

MOLECULAR LINE SURVEYS OF STAR-FORMING REGIONS WITH HERSCHEL (FIRST)

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ABSTRACT

The importance of spectral line surveys with the *Herschel Space Observatory* (FIRST) is discussed. An overview of recent line surveys of young stellar objects at submillimeter and infrared wavelengths obtained with ground-based telescopes and the *Infrared Space Observatory* is given, and chemical diagnostics at different evolutionary stages are identified. The need for the development of sophisticated radiative transfer models to infer the physical, chemical and dynamical conditions in star-forming regions is emphasized.

Key words: Stars: formation – Molecules – Interstellar Medium

1. INTRODUCTION

The earliest stages of star- and planet-formation occur deep inside molecular clouds of gas and dust, and can only be studied at long infrared and submillimeter wavelengths. Observations of the continuum emission from dust provide insight into the structure of star-forming regions (e.g., Motte et al. 1998, André, this volume), whereas the spectral energy distributions give an indication of the evolutionary state of the object (e.g., Lada 1999). However, the dynamics, physics and chemistry of the gas can only be studied through molecular line observations. The *Herschel Space Observatory* (previously known as FIRST) can make unique contributions in this area because of its complete spectral coverage over a wide, unexplored wavelength range unhindered by the Earth's atmosphere.

In the last two decades, the power of spectral surveys has been amply demonstrated. The main results include (i) an *unbiased* census of the principal atoms and molecules in the observed regions. This includes all phases of the interstellar–stellar lifecycle — from diffuse clouds to star-forming regions and outflow shocks, to the envelopes around late-type AGB stars and planetary nebulae and eventually supernova remnants (see Figure 1); (ii) use of ratios of lines of the same molecule to constrain the parameters of the different physical components in the beam, in particular temperature and density; (iii) use of the molecular abundances as diagnostics of the evolutionary state; (iv) probes of the different dynamical processes such as

shocks, turbulence and infall, by comparing high-spectral resolution line shapes of molecules which have different excitation and chemistry; (v) measurement of the total cooling rate of the gas, in particular the contributions from CO and H₂O; (vi) direct measurement of the contribution of the lines to the broad-band continuum, which can affect the determination of dust parameters; and (vii) opportunities for unexpected discoveries of new, sometimes exotic species.

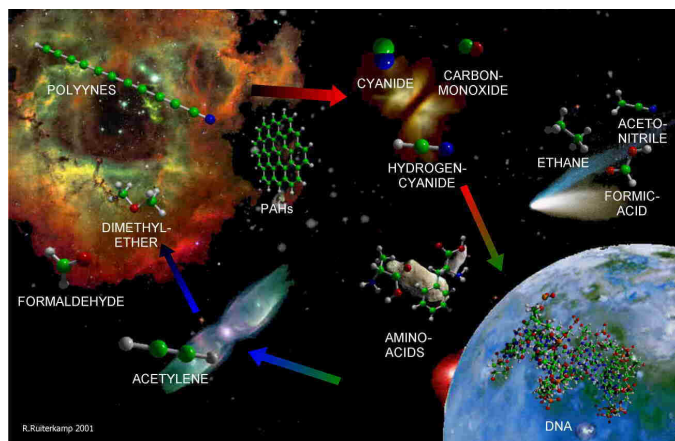


Figure 1. Illustration of the lifecycle of gas and dust to be probed by submillimeter and far-infrared observations (figure by R. Ruiterkamp, private communication; based on Ehrenfreund & Charnley 2000).

In the following, a brief history of molecular line surveys will be given, followed by an in-depth discussion of recent surveys at (sub-)millimeter wavelengths using large aperture ground-based telescopes, and at mid- and far-infrared wavelengths with the *Infrared Space Observatory* (ISO). Finally, the importance of line surveys with the *Herschel Space Observatory* will be emphasized. Previous reviews of line surveys include Schilke et al. (1997b, 1999), whereas the case for molecular line observations with *Herschel* (FIRST) has been made by, e.g., Phillips (1990), van Dishoeck & Helmich (1996), van Dishoeck (1997) and Cernicharo (1999). Line surveys of late-type stars are discussed by Guélin et al., this volume.

