in a cloud-cloud collision rather than from outflows and hot cores associated with recent star formation.

Despite the self-absorption present in the profiles abundances and kinetic temperatures have been calculated; however, it is important to note that the parameters derived are likely to be inaccurate. The HC$_3$N abundance in G1.6-0.025 seems particularly high, with the LTE value a factor of 3.6 times the median value for the entire sample (Table 6-3). The results of LVG modelling give a value more than an order of magnitude larger again. Although this transition is affected by self-absorption, with the results of both LVG and LTE abundance calculations being unreliable, the calculated values are likely to be a minimum in the presence of self-absorption, so it would seem that the HC$_3$N abundance is genuinely very high. The $T_{\text{kin}}$ from CO is 20 K, while the LVG modelling of HC$_3$N gives $T_{\text{kin}}$ of 45 K, close to the value of $>50$ K derived from NH$_3$ (Gardner et al. 1985). The good correspondence between $T_{\text{kin}}$ from HC$_3$N modelling and $T_{\text{kin}}$ from NH$_3$ suggest that perhaps the LVG value for the abundance of HC$_3$N may be accurate; the $T_{\text{ex}}$ for the individual transitions (Table A-29(e)) are consistent with the appearance and $T_{\text{ex}}$ from the rotation diagram. The lower $T_{\text{kin}}$ from CO suggests that there is a temperature gradient across the molecular cloud, and this in part may explain the self-absorption.

**G1.6-0.025 (Emission near 155 km s$^{-1}$)**

The emission near 155 km s$^{-1}$ has many similarities with that at 50 km s$^{-1}$, including the presence of the CH$_3$OH 3$_1$-4$_0$ A$^+$ transition in absorption, implying the presence of Type I maser emission, and strong SiO emission in both the (2-1) and (3-2) transitions. On the other hand, the emission at this velocity is not self-absorbed, except for HCN and HCO$^+$. Emission from SiO, CH$_3$OH and OCS is detected, in keeping with the presence of shocked gas, possibly resulting from a cloud-cloud collision.
Once again, the individual $T_{ex}$ obtained from LVG modelling are consistent with the shape and $T_{ex}$ obtained from the rotation diagram, however the abundance from the rotation diagram is more than an order of magnitude lower than that obtained from LVG modelling. High optical depth (not obvious on the shape of the rotation diagram) is a possible explanation, due the large abundance of HC$_3$N. The $T_{kin}$ from CO is consistent with that from LVG modelling of HC$_3$N (16 K and 20 K respectively).

As Table 6-3 shows, the molecular abundances for emission at this velocity are close to the median values for the entire sample, with the exception of OCS, HC$_3$N and probably CH$_3$OH.

**G1.6-0.025 (General Comments)**

There are several features of G1.6-0.025 worthy of further investigation. It is likely that this molecular cloud is composed of 2 clouds at different velocities undergoing a cloud-cloud collision. Both the CH$_3$OH $3_{1-4_0}$ A+ transition in absorption and strong SiO emission in both the (2-1) and (3-2) transitions are supportive of this scenario. There are no obvious signs of current of previous star formation, however the compression caused by the cloud-cloud collision will almost certainly lead to the onset of star formation, as is thought to have occurred in Sgr B2 (Hunt et al. 1999). G1.6-0.025 should be investigated at high resolution (e.g. with the ATCA at millimetre-wavelengths) as it provides an excellent opportunity to investigate the onset of the star-formation process resulting from a cloud-cloud collision in a Galactic Centre GMC.

Another feature of G1.6-0.025 worthy of investigation is the apparently high abundance of HC$_3$N discovered by LVG modelling. It appears that this molecular cloud has until very recently been quiescent, and it may be that the chemistry has developed along the lines of that of the cyanopolyene peak in TMC-1 (although the 2 clouds have very different masses and temperatures). The abundances of other cyanopolyenes (HC$_{n+1}$N) should be investigated as they may provide important results for use in theoretical chemistry models of quiescent molecular clouds.

**Corona Australis Dark Cloud**

The Corona Australis dark cloud complex is a highly elongated system of dark clouds, located at a distance of around 130 pc from the solar system (Marraco & Rydgren 1981). Rossano (1978) identified five condensations in the complex using stellar extinction measurements, which he labelled A to E. The condensations A and B together form what is generally known as the R Cr A dark cloud, named for the pre-main-sequence variable emission-line star R Cr A. R Cr A is a young active star forming region containing 24 YSOs located between condensations A and B (Wilking et al. 1992). The position of these observations is on the south-eastern edge of condensation B. No maser emission is detected towards the position observed here.

The spectra of Figures B-30(a) and (b) are narrow, as is typical of dark clouds (average width 0.5 km s$^{-1}$). There is no evidence for outflows on the line profiles
towards this position, nor is any OCS detected; however CH$_3$OH emission is detected, suggesting that the gas has been warmed due to nearby star formation. The line profile of HNC is self-absorbed, and this could be due to infalling gas. The ratio of HCN/HNC abundance is low, at 0.7, so it may be that HNC is particularly abundant and hence optically thick in this cloud. The HC$_3$N abundance ratio is a factor of 9.4 higher compared to the median for all clouds in the sample (Table 6-3), which may indicate dark cloud chemistry similar to that present at the cyanopolyene peak in TMC-1. The HCO$^+$ abundance is also high (a factor of 4.2 higher than the median), another indication of a predominantly quiescent, dark cloud chemistry.

$T_{\text{kin}}$ from LVG modelling of HC$_3$N is 30 K, compared to 15 K from CO, suggesting that a warm core is present. The individual $T_{\text{ex}}$ for the 2 detected transitions of HC$_3$N are consistent with the $T_{\text{ex}}$ from the rotation diagram.

It is likely that star formation is occurring at this position, perhaps still in the early stages, as suggested by the possible presence of infall in the line profile of HNC, and the lack of outflows and maser emission. Given the high relative abundance of HC$_3$N, the abundances of other cyanopolyenes (HC$_{n+1}$N) should be investigated towards this position.

**6.17**

This source was included only for the purposes of calibrating Mopra and the number of transitions available was limited. In particular, the 2-mm SEST transitions are missing and the energy range covered by the rotation diagrams is small in the case of HC$_3$N and OCS. The linear fit to the OCS rotation diagram is poor and the excitation temperature is an upper limit. The CH$_3$OH fit is fairly good as the 97-GHz transitions observed give good energy coverage.

**6.3. General Properties of Molecular Clouds in this Sample.**

As previously stated, the southern molecular clouds in this sample were chosen because of their strong emission in a variety of molecules. Consequently, the general properties found for this sample will be representative of the densest cores within molecular clouds.

The molecules CS, HCN, HCO$^+$ and HNC were detected in all the dense cores of the sample. The molecules C$_2$H, HC$_3$N and SO were each detected in all but one of the dense cores, although it was a different dense core for each molecule. These molecules are all formed in the gas phase, and should be found in dense cores (see Table 1-2; Section 1.2.6).

Table 6-7 summarises the discussion of section 6.2, giving a summary of some indicators of star formation and physical state in the molecular clouds of the sample.
Table 6-7  Summary of some indicators of star formation and physical state in the molecular clouds of the sample.

<table>
<thead>
<tr>
<th>Molecular Cloud</th>
<th>Self-absorption</th>
<th>Masers</th>
<th>Ultras-Compact H II Region</th>
<th>Detected Emission</th>
<th>Line Wings</th>
<th>Abundance Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>OH or CH$_3$OH</td>
<td>H$_2$O</td>
<td>CH$_3$OH (any)</td>
<td>CH$_3$OH (2$^1$S)</td>
<td>Blue</td>
<td>Red</td>
</tr>
<tr>
<td>HH 46 D.C.</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>265.1+1.5</td>
<td>Y</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Y</td>
<td>-</td>
</tr>
<tr>
<td>268.4-0.8</td>
<td>Y</td>
<td>-</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Cham D.C.</td>
<td>Y</td>
<td>-</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>291.3-0.7 (W)</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
</tr>
<tr>
<td>Coal Sack D.C.</td>
<td>-</td>
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<td>-</td>
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<td>-</td>
<td>Y</td>
</tr>
<tr>
<td>301.1+0.2</td>
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<td>Y</td>
<td>-</td>
<td>Y</td>
<td>-</td>
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<tr>
<td>305.4+0.2</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>311.6+0.3</td>
<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
</tr>
<tr>
<td>322.2+0.6</td>
<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Lupus D.C.</td>
<td>Y</td>
<td>-</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
</tr>
<tr>
<td>326.7+0.6</td>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
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</tr>
<tr>
<td>327.3-0.5</td>
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<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
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<tr>
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<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
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</tr>
<tr>
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<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>333.6-0.2</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
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<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>345.5+0.3</td>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>NGC 6334(CO)</td>
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<td>Y</td>
<td>-</td>
<td>Y</td>
<td>Y</td>
<td>-</td>
</tr>
<tr>
<td>NGC 6334(N)</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>NGC 6334(N1)</td>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
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<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
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<td>Y</td>
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<td>Y</td>
<td>Y</td>
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<td>1.6-0.025(50)</td>
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<tr>
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<td>Y</td>
<td>Y</td>
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</tr>
<tr>
<td>R Cr A</td>
<td>Y</td>
<td>-</td>
<td>-</td>
<td>Y</td>
<td>-</td>
<td>Y</td>
</tr>
</tbody>
</table>

Notes.
- Presence of line-wings and individual transitions difficult to determine due to wide, complex and self-absorbed line profiles.
- Y Emission detected.
- - Emission not detected.

6.3.1 CH$_3$OH Emission

CH$_3$OH was detected in all but 4 of the 31 positions sampled. As CH$_3$OH is thought to be formed on grain surfaces and returned to the gas phase by evaporation after heating by nearby star formation (see Section 1.2) this suggests that star formation is occurring or has recently occurred in most of the dense cores. Radio H II regions have previously been detected in all the GMCs of this sample, so it known that star
formation has occurred in these clouds. However, the detection of CH$_3$OH suggests that star formation has occurred within the last $10^5$ years or so, as after this time molecular abundances are thought to reset to quiescent cloud values (Charnley et al. 1992; Caselli et al. 1993).

CH$_3$OH is present in 2 of the 4 dark clouds in the sample. The median CH$_3$OH abundance for the entire sample (Table 6-2) is comparable with most other molecules observed.

It is perhaps not surprising that the densest cores in the southern hemisphere should almost all show signs of recent star formation (i.e. within the last $10^5$ years), although a priori it would be expected that more (perhaps up to 50%) would be in a pre-star-forming stage, with dense gas, but a quiescent cloud chemistry (and hence no CH$_3$OH). The molecules used for both the initial and final selection of the cloud sample (CO, CS, HCN, HCO$^+$; see chapter 4) are those that should be found in both dense quiescent gas and gas where star formation has occurred. However, it appears that using these molecules for the selection process has resulted in the sample predominantly consisting of molecular clouds where star formation has already taken place. There may be several reasons for this.

Firstly, dense molecular clouds in the final stages of collapse (before the gas has been warmed by a protostar or YSO) are thought to be severely depleted in all molecules (Brown et al. 1988), and these objects are less likely to have been selected for this sample. A study aimed at selecting dense molecular clouds in the pre-star-formation stage would make a good complement to the observations reported here. The molecules HCO$^+$, C$_2$H, C$_3$H$_2$ and N$_2$H$^+$, which are thought to trace quiescent gas could be used to select such a sample.

Secondly, some molecules that trace quiescent gas are enhanced in warm or shocked gas (e.g. CS, HCN and HC$_3$N; see section 1.2.5). The intensity of CS and HCN emission was used in the selection of both the initial and the final sample, so the sample is likely to be biased towards regions with warm or shocked gas (i.e. regions in which star formation has already taken place).

Thirdly, most of the sample consists of GMCs, which are large complexes of dense gas and H II regions. The GMCs in this sample all have radio H II regions (with the exception of Gl.6-0.025). It is possible that many different regions are sampled in a GMC within the telescope beam, and that at least some of this gas belongs to dense condensations associated with recently formed stars, hence the detection of CH$_3$OH in most molecular clouds. Observations at high resolution with the ATCA at millimetre-wavelengths should be used to investigate this possibility.

The high-energy $2_{1-1}$, $E$ transition of CH$_3$OH was detected towards only 7 of the observed positions (and also in the calibrator clouds M 17 and Orion KL), three of which, G345.5+1.5, NGC 6334(S), and NGC 6334(N1), have T$_{inh}$ between 65 to 100 K and may contain hot cores. This transition is particularly prominent in Orion KL (which has T$_{inh}$ between 60 K and 200 K for the different components) and is known to be emitted from hotter and denser regions than the other $2_{2-1}$k transitions (Liechti & Wilson 1996; Liechti & Walmsley 1997). The molecular clouds that have positive
detections of this transition should be investigated for the presence of 'hot core' molecules.

The excitation temperatures found for CH$_3$OH from the rotation diagrams (Tables A-1 to A-31(d)) are generally sub-thermal, with a median value of the ratio T$_{ex}$(CH$_3$OH)/T$_{kin}$ of 0.4, with a range of 0.1 to 1.9. Only 2 clouds, Orion KL and the Chameleon have T$_{ex}$(CH$_3$OH) > T$_{kin}$. Bachiller et al. (1995) have used statistical equilibrium calculations to show that CH$_3$OH will be very sub-thermal at densities below $\sim$ 10$^7$ cm$^{-3}$, and will (for their assumed T$_{kin}$ of 12 K and 100 K) approach 0.6-0.8 of T$_{kin}$ for densities of 10$^8$ cm$^{-3}$. The range of T$_{ex}$(CH$_3$OH)/T$_{kin}$ found for these molecular clouds suggests that the densities are generally less than 10$^8$ cm$^{-3}$, and this is confirmed by the values for n(H$_2$) found from LVG modelling (Tables A-1 to A-31(c)).

6.3.2 OCS Emission

OCS is not so ubiquitous within the sample as CH$_3$OH. OCS was not detected in 13 of the 31 positions, and significantly was not detected at any positions where CH$_3$OH was not detected. OCS was also only detected in dense cores where at least some spectra show either red or blue-shifted line wings, confirming that OCS is probably directly related to molecular outflows. OCS seems to be a good pointer to current star formation. It is formed both on grain mantles and in hot neutral gas, and so is expected to be abundant in warm gas after the onset of star formation. Sulphur-bearing molecules such as OSC and SO should be enhanced in shocked gas, with large amounts being formed in the gas phase in these high temperature regions (Neufeld & Dalgarno 1989). It seems likely that OCS is present in gas that has recently formed stars for a shorter period of time than CH$_3$OH, probably because the production in the gas phase requires a higher activation energy (and hence higher temperatures) than the production of CH$_3$OH (Blake et al. 1994). It is also possible that OCS is consumed in chemical reactions at a faster rate than CH$_3$OH. The median abundance of OCS for the entire sample is somewhat lower than most other molecules (Table 6-2).

The excitation temperatures derived from the OCS rotation diagrams (Tables A-1 to A-31(d)) are generally closer to T$_{kin}$ than those of CH$_3$OH (median = 0.8 times T$_{kin}$), although if the OCS emission is arising from a small area of shocked gas the T$_{kin}$ derived from HC$_3$N and CO may not represent T$_{kin}$ in the shocked gas.

6.3.3 HC$_3$N Emission

A comparison of the results from the LVG modelling and LTE rotation diagram analysis of HC$_3$N emission has been discussed in Section 5.3.5. HC$_3$N has on average lower abundances (by an order of magnitude: Table 6-2) than most of the other molecules observed, and as has already been stated it is believed to be optically thin in most clouds. An exception to this seems to be G1.6-0.025, which has an anomalously large abundance of HC$_3$N that deserves further investigation. The average T$_{ex}$(HC$_3$N)/T$_{kin}$ from the rotation diagrams is 0.6, with a range of 0.3 to 3.1.
6.3.4 HCN/HNC and SO/CS Abundance Ratios

The HCN/HNC abundance ratio is greater than unity for all but 6 molecular clouds of the sample. Three of these clouds are dark clouds, which are likely to have mainly cool gas within the telescope beam, however some of the 6 molecular clouds have obvious signs of star formation. Conversely, some molecular clouds with no signs, or few signs of star formation have HCN/HNC > 1 (e.g. HH 46). The median HNC abundance for the entire sample is low compared to most other molecules (Table 6-2), and this may be due to the sample composed of dense (and generally warm) cores. The SO/CS ratio has a median of 0.3 for the molecular clouds in the sample, but even more than for the HCN/HNC ratio there is no strict correlation between SO/CS and other signs of star formation. This effect may arise because a wide variety of gas may be sampled within the telescope beam, so that for single dish observations these are not reliable indicators of star formation status.

6.3.5 Molecular Abundances in this Sample

Table 6-2 presents the statistical properties of the molecular abundances within the sample. For each molecule, only clouds in which the molecule was detected were used for the statistical calculations. The most remarkable feature of Table 6-2 is the similar values for the median relative molecular abundances for many molecules within the sample. The median values for all molecules differ by more than an order of magnitude, ranging from (0.2 to 5.0) x 10^{-9}, although given the range of molecular clouds included this seems quite small. The molecular abundances in individual molecular clouds are also surprisingly similar (Tables 6-1, 6-3), except for CH$_3$OH and OCS, and are probably more closely related to the star formation history than to initial properties of the molecular gas from which the cloud formed. Given that most of these molecular clouds are spiral-arm clouds, and all are contained within the plane of the Galaxy, then it is possible that they formed from diffuse gas that is homogeneous and well mixed by previous generations of star formation, with a generally similar average star-formation history.

An investigation of the molecular abundances in high-velocity molecular clouds, which lie far from the Galactic plane, and may be composed of infalling gas from the intergalactic medium, would provide an excellent comparison for the molecular clouds studied in this sample.

6.3.6 Comparison of These Observations with Chemical Models

The predictions from models of chemistry in hot cores, GMCs and dark clouds, and associated with different stages of star formation, are discussed in Chapter 1 (Sections 1.2.2 to 1.2.6). The chemistry depends on the stage of star formation, temperature etc. (van Dishoeck & Blake 1998). Individual sources are discussed in Section 6.2 and the general properties of the molecular clouds and their individual
abundances and physical conditions are discussed above in Section 6.3.1 to 6.3.5. In both sections 6.2 and 6.3 the abundances derived are compared with the abundances expected from chemical models. Models (see e.g., Brown, Charnley & Millar 1988; Bergin, Langer & Goldsmith 1995; Bergin et al. 1997; Taylor, Morata & Williams 1998; Marwick & Millar 2000) do not predict large variations with time and physical conditions for most of the molecules observed in this thesis over much of the lifetime of a dense molecular core. (However, it should be noted that there is considerable disagreement between many of the models.) There are however some exceptions to this, as noted in both Chapters 1 and 6. The exceptions are the abundance of CH$_3$OH and OCS, which are expected to be found closer to the time of star formation, (sections 6.3.1 & 6.3.2). The CH$_3$OH and OCS abundances derived for the molecular clouds in this sample, and their implications for chemical models, have been discussed extensively in sections 6.3.1 & 6.3.2. Other molecular abundance parameters that are believed to vary with time evolution and physical state of the gas are the HCN/HNC ratio and the CS/SO ratio. These ratios have been discussed extensively in Chapter 1 as well as in this Chapter.

Referring to Table 6-2, which includes the normalised mean and standard deviation for the sample of molecules observed in this thesis, it can be seen from a comparison of these values for each molecule that the relative abundances (to H$_2$) of C$_2$H, CS, HC$_3$N, HCN, HCO$^+$ and HNC do not vary significantly for the dense cores in this sample. The standard deviation for each of the above molecules is similar to the average value of the abundance of the molecule itself. It must be noted that there will be selection effects operating on this sample (see Section 4.2) and most clouds may therefore be at similar stages of evolution. However, there is a more significant difference in the abundances of CH$_3$OH, SO and OCS. The standard deviation of CH$_3$OH is about 3 times that of the average value for this molecule in clouds of the sample, while OCS and SO have standard deviations of about twice their respective average values.

These results are in qualitative agreement with many chemical models, and certainly in agreement with the results of other observers. Bergin et al. (1997), in a study of the molecular clouds Orion A, M 17 and Cepheus A, found that although chemical differences did exist, the molecular composition of these dense clouds was remarkably homogeneous. In this thesis, for a significantly larger sample, the same conclusion is drawn. The molecular exceptions to this are CH$_3$OH, SO and OCS. Is this what the chemical models predict?

Qualitatively, as can be seen from Table 1-2 the models and observations used in the compilation of this table (see Sections 1.2.2 to 1.2.6 for references) are in agreement with the presence of C$_2$H, CS, HC$_3$N, HCN, HCO$^+$ and HNC throughout the star formation process. The presence of OCS and CH$_3$OH for a shorter period of time, and at a later stage of star formation is also supported by the greater variation in the abundance of these two molecules, as well as by the non-detections in a number of molecular clouds, particularly for OCS. SO, as has been previously stated, is also sensitive to the onset of star formation, which may
account for the larger variation in abundances for this molecule. On the other hand, SO is detected in all but one molecular cloud, and the predicted CS/SO abundance ratio with time evolution (see Section 6.3.4) during star formation was not found. Surprisingly, although the sample observed here contains 5 dark clouds, significant differences between the abundances in dark clouds and GMCs were not observed. The dark cloud cores in the sample are also expected to be cooler than the GMC cores, so the discussion below is most relevant to the GMCs.

More quantitatively, the time-dependent molecular evolution model of Charnley (1997) for hot core chemistry (at 100K) predicts that the molecules SO and CS will be present in the gas phase for most of the life of the hot core (a few times $10^5$ years), whereas OCS is likely to be present for about a third of the lifetime of a hot core. This prediction matches nicely with the finding of this thesis that about 1/3 of the molecular clouds had positive detections of OCS, whereas CS and SO are ubiquitous. However once again, the caveat is that although this sample consists of dense cores, there is no direct evidence that much of the sample contains gas at 100K, although given the presence of star formation in almost all dense cores it is very likely. Observations at higher resolution may help resolve the issue. Another time-dependent chemical model is that of Charnley and Rodgers (2001, hereafter CR) again for gas at 100 K, which predicts that CH$_3$OH will be present throughout the lifetime of the hot core, after the evaporation of the grain mantles. In fact, CR present two similar models with differences in the initial NH$_3$ abundance; however, for the molecules considered here the effect of the NH$_3$ abundance is not significant. Given the effects of beam dilution and consequent uncertainty about how much gas is present in the beam and how many different phases of star-formation are being observed simultaneously, the detection of CH$_3$OH emission in over 2/3 of the molecular clouds is probably consistent with this model. The relative number of detections of OCS and CH$_3$OH are certainly qualitatively consistent between the two models just discussed. The main discrepancy between the CR model and the observations of this thesis is that HC$_3$N is predicted to be detectable for only about 1/3 of the lifetime of the hot core. This is clearly at variance with the fact that HC$_3$N was detected in all but one molecular cloud. If the CR model was accurate for HC$_3$N, then it would be expected that there would be fewer detections of HC$_3$N than CH$_3$OH.

### 6.4 Summary

The molecular clouds of the sample have been discussed individually in terms of the observational results and derived parameters presented in Appendices A and B and previous observations. The results can be summarised as follows:

Most molecular clouds observed here show at least some evidence for recent or on-going star formation in these observations, as shown by the common presence of line wings, and the detection of CH$_3$OH and OCS.
Star formation seems to have occurred within the last \(10^2\) years towards most observed positions, in view of the detection of CH\(_3\)OH in most molecular clouds.

The presence of star formation in most of these dense cores is perhaps not surprising because the cores were selected on the basis that they had high brightness temperatures in previous observations.

The molecular clouds G265.1+1.5, G291.3-0.7 and G1.6-0.025 have self-absorbed line profiles in many molecules, suggesting a complex cloud structure and kinematics.

The observed positions in the Chameleon and Lupus dark clouds and towards NGC 6334(N1) show both self-absorption in one or more optically thick transitions and blue-shifted line wings, which may pinpoint infalling gas, although further investigation is required.

Detection of emission from the CH\(_3\)OH \(2_1-1_1\) E transition suggests that the positions G291.3-0.7, G345.5+1.5, NGC 6334(S), NGC 6334(N), NGC 6334(N1), G351.6-1.3 and G353.4-0.4 may contain hot cores or particularly dense gas. The positions G345.5+1.5, NGC 6334(S), and NGC 6334(N1) have \(T_{\text{kin}}\) from 65 to 100 K and probably contain hot cores.

OCS emission seems to be associated with current or at least very recent star formation. This molecule is only detected in molecular clouds with obvious signs of molecular outflow in line profiles.

The HCN/HNC and SO/CS abundance ratios do not seem to be good pointers to star formation status within this sample. This may be because the molecular clouds of the sample are all dense cores, most with a least some signs of active star formation. It may be necessary to include molecular clouds that are quiescent before these correlations become obvious, or it may be that beam dilution effects are masking the correlation.

The molecular cloud G1.6-0.025 is a peculiar cloud that needs further investigation. The observed CH\(_3\)OH and OCS abundance probably point more to a cloud-cloud collision than to star formation. HC\(_3\)N is particularly abundant in this molecular cloud, and the relationship between this and a possible cloud-cloud collision should be investigated.

The qualitative agreement between the chemical models discussed and summarized in Chapter 1 is good. Agreement between these observations and the two specific chemical models discussed in Section 6.3.6 is also generally good.
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Appendix A

Observed and Derived Parameters in Dense Cores

Molecules in Southern Molecular Clouds: A Millimetre-wave Study of Dense Cores

Maria R. Hunt
PLEASE NOTE

The greatest amount of care has been taken while scanning the following pages. The best possible results have been obtained.
Appendix A

Summary of Observed and Derived Parameters in Dense Cores

A molecular cloud is described by the combination of parameters required to build up a picture of the source. For this reason all observational and derived parameters are presented together on a source-by-source basis.

Figures A-1(a) – A-31(a). The left-hand figure shows a grey-scale plot of $\chi^2$ as a function of the log of the molecular hydrogen density ($\log[n(H_2)]$) and the log of the $HC_3N$ column density per unit velocity gradient ($\log[N(HC_3N)/(dv/dr)]$), for the kinetic temperature ($T_{\text{kin}}$) at $\chi^2_{\text{min}}$. The right-hand figure shows a grey-scale plot of $\chi^2$ as a function of $\log[n(H_2)]$ and $T_{\text{kin}}$ for $\log[N(HC_3N)/(dv/dr)]$ at $\chi^2_{\text{min}}$. The position of $\chi^2_{\text{min}}$ is marked with an X in each figure, while the solid line shows the boundary for plausible values at the 0.68 confidence level. The grey-scale contours are for $\Delta \chi^2 = 3.5$ (1σ), 6.25 (2σ), 11.3 (3σ), 25, 50, 75 and 100.