2. HISTORY

Massive star-forming regions such as Orion-KL and SgrB2 have traditionally been prime targets for line surveys owing to their bright molecular lines. Many surveys at millimeter (e.g., Johansson et al. 1984, Cummins et al. 1986, Turner 1991) and submillimeter (e.g., Jewell et al. 1989, Sutton et al. 1991) have appeared since the development of (sub-)millimeter telescopes, and they have contributed hugely to the inventory of lines and species.

The OVRO 1 millimeter survey of Orion-KL by Sutton et al. (1985) and Blake et al. (1986, 1987) has been particularly influential. These papers made a large impact not only because of the high quality of the data, but also because the data were accompanied by a detailed physical and chemical analysis. Based on the line shapes and excitation of the molecules, different physical components could be identified within the 30'' beam, such as the quiescent molecular ridge, the plateau outflow gas, the hot core near IRc2, and the so-called compact ridge — another hot and dense clump of gas. Temperatures were found to range from ~ 50 K for the quiescent gas to nearly 1000 K in the outflowing gas and hot core(s).

Second, the chemical composition of the individual components could be determined, and was found to vary considerably: the quiescent ridge contains only simple molecules, whereas the outflow is rich in SO and SO₂ and the hot cores in complex saturated organic molecules such as CH₃OCH₃ and CH₃CN. Blake et al. (1987) put forward a scenario in which the complexity of the spectra is caused by the interaction of the young massive star(s) with their surroundings through shocks, ultraviolet photons and passive radiative heating. The chemical variations were proposed to be due to varying elemental C/O ratios in the gas, which were thought to be linked to the freeze-out of molecules from the gas during the cold (pre-)collapse phase and subsequent evaporation of the ices.

Although the details have changed, the main aspects of this scenario have remained valid. In particular, the Orion survey has stimulated new chemical models appropriate for hot cores, in which a mixture of ices sublimates from the grains once the young star heats up its surroundings. The evaporated molecules subsequently drive a rapid high-temperature gas-phase chemistry for a period of $\sim 10^5$ yr, until the normal ion-molecule chemistry takes over (e.g., Charnley et al. 1992, 1995, Charnley 1997, Caselli et al. 1993). The main difference with the earlier work is the composition of the ices. Blake et al. assumed that evaporated H₂O is the main driver of the hot core chemistry, whereas Millar et al. (1991) and Charnley et al. (1992) showed that CH₃OH is much more effective in producing complex organic molecules. Thanks to the improvements in mid-infrared observations, CH₃OH is now known to be a major component of interstellar ices in at least some high-mass star-forming regions, with abundances up to 30% of H₂O-ice, or 10^{-5} with respect to H₂ (see summary

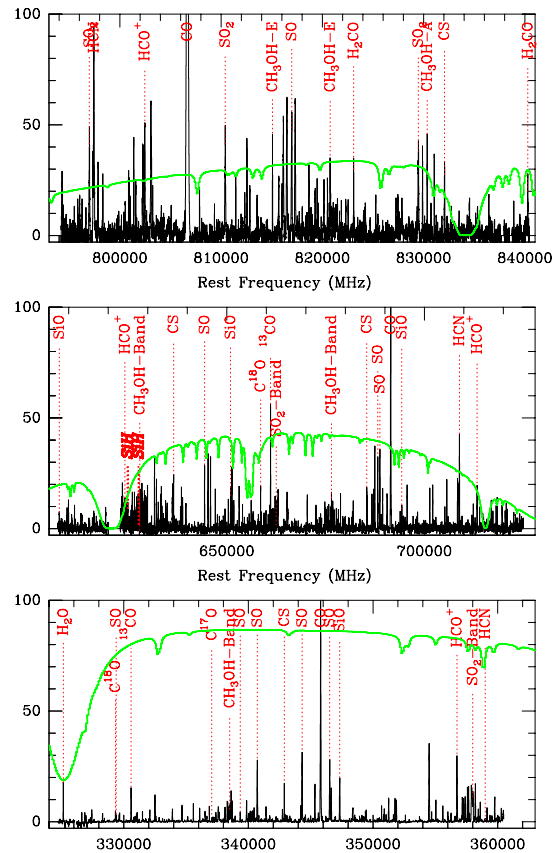


Figure 2. Top: CSO 794–840 GHz line survey by Mehringer et al. (2001); Middle: CSO 600–720 GHz survey by Schilke et al. (2001); Bottom: CSO 325–360 GHz line survey by Schilke et al. (1997).

by Dartois et al. 1999). Recent overviews of the chemistry in star-forming regions are given by van Dishoeck & Blake (1998) and Ehrenfreund & Charnley (2000).