Figures A-1(b) – A-31(b). Rotation diagrams for $HC_3N$, $CH_3OH$ and OCS (see section 5.3.3 for details).
Orion A

(a) Observed parameters

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<th>dv (km s⁻¹)</th>
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<th>JMBdv (K km s⁻¹)</th>
<th>JMBdv (K km s⁻¹)</th>
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Notes.
Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

(b) Derived parameters

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<th>Centre = 8.3 ± 0.1 km s⁻¹</th>
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(i) LVG models

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<th>( \Delta \chi^2 = 3.5 )</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{HC}_3\text{N} \ (25\text{km/s}) )</td>
<td>75</td>
<td>&gt;40</td>
<td>1E14</td>
<td>1E14</td>
<td>6.7E-10</td>
<td>3E5</td>
<td>&gt;1E</td>
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<tr>
<td>( \text{HC}_3\text{N} \ (4\text{km/s}) )</td>
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<td>15-85</td>
<td>1E14</td>
<td>1E14</td>
<td>6.7E-10</td>
<td>1E6</td>
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</tr>
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</table>

\[ \chi^2 \text{ for } n(H_2) \text{ and } N(\text{HC}_3\text{N}) \]

\[ \chi^2 \text{ for } n(H_2) \text{ and } T_{\text{kin}} \]

\[ \log[n(H_2)] \]

\[ \log[N(\text{HC}_3\text{N})/dv/dr] \]

\[ T_{\text{kin}} \]

\[ \chi^2 \text{ for } n(H_2) \text{ and } N(\text{HC}_3\text{N}) \]

\[ \chi^2 \text{ for } n(H_2) \text{ and } T_{\text{kin}} \]

\[ \log[n(H_2)] \]

\[ \log[N(\text{HC}_3\text{N})/dv/dr] \]

\[ T_{\text{kin}} \]

Figure A-1(a)
(ii) LTE models

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<th>MOLECULE</th>
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<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
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<th>$N_{tot}$ (cm$^{-2}$)</th>
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Notes.

$^*$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.

Excitation temperatures in brackets are assumed temperatures.

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<th>Transition</th>
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<td>16-15</td>
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Figure A-1(b)
### HH 46

(a) Observed parameters

#### Table A-2(a)  
**Observed Line Intensities in HH 46**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>(dv) (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB} dv) (K km s(^{-1}))</th>
<th>Total Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^13)CO</td>
<td>1-0</td>
<td>1.4</td>
<td>1.3</td>
<td>14.25</td>
<td>19.73</td>
<td>19.7 23</td>
</tr>
<tr>
<td>(^12)CO</td>
<td>1-0</td>
<td>4.0</td>
<td>0.9</td>
<td>6.90</td>
<td>6.62</td>
<td>6.6 08</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>4.5</td>
<td>0.6</td>
<td>1.08</td>
<td>0.69</td>
<td>0.7 03</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>4.4</td>
<td>2.0</td>
<td>0.97</td>
<td>0.25</td>
<td>0.7 03</td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
<td>1.1</td>
<td>0.8</td>
<td>0.39</td>
<td>0.43</td>
<td></td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>5.3</td>
<td>0.9</td>
<td>1.04</td>
<td>0.99</td>
<td>1.0 03</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>5.2</td>
<td>0.7</td>
<td>0.56</td>
<td>0.45</td>
<td>0.4 02</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0 F=2-1</td>
<td>5.3</td>
<td>1.1</td>
<td>0.87</td>
<td>1.02</td>
<td>1.8 03</td>
</tr>
<tr>
<td></td>
<td>1-0 F=1-1</td>
<td>(10.1)</td>
<td>1.0</td>
<td>0.38</td>
<td>0.40</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-0 F=0-1</td>
<td>(-1.7)</td>
<td>1.0</td>
<td>0.33</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>H(^{15})CN</td>
<td>1-0</td>
<td>-</td>
<td>0.31</td>
<td>0.78</td>
<td>0.8</td>
<td>0.8 02</td>
</tr>
<tr>
<td>H(_2)CN</td>
<td>1-0</td>
<td>5.2</td>
<td>0.9</td>
<td>0.72</td>
<td>0.67</td>
<td>0.7 03</td>
</tr>
<tr>
<td>H(_{13})C(^{15})N</td>
<td>1-0</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
<td></td>
<td>&lt;0.2</td>
</tr>
<tr>
<td>H(_{13})C(^{15})N</td>
<td>4(0,4)-3(0,3)</td>
<td>-</td>
<td>-</td>
<td>&lt;0.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>1-0</td>
<td>5.3</td>
<td>1.1</td>
<td>1.40</td>
<td>1.63</td>
<td>1.6 03</td>
</tr>
<tr>
<td>H(^{13})CO(^+)</td>
<td>1-0</td>
<td>4.9</td>
<td>1.0</td>
<td>0.39</td>
<td>0.41</td>
<td>0.4 01</td>
</tr>
<tr>
<td>H(^{18})O(^+)</td>
<td>1-0</td>
<td>-</td>
<td>-</td>
<td>&lt;0.14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{13})N</td>
<td>10-9</td>
<td>-</td>
<td>-</td>
<td>&lt;0.04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{13})N</td>
<td>11-10</td>
<td>-</td>
<td>-</td>
<td>&lt;0.07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{13})N</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{13})N</td>
<td>15-14</td>
<td>-</td>
<td>-</td>
<td>&lt;0.08</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{13})N</td>
<td>16-15</td>
<td>-</td>
<td>-</td>
<td>&lt;0.08</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>-</td>
<td>-</td>
<td>&lt;0.14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>-</td>
<td>-</td>
<td>&lt;0.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>&lt;0.23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH 2(0)-1(0) A(^+)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH 3(-1)-2(-1)E</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH 15(3)-14(4)A(^-)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>5.2</td>
<td>0.7</td>
<td>1.29</td>
<td>0.99</td>
<td>1.0 03</td>
</tr>
</tbody>
</table>

**Notes.**

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = 5.2 ± 0.2 km s⁻¹</th>
<th>$T_{\text{kin}}$ = 17.7 K</th>
<th>$N(H_2) = (3.9 \pm 0.4) \times 10^{21}$ cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 1.0 ± 0.1 km s⁻¹</td>
<td></td>
<td>$n(H_2) = 3.0 \times 10^2$ cm⁻³</td>
</tr>
</tbody>
</table>

(i) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm⁻³)</th>
<th>$N(X)/N(H_2)$</th>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm⁻³)</th>
<th>$N(X)/N(H_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>17.7$^A$</td>
<td>9.07E+15</td>
<td>1.81E-06</td>
<td>HCN</td>
<td>(4)</td>
<td>1.75E+13</td>
<td>3.51E-09</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>17.7$^A$</td>
<td>7.2E+14</td>
<td>1.44E-07</td>
<td>HCO$^+$</td>
<td>(4)</td>
<td>6.89E+12</td>
<td>1.38E-09</td>
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<tr>
<td>C₂H</td>
<td>(8)</td>
<td>1.75E+13</td>
<td>3.49E-09</td>
<td>HNC</td>
<td>(4)</td>
<td>6.57E+10</td>
<td>1.31E-11</td>
</tr>
<tr>
<td>CS</td>
<td>3.9</td>
<td>1.02E+12</td>
<td>2.04E-10</td>
<td>SO</td>
<td>(8)</td>
<td>1E+13</td>
<td>2E-09</td>
</tr>
</tbody>
</table>

Notes.

$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.

Excitation temperatures in brackets are assumed temperatures.
### G265.1+1.5 (RCW 36)

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Centre dv TMB J_TMBdv</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(km s^{-1}) (K) (K km s^{-1}) (K km s^{-1})</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(8.0) 2.8 21.44 63.94</td>
<td>114.0 13.5</td>
</tr>
<tr>
<td></td>
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<td>*(5.4) 1.2 13.50 17.25</td>
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<td>*(3.7) 2.6 11.85 32.62</td>
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<td>*(4.0) 1.6 3.56 3.79</td>
<td>38.2 4.5</td>
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<td>*(3.0) 1.8 10.63 29.42</td>
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<td>*(1.9) 1.8 2.60 4.98</td>
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<tr>
<td></td>
<td></td>
<td>*(6.0) 1.9 1.94 3.92</td>
<td>3.9 0.5</td>
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<tr>
<td></td>
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<td>*(7.1) 3.6 0.39 1.51</td>
<td>2.2 0.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(7.0) 3.7 0.20 0.77</td>
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<td>*(6.1) 1.2 0.98 1.28</td>
<td>5.1 0.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(13.6) 2.2 0.86 2.01</td>
<td>7.4 0.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(9.8) 3.3 0.59 2.07</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(7.9) 1.0 1.02 1.09</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(5.9) 1.0 0.91 0.97</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(0.7) 3.6 0.32 1.23</td>
<td></td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>*(13.6) 2.2 0.86 2.01</td>
<td>7.4 0.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(9.8) 3.3 0.59 2.07</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(7.9) 1.0 1.02 1.09</td>
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<tr>
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<td>*(5.9) 1.0 0.91 0.97</td>
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<tr>
<td></td>
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<td>*(0.7) 3.6 0.32 1.23</td>
<td></td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>*(5.9) 1.3 0.75 1.06</td>
<td>3.4 0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(8.2) 2.2 1.00 2.35</td>
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</tr>
<tr>
<td></td>
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<td>*(6.0) 4.8 0.12 0.61</td>
<td>0.6 0.2</td>
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<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>*(8.8) 2.0 2.02 4.31</td>
<td>5.2 0.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(5.8) 1.0 0.86 0.91</td>
<td></td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>*(5.8) 1.0 0.86 0.91</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(7.7) 2.1 0.39 0.87</td>
<td>0.9 0.1</td>
</tr>
<tr>
<td>HCN</td>
<td>10-9</td>
<td>*(7.1) 2.2 0.18 0.41</td>
<td>0.4 0.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(11.0) - - -</td>
<td>0.2 0.1</td>
</tr>
<tr>
<td>HCN</td>
<td>11-10</td>
<td>*(7.0) 2.8 0.14 0.43</td>
<td>0.4 0.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>*(15.14) - - -</td>
<td>0.2 0.1</td>
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<tr>
<td>OCS</td>
<td>7-6</td>
<td>*(7.6) - - -</td>
<td>&lt;0.3 0.3</td>
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<tr>
<td></td>
<td></td>
<td>*(8.7) - - -</td>
<td>&lt;0.2 0.2</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>*(9.8) - - -</td>
<td>&lt;0.3 0.3</td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>*(12.11) - - -</td>
<td>&lt;0.2 0.2</td>
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<tr>
<td>CH3OH</td>
<td>2(0)-1(0) A+</td>
<td>*(2.0) - - -</td>
<td>&lt;0.3 0.3</td>
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<tr>
<td>CH3OH</td>
<td>3(1)-2(1) E</td>
<td>*(3.1) - - -</td>
<td>&lt;0.3 0.3</td>
</tr>
<tr>
<td>CH3OH</td>
<td>15(3)-14(4) A+</td>
<td>*(15.3) - - -</td>
<td>&lt;0.1 0.1</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>(3.0) 2.1 0.58 1.34</td>
<td>1.3 0.3</td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-3(b)  

<table>
<thead>
<tr>
<th>Derived Physical Parameters of RCW 36</th>
</tr>
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<tbody>
<tr>
<td>Centre = 7.0 ± 0.3 km s⁻¹</td>
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<tr>
<td>Width = 2.1 ± 0.2 km s⁻¹</td>
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<td></td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-3(c)  

<table>
<thead>
<tr>
<th>Molecular Abundances in RCW 36</th>
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<tr>
<td>MOLECULE</td>
</tr>
<tr>
<td>----------------</td>
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<tr>
<td>HC₃N</td>
</tr>
</tbody>
</table>

Notes.  
² Fit not constrained by data. Limits are maximum and minimum values considered in model.

Figure A-3(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>24.9 *</td>
<td>7.1E+16</td>
<td>2.5E-06</td>
<td>HCN</td>
<td>(5)</td>
<td>1.7E+13</td>
<td>5.9E-10</td>
</tr>
<tr>
<td>$^{18}$O</td>
<td>24.9 *</td>
<td>5.5E+15</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(5)</td>
<td>1.8E+13</td>
<td>6.3E-10</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(13)</td>
<td>2.2E+14</td>
<td>7.6E-09</td>
<td>HNC</td>
<td>(5)</td>
<td>6.5E+12</td>
<td>2.2E-10</td>
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<tr>
<td>CS</td>
<td>5.2</td>
<td>1.5E+13</td>
<td>5.1E-10</td>
<td>SO</td>
<td>(13)</td>
<td>3.6E+13</td>
<td>1.3E-09</td>
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<td>HC$_3$N</td>
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<td>8.7E-11</td>
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</tbody>
</table>

Notes.

*Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and $^{18}$O.

**Table A-3(e)**

Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>29.2</td>
</tr>
<tr>
<td>11-10</td>
<td>28.7</td>
</tr>
<tr>
<td>12-11</td>
<td>28.9</td>
</tr>
<tr>
<td>15-14</td>
<td>24.2</td>
</tr>
<tr>
<td>16-15</td>
<td>16.7</td>
</tr>
</tbody>
</table>

**Figure A-3(b)**
### (a) Observed parameters

#### Table A-4(a) Observed Line Intensities in 268.4-0.8

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Centre (km s(^{-1})) dv (km s(^{-1})) (T_mB) (K) (\int T_{mB}dv) (K km s(^{-1})) (\delta\int T_{mB}dv) (K km s(^{-1}))</td>
<td>(\int T_{mB}dv) (K km s(^{-1})) (\delta\int T_{mB}dv) (K km s(^{-1}))</td>
</tr>
<tr>
<td>CO</td>
<td>1-0</td>
<td>*0.8 4.2 19.93 89.17 124.5 14.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>*5.8 2.7 12.29 35.34</td>
<td></td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>1.9 3.1 11.72 38.70 58.5 6.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0 7.3 2.54 19.75</td>
<td></td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>2.4 2.4 2.00 5.12 5.1 0.6</td>
<td></td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 (F=1-0)</td>
<td>2.6 2.5 0.79 2.10 3.6 0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 (F=2-1)</td>
<td>2.9 2.3 0.59 1.45</td>
<td></td>
</tr>
<tr>
<td>CS</td>
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<td>8-7</td>
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**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-4(b)  Derived Physical parameters of 268.4-0.8

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<tr>
<th>Parameter</th>
<th>Value</th>
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<td>Centre</td>
<td>$2.8 \pm 0.1$ km s$^{-1}$</td>
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<tr>
<td>Width</td>
<td>$3.0 \pm 0.2$ km s$^{-1}$</td>
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<td>$T_{\text{kin}}$</td>
<td>23.4 K</td>
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<tr>
<td>$N(\text{H}_2)$</td>
<td>$(3.7 \pm 0.7)\times10^{22}$ cm$^2$</td>
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<tr>
<td>$n(\text{H}_2)$</td>
<td>$2.9\times10^3$ cm$^3$</td>
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(i) LVG models

Table A-4(c)  Molecular Abundances in 268.4-0.8 LVG Models

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<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
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<td>$25-60$</td>
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<td>$1\times10^{13}$</td>
<td>$3\times10^{-10}$</td>
<td>$1\times10^{7}$</td>
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Figure A-4(a)
(ii) LTE models

Table A-4(d)
Molecular Abundances in 268.4-0.8
Optically Thin LTE Models

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<th>MOLECULE</th>
<th>T_ex (K)</th>
<th>N_tot (cm^-2)</th>
<th>f(X) [N(X)/N(H_2)]</th>
<th>MOLECULE</th>
<th>T_ex (K)</th>
<th>N_tot (cm^-2)</th>
<th>f(X) [N(X)/N(H_2)]</th>
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<td>^13CO</td>
<td>23.4^A</td>
<td>1.1E+17</td>
<td>3.1E-06</td>
<td>HCN</td>
<td>(12)</td>
<td>1.6E+14</td>
<td>4.5E-09</td>
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<tr>
<td>C^18O</td>
<td>23.4^A</td>
<td>6.9E+15</td>
<td>1.9E-07</td>
<td>HCO^+</td>
<td>(12)</td>
<td>1.1E+14</td>
<td>3.0E-09</td>
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<td>C_2H</td>
<td>(9)</td>
<td>9.2E+13</td>
<td>2.5E-09</td>
<td>HNC</td>
<td>(12)</td>
<td>1.5E+13</td>
<td>4.2E-10</td>
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<td>CH_3OH</td>
<td>9.1</td>
<td>3.7E+14</td>
<td>1.0E-08</td>
<td>OCS</td>
<td>29.2</td>
<td>2.9E+13</td>
<td>7.9E-10</td>
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<tr>
<td>CS</td>
<td>11.8</td>
<td>1.1E+14</td>
<td>2.9E-09</td>
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<td>(12)</td>
<td>7.4E+13</td>
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<td>3.5E-10</td>
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Notes.
^A Excitation temperature of ^13CO.
Excitation temperatures in brackets are assumed temperatures.

Table A-4(e)
Excitation Temperature of HC_3N Transitions from LVG Models

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<tr>
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<td>11-10</td>
<td>29.6</td>
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<td>12-11</td>
<td>29.7</td>
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<td>15-14</td>
<td>28.3</td>
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<td>16-15</td>
<td>23.2</td>
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Figure A-4(b)
(a) Observed parameters

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<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>TMB (K)</th>
<th>JTMBdv (K km s⁻¹)</th>
<th>δJTMBdv (K km s⁻¹)</th>
<th>Total Emission</th>
<th>(\tilde{J}T_{MB}dv)</th>
<th>(\delta\tilde{J}T_{MB}dv)</th>
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<td>0.77</td>
<td>0.3</td>
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**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

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<th>Derived Physical Parameters of Cham</th>
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<td>T_{kin} = 14.2 K</td>
</tr>
<tr>
<td>Width = 0.7 ± 0.1 km s⁻¹</td>
<td>(N(H_2) = (7.9 ± 2.1) \times 10^{21} \text{ cm}^{-2})</td>
</tr>
<tr>
<td></td>
<td>(n(H_2) = 6.1 \times 10^2 \text{ cm}^{-3})</td>
</tr>
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(i) LVG models

<table>
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<tr>
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<td>(\chi^2_{min})</td>
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<tr>
<td>HC₃N</td>
<td>(T_k) (K)</td>
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\(\chi^2\) for \(n(H_2)\) and \(N(HC_3N)\)

\(\chi^2\) for \(n(H_2)\) and \(T_{kin}\)

![Figure A-5(a)](image-url)
(i) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
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<tbody>
<tr>
<td>$^{12}\text{CO}$</td>
<td>14.2</td>
<td>1.3E+16</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(4)</td>
<td>5.0E+13</td>
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<tr>
<td>$\text{C}^{18}\text{O}$</td>
<td>14.2</td>
<td>2.7E+15</td>
<td>3.8E-07</td>
<td>HCO$^+$</td>
<td>(4)</td>
<td>2.5E+13</td>
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<tr>
<td>CH$_3$OH</td>
<td>7.3</td>
<td>5.6E+13</td>
<td>7.8E-09</td>
<td>HNC</td>
<td>(4)</td>
<td>7.1E+12</td>
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<tr>
<td>CS</td>
<td>3.9</td>
<td>3.0E+12</td>
<td>4.2E-10</td>
<td>SO</td>
<td>(7)</td>
<td>1.1E+13</td>
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Notes:
A Excitation temperature of $^{12}\text{CO}$.
Excitation temperatures in brackets are assumed temperatures.

Table A-5(e)

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<tr>
<th>Transition</th>
<th>$T_{\text{ex}}$ (K)</th>
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<td>11-10</td>
<td>13.1</td>
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<tr>
<td>12-11</td>
<td>13.1</td>
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<tr>
<td>15-14</td>
<td>-</td>
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<td>16-15</td>
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Figure A-5(b)
(a) Observed parameters

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<th>Molecule</th>
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<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB}dv) (K km s(^{-1}))</th>
<th>(\delta T_{MB}dv) (K km s(^{-1}))</th>
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<td>100.82</td>
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<td>12.12</td>
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<tr>
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<tr>
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<tr>
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<td>0.19</td>
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<td>0.9</td>
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<td>1.37</td>
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<td>4.7</td>
<td>0.27</td>
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<td>0.4</td>
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Notes.
* Emission self-absorbed
Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
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<tr>
<th>Centre = -23.2 ± 0.6 km s⁻¹</th>
<th>T_{kin} = 28.4 K</th>
<th>N(H₂) = (3.6 ± 0.8)E+22 cm⁻²</th>
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<tbody>
<tr>
<td>Width = 3.5 ± 0.2 km s⁻¹</td>
<td></td>
<td>n(H₂) = 2.8E+3 cm⁻³</td>
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</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>T_k (K)</th>
<th>T_k (K)</th>
<th>N_{tot} (cm⁻³)</th>
<th>N_{rot} (cm⁻³)</th>
<th>(f(X))</th>
<th>n(H₂) (cm⁻³)</th>
<th>n(H₂) (cm⁻³)</th>
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<tr>
<td>HCN</td>
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<td>&gt;10</td>
<td>3E12</td>
<td>1E12-3E14</td>
<td>9E-11</td>
<td>1E6</td>
<td>&gt;1E3</td>
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Notes.
A Fit not constrained by data. Limits are maximum and minimum values considered in model.
(ii) LTE models

<table>
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<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
</tr>
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<tr>
<td>$^{13}$CO</td>
<td>28.4</td>
<td>8.2E+16</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>35.8</td>
<td>3.9E+12</td>
<td>8.7E-11</td>
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<td>C$^{18}$O</td>
<td>28.4</td>
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<td>1.1E-07</td>
<td>HCN</td>
<td>(6)</td>
<td>5.4E+13</td>
<td>1.2E-09</td>
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<tr>
<td>C$_2$H</td>
<td>(19)</td>
<td>1.0E+15</td>
<td>2.3E-08</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>3.1E+13</td>
<td>6.9E-10</td>
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<tr>
<td>CH$_3$OH</td>
<td>18.8</td>
<td>1.1E+14</td>
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<td>(6)</td>
<td>4.7E+12</td>
<td>1.0E-10</td>
</tr>
<tr>
<td>CS</td>
<td>6.3</td>
<td>6.2E+13</td>
<td>1.4E-09</td>
<td>SO</td>
<td>(19)</td>
<td>9.8E+13</td>
<td>2.2E-09</td>
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</table>

Notes.
- A Excitation temperature of $^{13}$CO.
- Excitation temperatures in brackets are assumed temperatures.

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
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<td>10-9</td>
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<td>11-10</td>
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<td>15-14</td>
<td>19.7</td>
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<tr>
<td>16-15</td>
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Figure A-6(b)
### G291.3-0.7 (RCW 57(W))

(a) Observed parameters

<table>
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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>T_{MB} (K)</th>
<th>( \bar{J}_{MBdv} ) (K km s⁻¹)</th>
<th>( \delta \bar{J}_{MBdv} ) (K km s⁻¹)</th>
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</thead>
<tbody>
<tr>
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<td>3.8</td>
<td>10.67</td>
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<td>43.19</td>
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<td>(^{13}\text{CO})</td>
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<td>0.23</td>
<td>0.88</td>
<td>0.4</td>
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<td>-24.2</td>
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<td>1.22</td>
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<td>1.9</td>
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<td>-</td>
<td>-</td>
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<td>33.3</td>
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<td>2.0</td>
<td>0.77</td>
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<tr>
<td>(^{12}\text{HC}^{18}\text{O}^{+})</td>
<td>1-0</td>
<td>-22.4</td>
<td>4.1</td>
<td>0.45</td>
<td>1.96</td>
<td>1.3</td>
</tr>
<tr>
<td>(^{12}\text{HCN})</td>
<td>10-9</td>
<td>-23.9</td>
<td>2.9</td>
<td>1.15</td>
<td>3.58</td>
<td>3.6</td>
</tr>
<tr>
<td>(^{12}\text{HCN})</td>
<td>11-10</td>
<td>-23.9</td>
<td>3.2</td>
<td>0.71</td>
<td>2.41</td>
<td>2.4</td>
</tr>
<tr>
<td>(^{12}\text{HCN})</td>
<td>12-11</td>
<td>-23.0</td>
<td>2.7</td>
<td>0.60</td>
<td>1.71</td>
<td>1.7</td>
</tr>
<tr>
<td>(^{12}\text{HCN})</td>
<td>15-14</td>
<td>-24.2</td>
<td>2.1</td>
<td>0.50</td>
<td>1.10</td>
<td>1.1</td>
</tr>
<tr>
<td>(^{12}\text{OCS})</td>
<td>7-6</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
<td>&lt;0.5</td>
<td></td>
</tr>
<tr>
<td>(^{12}\text{OCS})</td>
<td>8-7</td>
<td>-21.3</td>
<td>3.5</td>
<td>0.07</td>
<td>0.26</td>
<td>0.26</td>
</tr>
<tr>
<td>(^{12}\text{OCS})</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
<td>&lt;0.6</td>
<td></td>
</tr>
<tr>
<td>(^{12}\text{OCS})</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
<td>&lt;0.3</td>
<td></td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>2(1)-1(1)E</td>
<td>-23.4</td>
<td>2.4</td>
<td>0.17</td>
<td>0.44</td>
<td>0.4</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>2(0)-1(0)E</td>
<td>-23.1</td>
<td>4.3</td>
<td>0.24</td>
<td>1.11</td>
<td>1.1</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>2(0)-1(0)A+</td>
<td>-23.5</td>
<td>3.3</td>
<td>0.98</td>
<td>3.45</td>
<td>3.4</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>2(-1)-1(-1)E</td>
<td>-23.2</td>
<td>3.9</td>
<td>0.66</td>
<td>2.71</td>
<td>2.7</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>3(0)-2(0)A+</td>
<td>-35.9</td>
<td>3.0</td>
<td>0.76</td>
<td>2.43</td>
<td>2.4</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>3(-1)-2(-1)E</td>
<td>-23.9</td>
<td>3.0</td>
<td>0.61</td>
<td>1.96</td>
<td>2.0</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>3(0)-2(0)E</td>
<td>-16.9</td>
<td>5.2</td>
<td>0.20</td>
<td>1.09</td>
<td>1.1</td>
</tr>
<tr>
<td>(^{12}\text{CH}_2\text{OH}^{97})</td>
<td>15(3)-14(4)A-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(^{12}\text{SO})</td>
<td>3(2)-2(1)</td>
<td>-23.7</td>
<td>4.2</td>
<td>1.26</td>
<td>5.61</td>
<td>9.3</td>
</tr>
<tr>
<td></td>
<td>20.0</td>
<td>3.4</td>
<td>1.04</td>
<td>3.74</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**
* Emission self-absorbed
* Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -23.3 ± 0.4 km s⁻¹</th>
<th>T_{kin} = 35.6 K</th>
<th>N(H₂) = (7.8 ± 0.5)E+22 cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 3.9 ± 0.4 km s⁻¹</td>
<td></td>
<td>n(H₂) = 6.0E+3 cm⁻³</td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>( T_k ) (K)</th>
<th>( T_k ) (K)</th>
<th>( N_{tot} ) (cm⁻³)</th>
<th>( N_{tot} ) (cm⁻³)</th>
<th>( f(X) )</th>
<th>n(H₂) (cm⁻³)</th>
<th>n(H₂) (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>36</td>
<td>&gt;20</td>
<td>1E13</td>
<td>1E13</td>
<td>1E-10</td>
<td>1E6</td>
<td>&gt;1E5</td>
</tr>
</tbody>
</table>

\[ \chi^2 \text{ for } n(H_2) \text{ and } N(HC_3N) \]

\[ \chi^2 \text{ for } n(H_2) \text{ and } T_{kin} \]

**Figure A-7(a)**
(ii) LTE models

Table A-7(d) Molecular Abundances in RCW 57(W) Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>T_ex (K)</th>
<th>N_tot (cm⁻³)</th>
<th>f(X)</th>
<th>MOLECULE</th>
<th>T_ex (K)</th>
<th>N_tot (cm⁻²)</th>
<th>f(X)</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹²CO</td>
<td>35.6</td>
<td>1.9E+17</td>
<td>2.2E-06</td>
<td>HCN</td>
<td>(8)</td>
<td>8.1E+13</td>
<td>9.1E-10</td>
</tr>
<tr>
<td>C¹⁸O</td>
<td>35.6⁺</td>
<td>1.7E+16</td>
<td>1.9E-07</td>
<td>HCO⁺</td>
<td>(8)</td>
<td>1.2E+14</td>
<td>1.4E-09</td>
</tr>
<tr>
<td>C₂H</td>
<td>(11)</td>
<td>2.4E+14</td>
<td>2.7E-09</td>
<td>HNC</td>
<td>(8)</td>
<td>1.1E+13</td>
<td>1.2E-10</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>11.0</td>
<td>3.3E+14</td>
<td>3.7E-09</td>
<td>OCS</td>
<td>(15)</td>
<td>1.9E+13</td>
<td>2.1E-10</td>
</tr>
<tr>
<td>CS</td>
<td>8.3</td>
<td>2.4E+14</td>
<td>2.7E-09</td>
<td>SO</td>
<td>(11)</td>
<td>1.1E+14</td>
<td>1.3E-09</td>
</tr>
<tr>
<td>HCN</td>
<td>15.1</td>
<td>1.4E+13</td>
<td>1.6E-10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes.

* Excitation temperature of ¹²CO.

Excitation temperatures in brackets are assumed temperatures.

---

Table A-7(e) Excitation Temperature of HCN Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>T_ex (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>32.1</td>
</tr>
<tr>
<td>11-10</td>
<td>30.7</td>
</tr>
<tr>
<td>12-11</td>
<td>30.1</td>
</tr>
<tr>
<td>15-14</td>
<td>18.4</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-7(b)
### Coalsack D.C.

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>TMB (K)</th>
<th>JΤMBdv (K km s⁻¹)</th>
<th>JΤMBdv (K km s⁻¹)</th>
<th>δJΤMBdv (K km s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹⁴CO</td>
<td>1-0</td>
<td>-5.0</td>
<td>1.2</td>
<td>11.36</td>
<td>14.51</td>
<td>36.8</td>
<td>4.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-3.2</td>
<td>6.2</td>
<td>3.37</td>
<td>22.24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>¹³CO</td>
<td>1-0</td>
<td>-5.7</td>
<td>0.9</td>
<td>8.97</td>
<td>8.60</td>
<td>8.6</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-5.2</td>
<td>0.6</td>
<td>2.00</td>
<td>1.28</td>
<td>1.3</td>
<td>0.3</td>
</tr>
<tr>
<td>C₂H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>0.30</td>
<td></td>
<td></td>
<td>&lt;0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>-4.6</td>
<td>0.7</td>
<td>2.37</td>
<td>1.74</td>
<td>4.5</td>
<td>0.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-3.4</td>
<td>5.3</td>
<td>0.44</td>
<td>2.48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HCN</td>
<td>1-0, F=2-1</td>
<td>-4.6</td>
<td>1.0</td>
<td>1.49</td>
<td>1.59</td>
<td>3.1</td>
<td>0.4</td>
</tr>
<tr>
<td></td>
<td>1-0, F=1-1</td>
<td>(0.3)</td>
<td>1.2</td>
<td>0.96</td>
<td>1.22</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-0, F=0-1</td>
<td>(-12.5)</td>
<td>1.0</td>
<td>0.24</td>
<td>0.25</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H¹³CN</td>
<td>1-0</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HNC</td>
<td>1-0</td>
<td>-4.6</td>
<td>1.1</td>
<td>2.40</td>
<td>2.74</td>
<td>2.7</td>
<td>0.4</td>
</tr>
<tr>
<td>HN¹³C</td>
<td>1-0</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>-4.6</td>
<td>0.5</td>
<td>0.33</td>
<td>0.18</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>HCO⁺</td>
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<td>-4.6</td>
<td>1.1</td>
<td>3.23</td>
<td>3.78</td>
<td>3.8</td>
<td>0.5</td>
</tr>
<tr>
<td>H¹³CO⁺</td>
<td>1-0</td>
<td>-4.2</td>
<td>0.5</td>
<td>2.47</td>
<td>1.39</td>
<td>1.4</td>
<td>0.2</td>
</tr>
<tr>
<td>HC¹⁸O⁺</td>
<td>1-0</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HC₃N</td>
<td>10-9</td>
<td>-4.6</td>
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<td>0.82</td>
<td>0.18</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>HC₅N</td>
<td>11-10</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HC₅N</td>
<td>12-11</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HC₅N</td>
<td>11-14</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.03</td>
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<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃OH</td>
<td>2(1)-1(1)E</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃OH</td>
<td>2(0)-1(0)E</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃OH</td>
<td>2(0)-1(0) A⁺</td>
<td>-4.3</td>
<td>2.5</td>
<td>1.08</td>
<td>2.85</td>
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<td>0.4</td>
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<tr>
<td>CH₃OH</td>
<td>2(-1)-1(-1)E</td>
<td>-4.5</td>
<td>2.6</td>
<td>0.84</td>
<td>2.33</td>
<td>2.3</td>
<td>0.4</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>3(0)-2(0)A⁺</td>
<td>-4.4</td>
<td>0.9</td>
<td>0.77</td>
<td>0.77</td>
<td>0.8</td>
<td>0.3</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>3(-1)-2(-1)E</td>
<td>-4.4</td>
<td>1.0</td>
<td>0.76</td>
<td>0.84</td>
<td>0.8</td>
<td>0.3</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>3(0)-2(0)E</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.12</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃OH</td>
<td>5(-1)-4(0)E</td>
<td>-</td>
<td></td>
<td></td>
<td>&lt;0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-4.5</td>
<td>0.9</td>
<td>0.98</td>
<td>0.89</td>
<td>0.9</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-8(b)  Derived Physical Parameters of Coalsack

<table>
<thead>
<tr>
<th>Centre = 4.6 ± 0.2 km s⁻¹</th>
<th>T_{kin} = 14.8 K</th>
<th>N(H₂) = (6.8 ± 0.9)E+21 cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 1.0 ± 0.2 km s⁻¹</td>
<td></td>
<td>n(H₂) = 5.3E+2 cm⁻³</td>
</tr>
</tbody>
</table>

(i) LTE models

Table A-8(d)  Molecular Abundances in Coalsack

Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>T_{ex} (K)</th>
<th>N_{tot} (cm⁻²)</th>
<th>f(X)</th>
<th>MOLECULE</th>
<th>T_{ex} (K)</th>
<th>N_{tot} (cm⁻²)</th>
<th>f(X)</th>
</tr>
</thead>
<tbody>
<tr>
<td>^12CO</td>
<td>14.8</td>
<td>1.45E+16</td>
<td>1.84E-06</td>
<td></td>
<td>HCN</td>
<td>(5)</td>
<td>5.31E+12</td>
</tr>
<tr>
<td>C¹⁸O</td>
<td>14.8</td>
<td>1.23E+15</td>
<td>1.56E-07</td>
<td></td>
<td>HCO⁺</td>
<td>(5)</td>
<td>2.91E+13</td>
</tr>
<tr>
<td>C₂H</td>
<td>(6)</td>
<td>≤ 5.58E+12</td>
<td>7.06E-10</td>
<td></td>
<td>HNC</td>
<td>(5)</td>
<td>6.87E+12</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>6.0</td>
<td>1.94E+14</td>
<td>2.46E-08</td>
<td></td>
<td>OCS</td>
<td>(15)</td>
<td>7.68E+12</td>
</tr>
<tr>
<td>CS</td>
<td>5.4</td>
<td>5.64E+12</td>
<td>7.14E-10</td>
<td></td>
<td>SO</td>
<td>(6)</td>
<td>8.19E+12</td>
</tr>
<tr>
<td>HCN</td>
<td>(15)</td>
<td>7.21E+11</td>
<td>9.13E-11</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes:

A Excitation temperature of ^12CO.

Excitation temperatures in brackets are assumed temperatures.

Figure A-8(b)
## G301.0+1.2 (RCW 65)

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>(dv) (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB}dv) (K km s(^{-1}))</th>
<th>(\delta T_{MB}dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-43.2</td>
<td>4.8</td>
<td>30.51</td>
<td>155.97</td>
<td>156.0</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>-43.7</td>
<td>3.8</td>
<td>10.57</td>
<td>42.80</td>
<td>42.8</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
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<td>4.3</td>
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<tr>
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</tr>
<tr>
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<td>2.3</td>
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<td>3.52</td>
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<td>13.0</td>
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<td>HCN</td>
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<tr>
<td>HNC</td>
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<td>-</td>
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<td>H(^{13})CO(^{+})</td>
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<td>3.3</td>
<td>0.41</td>
<td>1.46</td>
<td>1.5</td>
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<tr>
<td>H(^{15})O(^{+})</td>
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<td>-</td>
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<td>&lt;0.5</td>
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<td>-</td>
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<td>2.8</td>
<td>0.41</td>
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<td>-</td>
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<td>8-7</td>
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<td>&lt;0.7</td>
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<td>&lt;0.5</td>
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<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
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</tr>
<tr>
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<td>2(1)-1(1)E</td>
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<td>-</td>
<td>&lt;1.3</td>
<td>-</td>
<td>-</td>
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<tr>
<td></td>
<td>2(0)-1(0)E</td>
<td>-</td>
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<td>&lt;1.3</td>
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<tr>
<td></td>
<td>2(0)-1(0) A(^{+})</td>
<td>-42.9</td>
<td>3.5</td>
<td>0.29</td>
<td>1.15</td>
<td>1.2</td>
</tr>
<tr>
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<td>2(-1)-1(-1)E</td>
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<td>&lt;1.3</td>
<td>-</td>
<td>-</td>
</tr>
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<td>3(0)-2(0) A(^{+})</td>
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</tr>
<tr>
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<td>3(-1)-2(-1)E</td>
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<td>3.9</td>
<td>0.38</td>
<td>1.59</td>
<td>1.6</td>
</tr>
<tr>
<td></td>
<td>3(0)-2(0)E</td>
<td>-42.5</td>
<td>1.9</td>
<td>0.22</td>
<td>0.46</td>
<td>0.5</td>
</tr>
<tr>
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<td>5(-1)-4(0)E</td>
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<td>3.3</td>
<td>0.23</td>
<td>0.81</td>
<td>0.8</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-42.7</td>
<td>3.6</td>
<td>0.11</td>
<td>0.40</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Notes:

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-9(b) Derived Physical Parameters of RCW 65

<table>
<thead>
<tr>
<th>Centre = $-42.9 \pm 0.1$ km s$^{-1}$</th>
<th>$T_{\text{kin}} = 34.0$ K</th>
<th>$N(\text{H}_2) = (3.8 \pm 0.3) \times 10^{22}$ cm$^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = $3.5 \pm 0.2$ km s$^{-1}$</td>
<td></td>
<td>$n(\text{H}_2) = 2.9 \times 10^{3}$ cm$^{-3}$</td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-9(c) Molecular Abundances in RCW 65

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 1$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 1$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 1$</th>
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</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>$100$</td>
<td>&gt;20</td>
<td>3E12</td>
<td>3E12-3E13</td>
<td>8E-11</td>
<td>3E5</td>
</tr>
</tbody>
</table>

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$

$\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-9(a)
(ii) LTE models

Table A-9(d) Molecular Abundances in RCW 65 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>34.0$^A$</td>
<td>9.5E+16</td>
<td>2.3E-06</td>
<td>HC$_3$N</td>
<td>18.9</td>
<td>5.5E+12</td>
<td>1.3E-10</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>34.0$^A$</td>
<td>7.9E+15</td>
<td>1.9E-07</td>
<td>HCN</td>
<td>(7)</td>
<td>8.1E+13</td>
<td>1.9E-09</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(13)</td>
<td>7.1E+14</td>
<td>1.7E-08</td>
<td>HCO$^+$</td>
<td>(7)</td>
<td>4.3E+13</td>
<td>1.0E-09</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>13.4</td>
<td>1.6E+14</td>
<td>3.7E-09</td>
<td>HNC</td>
<td>(7)</td>
<td>9.2E+12</td>
<td>2.2E-10</td>
</tr>
<tr>
<td>CS</td>
<td>6.6</td>
<td>2.0E+14</td>
<td>4.7E-09</td>
<td>SO</td>
<td>(13)</td>
<td>1.7E+13</td>
<td>4.0E-10</td>
</tr>
</tbody>
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Notes.
$^A$ Excitation temperature of $^{12}$CO.
Excitation temperatures in brackets are assumed temperatures.

Table A-9(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
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<tbody>
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<td>10-9</td>
<td>76.1</td>
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<td>11-10</td>
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<tr>
<td>15-14</td>
<td>15.3</td>
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<tr>
<td>16-15</td>
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</tr>
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Figure A-9(b)
Table A-10(a)  Observed Line Intensities in 305.4+0.2

<table>
<thead>
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<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>Centre (km s(^{-1}))</td>
<td>dv (km s(^{-1}))</td>
</tr>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-35.1</td>
<td>4.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-39.9</td>
<td>4.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-45.4</td>
<td>2.7</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>-38.4</td>
<td>6.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-35.4</td>
<td>2.7</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>-37.0</td>
<td>5.9</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>-37.2</td>
<td>7.6</td>
</tr>
<tr>
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<td>1-0 3/2-1/2 F=2-1</td>
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<td>4.6</td>
</tr>
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<td>CS</td>
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<td>5.2</td>
</tr>
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<td>1.03</td>
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<tr>
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<td>2-1</td>
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</tr>
<tr>
<td>HCN</td>
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<td>(-34.5)</td>
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<td>0.37</td>
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<td>5.8</td>
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<td>4.0</td>
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<td>SO</td>
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<td>3.8</td>
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</table>

Notes: * Emission self-absorbed
Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{k}$ (K)</th>
<th>$T_{k}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>$n(H_2)$ (cm$^{-3}$)</th>
<th>$n(H_2)$ (cm$^{-3}$)</th>
</tr>
</thead>
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<td>&gt;30</td>
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<td>1E13</td>
<td>2E-10</td>
<td>1E6</td>
<td>&gt;3E4</td>
</tr>
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<td>10-200$^A$</td>
<td>3E13</td>
<td>1E13-1E15</td>
<td>6E-10</td>
<td>3E7</td>
<td>&gt;1E3$^A$</td>
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</tbody>
</table>

Notes.

$^A$ Fit not constrained by data. Limits are maximum and minimum values considered in model.

![Figure A-10(a)](image-url)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
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<td>1.9E-07</td>
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<td>(7)</td>
<td>1.4E+14</td>
<td>1.9E-09</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(15)</td>
<td>2.7E+14</td>
<td>3.6E-09</td>
<td>HCO$^+$</td>
<td>(7)</td>
<td>1.0E+14</td>
<td>1.4E-09</td>
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<td>1.3E-10</td>
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<td>CS</td>
<td>6.9</td>
<td>2.0E+14</td>
<td>2.8E-09</td>
<td>SO</td>
<td>(15)</td>
<td>1.6E+13</td>
<td>2.1E-10</td>
</tr>
</tbody>
</table>

Notes.
$^A$ Excitation temperature of $^{13}$CO.
Excitation temperatures in brackets are assumed temperatures.

Table A-10(e)

Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
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<tbody>
<tr>
<td>0=extended</td>
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<tr>
<td>10-9</td>
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<td>11-10</td>
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<td>12-11</td>
<td>58.1</td>
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<tr>
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<td>26.6</td>
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<tr>
<td>16-15</td>
<td>-</td>
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<tr>
<td>0=60$^o$</td>
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<td>11-10</td>
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<td>16-15</td>
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Figure A-10(b)
### G311.6+0.3

#### (a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>T_MB (K)</th>
<th>∫T_MBdv (K km s⁻¹)</th>
<th>∫∫T_MBdv (K km s⁻¹)</th>
<th>∂∫T_MBdv (K km s⁻¹)</th>
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<td>6.47</td>
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<td>CH_{3}OH</td>
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<td>-54.2</td>
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<td>0.87</td>
<td>1.89</td>
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<td>0.4</td>
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<td>CH_{3}OH</td>
<td>3(1)-2(1)E</td>
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<td>1.54</td>
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<td>3(0)-2(0)E</td>
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<td>0.2</td>
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<td>CH_{3}OH</td>
<td>5(1)-4(0)E</td>
<td>-54.3</td>
<td>4.4</td>
<td>0.14</td>
<td>0.63</td>
<td>0.6</td>
<td>0.1</td>
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<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
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<td>3.5</td>
<td>0.59</td>
<td>2.17</td>
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<td>0.4</td>
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<td>0.35</td>
<td>0.90</td>
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**Notes.**
- * Emission self-absorbed
- Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -48.8 ± 0.6, -55.9 ±/− 0.4</th>
<th>$T_{\text{kin}}$ = 10.7K</th>
<th>$N(\text{H}_2)$ = (4.0 ± 0.9)$\times 10^{22}$ cm$^{-2}$</th>
</tr>
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<tbody>
<tr>
<td>Width = 3.3 ± 0.2 km/s</td>
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<td>$n(\text{H}_2)$ = 3.1$\times 10^{3}$ cm$^{-3}$</td>
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</table>

(i) LVG models

<table>
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<th>Table A-11(c)</th>
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<td><strong>HC$_3$N Abundance in 311.6+0.3</strong></td>
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<th>$\Delta\chi^2 = 1$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 1$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 1$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 1$</th>
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<tr>
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<td>20</td>
<td>15-50</td>
<td>1$\times 10^{13}$</td>
<td>1$\times 10^{13}$</td>
<td>3$\times 10^{-10}$</td>
<td>3$\times 10^{12}$</td>
<td>3$\times 10^{12}$</td>
<td>$&gt;10^5$</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>35</td>
<td>20-70</td>
<td>1$\times 10^{13}$</td>
<td>1$\times 10^{13}$</td>
<td>3$\times 10^{-10}$</td>
<td>3$\times 10^{6}$</td>
<td>$&gt;10^5$</td>
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Figure A-11(a)
(i) LTE models

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<th>MOLECULE</th>
<th>$T_{	ext{ex}}$ (K)</th>
<th>$N_{\text{exp}}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{	ext{ex}}$ (K)</th>
<th>$N_{\text{exp}}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
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<td>10.7$^A$</td>
<td>1.2E+17</td>
<td>3.0E-06</td>
<td>HCN</td>
<td>(6)</td>
<td>3.5E+13</td>
<td>8.8E-10</td>
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<tr>
<td>C$^{18}$O</td>
<td>10.7$^A$</td>
<td>9.0E+15</td>
<td>2.2E-07</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>3.6E+13</td>
<td>9.1E-10</td>
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<tr>
<td>C$_2$H</td>
<td>(8)</td>
<td>5.9E+13</td>
<td>1.5E-09</td>
<td>HNC</td>
<td>(6)</td>
<td>8.3E+12</td>
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<td>OCS</td>
<td>(6)</td>
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<td>5.8</td>
<td>2.5E+13</td>
<td>6.2E-10</td>
<td>SO</td>
<td>(6)</td>
<td>2.5E+13</td>
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**Notes.**

$^A$ Excitation temperature of $^{12}$CO.

Excitation temperatures in brackets are assumed temperatures.

---

Table A-11(e)  
Excitation Temperature of HC$_3$N Transitions from LVG Models

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<th>Transition</th>
<th>$T_{\text{ex}}$(K)</th>
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<td>15-14</td>
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<td>16-15</td>
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<td>$\theta$=60°</td>
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Figure A-11(b)
(a) Observed parameters

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<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
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<td>dv (km s$^{-1}$)</td>
</tr>
<tr>
<td>$^{12}$CO</td>
<td>1-0</td>
<td>-57.1</td>
<td>4.4</td>
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<td>13-14</td>
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<td>2.1</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>15-14</td>
<td>-54.3</td>
<td>5.9</td>
</tr>
<tr>
<td>OCS</td>
<td>7-8</td>
<td>-54.5</td>
<td>8.0</td>
</tr>
<tr>
<td></td>
<td>8-7</td>
<td>-55.9</td>
<td>7.1</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-58.2</td>
<td>5.3</td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-54.7</td>
<td>4.0</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(2(1)-1(1))E</td>
<td>-56.2</td>
<td>5.3</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(2(0)-1(0))E</td>
<td>-54.6</td>
<td>5.8</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(2(1)-1(1))E</td>
<td>-54.4</td>
<td>4.3</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(3(0)-2(0))A+</td>
<td>-55.3</td>
<td>4.9</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(3(1)-2(1))E</td>
<td>-55.8</td>
<td>5.9</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(3(0)-2(0))E</td>
<td>-57.3</td>
<td>6.4</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(3(1)-4(0))A+</td>
<td>-57.9</td>
<td>3.6</td>
</tr>
<tr>
<td>SO</td>
<td>(2(2)-2(1))</td>
<td>-56.1</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Notes.
* Emission probably self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions
(b) Derived parameters

Table A-12(b)  Derived Physical Parameters of RCW 92

<table>
<thead>
<tr>
<th>Centre = -56.1 ± 0.3 km s⁻¹</th>
<th>$T_{\text{kin}} = 32.8$ K</th>
<th>$N(\text{H}_2) = (9.0 ± 2.0) \times 10^{22}$ cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 3.8 ± 0.3 km s⁻¹</td>
<td></td>
<td>$n(\text{H}_2) = 7.0 \times 10^3$ cm⁻³</td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-12(c)  Molecular Abundances in RCW 92

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>$T_k$ (K)</td>
<td>$T_x$ (K)</td>
<td>$N_{\text{tot}}$ (cm⁻³)</td>
<td>$N_{\text{tot}}$ (cm⁻³)</td>
<td>$f(X)$</td>
<td>$n(\text{H}_2)$ (cm⁻³)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>&gt;25</td>
<td>1E13</td>
<td>1E13</td>
<td>1E-10</td>
<td>1E6</td>
</tr>
</tbody>
</table>

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$  $\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

![Figure A-12(a)](image-url)
(ii) LTE models

Table A-12(d) Molecular Abundances in RCW 92 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>32.8*</td>
<td>2.6E+17</td>
<td>2.2E-06</td>
<td>HCN</td>
<td>(10)</td>
<td>2.0E+14</td>
<td>1.7E-09</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>32.8*</td>
<td>2.3E+16</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(10)</td>
<td>8.0E+13</td>
<td>6.7E-10</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(10)</td>
<td>7.2E+14</td>
<td>6.0E-09</td>
<td>HNC</td>
<td>(10)</td>
<td>5.9E+13</td>
<td>4.9E-10</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>9.9</td>
<td>5.0E+14</td>
<td>4.2E-09</td>
<td>OCS</td>
<td>19.8</td>
<td>4.9E+13</td>
<td>4.1E-10</td>
</tr>
<tr>
<td>CS</td>
<td>9.6</td>
<td>3.1E+14</td>
<td>2.6E-09</td>
<td>SO</td>
<td>(10)</td>
<td>5.4E+13</td>
<td>4.5E-10</td>
</tr>
<tr>
<td>HCN</td>
<td>19.4</td>
<td>1.9E+13</td>
<td>1.6E-10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes.

* $T_{ex}$ is the excitation temperature of $^{13}$CO.

Excitation temperatures in brackets are assumed temperatures.

Table A-12(e) Excitation Temperature of HCN Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>47.0</td>
</tr>
<tr>
<td>11-10</td>
<td>45.0</td>
</tr>
<tr>
<td>12-11</td>
<td>42.9</td>
</tr>
<tr>
<td>15-14</td>
<td>22.4</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-12(b)
Lupus D.C.