3. RECENT SUBMILLIMETER SURVEYS

The advent of large aperture (sub-)millimeter telescopes on high dry sites equipped with sensitive heterodyne SIS receivers has stimulated new and deeper surveys of star-forming regions. Compared with the older data, the new high frequency surveys refer to smaller beams of 10''–20'' compared with $\sim 1'$ and measure higher rotational transitions, thus probing directly the warmer and denser gas associated with the young stellar objects (YSOs) rather than the extended cloud. Also, a much larger variety of high-mass and low-mass objects has been observed at low- and/or high frequencies. Table 1 summarizes published (sub-)millimeter surveys since 1994, whereas Figures 2–4 illustrate the richness of the line spectra.

Table 1. Overview of millimeter and submillimeter line surveys of star-forming regions since 1994

Object	Frequency range (GHz)	Telescope	Reference
Orion-KL	125–138	TRAO	Kim et al. 1999
	138–147	TRAO	Lee et al. 1999
	325–360	CSO	Schilke et al. 1997a
	455–505	JCMT	Araki et al. 2000
	607–725	CSO	Schilke et al. 2001
	685–692	JCMT	Harris et al. 1996
	794–840	CSO	Mehring et al. 2001
	840–900	CSO	Comita et al. 2001
	200–900	CSO-FTS	Serabyn & Weisstein 1995
SgrB2 (N,M,NW)	30–116	Nobeyama 45m	Ohishi & Kaifu 1999
	218–263	SEST	Nummelin et al. 1998, 2000
G34.3+0.15	84.7–115.7	TRAO	Kim et al. 2000
	123.5–155.3	TRAO	Kim et al. 2000
	330–365	JCMT	Macdonald et al. 1996
G5.89-0.39	330–360	JCMT	Thompson & Macdonald 1999
TMC-1	8.8–50	Nobeyama 45m	Ohishi & Kaifu 1998
W3 IRS5, IRS4, W3 (OH/H ₂ O)	334–365	JCMT	Helmich & van Dishoeck 1997
<i>Selected settings*</i>			
Orion-KL	100	BIMA	Wright et al. 1996
	100	FCRAO	Ungerechts et al. 1997
	230	OVRO	Blake et al. 1996
	345	JCMT	Sutton et al. 1995
B5 IRS1	230,345	JCMT	Kelly et al. 1996
DM Tau, GG Tau	100,230,345	IRAM 30m	Dutrey et al. 1997
G327.3-0.6	100,150,230	SEST	Gibb et al. 2000
L1157	100,230	IRAM 30m	Bachiller & Perez-Gutierrez 1997
L134N	100	FCRAO	Dickens et al. 2000
LkCa15	100,230	OVRO	Qi et al. 2001
IRAS05338–0624	100,230	NRAO 12m, CSO, BIMA	McMullin et al. 1994
IRAS16293–2422	230,345	CSO, JCMT	Blake et al. 1994, van Dishoeck et al. 1995
M17, Cepheus A	100	FCRAO	Bergin et al. 1997
NGC 6334 I, I(N)	345	JCMT	McCutcheon et al. 2000
NGC 2264	230,245	JCMT	Schreyer et al. 1997
NGC 1333 IRAS4	230,345	CSO	Blake et al. 1995
Serpens S68	100,230,345	NRAO 12m, CSO, BIMA	McMullin et al. 2000
Serpens SMM1-4	230,345	JCMT	Hogerheijde et al. 1999
TMC-1	100	FCRAO	Pratap et al. 1997
UC HII regions (14)	230,345	JCMT	Hatchell et al. 1998
Massive YSOs (12)	230,345	JCMT	van der Tak, Boonman et al. 2001

* Selected settings covering ≥ 5 GHz total in atmospheric window(s) and/or a large number (>10) of different species

What have we learned from these data? First, the quality of the data is a testimony to the orders of magnitude advances in the technology since the early days of millimeter astronomy. Second, the lines are found to contribute 50% or more of the broadband continuum at 350–650 GHz in some objects, in particular hot cores (Groesbeck 1995). On the other hand, the contribution is less than 10% in

other objects, including the most line-rich low-mass YSO IRAS 16293–2422. Third, even with the smaller beams, the physical structure of the sources is still unresolved, but the different physical components can often be separated on the basis of excitation and line profiles. Moreover, the data are sensitive to regions as small as $1''$ such as hot cores in distant high-mass YSOs.