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>TMB (K)</th>
<th>(\int TMBdv) (K km s⁻¹)</th>
<th>(\delta \int TMBdv) (K km s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>4.9</td>
<td>1.9</td>
<td>16.14</td>
<td>32.66</td>
<td>32.66</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>4.2</td>
<td>1.1</td>
<td>10.95</td>
<td>12.82</td>
<td>12.82</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>4.5</td>
<td>0.7</td>
<td>2.60</td>
<td>1.94</td>
<td>1.94</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>5.1</td>
<td>0.5</td>
<td>1.41</td>
<td>0.75</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
<td>5.1</td>
<td>0.6</td>
<td>1.13</td>
<td>0.72</td>
<td>0.72</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>5.4</td>
<td>0.8</td>
<td>1.48</td>
<td>1.28</td>
<td>1.28</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>5.2</td>
<td>0.5</td>
<td>1.46</td>
<td>0.81</td>
<td>0.81</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0 F=0-1</td>
<td>(-2.2)</td>
<td>0.7</td>
<td>1.16</td>
<td>0.86</td>
<td>2.41</td>
</tr>
<tr>
<td></td>
<td>1-0 F=2-1</td>
<td>4.7</td>
<td>0.7</td>
<td>1.16</td>
<td>0.86</td>
<td>0.86</td>
</tr>
<tr>
<td></td>
<td>1-0 F=1-1</td>
<td>(9.7)</td>
<td>0.8</td>
<td>0.81</td>
<td>0.69</td>
<td>0.69</td>
</tr>
<tr>
<td>H(^{13})CN</td>
<td>1-0</td>
<td>3.9</td>
<td>0.4</td>
<td>0.99</td>
<td>0.46</td>
<td>0.5</td>
</tr>
<tr>
<td>HNC</td>
<td>1-0</td>
<td><em>4.5</em></td>
<td>0.3</td>
<td>3.07</td>
<td>1.13</td>
<td>2.44</td>
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<tr>
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<td></td>
<td><em>5.3</em></td>
<td>0.8</td>
<td>1.57</td>
<td>1.31</td>
<td></td>
</tr>
<tr>
<td>HN(^{13})C</td>
<td>1-0</td>
<td>3.8</td>
<td>0.7</td>
<td>1.28</td>
<td>0.92</td>
<td>0.9</td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>5.1</td>
<td>0.4</td>
<td>0.36</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>1-0</td>
<td>4.7</td>
<td>1.1</td>
<td>0.72</td>
<td>0.84</td>
<td>0.84</td>
</tr>
<tr>
<td>H(^{13})CO(^+)</td>
<td>1-0</td>
<td>4.2</td>
<td>0.4</td>
<td>3.23</td>
<td>1.30</td>
<td>1.3</td>
</tr>
<tr>
<td>H(^{18})O(^+)</td>
<td>1-0</td>
<td>5.6</td>
<td>0.24</td>
<td>-</td>
<td>(&lt;0.1)</td>
<td></td>
</tr>
<tr>
<td>HCN</td>
<td>10-9</td>
<td>4.9</td>
<td>0.4</td>
<td>3.01</td>
<td>1.18</td>
<td>1.18</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>11-10</td>
<td>5.3</td>
<td>0.5</td>
<td>2.10</td>
<td>1.03</td>
<td>1.03</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>12-11</td>
<td>5.1</td>
<td>0.3</td>
<td>2.36</td>
<td>0.81</td>
<td>0.81</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>15-14</td>
<td>5.2</td>
<td>0.4</td>
<td>0.69</td>
<td>0.32</td>
<td>0.32</td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>(&lt;0.1)</td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>(&lt;0.1)</td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>(&lt;0.2)</td>
<td></td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2(0)-1(0) A(^+)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>(&lt;0.2)</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>4.8</td>
<td>0.5</td>
<td>0.69</td>
<td>0.34</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Notes.
* Emission probably self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions
(b) Derived parameters

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>$T$ (K)</td>
<td>$T_k$ (K)</td>
<td>$N_{\text{tot}}$ (cm$^{-3}$)</td>
<td>$N_{\text{tot}}$ (cm$^{-3}$)</td>
<td>$f(X)$</td>
<td>$n(H_2)$ (cm$^{-3}$)</td>
<td>$n(H_2)$ (cm$^{-3}$)</td>
<td>$n(H_2)$ (cm$^{-3}$)</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>15</td>
<td>15-20</td>
<td>1E13</td>
<td>1E13</td>
<td>1E-9</td>
<td>1E6</td>
<td>3E5-3E8</td>
<td></td>
</tr>
</tbody>
</table>

---

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{\text{kin}}$ (K)</th>
<th>$N(H_2)$ (cm$^{-3}$)</th>
<th>$n(H_2)$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>19.6</td>
<td>(9.5 ± 1.0)E+2 cm$^{-3}$</td>
<td>7.3E+2 cm$^{-3}$</td>
</tr>
</tbody>
</table>

---

Figure A-13(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$ [N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$ [N(X)/N(H$_2$)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>19.6$^A$</td>
<td>2.8E+16</td>
<td>2.4E-06</td>
<td>HCN</td>
<td>(6)</td>
<td>1.5E+13</td>
<td>1.3E-09</td>
</tr>
<tr>
<td>C$^{13}$O</td>
<td>19.6$^A$</td>
<td>2.8E+15</td>
<td>2.3E-07</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>3.3E+13</td>
<td>2.7E-09</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(13)</td>
<td>6.1E+13</td>
<td>5.1E-09</td>
<td>HNC</td>
<td>(6)</td>
<td>3.5E+13</td>
<td>2.9E-09</td>
</tr>
<tr>
<td>CS</td>
<td>6.8</td>
<td>3.5E+12</td>
<td>3.0E-10</td>
<td>SO</td>
<td>(13)</td>
<td>4.5E+12</td>
<td>3.8E-10</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>13.3</td>
<td>6.3E+12</td>
<td>5.2E-10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes:
$^A$ Excitation temperature of $^{12}$CO.
Excitation temperatures in brackets are assumed temperatures.

Table A-13(e)
Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>13.8</td>
</tr>
<tr>
<td>11-10</td>
<td>13.2</td>
</tr>
<tr>
<td>12-11</td>
<td>13.1</td>
</tr>
<tr>
<td>15-14</td>
<td>10.8</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-13(b)
## Chapter A
### G326.7+0.6

**Table A-14(a)**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB} dv) (K km s(^{-1}))</th>
<th>(\delta T_{MB} dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>12CO</td>
<td>1-0</td>
<td>-39.9</td>
<td>10.2</td>
<td>22.13</td>
<td>240.40</td>
<td>257.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-25.1</td>
<td>2.8</td>
<td>5.66</td>
<td>16.88</td>
<td>6.0</td>
</tr>
<tr>
<td>13CO</td>
<td>1-0</td>
<td>-41.5</td>
<td>8.7</td>
<td>7.09</td>
<td>50.62</td>
<td>50.6</td>
</tr>
<tr>
<td>C18O</td>
<td>1-0</td>
<td>-41.1</td>
<td>4.8</td>
<td>1.32</td>
<td>6.76</td>
<td>8.8</td>
</tr>
<tr>
<td>C2H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>-38.1</td>
<td>6.0</td>
<td>0.34</td>
<td>2.17</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
<td>-35.8</td>
<td>5.4</td>
<td>0.22</td>
<td>1.33</td>
<td>1.3</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>-40.3</td>
<td>5.3</td>
<td>2.85</td>
<td>17.17</td>
<td>24.8</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>-44.6</td>
<td>7.5</td>
<td>0.34</td>
<td>2.71</td>
<td>11.9</td>
</tr>
<tr>
<td>(^{13})CS</td>
<td>2-1</td>
<td>-43.3</td>
<td>4.5</td>
<td>0.31</td>
<td>2.66</td>
<td>2.7</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>(-34.5)</td>
<td>8.7</td>
<td>1.49</td>
<td>13.77</td>
<td>35.6</td>
</tr>
<tr>
<td>H(^{15})CN</td>
<td>1-0</td>
<td>(-39.5)</td>
<td>16.6</td>
<td>1.23</td>
<td>21.74</td>
<td>4.2</td>
</tr>
<tr>
<td>HNC</td>
<td>1-0</td>
<td>-37.8</td>
<td>15.4</td>
<td>0.19</td>
<td>3.03</td>
<td>3.0</td>
</tr>
<tr>
<td>HN(^{13})C</td>
<td>1-0</td>
<td>-39.9</td>
<td>6.1</td>
<td>1.62</td>
<td>10.43</td>
<td>14.8</td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>-37.5</td>
<td>8.5</td>
<td>0.09</td>
<td>0.79</td>
<td>0.8</td>
</tr>
<tr>
<td>HCO+</td>
<td>1-0</td>
<td>-37.9</td>
<td>12.6</td>
<td>1.12</td>
<td>15.05</td>
<td>23.6</td>
</tr>
<tr>
<td>H(^{15})CO(^+)</td>
<td>1-0</td>
<td>-39.5</td>
<td>3.0</td>
<td>0.30</td>
<td>0.94</td>
<td>0.9</td>
</tr>
<tr>
<td>HC18O+</td>
<td>1-0</td>
<td>-39.6</td>
<td>5.2</td>
<td>0.44</td>
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<td>3.0</td>
</tr>
<tr>
<td>HC3N</td>
<td>10-9</td>
<td>-45.6</td>
<td>2.9</td>
<td>0.16</td>
<td>0.51</td>
<td>&lt;0.4</td>
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<tr>
<td>HC3N</td>
<td>11-10</td>
<td>-39.0</td>
<td>4.0</td>
<td>0.23</td>
<td>0.96</td>
<td>0.9</td>
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<tr>
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<td>12-11</td>
<td>-40.4</td>
<td>3.8</td>
<td>0.46</td>
<td>1.88</td>
<td>1.9</td>
</tr>
<tr>
<td>HC3N</td>
<td>15-14</td>
<td>-40.3</td>
<td>3.8</td>
<td>0.46</td>
<td>1.88</td>
<td>1.9</td>
</tr>
<tr>
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<td>7-6</td>
<td>-39.4</td>
<td>8.6</td>
<td>0.16</td>
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<td>1.49</td>
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<td>8-7</td>
<td>-40.4</td>
<td>8.6</td>
<td>0.53</td>
<td>3.56</td>
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<td>9-8</td>
<td>-40.1</td>
<td>8.9</td>
<td>0.56</td>
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<td>5.27</td>
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<tr>
<td>OCS</td>
<td>12-11</td>
<td>-38.1</td>
<td>7.2</td>
<td>0.57</td>
<td>4.41</td>
<td>4.4</td>
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<td>2(1)-1(1)E</td>
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<td>6.3</td>
<td>0.40</td>
<td>2.89</td>
<td>2.7</td>
</tr>
<tr>
<td>CH3OH</td>
<td>2(0)-1(0)E</td>
<td>-38.4</td>
<td>10.8</td>
<td>0.24</td>
<td>2.77</td>
<td>2.8</td>
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<td>CH3OH</td>
<td>2(0)-1(0)A+</td>
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<td>6.3</td>
<td>0.40</td>
<td>2.89</td>
<td>2.7</td>
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<tr>
<td>CH3OH</td>
<td>3(1)-2(1)E</td>
<td>-38.7</td>
<td>6.3</td>
<td>0.40</td>
<td>2.89</td>
<td>2.7</td>
</tr>
<tr>
<td>CH3OH</td>
<td>3(0)-2(0)E</td>
<td>-38.4</td>
<td>10.8</td>
<td>0.24</td>
<td>2.77</td>
<td>2.8</td>
</tr>
<tr>
<td>CH3OH</td>
<td>3(1)-4(0)A+</td>
<td>-38.7</td>
<td>6.3</td>
<td>0.40</td>
<td>2.89</td>
<td>2.7</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-39.4</td>
<td>8.9</td>
<td>0.36</td>
<td>3.38</td>
<td>3.4</td>
</tr>
</tbody>
</table>

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-14(b)  

<table>
<thead>
<tr>
<th>Derived physical parameters of 326.7+0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centre = -40.0 ± 0.3 km s(^{-1})</td>
</tr>
<tr>
<td>Width = 6 ± 1 km s(^{-1})</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-14(c)  

<table>
<thead>
<tr>
<th>Molecular Abundances in 326.7+0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLECULE</td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>HC(_3)N</td>
</tr>
</tbody>
</table>

Notes.  
\(^{\text{A}}\) Fit not constrained by data. Limits are maximum and minimum values considered in model.

\[ \chi^2 \] for \(n(\text{H}_2)\) and \(N(\text{HC}_3\text{N})\)

\[ \chi^2 \] for \(n(\text{H}_2)\) and \(T_{\text{kin}}\)

**Figure A-14(a)**
(ii) LTE models

Table A-14(d) Molecular Abundances in 326.7+0.6
Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>( T_{\text{ex}} ) (K)</th>
<th>( N_{\text{tot}} ) (cm(^{-2}))</th>
<th>( f(X) ) [( N(X)/N(H_2) )]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{13}\text{CO})</td>
<td>25.6(^{\text{A}})</td>
<td>8.5E+16</td>
<td>1.7E-06</td>
</tr>
<tr>
<td>(^{13}\text{N})</td>
<td>25.6(^{\text{A}})</td>
<td>9.7E+15</td>
<td>1.9E-07</td>
</tr>
<tr>
<td>(^{2}\text{H})</td>
<td>(20)</td>
<td>2.2E+14</td>
<td>4.4E-09</td>
</tr>
<tr>
<td>(\text{CH}_3\text{OH})</td>
<td>20.3</td>
<td>5.4E+14</td>
<td>1.1E-08</td>
</tr>
<tr>
<td>(\text{CS})</td>
<td>5.9</td>
<td>2.8E+14</td>
<td>5.4E-09</td>
</tr>
<tr>
<td>(\text{H}_2\text{N})</td>
<td>11.3</td>
<td>1.4E+13</td>
<td>2.7E-10</td>
</tr>
<tr>
<td>(\text{HCN})</td>
<td>(6)</td>
<td>1.0E+14</td>
<td>2.0E-09</td>
</tr>
<tr>
<td>(\text{HCO}^+)</td>
<td>(6)</td>
<td>2.4E+13</td>
<td>4.6E-10</td>
</tr>
<tr>
<td>(\text{HNC})</td>
<td>(6)</td>
<td>3.5E+13</td>
<td>6.9E-10</td>
</tr>
<tr>
<td>(\text{SO})</td>
<td>(20)</td>
<td>6.1E+13</td>
<td>1.2E-08</td>
</tr>
</tbody>
</table>

Notes.

\(^{\text{A}}\) Excitation temperature of \(^{13}\text{CO}\) is assumed for \(^{13}\text{CO}\) and \(^{13}\text{N}\).

Excitation temperatures in brackets are assumed temperatures.

Figure A-14(b)

Table A-14(e) Excitation Temperature of \(\text{HC}_2\text{N}\) Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>( T_{\text{ex}} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>14.4</td>
</tr>
<tr>
<td>11-10</td>
<td>12.8</td>
</tr>
<tr>
<td>12-11</td>
<td>11.9</td>
</tr>
<tr>
<td>15-14</td>
<td>9.0</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>
(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB} dv) (K km s(^{-1}))</th>
<th>(\int J T_{MB} dv) (K km s(^{-1}))</th>
<th>(\delta J T_{MB} dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-47.7</td>
<td>7.5</td>
<td>37.22</td>
<td>297.31</td>
<td>297.3</td>
<td>35.1</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>-48.4</td>
<td>5.9</td>
<td>17.15</td>
<td>107.74</td>
<td>107.7</td>
<td>12.7</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>-48.3</td>
<td>5.0</td>
<td>3.05</td>
<td>16.26</td>
<td>16.3</td>
<td>1.9</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>-46.6</td>
<td>5.8</td>
<td>0.96</td>
<td>5.94</td>
<td>9.7</td>
<td>1.2</td>
</tr>
<tr>
<td>1-0 3/2-1/2 F=2-1</td>
<td>-86.5</td>
<td>6.5</td>
<td>0.55</td>
<td>3.80</td>
<td>61.5</td>
<td>6.1</td>
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</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>-49.1</td>
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<td>3.36</td>
<td>18.85</td>
<td>51.5</td>
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<tr>
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<td>6.91</td>
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<tr>
<td>1-0</td>
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<td>4.90</td>
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</tr>
<tr>
<td>H(^{13})CN</td>
<td>1-0 F=2-1</td>
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<td>4.7</td>
<td>2.89</td>
<td>14.48</td>
<td>51.5</td>
<td>6.1</td>
</tr>
<tr>
<td>1-0 F=0-1</td>
<td>-51.1</td>
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</tr>
<tr>
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<tr>
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<td>1.08</td>
<td>5.11</td>
<td>8.7</td>
<td>1.3</td>
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<tr>
<td>1-0 F=0-1</td>
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<td>0.52</td>
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<td>71.5</td>
<td>7.1</td>
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</tr>
<tr>
<td>1-0 F=1-1</td>
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<td>0.62</td>
<td>2.41</td>
<td>71.5</td>
<td>7.1</td>
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</tr>
<tr>
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<td>-47.8</td>
<td>6.6</td>
<td>2.34</td>
<td>16.47</td>
<td>22.6</td>
<td>2.7</td>
</tr>
<tr>
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<td>1.74</td>
<td>6.09</td>
<td>1.1</td>
<td>0.3</td>
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</tr>
<tr>
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<td>-46.1</td>
<td>5.6</td>
<td>0.18</td>
<td>1.08</td>
<td>1.1</td>
<td>0.3</td>
</tr>
<tr>
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<td>0.42</td>
<td>0.4</td>
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<tr>
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<td>1.26</td>
<td>1.3</td>
<td>0.3</td>
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<tr>
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<td>-45.5</td>
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<tr>
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<td>0.57</td>
<td>0.6</td>
<td>0.2</td>
</tr>
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<td>0.55</td>
<td>2.24</td>
<td>3.7</td>
<td>0.5</td>
</tr>
<tr>
<td>11-10</td>
<td>-47.2</td>
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<td>0.13</td>
<td>1.47</td>
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<td>&lt;0.7</td>
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</tr>
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<tr>
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<td>2.9</td>
<td>0.4</td>
</tr>
<tr>
<td>OCS</td>
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<td>-47.5</td>
<td>4.2</td>
<td>0.09</td>
<td>0.39</td>
<td>0.4</td>
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</tr>
<tr>
<td>OCS</td>
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<td>-</td>
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<tr>
<td>OCS</td>
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<td>-45.4</td>
<td>2.3</td>
<td>0.15</td>
<td>0.38</td>
<td>0.4</td>
<td>0.1</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2(1)-1(1)E</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;1.1</td>
<td>&lt;1.1</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2(0)-1(0)E</td>
<td>-46.6</td>
<td>2.3</td>
<td>0.13</td>
<td>0.36</td>
<td>0.4</td>
<td>0.2</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2(0)-1(0) A+</td>
<td>-45.9</td>
<td>4.1</td>
<td>0.29</td>
<td>1.27</td>
<td>1.3</td>
<td>0.3</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2(1)-1(1)E</td>
<td>-45.7</td>
<td>6.3</td>
<td>0.30</td>
<td>1.56</td>
<td>1.8</td>
<td>0.3</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>3(0)-2(0)A+</td>
<td>-46.2</td>
<td>4.5</td>
<td>0.39</td>
<td>1.85</td>
<td>1.9</td>
<td>0.4</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>3(1)-2(1)E</td>
<td>-46.1</td>
<td>6.2</td>
<td>0.18</td>
<td>1.22</td>
<td>1.2</td>
<td>0.3</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>3(0)-2(0)E</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.7</td>
<td>&lt;0.7</td>
<td></td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>3(1)-4(0) A+</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;0.3</td>
<td>&lt;0.3</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-46.6</td>
<td>4.7</td>
<td>1.17</td>
<td>5.81</td>
<td>5.8</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Notes.
* Emission self-absorbed
  Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -47.3 ± 0.3 km s⁻¹</th>
<th>$T_{\text{kin}} = 40.7$ K</th>
<th>$N(\text{H}_2) = (1.2 ± 0.3) \times 10^{23}$ cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 4.7 ± 0.3 km s⁻¹</td>
<td></td>
<td>$n(\text{H}_2) = 9.3 \times 10^3$ cm⁻³</td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_k$ (K)</th>
<th>$N_{\text{tot}}$ (cm⁻²)</th>
<th>$T_k$ (K)</th>
<th>$N_{\text{tot}}$ (cm⁻²)</th>
<th>$f(X)$</th>
<th>$n(\text{H}_2)$ (cm⁻³)</th>
<th>$n(\text{H}_2)$ (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>45</td>
<td>20-200⁸</td>
<td>1E13</td>
<td>1E13</td>
<td>8E-11</td>
<td>1E6</td>
<td>&gt;1E5</td>
</tr>
</tbody>
</table>

Notes.

⁸ Fit not constrained by data. Limits are maximum and minimum values considered in model.

---

$x^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$

$x^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-15(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>f(X) $[N(X)/N(H_2)]$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>f(X) $[N(X)/N(H_2)]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>40.7A</td>
<td>3.1E+17</td>
<td>1.8E-06</td>
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<td>(10)</td>
<td>4.9E+14</td>
<td>2.8E-09</td>
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<tr>
<td>C$^{18}$O</td>
<td>40.7A</td>
<td>3.6E+16</td>
<td>2.1E-07</td>
<td>HCO$^+$</td>
<td>(10)</td>
<td>1.9E+14</td>
<td>1.1E-09</td>
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<tr>
<td>C$_2$H</td>
<td>(11)</td>
<td>5.0E+14</td>
<td>2.9E-09</td>
<td>HNC</td>
<td>(10)</td>
<td>6.9E+13</td>
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<td>CH$_3$OH</td>
<td>11.1</td>
<td>1.7E+14</td>
<td>1.0E-09</td>
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<td>3.1E+13</td>
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<td>CS</td>
<td>10.1</td>
<td>7.7E+14</td>
<td>4.5E-09</td>
<td>SO</td>
<td>(11)</td>
<td>7.0E+13</td>
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Notes:

A: Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-15(e)

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<td>11-10</td>
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<td>15-14</td>
<td>21.1</td>
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<td>16-15</td>
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Figure A-15(b)
**Table A-16(a) Observed Line Intensities in 331.5-0.1**

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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
<th></th>
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<tr>
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<td>dv (km s(^{-1}))</td>
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<td>5.94</td>
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<td>3.18</td>
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<td>-89.7</td>
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<td>12-11</td>
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<td>0.38</td>
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<td>-89.6</td>
<td>8.4</td>
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<td>8.4</td>
<td>0.05</td>
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<tr>
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<td>-95.5</td>
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<td>0.45</td>
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<td>3(0)-2(0)E</td>
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<td>0.11</td>
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<td>8.9</td>
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<td>5.6</td>
<td>0.33</td>
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**Notes.**
* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -100.8 ± 0.3, -89.3 ± 0.2 km s⁻¹</th>
<th>T_{kin} = 25.5 K</th>
<th>N(H₂) = (8.5 ± 1.3)E+22 cm⁻²</th>
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<tbody>
<tr>
<td>Width = 5 ± 1 km s⁻¹</td>
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<td>n(H₂) = 6.6E+3 cm⁻³</td>
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(i) LVG models

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<tr>
<th>MOLECULE</th>
<th>T_x (K)</th>
<th>T_x (K)</th>
<th>N_{tot} (cm⁻³)</th>
<th>N_{tot} (cm⁻³)</th>
<th>f(X)</th>
<th>n(H₂) (cm⁻³)</th>
<th>n(H₂) (cm⁻³)</th>
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</thead>
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<td>10-50</td>
<td>3E13</td>
<td>3E13</td>
<td>4E-10</td>
<td>1E8</td>
<td>&gt;1E4</td>
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</tbody>
</table>

\[ \chi^2 \text{ for } n(H_2) \text{ and } N(HC_3N) \]

\[ \chi^2 \text{ for } n(H_2) \text{ and } T_{kin} \]

Figure A-16(a)
(ii) LTE models

Table A-16(d) Molecular Abundances in 331.5-0.1 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>Teq (K)</th>
<th>Ntot [cm⁻³]</th>
<th>f(X)</th>
<th>MOLECULE</th>
<th>Teq (K)</th>
<th>Ntot [cm⁻³]</th>
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</thead>
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<tr>
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<td>25.5</td>
<td>2.0E+17</td>
<td>1.8E-06</td>
<td>HC₃N</td>
<td>14.5</td>
<td>1.4E+13</td>
</tr>
<tr>
<td>C¹⁸O</td>
<td>25.5</td>
<td>2.4E+16</td>
<td>2.2E-07</td>
<td>HCN</td>
<td>(8)</td>
<td>9.3E+12</td>
</tr>
<tr>
<td>C₂H</td>
<td>(8)</td>
<td>2.2E+14</td>
<td>2.0E-09</td>
<td>HCO⁺</td>
<td>(8)</td>
<td>1.2E+13</td>
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<tr>
<td>CH₃OH</td>
<td>8.4</td>
<td>3.0E+14</td>
<td>2.7E-09</td>
<td>HNC</td>
<td>(8)</td>
<td>8.0E+12</td>
</tr>
<tr>
<td>CS</td>
<td>5.6</td>
<td>1.9E+13</td>
<td>1.7E-10</td>
<td>OCS</td>
<td>(15)</td>
<td>6.3E+13</td>
</tr>
</tbody>
</table>

Notes:
A: Excitation temperature of ¹²CO is assumed for ¹³CO and C¹⁸O.
- Excitation temperatures in brackets are assumed temperatures.