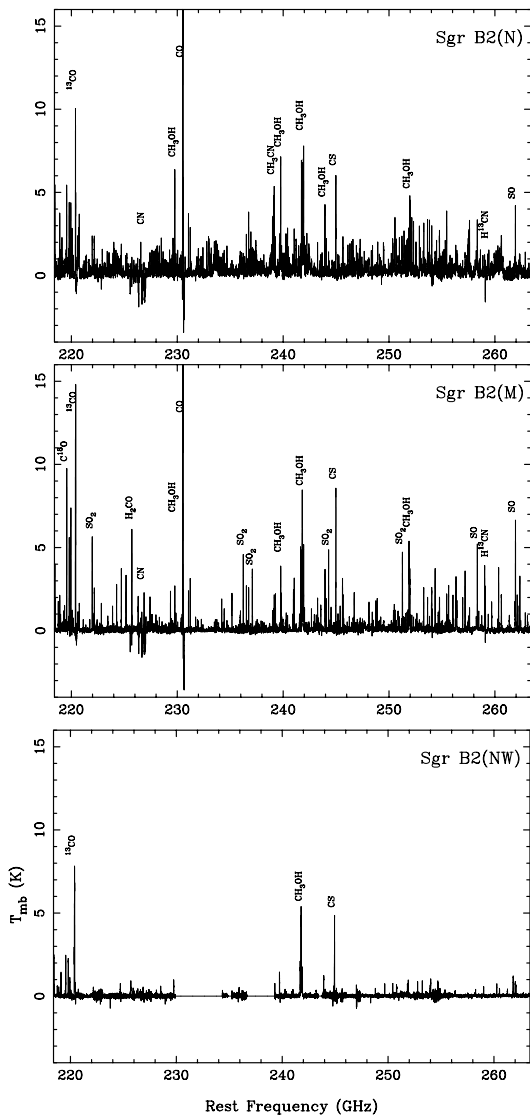


Figure 3. SEST 218–267 GHz line survey by Nummelin et al. (1998, 2000). Note the chemical differences between the N, M and NW positions.

Fourth, the chemical variations found for Orion are not unique: other regions have been found in which the chemistry clearly differs from position to position. Recent examples include the N, M and NW positions in SgrB2 (Nummelin et al. 1998, 2000, see Figure 3) and the IRS4, IRS5 and H₂O-maser positions in W 3 (Helmich & van Dishoeck 1997). Fifth, most of the diagnostic information is derived from weak features: surveys need to be sensitive — down to the confusion limit or such that typical abundance limits are $< 10^{-10}$ — to be of value. Finally, the line surveys have stimulated the development of laboratory spectroscopy and line catalogues (e.g., Lovas et al. 1992, Pickett et al. 1998, Oesterling et al. 1999), as well as associated software for analysis (Groesbeck 1995, Schilke et al. 2001). In addition, the radiative transfer methods

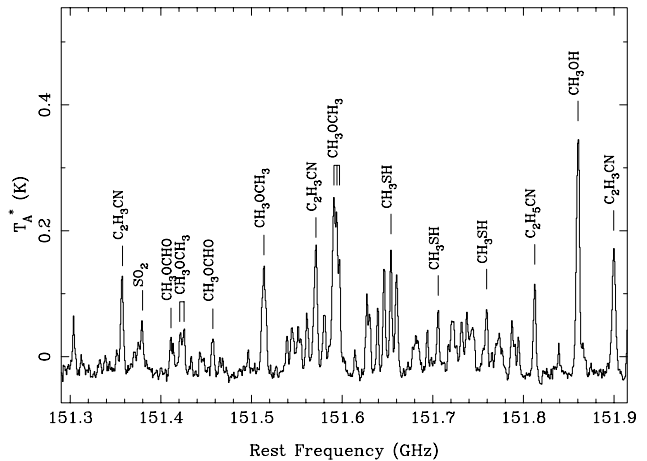


Figure 4. Part of the SEST line survey by Gibb et al. (2000) of the hot core G327.3-0.6, illustrating the rich spectrum due to complex organic molecules in hot cores.

have evolved from simple large velocity gradient or constant excitation temperature models (e.g., Irvine et al. 1987) to full 2D or even 3D accelerated Monte-Carlo or Lambda Iteration models in which realistic physical models are coupled with the molecular excitation (e.g., Juvola 1997, Yates et al. 1997, Hogerheijde & van der Tak 2000, see Figure 5). Together, these data and analyses have led to a more comprehensive picture of the physical and chemical evolution of star-forming regions, as outlined in Table 2.

4. MID- AND FAR-INFRARED SURVEYS

In the last five years, the Short Wavelength Spectrometer (SWS, $R = \lambda/\Delta\lambda \approx 500 - 2000$, beam $\sim 20''$) and Long Wavelength Spectrometer (LWS, $R \approx 200$, beam $\sim 80''$) on ISO have opened up the 2.5–200 μm for spectroscopic surveys of star-forming regions. Although the spectral resolutions are lower and the beams larger than those of submillimeter surveys, the wide wavelength coverage allows a number of unique features to be observed. In particular, solid-state features such as silicates and ices and large molecules such as PAHs are uniquely observed in this wavelength range. Moreover, atomic and ionic fine-structure lines, as well as the vibration-rotation transitions of gas-phase molecules, are prominent in the mid-infrared, whereas the high- J pure-rotational lines of CO, OH and H₂O occur at far-infrared wavelengths.

In its 2.4 yr lifetime, ISO made complete SWS 2.4–45 μm scans of at least 50 star-forming regions, primarily of high- and intermediate mass YSOs at different stages of evolution (flux > 10 Jy at 15 μm , $L > 10^2 L_\odot$) (see van Dishoeck et al. 1999, Cox et al. 1999, van Dishoeck & Tielens 2001 for reviews). The LWS obtained 44–197 μm spectra of a similar number of objects, including some deeply embedded low-mass YSOs (Saraceno et al. 1999).

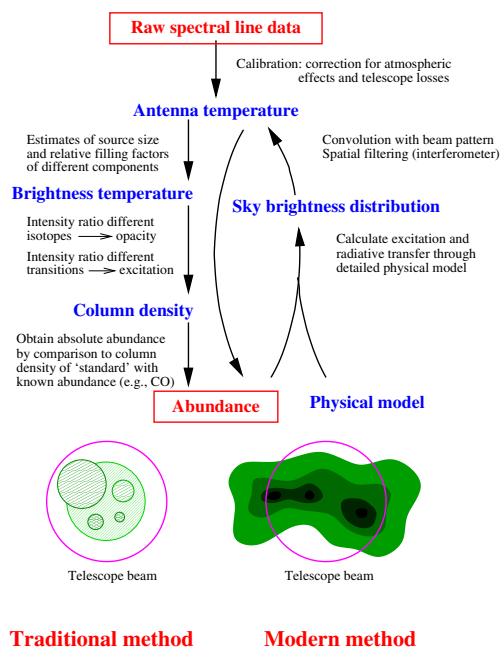


Figure 5. The steps involved in deriving molecular abundances from spectral line data. The left-hand side shows the ‘homogeneous’ approach as outlined by Irvine et al. (1987); the right-hand side shows the more modern ‘detailed’ approach from which abundance profiles can be derived (from van Dishoeck & Hogerheijde 1999).

Figures 6–7 contain representative spectra of sources at different stages.

Based on these spectra, a number of infrared diagnostic features can be identified, which complement the sub-millimeter diagnostics noted in §3 (see Table 2). In the youngest deeply-embedded objects, strong ice and silicate absorptions are found, whereas in the more evolved YSOs emerging from their molecular cocoons, PAH features and atomic and ionic lines become prominent (Figure 7). At longer wavelengths, strong H₂O lines in the earliest phases are replaced by OH lines at later stages (Figure 6). Once the envelope has disappeared, amorphous and crystalline silicate emission from circumstellar disks becomes prominent (Figure 8). The latter can resemble that of solar system objects such as comets.

The complete infrared spectral surveys have led to the identification of several new lines and features:

- Observation of many new thermal emission lines of H₂O and OH with both the SWS and LWS (see Figures 6 and 9). The H₂O abundance is found to increase from $< 10^{-7}$ with respect to H₂ to at least 10^{-4} in warm gas, due to the combined effects of the evaporation of icy mantles and high-temperature reactions driving atomic oxygen into H₂O. However, except perhaps in localized regions, H₂O is not a major coolant of the gas compared with CO (Saraceno et al. 1999).