Table A-16(e) Excitation Temperature of HC₃N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>Teq (K)</th>
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<tbody>
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<td>11-10</td>
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<td>12-11</td>
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<tr>
<td>15-14</td>
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<td>16-15</td>
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Figure A-16(b)
### (a) Observed parameters

#### Table A-17(a) Observed Line Intensities in 333.0-0.6

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>Gaussian Components of fit</th>
<th>Total Emission (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(km s(^{-1})) dv (km s(^{-1}))</td>
<td>TMB (K)</td>
<td>fTMBdv (K km s(^{-1}))</td>
</tr>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-72.0 4.4 2.55</td>
<td>11.94</td>
<td>410.2 48.4</td>
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<td>54.45</td>
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<td>329.33</td>
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<td>(^{13})CO</td>
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<td>-52.8 5.1 17.88</td>
<td>97.13</td>
<td>177.5 21.0</td>
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<td>-52.3 5.0 0.22</td>
<td>1.16</td>
<td>1.2 0.3</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>2(0)-1(0) A(^{+})</td>
<td>-53.3 18.0 0.32</td>
<td>6.18</td>
<td>8.0 1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-50.8 2.6 0.63</td>
<td>1.78</td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>2(1)-1(1) E</td>
<td>-50.9 4.4 0.36</td>
<td>1.78</td>
<td>1.8 0.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-55.4 5.1 1.25</td>
<td>6.86</td>
<td>6.9 1.1</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(1)-2(1) E</td>
<td>-52.1 5.4 1.06</td>
<td>6.09</td>
<td>6.1 0.9</td>
</tr>
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<td></td>
<td></td>
<td>-52.3 5.1 0.49</td>
<td>2.62</td>
<td>2.6 0.4</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(0)-2(0) E</td>
<td>-53.2 2.2 0.21</td>
<td>0.51</td>
<td>0.5 0.1</td>
</tr>
<tr>
<td>SO(^{15})</td>
<td>3(2)-2(1)</td>
<td>-51.3 3.2 1.36</td>
<td>4.61</td>
<td>5.4 0.7</td>
</tr>
</tbody>
</table>
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -51.5 ± 0.2 km s⁻¹</th>
<th>Derived physical parameters of 333.0-0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 4.3 ± 0.6 km s⁻¹</td>
<td></td>
</tr>
<tr>
<td>$T_{\text{kin}} = 31.6 \text{ K}$</td>
<td>$N(\text{H}_2) = (1.9 \pm 0.5) \times 10^{23} \text{ cm}^{-2}$</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta \chi^2 = 3.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>200</td>
<td>&gt;35</td>
<td>1E13</td>
<td>1E13</td>
<td>5E-11</td>
<td>3E5</td>
<td>&gt;3E5</td>
<td></td>
</tr>
</tbody>
</table>

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$

$\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-17(a)
(ii) LTE models

### Table A-17(d)

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>( T_{\text{ex}} ) (K)</th>
<th>( N_{\text{tot}} ) (cm(^{-2}))</th>
<th>( f(X) )</th>
<th>MOLECULE</th>
<th>( T_{\text{ex}} ) (K)</th>
<th>( N_{\text{tot}} ) (cm(^{-2}))</th>
<th>( f(X) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{13})CO</td>
<td>31.6(^{A})</td>
<td>4.74E+17</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(12)</td>
<td>6.5E+14</td>
<td>2.5E-09</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>31.6(^{A})</td>
<td>5.98E+16</td>
<td>2.3E-07</td>
<td>HCO(^+)</td>
<td>(12)</td>
<td>3.5E+14</td>
<td>1.4E-09</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>(13)</td>
<td>4.9E+14</td>
<td>1.9E-09</td>
<td>HNC</td>
<td>(12)</td>
<td>1.8E+14</td>
<td>6.8E-10</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>13.1</td>
<td>6.6E+14</td>
<td>2.5E-09</td>
<td>OCS</td>
<td>(22)</td>
<td>7.2E+13</td>
<td>2.8E-10</td>
</tr>
<tr>
<td>CS</td>
<td>12.3</td>
<td>1.6E+15</td>
<td>6.1E-09</td>
<td>SO</td>
<td>(13)</td>
<td>7.2E+13</td>
<td>2.8E-10</td>
</tr>
<tr>
<td>H(_2)CN</td>
<td>22.1</td>
<td>2.7E+13</td>
<td>1.0E-10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**

*\(^{A}\) Excitation temperature of \(^{12}\)CO is assumed for \(^{13}\)CO and C\(^{18}\)O.*

Excitation temperatures in brackets are assumed temperatures.

### Table A-17(e)

<table>
<thead>
<tr>
<th>Transition</th>
<th>( T_{\text{ex}} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>151.4</td>
</tr>
<tr>
<td>11-10</td>
<td>106.3</td>
</tr>
<tr>
<td>12-11</td>
<td>52.7</td>
</tr>
<tr>
<td>15-14</td>
<td>16.6</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

**Figure A-17(b)**
### (a) Observed parameters

#### Table A-18(a) Observed Line Intensities in 333.4-0.4

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s⁻¹)</th>
<th>dv (km s⁻¹)</th>
<th>TMB (K)</th>
<th>∫TMBdv (K km s⁻¹)</th>
<th>Total Emission ∫TMBdv (K km s⁻¹)</th>
<th>∫TMBdv (K km s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹²CO</td>
<td>1-0</td>
<td>-50.2</td>
<td>3.6</td>
<td>27.73</td>
<td>106.31</td>
<td>408.5</td>
<td>48.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-54.6</td>
<td>6.8</td>
<td>30.57</td>
<td>221.39</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-44.0</td>
<td>11.1</td>
<td>6.84</td>
<td>80.81</td>
<td></td>
<td></td>
</tr>
<tr>
<td>¹³CO</td>
<td>1-0</td>
<td>-53.1</td>
<td>7.0</td>
<td>18.53</td>
<td>333.17</td>
<td>143.9</td>
<td>17.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-45.1</td>
<td>2.2</td>
<td>2.43</td>
<td>5.69</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C¹⁸O</td>
<td>1-0</td>
<td>-52.8</td>
<td>5.7</td>
<td>4.29</td>
<td>26.06</td>
<td>26.1</td>
<td>3.1</td>
</tr>
<tr>
<td>C₂H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>-52.3</td>
<td>6.7</td>
<td>1.29</td>
<td>9.24</td>
<td>38.5</td>
<td>4.5</td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
<td>-92.7</td>
<td>4.6</td>
<td>0.86</td>
<td>4.23</td>
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<td></td>
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<tr>
<td>CS</td>
<td>2-1</td>
<td>-51.4</td>
<td>4.8</td>
<td>2.95</td>
<td>15.09</td>
<td>13.5</td>
<td>1.6</td>
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<td>3-2</td>
<td>-52.1</td>
<td>6.1</td>
<td>4.32</td>
<td>27.89</td>
<td>27.9</td>
<td>4.8</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>(-56.0)</td>
<td>9.8</td>
<td>1.61</td>
<td>18.85</td>
<td>23.7</td>
<td>2.8</td>
</tr>
<tr>
<td>H¹³CN</td>
<td>1-0</td>
<td>(-53.9)</td>
<td>3.7</td>
<td>0.37</td>
<td>1.45</td>
<td>4.9</td>
<td>3.8</td>
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<td>4.3</td>
<td>1.60</td>
<td>7.31</td>
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<tr>
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<td>-53.5</td>
<td>3.2</td>
<td>0.34</td>
<td>1.15</td>
<td>1.2</td>
<td>0.3</td>
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<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>-52.5</td>
<td>6.0</td>
<td>0.17</td>
<td>1.11</td>
<td>1.1</td>
<td>0.3</td>
</tr>
<tr>
<td>HCO⁺</td>
<td>1-0</td>
<td>-49.6</td>
<td>4.1</td>
<td>2.80</td>
<td>12.21</td>
<td>21.8</td>
<td>2.6</td>
</tr>
<tr>
<td>H¹³CO⁺</td>
<td>1-0</td>
<td>-54.9</td>
<td>6.6</td>
<td>1.37</td>
<td>9.62</td>
<td>6.1</td>
<td>0.7</td>
</tr>
<tr>
<td>HC³N</td>
<td>1-0</td>
<td>-52.7</td>
<td>2.6</td>
<td>0.09</td>
<td>0.24</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>HCN</td>
<td>10-9</td>
<td>-52.5</td>
<td>5.7</td>
<td>0.35</td>
<td>2.13</td>
<td>2.1</td>
<td>0.3</td>
</tr>
<tr>
<td>HCN</td>
<td>12-11</td>
<td>-52.0</td>
<td>4.1</td>
<td>0.33</td>
<td>1.41</td>
<td>1.4</td>
<td>0.3</td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>-52.8</td>
<td>5.1</td>
<td>0.09</td>
<td>0.46</td>
<td>0.5</td>
<td>0.2</td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>-52.1</td>
<td>4.4</td>
<td>0.10</td>
<td>0.45</td>
<td>0.5</td>
<td>0.1</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-53.7</td>
<td>1.4</td>
<td>0.17</td>
<td>0.26</td>
<td>0.3</td>
<td>0.2</td>
</tr>
<tr>
<td>CH₂OH</td>
<td>2(1)-1(1)E</td>
<td>-50.8</td>
<td>5.9</td>
<td>0.64</td>
<td>4.46</td>
<td>&lt;0.5</td>
<td></td>
</tr>
<tr>
<td>CH₂OH</td>
<td>2(0)-1(0)E</td>
<td>-51.5</td>
<td>3.1</td>
<td>0.39</td>
<td>1.43</td>
<td>1.3</td>
<td>0.5</td>
</tr>
<tr>
<td>CH₂OH</td>
<td>2(0)-1(0) A⁺</td>
<td>-52.7</td>
<td>4.4</td>
<td>0.81</td>
<td>4.28</td>
<td>3.9</td>
<td>0.5</td>
</tr>
<tr>
<td>CH₂OH</td>
<td>3(1)-2(1)E</td>
<td>-52.1</td>
<td>1.3</td>
<td>1.03</td>
<td>1.58</td>
<td>1.4</td>
<td>0.3</td>
</tr>
<tr>
<td>CH₂OH</td>
<td>3(0)-2(0)E</td>
<td>-52.9</td>
<td>4.6</td>
<td>0.33</td>
<td>1.82</td>
<td>&lt;1.3</td>
<td></td>
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<tr>
<td>CH₂OH</td>
<td>5(1)-4(0)E</td>
<td>-52.9</td>
<td>4.6</td>
<td>0.33</td>
<td>1.82</td>
<td>1.6</td>
<td>0.3</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-52.4</td>
<td>2.2</td>
<td>0.30</td>
<td>0.79</td>
<td>4.2</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-52.5</td>
<td>6.2</td>
<td>0.52</td>
<td>3.82</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -52.5 ± 0.4 km s⁻¹</th>
<th>$T_{\text{kin}} = 34.1$ K</th>
<th>$N(\text{H}_2) = (1.7 ± 0.4)\times10^{23}$ cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 5.7 ± 0.3 km s⁻¹</td>
<td></td>
<td>$n(\text{H}_2) = 1.3E+4$ cm⁻³</td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>Table A-18(c)</th>
<th>Molecular Abundances in 333.4-0.4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LVG Models</td>
</tr>
<tr>
<td>MOLECULE</td>
<td>$\chi^2_{\text{min}}$</td>
</tr>
<tr>
<td></td>
<td>$T_k$ (K)</td>
</tr>
<tr>
<td>HC₃N</td>
<td>15</td>
</tr>
</tbody>
</table>

Notes:
^ Fit not constrained by data. Limits are maximum and minimum values considered in model.

Figure A-18(a)
(ii) LTE models

Table A-18(d) Molecular Abundances in 333.4-0.4 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>T$_{ex}$ (K)</th>
<th>N$_{tot}$ (cm$^{-2}$)</th>
<th>f(X)</th>
<th>MOLECULE</th>
<th>T$_{ex}$ (K)</th>
<th>N$_{tot}$ (cm$^{-2}$)</th>
<th>f(X)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>34.1$^A$</td>
<td>4.0E+17</td>
<td>1.8E-08</td>
<td>HCN</td>
<td>(6)</td>
<td>1.7E+14</td>
<td>7.5E-10</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>34.1$^A$</td>
<td>5.1E+16</td>
<td>2.3E-07</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>1.4E+14</td>
<td>6.1E-10</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(7)</td>
<td>3.0E+14</td>
<td>1.4E-09</td>
<td>HNC</td>
<td>(6)</td>
<td>4.4E+13</td>
<td>2.0E-10</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>7.4</td>
<td>2.8E+14</td>
<td>1.3E-09</td>
<td>OCS</td>
<td>9.0</td>
<td>5.3E+13</td>
<td>2.4E-10</td>
</tr>
<tr>
<td>CS</td>
<td>6.1</td>
<td>3.1E+14</td>
<td>1.4E-09</td>
<td>SO</td>
<td>(7)</td>
<td>4.0E+13</td>
<td>1.8E-10</td>
</tr>
<tr>
<td>HCN</td>
<td>12.9</td>
<td>1.1E+13</td>
<td>5.2E-11</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes:
$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-18(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>T$_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>15.0</td>
</tr>
<tr>
<td>11-10</td>
<td>-</td>
</tr>
<tr>
<td>12-11</td>
<td>15.0</td>
</tr>
<tr>
<td>15-14</td>
<td>-</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-18(b)
## (a) Observed parameters

### Table A-19(a) Observed Line Intensities in G333.6-0.2

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
<th>( f T_{MB} dv )</th>
<th>( \delta f T_{MB} dv )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Centre (km s(^{-1}))</td>
<td>dv (km s(^{-1}))</td>
<td>( T_{MB} ) (K)</td>
<td>( f T_{MB} dv ) (K km s(^{-1}))</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>(-51.1)</td>
<td>3.5</td>
<td>19.42</td>
<td>72.38</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-54.4)</td>
<td>6.4</td>
<td>13.66</td>
<td>93.24</td>
</tr>
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<td></td>
<td></td>
<td>(-47.0)</td>
<td>1.4</td>
<td>9.28</td>
<td>13.83</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>(-49.7)</td>
<td>9.3</td>
<td>9.98</td>
<td>98.84</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-42.7)</td>
<td>1.5</td>
<td>2.78</td>
<td>4.44</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(-40.3)</td>
<td>1.7</td>
<td>1.58</td>
<td>2.86</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>(-48.1)</td>
<td>8.3</td>
<td>2.30</td>
<td>20.32</td>
</tr>
<tr>
<td>C(_2)H</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>(-49.1)</td>
<td>8.0</td>
<td>0.57</td>
<td>4.85</td>
</tr>
<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
<td>(-89.2)</td>
<td>6.7</td>
<td>0.38</td>
<td>2.71</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>(-48.5)</td>
<td>5.6</td>
<td>4.68</td>
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<td>(-47.9)</td>
<td>5.7</td>
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<td>(-47.0)</td>
<td>12.1</td>
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<td>0.81</td>
<td>7.16</td>
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<td>(-47.9)</td>
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<td>5.56</td>
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<td>6.4</td>
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<td>HC(^{18})O(^*)</td>
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<td>HC(_3)N</td>
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<tr>
<td>OCS</td>
<td>8-7</td>
<td>-</td>
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<td>&lt;0.3</td>
<td></td>
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<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>&lt;0.8</td>
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<tr>
<td>OCS</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.6</td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>2(0)-1(0) A+</td>
<td>-</td>
<td>-</td>
<td>&lt;2.1</td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(-1)-2(-1)E</td>
<td>-</td>
<td>-</td>
<td>&lt;1.2</td>
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</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(1)-4(0) A+</td>
<td>-</td>
<td>-</td>
<td>&lt;0.7</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>(-48.0)</td>
<td>11.2</td>
<td>0.36</td>
<td>4.30</td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-19(b) Derived physical parameters of 333.6-0.2

| Centre = -48.3 ± 0.2 km s⁻¹ | $T_{\text{kin}} = 22.9$ K | $N(\text{H}_2) = (8.2 ± 2.2) \times 10^{22}$ cm⁻² |
| Width = 6.5 ± 0.6 km s⁻¹ | $n(\text{H}_2) = 6.3 \times 10^3$ cm⁻³ |

(i) LVG models

Table A-19(c) Molecular Abundances in 333.6-0.2 LVG Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$T_k$ (K)</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$T_k$ (K)</th>
<th>$N_{\text{tot}}$ (cm⁻³)</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$f(\chi)$</th>
<th>$N(\text{H}_2)$ (cm⁻³)</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$n(\text{H}_2)$ (cm⁻³)</th>
<th>$\Delta \chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$n(\text{H}_2)$ (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>0.0</td>
<td>&gt;15</td>
<td>3E13</td>
<td>3E13</td>
<td>&gt;15</td>
<td>3E13-3E14</td>
<td>0=extended</td>
<td>4E-10</td>
<td>3E10</td>
<td>&gt;3E4</td>
<td>4E-10</td>
<td>3E10</td>
<td>&gt;3E4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HC₃N</td>
<td>95</td>
<td>&gt;35</td>
<td>3E13</td>
<td>3E13</td>
<td>&gt;35</td>
<td>3E13-3E14</td>
<td>0=60°</td>
<td>4E-10</td>
<td>1E6</td>
<td>&gt;3E5</td>
<td>4E-10</td>
<td>1E6</td>
<td>&gt;3E5</td>
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Figure A-19(a)
(ii) LTE models

Table A-19(d) Molecular Abundances in 333.6-0.2
Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>22.9$^A$</td>
<td>1.9E+17</td>
<td>1.9E-06</td>
<td>HCN</td>
<td>(8)</td>
<td>3.1E+14</td>
<td>3.1E-09</td>
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<tr>
<td>C$^{18}$O</td>
<td>22.9$^A$</td>
<td>2.7E+16</td>
<td>2.7E-07</td>
<td>HCO$^+$</td>
<td>(8)</td>
<td>2.9E+14</td>
<td>2.9E-09</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(23)</td>
<td>9.5E+14</td>
<td>9.5E-09</td>
<td>HNC</td>
<td>(8)</td>
<td>9.7E+13</td>
<td>9.7E-10</td>
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<tr>
<td>CS</td>
<td>7.8</td>
<td>4.1E+14</td>
<td>4.1E-09</td>
<td>SO</td>
<td>(23)</td>
<td>1.4E+14</td>
<td>1.4E-09</td>
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<tr>
<td>HC$_3$N</td>
<td>36.9</td>
<td>3.6E+13</td>
<td>3.6E-10</td>
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</tr>
</tbody>
</table>

Notes.

$^A$ Excitation temperature of $^{13}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-19(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{\text{ex}}$ (K)</th>
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<tbody>
<tr>
<td>$\theta$=extended</td>
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</tr>
<tr>
<td>10-9</td>
<td>30.0</td>
</tr>
<tr>
<td>11-10</td>
<td>30.0</td>
</tr>
<tr>
<td>12-11</td>
<td>30.0</td>
</tr>
<tr>
<td>15-14</td>
<td>30.0</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
<tr>
<td>$\theta$=60$^\circ$</td>
<td></td>
</tr>
<tr>
<td>10-9</td>
<td>94.8</td>
</tr>
<tr>
<td>11-10</td>
<td>98.1</td>
</tr>
<tr>
<td>12-11</td>
<td>75.5</td>
</tr>
<tr>
<td>15-14</td>
<td>30.7</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
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</table>

Figure A-19(b)
## IRAS 16562

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
<th>$\int T_{mb} dv$</th>
<th>$\delta T_{mb} dv$</th>
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<td></td>
<td></td>
<td>Centre (km s$^{-1}$)</td>
<td>$dv$ (km s$^{-1}$)</td>
<td>$T_{mb}$ (K)</td>
<td>$\int T_{mb} dv$ (K km s$^{-1}$)</td>
</tr>
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<td>-13.3</td>
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<td>60.00</td>
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<td>C$^{18}$O</td>
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<td>-12.7</td>
<td>3.9</td>
<td>2.59</td>
<td>10.77</td>
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<td>4.1</td>
<td>2.58</td>
<td>11.28</td>
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<td>4.1</td>
<td>1.37</td>
<td>5.99</td>
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<td>4.0</td>
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<td>13.28</td>
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<td>1.44</td>
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<td>3.6</td>
<td>2.31</td>
<td>8.85</td>
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<td>3.7</td>
<td>2.43</td>
<td>9.62</td>
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<td>4.0</td>
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<td>8.89</td>
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<td>1.26</td>
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<td>4.6</td>
<td>0.29</td>
<td>1.40</td>
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<td>0.25</td>
<td>0.62</td>
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<tr>
<td>OCS</td>
<td>12-11</td>
<td>-11.6</td>
<td>2.9</td>
<td>0.27</td>
<td>0.85</td>
</tr>
<tr>
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<td>2.6</td>
<td>0.31</td>
<td>0.86</td>
</tr>
<tr>
<td>CH$_2$OH</td>
<td>2(0)-1(0)E</td>
<td>-12.0</td>
<td>3.5</td>
<td>0.62</td>
<td>2.28</td>
</tr>
<tr>
<td>CH$_2$OH</td>
<td>2(0)-1(0) A+</td>
<td>-12.4</td>
<td>3.6</td>
<td>2.64</td>
<td>9.97</td>
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<tr>
<td>CH$_2$OH</td>
<td>2(1)-1(1)E</td>
<td>-12.5</td>
<td>6.5</td>
<td>1.98</td>
<td>13.77</td>
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<tr>
<td>CH$_2$OH</td>
<td>3(0)-2(0)A+</td>
<td>-11.3</td>
<td>4.7</td>
<td>3.74</td>
<td>18.85</td>
</tr>
<tr>
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<td>3(1)-2(1)E</td>
<td>-11.4</td>
<td>4.0</td>
<td>3.53</td>
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<td>-11.9</td>
<td>4.9</td>
<td>1.47</td>
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<td>3(1)-4(0) A+</td>
<td>-</td>
<td></td>
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<td>6.76</td>
</tr>
<tr>
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<td>9.0</td>
<td>0.53</td>
<td>5.05</td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-20(b) Derived physical parameters of IRAS 16562

<table>
<thead>
<tr>
<th>Centre = $-11.9 \pm 0.2$ km s$^{-1}$</th>
<th>$T_{\text{kin}} = 37.9$ K</th>
<th>$N(H_2) = (7.8 \pm 1.1) \times 10^{22}$ cm$^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = $4.0 \pm 0.2$ km s$^{-1}$</td>
<td>$n(H_2) = 5.9 \times 10^3$ cm$^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-20(c) Molecular Abundances in IRAS 16562

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_k$ (K)</th>
<th>$T_x$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>$n(H_2)$ (cm$^{-3}$)</th>
<th>$n(H_3)$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>105</td>
<td>40-200</td>
<td>3E13</td>
<td>3E13</td>
<td>4E-10</td>
<td>3E5</td>
</tr>
</tbody>
</table>

$\chi^2$ for $n(H_2)$ and $N(HC_3N)$

$\chi^2$ for $n(H_2)$ and $T_{\text{kin}}$

Figure A-20(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
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<tr>
<td>$^{12}$CO</td>
<td>37.9$^A$</td>
<td>1.5E+17</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(14)</td>
<td>8.3E+14</td>
<td>9.9E-09</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>37.9$^A$</td>
<td>2.2E+16</td>
<td>2.6E-07</td>
<td>HCO$^+$</td>
<td>(14)</td>
<td>5.2E+14</td>
<td>6.2E-09</td>
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<tr>
<td>C$_2$H</td>
<td>(10)</td>
<td>5.5E+14</td>
<td>6.6E-09</td>
<td>HNC</td>
<td>(14)</td>
<td>2.3E+14</td>
<td>2.7E-09</td>
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<tr>
<td>CH$_3$OH</td>
<td>10.4</td>
<td>1.5E+15</td>
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<td>19.7</td>
<td>1.9E+13</td>
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<td>(10)</td>
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Notes:
$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

![Figure A-20(b)](image-url)
### (a) Observed parameters

#### Table A-21(a) Observed Line Intensities in 345.5+0.3

<table>
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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
<th>Centre</th>
<th>dv</th>
<th>$T_{MB}$</th>
<th>$J_{MBdv}$</th>
<th>$\delta J_{MBdv}$</th>
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<td>$^{12}$CO</td>
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<td>-19.1 4.5 19.33 92.64</td>
<td>233.9 27.6</td>
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<td>-15.4 8.7 15.24 141.24</td>
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<td>-18.0 2.1 0.11 0.24</td>
<td>0.2 0.1</td>
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<td>-17.2 1.7 0.29 0.53</td>
<td>0.5 0.2</td>
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<td>4.8 0.6</td>
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<td>2.6 0.5</td>
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<tr>
<td>CH$_3$OH</td>
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<td>3.5 0.4</td>
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<td>SO</td>
<td>3(2)-2(1)</td>
<td>-17.3 5.0 0.91 4.78</td>
<td>4.8 0.6</td>
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</table>

**Notes.**
- Emission self-absorbed
- Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
(b) Derived parameters

Table A-21(b) Derived physical parameters of 345.5+0.3

<table>
<thead>
<tr>
<th>Centre = -17.8 ± 0.4 km s⁻¹</th>
<th>( T_{\text{kin}} = 22.8 ) K</th>
<th>( N(\text{H}_2) = (8.6 \pm 2.1) \times 10^{22} ) cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 4.5 ± 0.3 km s⁻¹</td>
<td></td>
<td>( n(\text{H}_2) = 7.4 \times 10^3 ) cm⁻³</td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-21(c) Molecular Abundances in 345.5+0.3

<table>
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<tr>
<th>MOLECULE</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>( \chi^2_{\text{min}} )</th>
<th>( \Delta \chi^2 = 3.5 )</th>
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</thead>
<tbody>
<tr>
<td>HC₃N</td>
<td>50</td>
<td>&gt;25</td>
<td>1E13</td>
<td>1E13</td>
<td>1E-10</td>
<td>1E6</td>
</tr>
<tr>
<td></td>
<td>( T_k ) (K)</td>
<td>( T_k ) (K)</td>
<td>( N_{\text{tot}} ) (cm⁻³)</td>
<td>( N_{\text{tot}} ) (cm⁻³)</td>
<td>( f(X) )</td>
<td>( n(\text{H}_2) ) (cm⁻³)</td>
</tr>
</tbody>
</table>

\( \chi^2 \) for \( n(\text{H}_2) \) and \( N(\text{HC}_3\text{N}) \)

\( \chi^2 \) for \( n(\text{H}_2) \) and \( T_{\text{kin}} \)

Figure A-21(a)
(ii) LTE models

Table A-21(d) Molecular Abundances in 345.5±0.3 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{rot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{rot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>22.8$^A$</td>
<td>2.8E+17</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(9)</td>
<td>2.9E+14</td>
<td>2.0E-09</td>
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<tr>
<td>C$^{18}$O</td>
<td>22.8$^A$</td>
<td>2.8E+16</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(9)</td>
<td>1.9E+14</td>
<td>1.4E-09</td>
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<tr>
<td>C$_2$H</td>
<td>(15)</td>
<td>5.1E+14</td>
<td>3.8E-09</td>
<td>HNC</td>
<td>(9)</td>
<td>7.8E+13</td>
<td>5.8E-10</td>
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<tr>
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<td>5.3E-09</td>
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<td>4.8E+13</td>
<td>3.5E-10</td>
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<tr>
<td>CS</td>
<td>8.7</td>
<td>4.1E+14</td>
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<td>(15)</td>
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Notes.