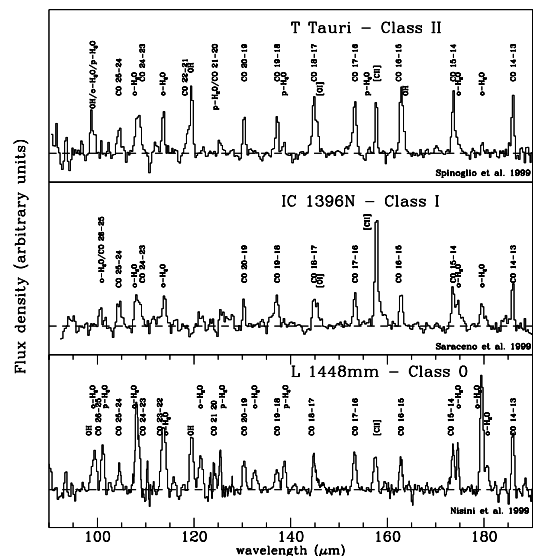


Figure 6. ISO-LWS spectra of three low-mass YSOs at different evolutionary stages. Note the strong gas-phase H₂O lines in the class 0 object L1448mm and the strong OH lines in the class II object T Tau (from Spinoglio et al. 2000, Saraceno et al. 1999 and Nisini et al. 1999).

Atomic O is surprisingly abundant in dense (translucent?) clouds based on the detection of the 63 μm [O I] line in absorption, containing at least 40% of the gas-phase oxygen budget (Baluteau et al. 1997, Poglitsch et al. 1996, Keene et al. 1999).

- Several new simple gas-phase molecules have been detected by ISO including interstellar CO₂ (van Dishoeck et al. 1996), HF (Neufeld et al. 1997), C₃ (Cernicharo et al. 2000) and CH₃ (Feuchtgruber et al. 2000) and circumstellar C₆H₂ and C₆H₆ (Cernicharo et al. 2001), which provide tests of the basic chemical networks. New far-infrared lines of known molecules have been observed for CH⁺ (Cernicharo et al. 1997), CO⁺ (Ceccarelli et al. 1998), NH, NH₂ and H₃O⁺ (Goicoechea & Cernicharo, this conference), allowing these molecules to be observed in different environments than probed by, e.g., optical absorption lines.
- The fundamental $J=1 \rightarrow 0$ emission line of HD at 112 μm has been detected toward the Orion Bar (Wright et al. 1999, Figure 11), whereas the $J=6 \rightarrow 5$ line at 19 μm has been seen in the Orion shock (Bertoldi et al. 1999). These data allow the first determination of the [D]/[H] ratio in an active star-forming region. The resulting value of $(0.7-1) \times 10^{-5}$ is nearly a factor of two lower than that found in the local diffuse interstellar medium.
- Line surveys of FU-Orionis objects — a class of YSOs which go through a phase of high accretion rate — have revealed unexpected emission from the [N II] 122 μm line, probably originating in an extended low-density region ($n_e \leq 100 \text{ cm}^{-3}$) ionized by ultraviolet photons

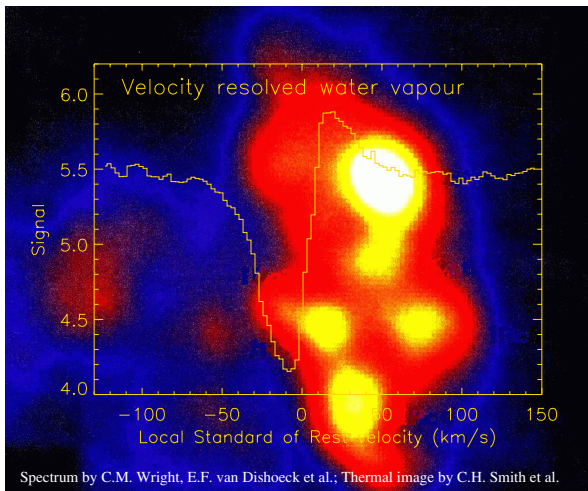


Figure 10. ISO-SWS Fabry-Perot spectrum of the $o\text{-H}_2\text{O } 4_{32} - 3_{03} 40.69 \mu\text{m}$ line toward Orion-KL, showing a P-Cygni line profile from the expanding plateau gas (from Wright et al. 2000).

and are sensitive to the ionization state and amount of hydrogenation of the carrier molecules.