$^A$ Excitation temperature of $^{13}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-21(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

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<td>11-10</td>
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<td>22.3</td>
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<td>16-15</td>
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Figure A-21(b)
### NGC 6334(S)

**(a) Observed parameters**

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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s$^{-1}$)</th>
<th>dv (km s$^{-1}$)</th>
<th>$T_{MB}$ (K)</th>
<th>$\tilde{J}$</th>
<th>Total Emission $\tilde{J}$</th>
<th>$\tilde{J}$</th>
<th>$\delta\tilde{J}$</th>
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<td></td>
<td>(K km s$^{-1}$)</td>
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<td>(K km s$^{-1}$)</td>
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<td>1.7</td>
<td>8.35</td>
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<td>15.52</td>
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<td>16.02</td>
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<td>90.4</td>
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<td>1-0</td>
<td>-6.9</td>
<td>4.3</td>
<td>2.59</td>
<td>11.86</td>
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<td>4.0</td>
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<td>0.78</td>
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<td>3.8</td>
<td>1.45</td>
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<td>4.2</td>
<td>1.95</td>
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<td>8.8</td>
<td>1.4</td>
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<td>3.5</td>
<td>1.71</td>
<td>6.46</td>
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<td></td>
<td>-7.8</td>
<td>9.7</td>
<td>0.60</td>
<td>6.17</td>
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</table>
Notes.
* Emission self-absorbed velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -6.5 ± 0.1 km s⁻¹</th>
<th>$T_{\text{kin}} = 28.8$ K</th>
<th>N(H₂) = (8.6 ± 0.6)E+22 cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 4.3 ± 0.2 km s⁻¹</td>
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<td>n(H₂) = 6.7E+3 cm⁻³</td>
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(i) LVG models

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<th>MOLECULE</th>
<th>$\chi^2_{\min}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
<th>$\chi^2_{\min}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
<th>$\chi^2_{\min}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
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<td>3E13</td>
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Figure A-22(a)
(ii) LTE models

Table A-22(d)

Molecular Abundances in NGC 6334(S)
Optically Thin LTE Models

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<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
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<tbody>
<tr>
<td>$^{12}$CO</td>
<td>28.8$^a$</td>
<td>2.2E+17</td>
<td>2.2E-06</td>
<td>HCN</td>
<td>(9)</td>
<td>1.1E+15</td>
<td>1.1E-08</td>
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<tr>
<td>C$^{18}$O</td>
<td>28.8$^a$</td>
<td>1.9E+16</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(9)</td>
<td>5.1E+14</td>
<td>5.1E-09</td>
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<td>6.8E+14</td>
<td>6.8E-09</td>
<td>HNC</td>
<td>(9)</td>
<td>2.0E+14</td>
<td>2.0E-09</td>
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<tr>
<td>CH$_3$OH</td>
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<td>1.6E+15</td>
<td>1.6E-08</td>
<td>OCS</td>
<td>38.9</td>
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<td>8.2E-09</td>
<td>SO</td>
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<td>5.7E+13</td>
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Notes.

$^a$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.

$^b$ Excitation temperatures in brackets are assumed temperatures.

Table A-22(e)

Excitation Temperature of HC$_3$N Transitions from LVG Models

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<td>11-10</td>
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<td>15-14</td>
<td>30.6</td>
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<td>16-15</td>
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Figure A-22(b)
## Observed Parameters

### Table A-23(a)

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<th>Gaussian Components of fit</th>
<th>Total Emission</th>
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<td></td>
<td></td>
<td>(km s⁻¹) (km s⁻²) (K)</td>
<td>(K km s⁻¹)</td>
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<td>(K km s⁻¹) (K km s⁻¹)</td>
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<td>2.4</td>
<td>5.8 39.40 243.37</td>
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<td>6.5 0.8</td>
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</tbody>
</table>

**Notes.** * Emission self-absorbed; * Hyperfine components of transition blended; Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
* Emission self-absorbed
  velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

B. Hyperfine components of transition blended.

(b) Derived parameters

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<th>Table A-23(b)</th>
<th>Derived physical parameters of NGC 6334(CO)</th>
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<tr>
<td>Centre = -1.1 ± 0.2, -4.4 +/- 0.1 km s⁻¹</td>
<td>( T_{\text{kin}} = 42.9 ) K</td>
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<td>Width = 3.8 ± 0.4 km s⁻¹</td>
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</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>Table A-23(c)</th>
<th>Molecular Abundances in NGC 6334(CO)</th>
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<tbody>
<tr>
<td>MOLECULE</td>
<td>( \chi^2_{\text{min}} )</td>
</tr>
<tr>
<td>HCN</td>
<td>( T_k ) (K)</td>
</tr>
<tr>
<td></td>
<td>15</td>
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</tbody>
</table>

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } N(\text{HC}_3\text{N}) \]

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } T_{\text{kin}} \]

Figure A-23(a)
(ii) LTE models

Table A-23(d) Molecular Abundances in NGC 6334(CO) Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-3}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (N(H$_2$))/N(X)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>42.9$^A$</td>
<td>2.8E+17</td>
<td>1.8E-08</td>
<td>HCN</td>
<td>(14)</td>
<td>8.0E+14</td>
<td>5.4E-09</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>42.9$^A$</td>
<td>3.0E+16</td>
<td>2.0E-07</td>
<td>HCO$^+$</td>
<td>(14)</td>
<td>3.2E+14</td>
<td>2.2E-09</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>(15)</td>
<td>8.8E+14</td>
<td>5.9E-09</td>
<td>HNC</td>
<td>(14)</td>
<td>2.2E+14</td>
<td>1.5E-09</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>8.8</td>
<td>4.5E+14</td>
<td>3.0E-09</td>
<td>OCS</td>
<td>37.9</td>
<td>5.7E+13</td>
<td>3.8E-10</td>
</tr>
<tr>
<td>CS</td>
<td>14.1</td>
<td>1.5E+15</td>
<td>9.7E-09</td>
<td>SO</td>
<td>(15)</td>
<td>1.4E+14</td>
<td>9.8E-10</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>36.6</td>
<td>2.3E+13</td>
<td>1.5E-10</td>
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</tr>
</tbody>
</table>

Notes:
$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-23(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>-</td>
</tr>
<tr>
<td>11-10</td>
<td>15.0</td>
</tr>
<tr>
<td>12-11</td>
<td>15.0</td>
</tr>
<tr>
<td>15-14</td>
<td>15.0</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-23(b)
NGC 6334(N)

(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{mb}) (K)</th>
<th>(\int T_{mb} dv) (K km s(^{-1}))</th>
<th>Total Emission (\int T_{mb} dv) (K km s(^{-1}))</th>
<th>(\delta \int T_{mb} dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>^{12}\text{CO}</td>
<td>1-0</td>
<td>-8.1</td>
<td>6.2</td>
<td>37.55</td>
<td>247.93</td>
<td>473.0</td>
<td>55.8</td>
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<tr>
<td></td>
<td></td>
<td>-2.9</td>
<td>5.9</td>
<td>33.26</td>
<td>208.97</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>6.1</td>
<td>1.7</td>
<td>8.91</td>
<td>16.14</td>
<td></td>
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</tr>
<tr>
<td>^{13}\text{CO}</td>
<td>1-0</td>
<td>-7.5</td>
<td>5.0</td>
<td>22.68</td>
<td>120.75</td>
<td>169.2</td>
<td>20.0</td>
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<td></td>
<td></td>
<td>-3.7</td>
<td>3.6</td>
<td>12.62</td>
<td>48.40</td>
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<td></td>
</tr>
<tr>
<td>C(^{18}\text{O})</td>
<td>1-0</td>
<td>-7.3</td>
<td>4.1</td>
<td>4.21</td>
<td>18.37</td>
<td>26.5</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-3.7</td>
<td>3.3</td>
<td>2.32</td>
<td>8.14</td>
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<td></td>
</tr>
<tr>
<td>C(_2\text{H})</td>
<td>1-0 3/2-1/2 F=1-0</td>
<td>-5.4</td>
<td>6.5</td>
<td>1.71</td>
<td>11.88</td>
<td>19.1</td>
<td>2.3</td>
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<tr>
<td></td>
<td>1-0 3/2-1/2 F=2-1</td>
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<td>6.2</td>
<td>1.09</td>
<td>7.20</td>
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<td>3-2</td>
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<td>2.9</td>
<td>6.40</td>
<td>19.61</td>
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<td>7.4</td>
<td>1.17</td>
<td>8.8</td>
<td>8.8</td>
<td>1.1</td>
</tr>
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<td>HCN</td>
<td>1-0\textsuperscript{a}</td>
<td>-6.5</td>
<td>8.0</td>
<td>6.95</td>
<td>59.20</td>
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<td>3.54</td>
<td>19.22</td>
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<tr>
<td>H(^{15}\text{CN})</td>
<td>1-0\textsuperscript{a}</td>
<td>-12.8</td>
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<td>0.24</td>
<td>0.85</td>
<td>15.1</td>
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<td>(-2.8)</td>
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<td>0.91</td>
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<tr>
<td>HNC</td>
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<td>4.17</td>
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<td>0.29</td>
<td>0.69</td>
<td>0.7</td>
<td>0.3</td>
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<td>49.9</td>
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<td>4.29</td>
<td>40.17</td>
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<tr>
<td>H(^{14}\text{CO})^{+}</td>
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<td>3.8</td>
<td>1.39</td>
<td>5.65</td>
<td>7.3</td>
<td>1.1</td>
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<td>2.4</td>
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<td>HC(^{18}\text{O})^{+}</td>
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<td>0.61</td>
<td>0.6</td>
<td>0.2</td>
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<tr>
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<td>1.91</td>
<td>2.81</td>
<td>12.1</td>
<td>1.5</td>
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<td>0.91</td>
<td>3.81</td>
<td>7.2</td>
<td>0.9</td>
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<td>-2.8</td>
<td>1.8</td>
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<td>3.39</td>
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<td>7.1</td>
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<td>1.2</td>
<td>1.25</td>
<td>1.63</td>
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<td>2.4</td>
<td>0.14</td>
<td>0.36</td>
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<tr>
<td>HC(_5\text{N})</td>
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<td>5.2</td>
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<td>0.8</td>
<td>0.09</td>
<td>0.07</td>
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<td>0.56</td>
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<td>7-6</td>
<td>-6.4</td>
<td>2.5</td>
<td>0.15</td>
<td>0.40</td>
<td>0.4</td>
<td>0.2</td>
</tr>
<tr>
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<td>8-7</td>
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<td>6.4</td>
<td>5.6</td>
<td>0.18</td>
<td>1.08</td>
<td>1.1</td>
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<td>9-8</td>
<td>-7.1</td>
<td>4.5</td>
<td>0.24</td>
<td>1.13</td>
<td>1.1</td>
<td>0.3</td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-5.4</td>
<td>6.0</td>
<td>0.14</td>
<td>0.88</td>
<td>0.9</td>
<td>0.2</td>
</tr>
<tr>
<td>CH(_3\text{OH})</td>
<td>2(1)-1(1)E</td>
<td>-6.5</td>
<td>3.0</td>
<td>0.26</td>
<td>0.85</td>
<td>0.9</td>
<td>0.3</td>
</tr>
<tr>
<td>CH(_3\text{OH})</td>
<td>2(0)-1(0)E</td>
<td>-5.6</td>
<td>6.0</td>
<td>0.63</td>
<td>4.04</td>
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<td>0.5</td>
</tr>
<tr>
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<td>-5.9</td>
<td>6.0</td>
<td>1.99</td>
<td>12.69</td>
<td>12.7</td>
<td>1.5</td>
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<tr>
<td>CH(_3\text{OH})</td>
<td>2(1)-1(1)E</td>
<td>-5.9</td>
<td>6.0</td>
<td>1.71</td>
<td>10.89</td>
<td>10.89</td>
<td>1.3</td>
</tr>
<tr>
<td>CH(_3\text{OH})</td>
<td>3(0)-2(0) A(^+)</td>
<td>-6.3</td>
<td>3.0</td>
<td>1.79</td>
<td>5.81</td>
<td>5.8</td>
<td>0.9</td>
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</table>
Table A-24(a)

<table>
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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre</th>
<th>dv</th>
<th>$T_{MB}$</th>
<th>$\int T_{MB} dv$</th>
<th>Total Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(km s$^{-1}$)</td>
<td>(km s$^{-1}$)</td>
<td>(K)</td>
<td>(K km s$^{-1}$)</td>
<td>(K km s$^{-1}$)</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(-1)-2(-1)E</td>
<td>-6.3</td>
<td>2.8</td>
<td>1.38</td>
<td>4.07</td>
<td>4.1</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(0)-2(0)E</td>
<td>-6.5</td>
<td>2.4</td>
<td>0.42</td>
<td>1.06</td>
<td>1.1</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(1)-4(0) A+</td>
<td>-</td>
<td></td>
<td>-</td>
<td>&lt;0.5</td>
<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-6.6</td>
<td>3.5</td>
<td>2.88</td>
<td>10.60</td>
<td>13.6</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-3.2</td>
<td>2.1</td>
<td>1.23</td>
<td>2.78</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Notes:

A. Emission self-absorbed
B. Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.
C. Hyperfine components of transition blended.

(b) Derived parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Derived physical parameters of NGC 6334(N)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Centre = -7.1 ± 0.2, 3.4 +/- 0.1 km s$^{-1}$</td>
</tr>
<tr>
<td></td>
<td>Width = 4.2 ± 0.4 km s$^{-1}$</td>
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<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{min}$</th>
<th>$\Delta \chi^2$ = 3.5</th>
<th>$\chi^2_{min}$</th>
<th>$\Delta \chi^2$ = 3.5</th>
<th>$\chi^2_{min}$</th>
<th>$\Delta \chi^2$ = 3.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>$T_k$ (K)</td>
<td>$T_k$ (K)</td>
<td>$N_{tot}$ (cm$^{-3}$)</td>
<td>$N_{tot}$ (cm$^{-3}$)</td>
<td>f(X)</td>
<td>n($H_2$) (cm$^{-3}$)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>20.55</td>
<td>3E13</td>
<td>3E13</td>
<td>2E-10</td>
<td>3E6</td>
</tr>
</tbody>
</table>

$\chi^2$ for n($H_2$) and N(HC$_3$N) $\chi^2$ for n($H_2$) and $T_{kin}$

Figure A-24(a)
(ii) LTE models

Table A-24(d) Molecular Abundances in NGC 6334(N) Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ [N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{\text{ex}}$ (K)</th>
<th>$N_{\text{tot}}$ [N(X)/N(H$_2$)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>41.1$^a$</td>
<td>5.6E+17</td>
<td>HCN</td>
<td>(13)</td>
<td>4.2E+14</td>
</tr>
<tr>
<td>$^{18}$O</td>
<td>6.0E+16</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(13)</td>
<td>1.5E+14</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>(7)</td>
<td>4.3E-14</td>
<td>HNC</td>
<td>(13)</td>
<td>7.6E+13</td>
</tr>
<tr>
<td>CS</td>
<td>7.4</td>
<td>1.0E+15</td>
<td>OCS</td>
<td>29.5</td>
<td>8.4E+13</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>12.9</td>
<td>1.6E+15</td>
<td>SO</td>
<td>(7)</td>
<td>1.3E+14</td>
</tr>
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</table>

Notes.

$^a$ Excitation temperature of $^{12}$CO is assumed for $^{18}$CO and $^{18}$O.

Excitation temperatures in brackets are assumed temperatures.

Table A-24(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
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<tr>
<th>Transition</th>
<th>$T_{\text{ex}}$ (K)</th>
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</tr>
<tr>
<td>11-10</td>
<td>19.1</td>
</tr>
<tr>
<td>12-11</td>
<td>19.1</td>
</tr>
<tr>
<td>15-14</td>
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<td>16-15</td>
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</table>

Figure A-24(b)
### NGC 6334(N1)

#### (a) Observed parameters

**Table A-25(a)**

<table>
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<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-2}))</th>
<th>(T_M) (K)</th>
<th>(\int T_M dv) (K km s(^{-1}))</th>
<th>(\delta \int T_M dv) (K km s(^{-1}))</th>
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<tr>
<td>(^{12})CO</td>
<td>1-0</td>
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<td>8.26</td>
<td>22.87</td>
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<td>3(1)-2(0)E</td>
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<td>4.8</td>
<td>2.14</td>
<td>11.03</td>
<td>22.7</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(1)-4(0) A(^{+})</td>
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<td>4.7</td>
<td>4.42</td>
<td>22.06</td>
<td>22.1</td>
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<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
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<td>4.7</td>
<td>4.42</td>
<td>22.06</td>
<td>2.6</td>
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</table>
(b) Derived parameters

<table>
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<th>Centre = -4.6 ± 0.3 km s⁻¹</th>
<th>$T_{\text{kin}} = 35.0$ K</th>
<th>( N(\text{H}_2) = (1.9 \pm 0.7) \times 10^{23}$ cm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 4.5 ± 0.3 km s⁻¹</td>
<td>( n(\text{H}_2) = 1.5 \times 10^4$ cm⁻³</td>
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</table>

(i) LVG models

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<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>$\chi^2_{\text{min}}$</th>
<th>( \Delta \chi^2 = 3.5 )</th>
<th>$\chi^2_{\text{min}}$</th>
<th>( \Delta \chi^2 = 3.5 )</th>
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</thead>
<tbody>
<tr>
<td>HCN</td>
<td>$T_k$ (K)</td>
<td>$T_k$ (K)</td>
<td>$N_{\text{tot}}$ (cm⁻³)</td>
<td>$N_{\text{tot}}$ (cm⁻³)</td>
<td>$f(X)$</td>
<td>$n(\text{H}_2)$ (cm⁻³)</td>
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<td>65</td>
<td>&gt;50</td>
<td>3E13</td>
<td>3E13</td>
<td>2E-10</td>
<td>1E6</td>
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</table>

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } N(\text{HC}_3\text{N}) \]

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } T_{\text{kin}} \]

Figure A-25(a)
(ii) LTE models

<table>
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<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>[N(X)/N(H$_2$)]</th>
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<tbody>
<tr>
<td>$^{12}$CO</td>
<td>35.0$^A$</td>
<td>8.7E+17</td>
<td>2.8E-06</td>
<td>HCN</td>
<td>(16)</td>
<td>1.5E+15</td>
<td>7.9E-08</td>
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<tr>
<td>C$^{18}$O</td>
<td>35.0$^A$</td>
<td>4.5E+16</td>
<td>1.9E-07</td>
<td>HCO$^+$</td>
<td>(16)</td>
<td>8.4E+14</td>
<td>3.5E-09</td>
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<tr>
<td>CO</td>
<td>(12)</td>
<td>1.0E+15</td>
<td>4.3E-09</td>
<td>HNC</td>
<td>(16)</td>
<td>5.8E+14</td>
<td>2.4E-09</td>
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<tr>
<td>CH$_3$OH</td>
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<td>2.9E+15</td>
<td>1.2E-08</td>
<td>OCS</td>
<td>35.3</td>
<td>2.2E+14</td>
<td>9.1E-10</td>
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<td>16.0</td>
<td>3.1E+15</td>
<td>1.3E-08</td>
<td>SO</td>
<td>(12)</td>
<td>3.6E+14</td>
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<td>HC$_3$N</td>
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<td>7.1E+13</td>
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Notes.

$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.

Excitation temperatures in brackets are assumed temperatures.

---

Table A-25(e)

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Figure A-25(b)
### Table A-26(a) Observed Line Intensities in RCW 122

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<th>dv (km s(^{-1}))</th>
<th>(T_{\text{mb}}) (K)</th>
<th>(\int T_{\text{mb}}dv) (K km s(^{-1}))</th>
<th>(\delta\int T_{\text{mb}}dv) (K km s(^{-1}))</th>
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<td>1-0</td>
<td>-12.0</td>
<td>6.9</td>
<td>6.16</td>
<td>45.24</td>
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<tr>
<td></td>
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<td>-13.3</td>
<td>3.8</td>
<td>0.36</td>
<td>1.46</td>
<td>8.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10.0</td>
<td>3.7</td>
<td>1.78</td>
<td>7.01</td>
<td>1.0</td>
</tr>
<tr>
<td>HC(^{18})O(^{+})</td>
<td>1-0</td>
<td>-11.9</td>
<td>3.2</td>
<td>0.22</td>
<td>0.73</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-12.5</td>
<td>17.1</td>
<td>0.14</td>
<td>2.56</td>
<td>0.9</td>
</tr>
<tr>
<td>H(^{13})C(^{18})N</td>
<td>11-10</td>
<td>-11.5</td>
<td>4.2</td>
<td>0.78</td>
<td>3.39</td>
<td>3.4</td>
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<td>3.7</td>
<td>0.64</td>
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<td>OCS</td>
<td>7-6</td>
<td>-11.1</td>
<td>5.4</td>
<td>0.17</td>
<td>0.99</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>8-7</td>
<td>-11.3</td>
<td>6.2</td>
<td>0.12</td>
<td>0.81</td>
<td>0.8</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-10.8</td>
<td>8.0</td>
<td>0.13</td>
<td>1.07</td>
<td>1.1</td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-11.1</td>
<td>6.9</td>
<td>0.15</td>
<td>1.08</td>
<td>1.1</td>
</tr>
<tr>
<td>CH(^{3})OH</td>
<td>2(1)-1(1)E</td>
<td>-12.1</td>
<td>6.8</td>
<td>0.66</td>
<td>4.77</td>
<td>4.8</td>
</tr>
<tr>
<td></td>
<td>2(0)-1(0)E</td>
<td>-11.0</td>
<td>4.1</td>
<td>0.42</td>
<td>1.81</td>
<td>0.3</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-12.3</td>
<td>5.0</td>
<td>1.15</td>
<td>6.17</td>
<td>7.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-11.1</td>
<td>22.7</td>
<td>0.05</td>
<td>1.15</td>
<td>0.9</td>
</tr>
</tbody>
</table>

### Notes.

* Emission self-absorbed

velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

Hyperfine components of transition blended. Velocity corrected to frequency of the F=2-1 hyperfine component.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = -12.0 ± 0.2 km s(^{-1})</th>
<th>(T_{\text{Kin}} = 38.3) K</th>
<th>(N(H_2) = (1.0 \pm 0.2)\times 10^{23}) cm(^{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 5.0 ± 0.4 km s(^{-1})</td>
<td>(n(H_2) = 7.7\times 10^3) cm(^{-3})</td>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>(T_{\text{X}}) (K)</th>
<th>(T_{\text{X}}) (K)</th>
<th>(N_{\text{tot}}) (cm(^{-3}))</th>
<th>(N_{\text{tot}}) (cm(^{-3}))</th>
<th>(f(X))</th>
<th>(n(H_2)) (cm(^{-3}))</th>
<th>(n(H_2)) (cm(^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(HC_3N)</td>
<td>15</td>
<td>3E11</td>
<td>3E13</td>
<td>3E13</td>
<td>3E10</td>
<td>3E10</td>
<td>&gt;3E4</td>
</tr>
</tbody>
</table>

\(\chi^2\) for \(n(H_2)\) and \(N(HC_3N)\)  
\(\chi^2\) for \(n(H_2)\) and \(T_{\text{kin}}\)  

**Figure A-26(a)**
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$N(X)/N(H_2)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$N(X)/N(H_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>38.3$^A$</td>
<td>2.0E+17</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(11)</td>
<td>8.4E+14</td>
<td>7.7E-09</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>38.3$^A$</td>
<td>3.1E+16</td>
<td>2.6E-07</td>
<td>HCO$^+$</td>
<td>(11)</td>
<td>3.9E+14</td>
<td>3.6E-09</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>5.6</td>
<td>3.4E+14</td>
<td>3.1E-09</td>
<td>HNC</td>
<td>(11)</td>
<td>1.6E+14</td>
<td>1.4E-09</td>
</tr>
<tr>
<td>CS</td>
<td>11.4</td>
<td>1.6E+15</td>
<td>1.4E-08</td>
<td>OCS</td>
<td>33.4</td>
<td>8.9E+13</td>
<td>8.1E-10</td>
</tr>
<tr>
<td>HCN</td>
<td>25.1</td>
<td>1.8E+13</td>
<td>1.6E-10</td>
<td>SO</td>
<td>(11)</td>
<td>2.2E+14</td>
<td>2.0E-09</td>
</tr>
</tbody>
</table>

Notes.
$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-26(e)

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>15.0</td>
</tr>
<tr>
<td>11-10</td>
<td>15.0</td>
</tr>
<tr>
<td>12-11</td>
<td>15.0</td>
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<tr>
<td>15-14</td>
<td>15.0</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-26(b)
### Observed Line Intensities in 351.6-1.3

#### Table A-27(a)

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB}dv) (K km s(^{-1}))</th>
<th>(\delta \int T_{MB}dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-14.2</td>
<td>15.5</td>
<td>8.82</td>
<td>145.60</td>
<td>334.6</td>
</tr>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>-10.4</td>
<td>6.5</td>
<td>27.31</td>
<td>189.02</td>
<td>98.1</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>-10.7</td>
<td>3.5</td>
<td>2.25</td>
<td>8.40</td>
<td>22.2</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>-9.8</td>
<td>2.5</td>
<td>2.48</td>
<td>6.72</td>
<td>29.5</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>-12.1</td>
<td>3.1</td>
<td>4.47</td>
<td>14.93</td>
<td>22.2</td>
</tr>
<tr>
<td>(^{13})CS</td>
<td>2-1</td>
<td>8.9</td>
<td>0.20</td>
<td>1.8</td>
<td>1.8</td>
<td>0.3</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0</td>
<td>(-9.5)</td>
<td>11.6</td>
<td>2.88</td>
<td>35.28</td>
<td>37.6</td>
</tr>
<tr>
<td>H(^{13})CN</td>
<td>1-0</td>
<td>-7.8</td>
<td>17.8</td>
<td>0.26</td>
<td>4.89</td>
<td>4.9</td>
</tr>
<tr>
<td>HNC</td>
<td>1-0</td>
<td>-14.0</td>
<td>3.0</td>
<td>0.96</td>
<td>3.10</td>
<td>12.8</td>
</tr>
<tr>
<td>HN(^{13})C</td>
<td>1-0</td>
<td>-12.1</td>
<td>7.0</td>
<td>0.17</td>
<td>1.28</td>
<td>1.3</td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>&lt;0.02</td>
<td>&lt;0.00</td>
<td>&lt;0.00</td>
<td>&lt;0.4</td>
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</tr>
<tr>
<td>HCO(^{+})</td>
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<td>-9.7</td>
<td>3.9</td>
<td>3.07</td>
<td>12.75</td>
<td>20.1</td>
</tr>
<tr>
<td>H(^{18})CO(^{+})</td>
<td>1-0</td>
<td>-14.5</td>
<td>4.1</td>
<td>0.34</td>
<td>1.52</td>
<td>3.0</td>
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<tr>
<td>HC(^{18})O(^{+})</td>
<td>1-0</td>
<td>-10.6</td>
<td>2.3</td>
<td>0.61</td>
<td>1.48</td>
<td>1.0</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>10-9</td>
<td>-12.5</td>
<td>6.0</td>
<td>0.27</td>
<td>1.76</td>
<td>1.8</td>
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<tr>
<td>HC(_3)N</td>
<td>11-10</td>
<td>-10.9</td>
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<td>0.13</td>
<td>0.67</td>
<td>0.7</td>
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<tr>
<td>HC(_3)N</td>
<td>12-11</td>
<td>-10.2</td>
<td>4.5</td>
<td>0.28</td>
<td>1.34</td>
<td>1.3</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>15-14</td>
<td>-</td>
<td>-</td>
<td>&lt;0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>-</td>
<td>-</td>
<td>&lt;0.3</td>
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<td></td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
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</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>&lt;0.7</td>
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<td></td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>2(1)-1(1)E</td>
<td>-52.5</td>
<td>2.1</td>
<td>0.21</td>
<td>0.46</td>
<td>0.5</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>2(0)-1(0)E</td>
<td>-14.3</td>
<td>2.4</td>
<td>0.23</td>
<td>0.59</td>
<td>0.6</td>
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<td>CH(_3)OH</td>
<td>2(0)-1(0) A+</td>
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<td>3.2</td>
<td>0.51</td>
<td>1.76</td>
<td>1.8</td>
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<tr>
<td>CH(_3)OH</td>
<td>2(-1)-1(-1)E</td>
<td>-4.0</td>
<td>2.6</td>
<td>0.35</td>
<td>0.96</td>
<td>1.0</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(1)-2(1)E</td>
<td>-</td>
<td>-</td>
<td>&lt;0.9</td>
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<tr>
<td>CH(_3)OH</td>
<td>5(-1)-4(0)E</td>
<td>-</td>
<td>-</td>
<td>&lt;0.4</td>
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<td></td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
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<td>2.9</td>
<td>1.16</td>
<td>3.56</td>
<td>5.9</td>
</tr>
<tr>
<td>SO</td>
<td>-13.0</td>
<td>3.8</td>
<td>0.58</td>
<td>2.34</td>
<td>0.7</td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**
- Emission self-absorbed
- Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions. Hyperfine components of transition blended. Velocity corrected to frequency of the F-2-1 hyperfine component.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre</th>
<th>Width</th>
<th>$T_{\text{kin}}$</th>
<th>$N(\text{H}_2)$</th>
<th>$n(\text{H}_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-14.0 \pm 0.3$, $-10.4 \pm 0.2$ km s$^{-1}$</td>
<td>$4.1 \pm 0.4$ km s$^{-1}$</td>
<td>30.8 K</td>
<td>$(8.6 \pm 0.5) \times 10^{22}$ cm$^{-2}$</td>
<td>$6.7 \times 10^3$ cm$^{-3}$</td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\Delta\chi^2 = 3.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$\text{C}_2$N</td>
<td>$T_k$ (K)</td>
<td>$T_k$ (K)</td>
<td>$N_{\text{tot}}$ (cm$^{-3}$)</td>
<td>$N_{\text{tot}}$ (cm$^{-3}$)</td>
<td>$f(X)$</td>
<td>$n(\text{H}_2)$ (cm$^{-3}$)</td>
</tr>
<tr>
<td>HC$_2$N</td>
<td>40</td>
<td>5-100$^a$</td>
<td>3E12</td>
<td>1E11-1E14</td>
<td>3E-11</td>
<td>3E5</td>
</tr>
</tbody>
</table>

Notes.