5. COBE-FIRAS SURVEY OF THE DIFFUSE MEDIUM

The Far-Infrared Absolute Spectrophotometer (FIRAS) on the Cosmic Background Explorer (COBE) has provided the first complete spectral survey from 1 cm to 100 μm of the diffuse medium in our Galaxy (Wright et al. 1991, Fixsen et al. 1999). Although the spectral resolution was low, $R \approx 100$, and the beam large, 7° , it provides a global overview of the strongest emission lines. In particular, [C II] is found to be the main coolant of the gas, whereas CO emission lines are present with a low excitation temperature characteristic of translucent clouds (i.e., low-density PDRs). The [N II] lines at 205 and 122 μm are seen as well, and can be used to probe the diffuse ionized gas and disentangle the contributions from the [C II] to the neutral and ionized medium.

6. PROSPECTS FOR HERSCHEL

The preceding sections have shown that ground-based submillimeter and space-based ISO observations have started to unravel the physical and chemical characteristics of star-forming regions. Clear variations in physical and chemical parameters have been found during the evolution from molecular clouds to circumstellar disks. Also, the value of complete line surveys for discovering new and unexpected features has been demonstrated. However, much remains to be learned since the existing data suffer from (i) inaccurate calibration with at least 30% uncertainty; (ii) poor weather statistics for ground-based surveys, which often take more than a year to complete for a single source; (iii) poor sensitivity at far-infrared wavelengths, so that only

the strongest, optically thick lines have been detected; (iv) poor spatial resolution, especially at far-infrared wavelengths (80'' LWS beam); (v) poor spectral resolution, so that the far-infrared lines are unresolved and cannot distinguish self-absorbed, outflow, or quiescent profiles; (vi) lack of coverage at ~ 1 THz, where the lowest- J lines of hydrides and the low-frequency bending modes of large molecules occur.

The *Herschel* Space Observatory will improve on each of these aspects by 1–2 orders of magnitude, especially at the higher frequencies (≥ 900 GHz, $\leq 300 \mu\text{m}$), where there is no competition from ground-based instruments and where SOFIA is at least an order of magnitude less sensitive. While SOFIA can give an initial impression of the complexity of spectra at shorter wavelengths, only space-based observatories such as *Herschel* with long, uninterrupted integration times unhindered by the Earth's atmosphere can properly survey the 60–500 μm range. A program covering at least three dozen sources ranging from diffuse gas to circumstellar disks should be a major goal of *Herschel* (see also the summary of the discussion panel on Astrochemistry). About 12–24 hr per source will be required to cover the full frequency range of HIFI down to 30–100 mK rms, whereas a complete PACS 60–210 μm line scan at $R \approx 1500$ down to $\sim 1 \times 10^{-17} \text{ W m}^{-2} 1\sigma$ (1σ) takes about 2–3 hrs per object. SPIRE can survey the 200–400 μm region at $R \geq 100$ in ~ 1 hr per object down to a similar 1σ sensitivity.

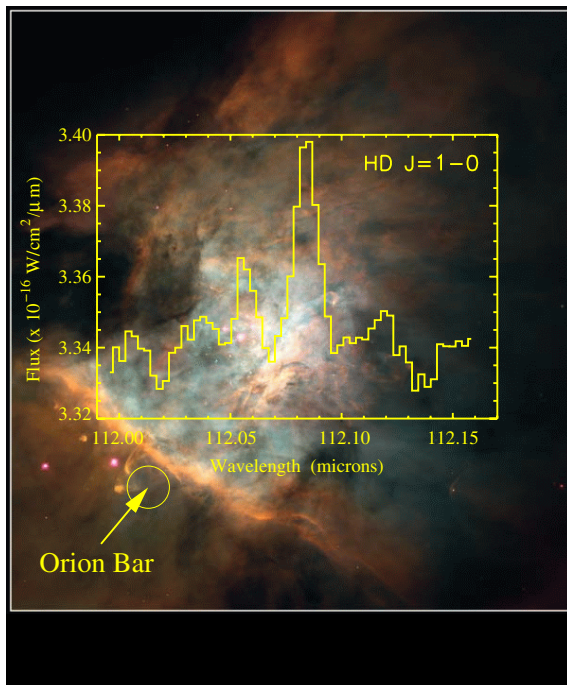
Such surveys could address several major questions in star-formation research. How does the chemical composition depend on the mass and luminosity of the object? What are the major mechanisms and time scales for various processes such as the clearing of the envelope? What is the role of outflows versus radiation? Which molecules are produced on grains and which are due to second generation 'hot core' chemistry? How far does the chemical complexity go? What is the role of water, both in the chemistry and in the cooling? Is O_2 ever the dominant form of gas-phase oxygen in molecular clouds, and if not, what does this imply for the structure of molecular clouds and envelopes around YSOs? Is the H_2O in disks primarily in gaseous or solid form, and how is this related to the amount of crystalline silicate material?