$^a$ Fit not constrained by data. Limits are maximum and minimum values considered in model.

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{H}_2)$

$\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-27(a)
(ii) LTE models

Table A-27(d) Molecular Abundances in 351.6-1.3 Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>30.8$^A$</td>
<td>2.0E+17</td>
<td>1.8E-06</td>
<td>HC$_3$N</td>
<td>14.0</td>
<td>6.9E+12</td>
<td>6.3E-11</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>30.8$^A$</td>
<td>2.1E+16</td>
<td>1.9E-07</td>
<td>HCN</td>
<td>(6)</td>
<td>1.6E+14</td>
<td>1.5E-09</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>20.3</td>
<td>3.0E+14</td>
<td>2.7E-09</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>7.6E+13</td>
<td>6.9E-10</td>
</tr>
<tr>
<td>CS</td>
<td>6.4</td>
<td>1.9E+14</td>
<td>1.7E-09</td>
<td>HNC</td>
<td>(6)</td>
<td>4.9E+13</td>
<td>4.4E-10</td>
</tr>
</tbody>
</table>

Notes.

$^A$ Excitation temperature of $^{13}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

---

Table A-27(e) Excitation Temperature of HC$_3$N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>28.2</td>
</tr>
<tr>
<td>11-10</td>
<td>24.5</td>
</tr>
<tr>
<td>12-11</td>
<td>21.7</td>
</tr>
<tr>
<td>15-14</td>
<td>12.1</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-27(b)
(a) Observed parameters

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>T(_{mb}) (K)</th>
<th>(\Delta T_{mb}) (K km s(^{-1}))</th>
<th>Total Emission (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^13)CO</td>
<td>1-0</td>
<td>-20.0</td>
<td>4.2</td>
<td>19.97</td>
<td>89.30</td>
<td>231.3</td>
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<tr>
<td></td>
<td></td>
<td>-14.6</td>
<td>6.3</td>
<td>21.17</td>
<td>142.03</td>
<td>27.3</td>
</tr>
<tr>
<td>(^13)CO</td>
<td>1-0</td>
<td>-17.7</td>
<td>5.6</td>
<td>14.03</td>
<td>83.69</td>
<td>93.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-20.1</td>
<td>1.5</td>
<td>5.83</td>
<td>9.31</td>
<td>11.0</td>
</tr>
<tr>
<td>C(^18)O</td>
<td>1-0</td>
<td>-17.8</td>
<td>4.3</td>
<td>4.88</td>
<td>22.34</td>
<td>22.3</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>-14.4</td>
<td>4.0</td>
<td>2.65</td>
<td>11.36</td>
<td>27.2</td>
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<td>CS</td>
<td>3-2</td>
<td>-18.4</td>
<td>3.4</td>
<td>1.58</td>
<td>5.70</td>
<td>21.5</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>-14.9</td>
<td>4.7</td>
<td>3.18</td>
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<td>0.51</td>
<td>0.5</td>
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<td>0.28</td>
<td>0.63</td>
<td>0.6</td>
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<td>4.3</td>
<td>1.97</td>
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<td>9.1</td>
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<td>2(-1)-1(-1)E</td>
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<td>4.9</td>
<td>1.59</td>
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<td>3(2)-2(1)</td>
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<td>4.1</td>
<td>1.41</td>
<td>6.16</td>
<td>10.8</td>
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<td>8.2</td>
<td>0.53</td>
<td>4.63</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Notes.

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions. B. Hyperfine components of transition blended. Velocity corrected to frequency of the F=2-1 hyperfine component.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre</th>
<th>Width</th>
<th>$T_{\text{kin}}$</th>
<th>$N(\text{H}_2)$</th>
<th>$n(\text{H}_2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-17.5 \pm 0.5$ km s$^{-1}$</td>
<td>$4.2 \pm 0.4$ km s$^{-1}$</td>
<td>24.6 K</td>
<td>$(9.9 \pm 2.8) \times 10^{22}$ cm$^{-2}$</td>
<td>$7.7 \times 10^{3}$ cm$^{-3}$</td>
</tr>
</tbody>
</table>

(i) LVG models

Table A-28(c)

<table>
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<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\chi^2$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\chi^2$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\chi^2$</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>15</td>
<td>$&gt;15$</td>
<td>3E13</td>
<td>3E13-1E14</td>
<td>3E-10</td>
<td>1E7</td>
<td>$&gt;3E4$</td>
<td></td>
</tr>
</tbody>
</table>

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$

$\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-28(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$CO</td>
<td>24.6</td>
<td>2.04E+17</td>
<td>1.19E-06</td>
<td>HCN</td>
<td>(6)</td>
<td>1.6E+14</td>
<td>9.28E-10</td>
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<tr>
<td>C$^{18}$O</td>
<td>24.6</td>
<td>3.4E+16</td>
<td>1.98E-07</td>
<td>HCO$^+$</td>
<td>(6)</td>
<td>2.11E+14</td>
<td>1.23E-09</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>8.1</td>
<td>3.92E+15</td>
<td>2.28E-08</td>
<td>HNC</td>
<td>(6)</td>
<td>1.28E+14</td>
<td>7.43E-10</td>
</tr>
<tr>
<td>CS</td>
<td>6.0</td>
<td>9.11E+13</td>
<td>5.3E-10</td>
<td>OCS</td>
<td>24.3</td>
<td>6.11E+13</td>
<td>3.55E-10</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>14.4</td>
<td>3.8E+13</td>
<td>2.09E-10</td>
<td>SO</td>
<td>(6)</td>
<td>1.75E+14</td>
<td>1.02E-09</td>
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**Notes.**

$^A$ Excitation temperature of $^{13}$CO is assumed for $^{13}$CO and C$^{18}$O.

Excitation temperatures in brackets are assumed temperatures.

**Figure A-28(b)**

**Table A-28(e)**

<table>
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<th>Transition</th>
<th>$T_{ex}$ (K)</th>
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<tr>
<td>11-10</td>
<td>14.8</td>
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<td>12-11</td>
<td>14.8</td>
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<td>15-14</td>
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<tr>
<td>16-15</td>
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</tbody>
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### Table A-29(a)

**Observed Line Intensities in G1.6-0.025 (50 km s\(^{-1}\)) Emission near 50 km s\(^{-1}\)**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
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</thead>
<tbody>
<tr>
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<td>Centre (km s(^{-1}))</td>
<td>dv (km s(^{-1}))</td>
<td>T(_{MB}) (K)</td>
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<td>1-0</td>
<td>59.9</td>
<td>19.6</td>
<td>16.4</td>
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<td>61.3</td>
<td>15.9</td>
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<td>45.3</td>
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</tr>
<tr>
<td>^13CO</td>
<td>1-0</td>
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<td>24.9</td>
<td>2.4</td>
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<td>$\delta T_{MB dv}$</td>
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<td>(K)</td>
<td>(K km s$^{-1}$)</td>
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<td>0.37</td>
<td>7.24</td>
</tr>
<tr>
<td>SiO</td>
<td>2-1</td>
<td>43.0 8.2</td>
<td>0.50</td>
<td>4.40</td>
</tr>
<tr>
<td>SiO</td>
<td>3-2</td>
<td>58.7 16.3</td>
<td>0.37</td>
<td>10.28</td>
</tr>
<tr>
<td>SiO</td>
<td>58.1 16.3</td>
<td>0.36</td>
<td>3.08</td>
<td>9.6 1.2</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>2(0,2)-1</td>
<td>42.5 8.1</td>
<td>0.56</td>
<td>4.87</td>
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<tr>
<td>H$_2$CO</td>
<td>2(1,1)-1</td>
<td>58.2 14.2</td>
<td>0.36</td>
<td>5.47</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>62.6 16.9</td>
<td>0.36</td>
<td>5.24</td>
<td>13.6 1.6</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>2(1,2)-1</td>
<td>41.9 7.7</td>
<td>0.63</td>
<td>6.17</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>59.5 14.4</td>
<td>0.40</td>
<td>6.17</td>
<td>18.85303 2.2</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>62.6 16.9</td>
<td>0.12</td>
<td>9.6</td>
<td>6.81</td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>58.2 8.3</td>
<td>0.29</td>
<td>4.90</td>
<td></td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>67.4 9.8</td>
<td>0.38</td>
<td>4.06</td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**

* Emission self-absorbed

Velocities shown in brackets have not been corrected for the frequency of hyperfine transitions. **Hyperfine components of transition blended. Velocity corrected to frequency of the P=2-1 hyperfine component.
(b) Derived parameters

Table A-29(b)  Derived physical parameters of G1.6-0.025 (60 km s\(^{-1}\))

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centre</td>
<td>47 ± 1, 60 +/- 1 km s(^{-1})</td>
</tr>
<tr>
<td>(T_{\text{kin}})</td>
<td>19.9K</td>
</tr>
<tr>
<td>(N(H_2))</td>
<td>(7 ± 2)E+22 cm(^{-2})</td>
</tr>
<tr>
<td>Width</td>
<td>9.1 ± 0.9, 18 +/- 2 km s(^{-1})</td>
</tr>
</tbody>
</table>

(i) LVG models

**Emission near 50 km s\(^{-1}\)**

Table A-29(c)  Molecular Abundances in G1.6-0.025 (60 km s\(^{-1}\)) LVG Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>(T_K) (K)</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(\chi^2_{\text{min}})</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(\chi^2_{\text{min}})</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(\chi^2_{\text{min}})</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(\chi^2_{\text{min}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC(_3)N</td>
<td>45</td>
<td>40-50</td>
<td>3E15</td>
<td>&gt;3E15</td>
<td>4E-8</td>
<td>3E4</td>
<td>3E3-3E4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(\chi^2\) for \(n(H_2)\) and \(N(HC_3N)\)  
\(\chi^2\) for \(n(H_2)\) and \(T_{\text{kin}}\)

Figure A-29(a) (50 km/s)
(ii) LTE models

Emission near 50 km s\(^{-1}\)

Table A-29(d)

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>(T_{ex}) (K)</th>
<th>(N_{rot}) (cm(^{-2}))</th>
<th>([N(X)/N(H_2)])</th>
<th>MOLECULE</th>
<th>(T_{ex}) (K)</th>
<th>(N_{rot}) (cm(^{-2}))</th>
<th>([N(X)/N(H_2)])</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>19.9 (^A)</td>
<td>8.53E+16</td>
<td>1.22E-06</td>
<td>HCN</td>
<td>(4)</td>
<td>1.79E+14</td>
<td>1.63E-09</td>
</tr>
<tr>
<td>(^{18})CO</td>
<td>19.9 (^A)</td>
<td>1.58E+16</td>
<td>2.26E-07</td>
<td>HCO(^+)</td>
<td>(4)</td>
<td>1.57E+14</td>
<td>1.43E-09</td>
</tr>
<tr>
<td>CS</td>
<td>4.2</td>
<td>3.2E+14</td>
<td>2.91E-09</td>
<td>HNC</td>
<td>(4)</td>
<td>1.54E+14</td>
<td>1.4E-09</td>
</tr>
<tr>
<td>(\text{HC}_3\text{N})</td>
<td>12.2</td>
<td>8.3E+13</td>
<td>7.54E-10</td>
<td>SO</td>
<td>(8)</td>
<td>1.11E+14</td>
<td>1.01E-09</td>
</tr>
</tbody>
</table>

Notes.

\(^A\) Excitation temperature of \(^{12}\)CO.
Excitation temperatures in brackets are assumed temperatures.

Table A-29(e)

<table>
<thead>
<tr>
<th>Transition</th>
<th>(T_{ex}) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>17.8</td>
</tr>
<tr>
<td>11-10</td>
<td>15.6</td>
</tr>
<tr>
<td>12-11</td>
<td>13.3</td>
</tr>
<tr>
<td>15-14</td>
<td>6.7</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-29(b) (50 km/s)
<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>(T_{MB}) (K)</th>
<th>(\int T_{MB}dv) (K km s(^{-1}))</th>
<th>(\delta \int T_{MB}dv) (K km s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>157.5</td>
<td>33.4</td>
<td>13.03</td>
<td>463.57</td>
<td>463.6</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>162.3</td>
<td>29.8</td>
<td>1.55</td>
<td>49.08</td>
<td>49.1</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>167.3</td>
<td>30.0</td>
<td>0.59</td>
<td>54.30</td>
<td>18.0</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>156.5</td>
<td>28.7</td>
<td>1.27</td>
<td>38.86</td>
<td>38.9</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>155.6</td>
<td>26.3</td>
<td>0.96</td>
<td>26.77</td>
<td>26.8</td>
</tr>
<tr>
<td>(^{33})CS</td>
<td>2-1</td>
<td>162.9</td>
<td>33.6</td>
<td>0.12</td>
<td>4.11</td>
<td>4.1</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0(^a)</td>
<td>(145.9)</td>
<td>25.9</td>
<td>2.56</td>
<td>70.80</td>
<td>108.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(175.6)</td>
<td>22.4</td>
<td>1.60</td>
<td>38.05</td>
<td>38.0</td>
</tr>
<tr>
<td>HCN</td>
<td>3-2(^a)</td>
<td>(149.5)</td>
<td>21.7</td>
<td>1.15</td>
<td>26.64</td>
<td>30.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(170.9)</td>
<td>8.3</td>
<td>0.43</td>
<td>3.79</td>
<td>4.7</td>
</tr>
<tr>
<td>H(^{13})CN</td>
<td>1-0</td>
<td>136.8</td>
<td>6.0</td>
<td>0.19</td>
<td>1.19</td>
<td>10.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>153.5</td>
<td>15.8</td>
<td>0.48</td>
<td>8.14</td>
<td>5.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>171.9</td>
<td>8.8</td>
<td>0.16</td>
<td>1.45</td>
<td></td>
</tr>
<tr>
<td>HNC</td>
<td>1-0</td>
<td>154.2</td>
<td>24.7</td>
<td>2.71</td>
<td>67.81</td>
<td>67.8</td>
</tr>
<tr>
<td>HN(^{13})C</td>
<td>1-0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;2.7</td>
<td></td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>157.9</td>
<td>25.2</td>
<td>0.23</td>
<td>6.17</td>
<td>6.2</td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>1-0</td>
<td>155.5</td>
<td>36.4</td>
<td>1.24</td>
<td>48.27</td>
<td>56.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>161.0</td>
<td>17.9</td>
<td>0.41</td>
<td>7.73</td>
<td>7.7</td>
</tr>
<tr>
<td>HCO(^+)</td>
<td>3-2</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;5.6</td>
<td></td>
</tr>
<tr>
<td>H(^{13})CO(^+)</td>
<td>1-0</td>
<td>159.3</td>
<td>38.2</td>
<td>0.11</td>
<td>4.35</td>
<td>4.4</td>
</tr>
<tr>
<td>HC(^{18})O(^+)</td>
<td>1-0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;2.7</td>
<td></td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>10-9</td>
<td>157.8</td>
<td>19.7</td>
<td>0.71</td>
<td>14.85</td>
<td>14.9</td>
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<td>11-10</td>
<td>157.7</td>
<td>21.4</td>
<td>0.63</td>
<td>14.40</td>
<td>14.4</td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>12-11</td>
<td>158.5</td>
<td>22.1</td>
<td>0.51</td>
<td>12.02</td>
<td>12.0</td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>14-13</td>
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<td>18.3</td>
<td>0.39</td>
<td>7.86</td>
<td>7.7</td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>15-14</td>
<td>157.5</td>
<td>19.5</td>
<td>0.43</td>
<td>8.92</td>
<td>8.9</td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>16-15</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;2.3</td>
<td></td>
</tr>
<tr>
<td>HC(_2)N</td>
<td>17-16</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;2.7</td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>158.6</td>
<td>21.2</td>
<td>0.27</td>
<td>6.06</td>
<td>6.1</td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>159.4</td>
<td>24.6</td>
<td>0.22</td>
<td>5.67</td>
<td>5.7</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>160.5</td>
<td>25.7</td>
<td>0.26</td>
<td>7.03</td>
<td>7.0</td>
</tr>
<tr>
<td>OCS</td>
<td>11-10</td>
<td>156.4</td>
<td>22.1</td>
<td>0.28</td>
<td>6.60</td>
<td>6.6</td>
</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>156.9</td>
<td>21.6</td>
<td>0.18</td>
<td>4.22</td>
<td>4.2</td>
</tr>
<tr>
<td>CH(_2)OH</td>
<td>2-1(^a)</td>
<td>159.7</td>
<td>28.7</td>
<td>1.93</td>
<td>58.80</td>
<td>58.8</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>3(1)-4(0)(^a)</td>
<td>158.8</td>
<td>18.0</td>
<td>-0.13</td>
<td>-2.49</td>
<td>-2.5</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>5.36</td>
<td>5.4</td>
</tr>
<tr>
<td>SO</td>
<td>2(3)-1(2)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;2.4</td>
<td></td>
</tr>
<tr>
<td>SIO</td>
<td>2-1</td>
<td>156.0</td>
<td>27.7</td>
<td>0.54</td>
<td>15.84</td>
<td>15.8</td>
</tr>
<tr>
<td>SIO</td>
<td>3-2</td>
<td>154.8</td>
<td>24.4</td>
<td>0.45</td>
<td>11.79</td>
<td>11.8</td>
</tr>
<tr>
<td>H(_2)CO</td>
<td>2(0,2)-1</td>
<td>154.7</td>
<td>22.1</td>
<td>0.29</td>
<td>6.80</td>
<td>6.8</td>
</tr>
<tr>
<td>H(_2)CO</td>
<td>2(1,1)-1</td>
<td>155.9</td>
<td>27.5</td>
<td>0.51</td>
<td>14.92</td>
<td>14.9</td>
</tr>
<tr>
<td>H(_2)CO</td>
<td>2(1,2)-1</td>
<td>153.7</td>
<td>28.9</td>
<td>0.86</td>
<td>24.53</td>
<td>24.5</td>
</tr>
<tr>
<td>H(^{13})CO</td>
<td>2(1,2)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>&lt;1.5</td>
<td></td>
</tr>
</tbody>
</table>
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = 157 ± 1 km s(^{-1})</th>
<th>(T_{\text{kin}} = 16.4\text{K})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width = 27 ± 1 km s(^{-1})</td>
<td>(N(\text{H}_2) = (6.8 \pm 2.5) \times 10^{22} \text{cm}^{-2})</td>
</tr>
</tbody>
</table>

(i) LVG models

Emission near 155 km s\(^{-1}\)

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>(X_{\text{min}})</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(Y_{\text{min}})</th>
<th>(\Delta Y^2 = 3.5)</th>
<th>(X_{\text{min}})</th>
<th>(\Delta X^2 = 3.5)</th>
<th>(Y_{\text{min}})</th>
<th>(\Delta Y^2 = 3.5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC(_3)N</td>
<td>20</td>
<td>20-25</td>
<td>3E15</td>
<td>3E15</td>
<td>4E-8</td>
<td>3E6</td>
<td>&gt;3E5</td>
<td></td>
</tr>
</tbody>
</table>

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } N(\text{HC}_3\text{N}) \]

\[ \chi^2 \text{ for } n(\text{H}_2) \text{ and } T_{\text{kin}} \]

Figure A-29(c) (155 km/s)
(ii) LTE models

**Emission near 155 km s\(^{-1}\)**

Table A-29(i) Molecular Abundances in G1.6-0.025 (150 km s\(^{-1}\))

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>(T_\text{ex}) (K)</th>
<th>(N_\text{tot}) (\text{cm}^{-2})</th>
<th>(f(X))</th>
<th>MOLECULE</th>
<th>(T_\text{ex}) (K)</th>
<th>(N_\text{tot}) (\text{cm}^{-2})</th>
<th>(f(X))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{13}\text{CO})</td>
<td>16.4 (^{A})</td>
<td>4.92E+16</td>
<td>7.24E-07</td>
<td>(^{13}\text{CO})</td>
<td>(4)</td>
<td>9.53E+13</td>
<td>8.66E-10</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>16.4 (^{A})</td>
<td>1.73E+16</td>
<td>2.55E-07</td>
<td>HNC</td>
<td>(4)</td>
<td>4.3E+13</td>
<td>3.91E-10</td>
</tr>
<tr>
<td>CS</td>
<td>4.2</td>
<td>3.47E+14</td>
<td>3.16E-09</td>
<td>OCS</td>
<td>20.7</td>
<td>5.25E+14</td>
<td>4.78E-09</td>
</tr>
<tr>
<td>HCN</td>
<td>21.6</td>
<td>6.14E+13</td>
<td>5.58E-10</td>
<td>SO</td>
<td>(12)</td>
<td>6.1E+13</td>
<td>5.54E-10</td>
</tr>
<tr>
<td>HCN</td>
<td>(4)</td>
<td>2.41E+14</td>
<td>3.55E-09</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**

\(^{A}\) Excitation temperature of \(^{13}\text{CO}\) is assumed for \(^{13}\text{CO}\) and C\(^{18}\)O.

Excitation temperatures in brackets are assumed temperatures.