Herschel will allow far-infrared diagnostics to be developed which will be complementary and unique compared with those observed at mid-infrared wavelengths by ISO and in the future by SIRTf and NGST, and with those at submillimeter wavelengths obtained with single-dish submillimeter telescopes and in the future by ALMA.

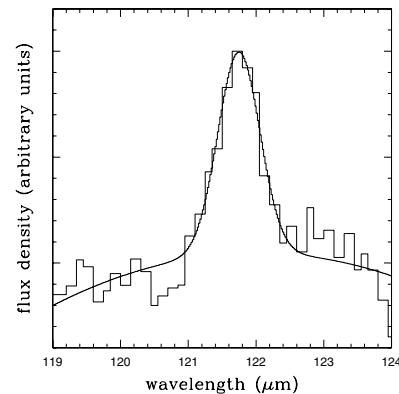
The requirements for the *Herschel* instruments include as complete wavelength coverage as possible (especially in the regions with H_2O gas phase lines), stable and accurate calibration (preferably better than 10%) and accurate pointing (both absolute and relative). Every effort should be made to cover unique spectral features such as the HD 112 μm line (HIFI) and the crystalline H_2O ice feature

Table 2. Chemical characteristics of massive star-forming regions

Component	Chemical characteristics	Submillimeter diagnostics	Infrared diagnostics	Examples
Dense cloud	Low-T chemistry	Ions, long-chains (HC ₅ N, ...)	Simple ices (H ₂ O, CO ₂)	SgrB2 (NW)
Cold envelope	Low-T chemistry, Heavy depletions	Simple species (CS, H ₂ CO)	Ices (H ₂ O, CO ₂ , CH ₃ OH)	N7538 IRS9, W 33A
Inner warm envelope	Evaporation, High-T chemistry	High T _{ex} (CH ₃ OH)	High gas/solid, High T _{ex} , Heated ices (C ₂ H ₂ , H ₂ O, CO ₂)	GL 2591, GL 2136
Hot core	Hot-core chemistry	Complex organics (CH ₃ OCH ₃ , CH ₃ CN, vib. excited mol.)	Hydrides (OH, H ₂ O)	Orion hot core, SgrB2(N), G34.3 W 3(H ₂ O)
Outflow: Direct impact	Shock chemistry, Sputtering	Si- and S-species (SiO, SO ₂)	Atomic lines, Hydrides ([S I], H ₂ O)	W 3 IRS5, SgrB2(M)
PDR, Compact H II regions	Photodissociation, Photoionization	Ions, radicals (CN/HCN, CO ⁺)	Ionic lines, PAHs ([NeII], [CII])	S 140, W 3 IRS4

Figure 11. Detection of the HD $J=1\rightarrow 0$ line at $112\ \mu\text{m}$ using the ISO-LWS toward the Orion Bar (from Wright et al. 1999).

(PACS). To have a maximum impact, the *Herschel* observations need to be accompanied by a thorough physical and chemical analysis. This requires not only laboratory and theoretical work to provide complete line catalogs up to a few THz, collisional excitation rate coefficients and other molecular data, but also further development of the new generation of radiative transfer models coupled with realistic physical structures and chemical codes.

Figure 12. Continuum-subtracted average spectrum of a sample FU Orionis objects, showing the detection of the $[\text{N II}]$ $121.8\ \mu\text{m}$ line (from Lorenzetti et al. 2000).

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