---

**Figure A-29(d) 155 (km/s)**

![Graph](#)

Table A-28(j)

<table>
<thead>
<tr>
<th>Transition</th>
<th>(T_\text{ex}) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>19.7</td>
</tr>
<tr>
<td>11-10</td>
<td>19.6</td>
</tr>
<tr>
<td>12-11</td>
<td>19.7</td>
</tr>
<tr>
<td>15-14</td>
<td>18.0</td>
</tr>
<tr>
<td>16-15</td>
<td>14.8</td>
</tr>
</tbody>
</table>
## Table A-30(a) Observed Line Intensities in R Cr A

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Centre (km s(^{-1}))</th>
<th>dv (km s(^{-1}))</th>
<th>T(_{MB}) (K)</th>
<th>(\int T_{MB}dv) (K km s(^{-1}))</th>
<th>(\delta \int T_{MB}dv) (K km s(^{-1}))</th>
<th>Total Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>4.9</td>
<td>0.9</td>
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<tr>
<td>(^{13})CO</td>
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<td>C(^{18})O</td>
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<td>0.6</td>
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<tr>
<td>(^{13})CS</td>
<td>2-1</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
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<tr>
<td>HCN</td>
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<td>0.8</td>
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<tr>
<td>HCN</td>
<td>1-0 F=0-1</td>
<td>(-1.5)</td>
<td>0.8</td>
<td>0.99</td>
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</tr>
<tr>
<td>H(^{13})CN</td>
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<td>-</td>
<td>-</td>
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<td></td>
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<td>HNC</td>
<td>1-0</td>
<td>*5.2</td>
<td>0.4</td>
<td>3.10</td>
<td>1.47</td>
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<td>HNC</td>
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<td>*6.8</td>
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<tr>
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<td>0.5</td>
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<td>0.34</td>
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<td>HNCO</td>
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<td>5.8</td>
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<td>0.25</td>
<td>0.13</td>
<td>0.1</td>
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<td>HCO(^{+})</td>
<td>1-0</td>
<td>5.4</td>
<td>1.4</td>
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<td>0.74</td>
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</tr>
<tr>
<td>HC(^{18})O(^{+})</td>
<td>1-0</td>
<td>-</td>
<td>-</td>
<td>0.00</td>
<td>&lt;0.1</td>
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</tr>
<tr>
<td>HC(_{3})N</td>
<td>10-9</td>
<td>5.6</td>
<td>0.4</td>
<td>1.93</td>
<td>0.78</td>
<td>0.8</td>
<td>0.3</td>
</tr>
<tr>
<td>HC(_{3})N</td>
<td>11-10</td>
<td>5.7</td>
<td>0.4</td>
<td>1.21</td>
<td>0.54</td>
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<td>0.2</td>
</tr>
<tr>
<td>HC(_{3})N</td>
<td>12-11</td>
<td>-</td>
<td>-</td>
<td>&lt;0.1</td>
<td></td>
<td></td>
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<tr>
<td>HC(_{3})N</td>
<td>15-14</td>
<td>-</td>
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<tr>
<td>OCS</td>
<td>7-8</td>
<td>-</td>
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<td>&lt;0.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>-</td>
<td>-</td>
<td>&lt;0.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_{3})OH</td>
<td>2(1)-1(1)E</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>CH(_{3})OH</td>
<td>2(0)-1(0)E</td>
<td>-</td>
<td>-</td>
<td>&lt;0.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_{3})OH</td>
<td>2(0)-1(0) A(^{+})</td>
<td>5.6</td>
<td>0.5</td>
<td>2.82</td>
<td>1.54</td>
<td>1.5</td>
<td>0.3</td>
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<tr>
<td>CH(_{3})OH</td>
<td>2(1)-1(-1)E</td>
<td>5.6</td>
<td>0.5</td>
<td>2.19</td>
<td>1.18</td>
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<td>CH(_{3})OH</td>
<td>3(0)-2(0)A(^{+})</td>
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<td>0.3</td>
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<tr>
<td>CH(_{3})OH</td>
<td>3(1)-2(-1)E</td>
<td>5.8</td>
<td>0.5</td>
<td>0.82</td>
<td>0.41</td>
<td>0.4</td>
<td>0.2</td>
</tr>
<tr>
<td>CH(_{3})OH</td>
<td>3(0)-2(0)E</td>
<td>-</td>
<td>-</td>
<td>&lt;0.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_{3})OH</td>
<td>3(1)-4(0) A(^{+})</td>
<td>-</td>
<td>-</td>
<td>&lt;0.05</td>
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<td></td>
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<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>5.2</td>
<td>0.6</td>
<td>2.46</td>
<td>1.57</td>
<td>1.6</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Notes:**

* Emission self-absorbed

**Emission velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

** Hyperfine components of transition blended. Velocity corrected to frequency of the F=2-1 hyperfine component.
(b) Derived parameters

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>Derived physical conditions of R Cr A</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Centre = 5.4 ± 0.3 km s(^{-1})</td>
</tr>
<tr>
<td></td>
<td>Width = 0.5 ± 0.1 km s(^{-1})</td>
</tr>
<tr>
<td></td>
<td>(T_{\text{kin}} = 15.9) K</td>
</tr>
<tr>
<td></td>
<td>(N(\text{H}_2) = (6.8 \pm 3.3) \times 10^{21}) cm(^{-2})</td>
</tr>
<tr>
<td></td>
<td>(n(\text{H}_2) = 5.3 \times 10^2) cm(^{-3})</td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>Molecular Abundances in R Cr A</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LVG Models</td>
</tr>
<tr>
<td></td>
<td>(\chi^2 = 1)</td>
</tr>
<tr>
<td></td>
<td>(\Delta\chi^2 = 1)</td>
</tr>
<tr>
<td></td>
<td>(\chi^2) (\chi^2)</td>
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<tr>
<td></td>
<td>(\chi^2) (\Delta\chi^2 = 1)</td>
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<tr>
<td>(\text{HC}_3\text{N})</td>
<td>(T_{\text{kin}} = 15.9) K</td>
</tr>
<tr>
<td></td>
<td>(N_{\text{tot}} = 5.25-35)</td>
</tr>
<tr>
<td></td>
<td>(N_{\text{tot}} = 3 \times 10^3)</td>
</tr>
<tr>
<td></td>
<td>(f(X) = 3 \times 10^2) cm(^{-3})</td>
</tr>
<tr>
<td></td>
<td>(n(\text{H}_2) = 4.4 \times 10^8)</td>
</tr>
<tr>
<td></td>
<td>(n(\text{H}_2) = 1 \times 10^4)</td>
</tr>
</tbody>
</table>

\(\chi^2\) for \(n(\text{H}_2)\) and \(N(\text{HC}_3\text{N})\)

\(\chi^2\) for \(n(\text{H}_2)\) and \(T_{\text{kin}}\)

Figure A-30(a)
(ii) LTE models

Table A-30(d) Molecular Abundances in R Cr A Optically Thin LTE Models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>( T_{\text{ex}} ) (K)</th>
<th>( N_{\text{tot}} ) (cm(^{-2}))</th>
<th>( f(X) )</th>
<th>MOLECULE</th>
<th>( T_{\text{ex}} ) (K)</th>
<th>( N_{\text{tot}} ) (cm(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{12})CO</td>
<td>15.0(^{a})</td>
<td>9.6E+15</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(7)</td>
<td>1.1E+13</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>15.0(^{a})</td>
<td>3.0E+15</td>
<td>5.7E-07</td>
<td>HCO(^{+})</td>
<td>(7)</td>
<td>3.2E+13</td>
</tr>
<tr>
<td>CH(_3)OH</td>
<td>5.9</td>
<td>1.2E+14</td>
<td>2.3E-08</td>
<td>HNC</td>
<td>(7)</td>
<td>1.5E+13</td>
</tr>
<tr>
<td>CS</td>
<td>6.7</td>
<td>1.6E+13</td>
<td>3.0E-09</td>
<td>SO</td>
<td>(6)</td>
<td>1.4E+13</td>
</tr>
<tr>
<td>HC(_3)N</td>
<td>8.7</td>
<td>7.0E+12</td>
<td>1.0E-09</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes.
\(^{a}\) Excitation temperature of \(^{12}\)CO is assumed for \(^{13}\)CO and C\(^{18}\)O.
Excitation temperatures in brackets are assumed temperatures.

Table A-30(e) Excitation Temperature of HC\(_3\)N Transitions from LVG Models

<table>
<thead>
<tr>
<th>Transition</th>
<th>( T_{\text{ex}} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>5.9</td>
</tr>
<tr>
<td>11-10</td>
<td>5.4</td>
</tr>
<tr>
<td>12-11</td>
<td></td>
</tr>
<tr>
<td>15-14</td>
<td></td>
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<tr>
<td>16-15</td>
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Figure A-30(b)
## M 17

(a) Observed parameters

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<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Gaussian Components of fit</th>
<th>Total Emission</th>
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</thead>
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<tr>
<td></td>
<td></td>
<td>Centre (km s(^{-1}))</td>
<td>dv (km s(^{-1}))</td>
</tr>
<tr>
<td>(^{12})CO</td>
<td>1-0</td>
<td>20.5</td>
<td>19.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>19.9</td>
<td>6.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>24.7</td>
<td>1.1</td>
</tr>
<tr>
<td>(^{13})CO</td>
<td>1-0</td>
<td>18.4</td>
<td>4.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.5</td>
<td>2.6</td>
</tr>
<tr>
<td>C(^{18})O</td>
<td>1-0</td>
<td>18.9</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22.8</td>
<td>1.9</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>19.5</td>
<td>6.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>19.3</td>
<td>3.1</td>
</tr>
<tr>
<td>HCN</td>
<td>1-0 F=2-1</td>
<td>19.7</td>
<td>4.4</td>
</tr>
<tr>
<td></td>
<td>1-0 F=1-1</td>
<td>(12.6)</td>
<td>4.7</td>
</tr>
<tr>
<td></td>
<td>1-0 F=0-1</td>
<td>(25.7)</td>
<td>3.7</td>
</tr>
<tr>
<td>H(^{13})CN</td>
<td>1-0 F=2-1</td>
<td>19.4</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>1-0 F=1-1</td>
<td>(12.5)</td>
<td>5.0</td>
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<td></td>
<td>1-0 F=0-1</td>
<td>(24.0)</td>
<td>4.3</td>
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<tr>
<td>HN(^{13})C</td>
<td>1-0</td>
<td>19.4</td>
<td>3.3</td>
</tr>
<tr>
<td>HNCO</td>
<td>4(0,4)-3(0,3)</td>
<td>19.8</td>
<td>3.3</td>
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<tr>
<td>HCO(^{+})</td>
<td>1-0</td>
<td>20.0</td>
<td>5.0</td>
</tr>
<tr>
<td>H(^{13})CO(^{+})</td>
<td>1-0</td>
<td>22.8</td>
<td>2.5</td>
</tr>
<tr>
<td>HC(^{18})O(^{+})</td>
<td>1-0</td>
<td>19.1</td>
<td>3.1</td>
</tr>
<tr>
<td>HCN</td>
<td>10-9</td>
<td>22.1</td>
<td>1.2</td>
</tr>
<tr>
<td>HCN</td>
<td>12-11</td>
<td>19.2</td>
<td>3.2</td>
</tr>
<tr>
<td>OCS</td>
<td>7-8</td>
<td>23.3</td>
<td>4.4</td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>19.0</td>
<td>8.7</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_{3})OH</td>
<td>2(1)-1(1)E</td>
<td>19.6</td>
<td>9.2</td>
</tr>
<tr>
<td>CH(_{2})OH</td>
<td>2(0)-1(0)E</td>
<td>18.5</td>
<td>5.0</td>
</tr>
<tr>
<td>CH(_{2})OH</td>
<td>2(0)-1(0) A+</td>
<td>18.9</td>
<td>4.1</td>
</tr>
<tr>
<td>CH(_{2})OH</td>
<td>2(-1)-1(-1)E</td>
<td>18.9</td>
<td>4.4</td>
</tr>
</tbody>
</table>

* Emission self-absorbed

... velocities shown in brackets have not been corrected for the frequency of hyperfine transitions.

* ... Hyperfine components of transition blended. Velocity corrected to frequency of the F=2-1 hyperfine component.
(b) Derived parameters

<table>
<thead>
<tr>
<th>Centre = $19.3 \pm 0.5$ km s$^{-1}$</th>
<th>$T_{\text{kin}} = 44.2$ K</th>
<th>$N(\text{H}_2) = (1.4 \pm 0.2) \times 10^{23}$ cm$^{-3}$</th>
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<td>Width = $4.0 \pm 0.4$ km s$^{-1}$</td>
<td>$n(\text{H}_2) = 1.1 \times 10^4$ cm$^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>

(i) LVG models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$\chi^2_{\text{min}}$</th>
<th>$T_K$ (K)</th>
<th>$T_K$ (K)</th>
<th>$N_{\text{tot}}$ (cm$^{-3}$)</th>
<th>$N_{\text{tot}}$ (cm$^{-3}$)</th>
<th>$f(X)$</th>
<th>$n(\text{H}_2)$ (cm$^{-3}$)</th>
<th>$n(\text{H}_2)$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC$_3$N</td>
<td>15</td>
<td>15-20</td>
<td>1E14</td>
<td>1E14</td>
<td>7E-10</td>
<td>3E6</td>
<td>$&gt;3E5$</td>
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</tr>
</tbody>
</table>

$\chi^2$ for $n(\text{H}_2)$ and $N(\text{HC}_3\text{N})$

$\chi^2$ for $n(\text{H}_2)$ and $T_{\text{kin}}$

Figure A-31(a)
(ii) LTE models

<table>
<thead>
<tr>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-3}$)</th>
<th>$f(X)$</th>
<th>MOLECULE</th>
<th>$T_{ex}$ (K)</th>
<th>$N_{tot}$ (cm$^{-2}$)</th>
<th>$f(X)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}$CO</td>
<td>44.2$^A$</td>
<td>3.4E+17</td>
<td>1.8E-06</td>
<td>HCN</td>
<td>(14)</td>
<td>1.1E+15</td>
<td>5.</td>
</tr>
<tr>
<td>C$^{18}$O</td>
<td>44.2$^A$</td>
<td>3.9E+16</td>
<td>2.0E-07</td>
<td>HCO$^+$</td>
<td>(14)</td>
<td>7.0E+14</td>
<td>3.</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>25.5</td>
<td>9.5E+14</td>
<td>5.0E-09</td>
<td>HNC</td>
<td>(14)</td>
<td>2.1E+14</td>
<td>1.</td>
</tr>
<tr>
<td>CS</td>
<td>13.6</td>
<td>2.3E+14</td>
<td>1.2E-09</td>
<td>OCS</td>
<td>29.2</td>
<td>8.3E+13</td>
<td>4.</td>
</tr>
<tr>
<td>HC$_3$N</td>
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<td>5.1E+13</td>
<td>2.7E-10</td>
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</tr>
</tbody>
</table>

Notes.

$^A$ Excitation temperature of $^{12}$CO is assumed for $^{13}$CO and C$^{18}$O.
Excitation temperatures in brackets are assumed temperatures.

Table A-31(e)

<table>
<thead>
<tr>
<th>Transition</th>
<th>$T_{ex}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-9</td>
<td>14.7</td>
</tr>
<tr>
<td>11-10</td>
<td>-</td>
</tr>
<tr>
<td>12-11</td>
<td>14.5</td>
</tr>
<tr>
<td>15-14</td>
<td>-</td>
</tr>
<tr>
<td>16-15</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure A-31(b)
Appendix B

Observed Spectra of Dense Cores

Molecules in Southern Molecular Clouds: A Millimetre-wave Study of Dense Cores

Maria R. Hunt
Figure B-1 (a)

Spectra of HH 46
Figure B-1 (b)  

Spectra of HH 46
Figure B-2 (a)

Spectra of G265.1+1.5
(RCW 36)
Figure B-3 (a)

Spectra of G268.4-0.8
Figure B-3 (b)
Figure B-4 (a)

Spectra of Cham D.C.
(Cha 4)
Figure B-5 (a)

Spectra of G291.3-0.7
(RCW 57 (E))
Spectra of G291-3.0.7 (RCW 57(E))

Figure B-5 (b)
Figure B-6 (a)

Spectra of G291.3-0.7
(RCW 57 (W))
Figure B-7 (a)

Spectra of Coalsack D.C. (CS 1)
Figure B-8 (a)

Spectra of G301.0+1.2 (RCW 65)
Figure B-8 (b) Spectra of G301.0+1.2 (RCW 65)
Figure B-9 (a)

Spectra of G305.4+0.2
Figure B-10 (a)

Spectra of G311.6+0.3
Spectra of G31.1+0.3

Figure B-10 (b)
**Figure B-11 (a)**

Spectra of G322.2+0.6 (RCW 92)
Spectra of G322.2+0.6 (RCW 92)

Figure B-11 (b)

velocities (km/s)
Figure B-12 (a)

Spectra of Lupus D.C. (Lup 4)
Figure B-12 (b) Spectra of Lupus D.C. (Lup 4)

Velocity (km/s)

CS2-1
CS3-2
HNC1-0
HC3N10-9
HC3N11-0
HC3N12-11
HC3N15-4
SO3(2)-O(1)
CH3OH 2(0)-1(0)
Figure B-13 (a)

Spectra of G326.7+0.6
Figure B-14 (a)

Spectra of G327.3-0.5
Figure B-15 (a)

Spectra of G331.5-0.1
Spectra of G333.0-0.6

Figure B-16 (a)
Figure B-17 (a)

Spectra of G333.4-0.4
Spectra of G333.4-4.4

Figure B-17 (b)

- CS3-1
- CS3-2
- HCN1-0
- HCS1-1
Figure B-18 (a)

Spectra of G333.6-0.2
Figure B-19 (a)

Spectra of IRAS 16562
Figure B-19 (b)
Figure B-20 (a)

Spectra of G345.5+0.3
Figure B-21 (a)

Spectra of NGC 6334 (S)
Figure B-22 (a)

Spectra of NGC 6334 (CO)
Figure B-23 (a)

Spectra of NGC 6334 (N)
Figure B-24 (a)

Spectra of NGC 6334 (NI)
Figure B-25 (a)

Spectra of G348.7-1.0 (RCW 122)
Figure B-26 (a)
*Spectra of G351.6-1.3*
Figure B.26 (b)

Spectra of C3H1.3
Figure B-27 (a)
Spectra of G353.4-0.4
Figure B-27 (b)  
Spectra of G353.4-0.4
Figure B-28 (a)

Spectra of G1.6-0.025
Figure B-29 (a)

Spectra of G1.6-0.025
Figure B-30 (a)

Spectra of Cor Aust D.C. (RCrA)
Figure B-30 (b)  
Spectra of Cor Aust D.C. (RCrA)
Figure B-31 (a)

Spectra of M17 (M17 SW)
Appendix C

Partition Functions and Einstein A Coefficients

Molecules in Southern Molecular Clouds:
A Millimetre-wave Study of Dense Cores

Maria R. Hunt
Chapter C Appendix C
Partition Functions and Einstein A Coefficients

Partition functions and Einstein A coefficients used in this thesis have been calculated from data in the on-line Caltech Submillimeter, Millimeter, and Microwave Spectral Line Catalog of Pickett et al. (1998) and are tabulated in this appendix.

C.1 Partition Functions

The Boltzmann distribution describes the energy level population distribution for a gas in thermodynamic equilibrium and is given by (2.14) and repeated here.

\[ \frac{N_i}{N} = \frac{g_i}{U} e^{-\frac{E_i}{kT}} \quad \text{(C.1)} \]

where \( N_i \) = the number of particles in state \( i \)
\( N = \) the total number of particles over all states
\( E_i = \) the energy of level \( i \)
\( g_i = \) statistical weight (number of degenerate states)
\( U = \) the partition function

The partition function is a sum over all energy states that normalizes the distribution (i.e. ensures that the sum of the terms \( N_i \) totals to \( N \)) and is given by

\[ U = \sum_i g_i e^{-\frac{E_i}{kT}} \quad \text{(C.2)} \]

The partition function is temperature dependent and Pickett et al. (1998), have calculated the sum over states for 7 temperatures between 9 and 300 K for the molecules in their catalogue. The values given in Pickett et al. have been used to find the temperature dependence of the partition function for the molecules used in this thesis and the derived equations are given in Table C-1. These equations have been used to calculate the partition function for the molecular abundance calculations in this thesis.

Calculating the sum over states is the most accurate way to find the partition function if the information is available. However, until recently, analytical approximations to the
partition function have generally been used. Analytical expressions for calculating the partition function can be found in Townes and Schawlow (1975) and Emerson (1996).

**Table C-1 Temperature dependent expression for partition function.**

All equations are calculated from the data of Pickett et al. (1998), and have correlation coefficient $r^2 = 1$.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Partition Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>C$_2$H</td>
<td>$Q = (1.9158)T$</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>$Q = (1.2343)T^{1.5}$</td>
</tr>
<tr>
<td>CS</td>
<td>$Q = (0.8524)T$</td>
</tr>
<tr>
<td>$^{13}$CS</td>
<td>$Q = (0.9029)T$</td>
</tr>
<tr>
<td>HCN</td>
<td>$Q = (1.4158)T$</td>
</tr>
<tr>
<td>H$^{13}$CN</td>
<td>$Q = (1.4531)T$</td>
</tr>
<tr>
<td>HNC</td>
<td>$Q = (0.4615)T$</td>
</tr>
<tr>
<td>HN$^{13}$C</td>
<td>$Q = (0.4802)T$</td>
</tr>
<tr>
<td>HCO$^+$</td>
<td>$Q = (0.4798)T$</td>
</tr>
<tr>
<td>H$^{13}$CO$^+$</td>
<td>$Q = (0.4821)T$</td>
</tr>
<tr>
<td>HCO$^+$</td>
<td>$Q = (0.491)T$</td>
</tr>
<tr>
<td>HC$_3$N</td>
<td>$Q = (13.749)T$</td>
</tr>
<tr>
<td>OCS</td>
<td>$Q = (3.4285)T$</td>
</tr>
<tr>
<td>SO</td>
<td>$Q = (2.8052)T$</td>
</tr>
</tbody>
</table>

**C.2 Einstein A coefficients**

The Einstein A coefficient ($A_{ul}$) is the probability (per second per unit volume) of a spontaneous radiative transition from energy level $u$ to energy level $l$. In terms of molecular properties $A_{ul}$ is given by

$$A_{ul} = \frac{64\pi^4}{3hc^3} \left| \mu_{ul} \right|^2$$ (C.3)

where $u$ and $l$ are the upper and lower levels respectively,

$\mu = \text{mean electric dipole moment of the molecule}$

$|\mu_{ul}| = \text{the dipole moment matrix for the transition}$,

and all units are cgs.

Equations for calculating the dipole moment matrix for linear, symmetric top and asymmetric top molecules can be found in Townes and Schawlow (1975), Rohlfs and Wilson (1996) and Emerson (1996).
The values for $A_{ul}$ used in this thesis have been calculated from data of Pickett et al. (1998), using the equation given in the catalogue

$$A_{ul} = I_{ul}(T_0) \nu_{ul} \left[ \frac{Q_u(T_0)}{g_u} \right] \frac{-E_u}{kT_0} \left( 1.748 \times 10^{-9} \right) \quad (C.4)$$

$A_{ul}$ is the Einstein coefficient for a spontaneous radiative transition between upper level, u, and lower level, l, in units of s$^{-1}$,

$I_{ul}(T_0)$ is the line intensity at 300 K in units of nm$^2$ MHz,

$\nu_{ul}$ is the frequency of the transition in MHz,

$Q_u(T_0)$ is the partition function evaluated at 300 K,

$g_u$ is the statistical weight of the upper level,

$E_u$ is the energy of the upper level above the ground state in cm$^{-1}$,

$T_0$ is 300 K, and

$k$ is Boltzmann’s constant (0.69501 cm$^{-1}$ K$^{-1}$).

The dipole matrix enters (C.3) through the line intensity (the quantity catalogued), which is calculated using the dipole matrix.

The values of $A_{ul}$ used in this thesis are listed in Table C-2.
Table C-2. Einstein A coefficients for molecular lines observed in this thesis.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Rest Frequency (GHz)</th>
<th>$A_d$ (s⁻¹)</th>
<th>Critical Density (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>1-0</td>
<td>115.271204</td>
<td>7.40E-08</td>
<td>7.4E+02</td>
</tr>
<tr>
<td>$^{13}$CO</td>
<td>1-0</td>
<td>110.201353</td>
<td>6.50E-08</td>
<td>6.5E+02</td>
</tr>
<tr>
<td>C$^3$O</td>
<td>1-0</td>
<td>109.78216</td>
<td>6.50E-08</td>
<td>6.5E+02</td>
</tr>
<tr>
<td>CS</td>
<td>2-1</td>
<td>97.980968</td>
<td>2.20E-05</td>
<td>2.2E+05</td>
</tr>
<tr>
<td>CS</td>
<td>3-2</td>
<td>146.969049</td>
<td>6.34E-05</td>
<td>6.3E+05</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>2(1)-1(1) E</td>
<td>96.73939</td>
<td>2.39E-06</td>
<td>2.4E+04</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>2(0)-1(0) A⁺</td>
<td>96.74142</td>
<td>3.25E-06</td>
<td>3.3E+04</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>2(0)-1(0) E</td>
<td>96.74458</td>
<td>3.11E-06</td>
<td>3.1E+04</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>2(1)-1(1) E</td>
<td>96.75551</td>
<td>2.27E-06</td>
<td>2.3E+04</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(1)-4(0) A⁺</td>
<td>107.01385</td>
<td>5.55E-06</td>
<td>5.5E+04</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(0)-2(0) E</td>
<td>145.09375</td>
<td>1.10E-05</td>
<td>1.1E+05</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>3(-1)-2(-1)E</td>
<td>145.09747</td>
<td>1.01E-05</td>
<td>1.0E+05</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>5(-1)-4(0)E</td>
<td>84.52121</td>
<td>1.65E-06</td>
<td>1.6E+04</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.284156</td>
<td>2.79E-07</td>
<td>2.8E+03</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.316925</td>
<td>1.64E-06</td>
<td>1.6E+04</td>
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<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.328624</td>
<td>1.36E-06</td>
<td>1.4E+04</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.402004</td>
<td>1.37E-06</td>
<td>1.4E+04</td>
</tr>
<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.407165</td>
<td>1.65E-06</td>
<td>1.6E+04</td>
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<tr>
<td>C$_2$H</td>
<td>1-0</td>
<td>87.446512</td>
<td>2.80E-07</td>
<td>2.8E+03</td>
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<tr>
<td>C$_2$H$_2$</td>
<td>2(1,2)-1(0,1)</td>
<td>85.338905</td>
<td>2.52E-05</td>
<td>2.5E+05</td>
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<tr>
<td>HCO⁺</td>
<td>1-0</td>
<td>89.188518</td>
<td>3.00E-05</td>
<td>3.0E+05</td>
</tr>
<tr>
<td>HCO⁺</td>
<td>3-2</td>
<td>267.557625</td>
<td>1.00E-03</td>
<td>1.0E+07</td>
</tr>
<tr>
<td>HC$^{18}$O⁺</td>
<td>1-0</td>
<td>85.162256</td>
<td>2.80E-05</td>
<td>2.8E+05</td>
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<tr>
<td>HCN</td>
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<td>88.631847</td>
<td>2.43E-05</td>
<td>2.4E+05</td>
</tr>
<tr>
<td>HCN</td>
<td>2-2</td>
<td>265.886432</td>
<td>8.45E-04</td>
<td>8.4E+06</td>
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<tr>
<td>HNC</td>
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<td>90.663574</td>
<td>2.70E-05</td>
<td>2.7E+05</td>
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<tr>
<td>HNC</td>
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<td>271.981067</td>
<td>9.20E-04</td>
<td>9.2E+06</td>
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<tr>
<td>HC$_3$N</td>
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<tr>
<td>HC$_3$N</td>
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<td>100.076389</td>
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<td>HC$_3$N</td>
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<td>109.173634</td>
<td>9.43E-05</td>
<td>9.4E+05</td>
</tr>
<tr>
<td>HC$_3$N</td>
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<td>136.4644</td>
<td>1.86E-04</td>
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<td>HC$_3$N</td>
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<td>145.560946</td>
<td>2.26E-04</td>
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</tr>
<tr>
<td>OCS</td>
<td>12-11</td>
<td>145.946812</td>
<td>8.74E-06</td>
<td>8.7E+04</td>
</tr>
<tr>
<td>OCS</td>
<td>7-6</td>
<td>85.139108</td>
<td>1.69E-06</td>
<td>1.7E+04</td>
</tr>
<tr>
<td>OCS</td>
<td>8-7</td>
<td>97.3012085</td>
<td>2.54E-06</td>
<td>2.5E+04</td>
</tr>
<tr>
<td>OCS</td>
<td>9-8</td>
<td>109.463063</td>
<td>3.64E-06</td>
<td>3.6E+04</td>
</tr>
<tr>
<td>SO</td>
<td>3(2)-2(1)</td>
<td>99.299879</td>
<td>1.17E-05</td>
<td>1.2E+05</td>
</tr>
</tbody>
</table>