HIFI Core Science Program
The interstellar medium

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commented and edited by J. Stutzki

Introduction

JSt: add paragraphs to intro to give

- short overview of topics and their relation to other HIFI core sciene areas

- give goals of document (scientific justification of each topic; HIFI uniqueness of proposed observations; coherent time estimate; identify prep work necessary)

- general comments on HIFI uniqueness:
–first time high spectral resolution observations throughout the FIR;
—-for submm: first time without earth atmosphere, hence unprecedented sensitivity (except for a few KAO observations);
—-for FIR: first time at all!
–SOFIA is complementary: has still residual atmosphere in many places; but may have better mapping capabilities for some strong lines; HOW DO WE DEAL WITH THIS IN THE PROPOSED HIFI CORE SCIENCE?
–other HIFI instruments: PACS: crossover resolution (equal sensitivity per spectral and spatial point) at about 30-100 km/s, and is going to have only resolution of about 100 km/s anyway. But spatial multiplexing advantage! SPIRE only very low spectral resolution and thus impossible to perform observations presented here (but both PACS and SPIRE necessary for complementary observations: broad band dust spectra, important lines beyond the spectral range of HIFI

- give rules for time estimate used throughout proposal (following Volker's suggestions).

then go to the scientific overview

The study of the interstellar medium (ISM) is critical for an understanding of both star formation and the evolution of galaxies. HIFI is a unique instrument to accomplish this, since for local sources most important spectral structures are obscured by the Earth atmosphere.

The formation of new stars in galaxies releases such large amounts of radiative and kinetic energy in the interstellar medium that matter continuously cycles between the dense and diffuse phases of the medium. The chemical evolution of matter in space and the formation of stars must be investigated within this broad context. Gas phase abundances of elements such as Si and Fe show that a significant fraction of matter accreted onto dust in molecular clouds is released back to the gas within the low density phases of the ISM. At the opposite, the detection of numerous molecular clouds at high Galactic latitude and of large abundances of molecules in the diffuse ISM show that the condensation of gas from the warm to cold phases is easily followed by the formation of molecules. Molecular abundances in these low column density molecular clouds are not readily explained with state of the art gas phase chemistry and alternative formation processes may be effective. For instance, The decrease of turbulent line widths from the warm phases to atomic clouds and from atomic to molecular clouds suggests that the condensation process of clouds goes with a dissipation of turbulent kinetic energy. The dissipation process may be able to greatly enhance the abundance of some species (e.g. CH^+).

The proposal is organised as follows :

Section 1 deals with the ISM structure, the role of HIFI for studying physical and chemical processes in the Warm and dense ISM is described in Section 2, Section 3 presents observations probing the transition from atomic to molecular gas, especially the formation of hydrides, while complex molecules are the subject of Section 4.

1 ISM structure

JST: I think this section title is not very well choosen; what "structure" do we have in minde? Spatial/velocity structure? Phases of the ISM? we have to find some better section title!

1.1 HIFI studies of the ISM phases

The interstellar medium (ISM) exists in different phases. Traditionally one distinguishes the warm ionized medium (WIM), the warm neutral medium (WNM) and the cold neutral medium (CNM). All three phases play an important role in the evolutionary cycle of interstellar matter, which overall controls the evolution of galaxies. A full understanding of the physical and chemical processes controling the ISM phases and their composition is thus of fundamental importance to astrophysics.

Due to their specific excitation conditions the various phases have different strandard tracers. The WIM is best studied in the optical and UV, in particular through its diffuse Hα emission, the WNM and CNM in the HI 21cm line and, for its densest component in the rotational lines of CO and other heavy molecules. The WNM is best traces by the strong cooling lines of C^+, CI, OI (for the denser parts) and other tracers such as N^+. Due to the complex spatial and kinematic structure of the turbulent ISM, high spatial resolution and the velocity information present in the line profiles have proven to be crucial for understanding of the ISM, allowing to separate otherwise overlapping components along the line of sight.

Over the years dedicated efforts have been conducted and significant progress has been made in the understanding of the ISM, in particular with the HST/GHRS, COBE/FIRAS and ISO/LWS and ISOCAM instruments, and more recently through UV absorption studies with FUSE. **JST: include the Japanes CII balloon BICE**

JST: I suggest to add here a more detailed overview of what the limitations are of the present data, and where HIFI is going to improve: e.g.:
FIR line observations (mostly CII, NII only from COBE and one single KAO observation in an external galaxy) limited to
(i) small telescopes (KAO, BICE, ISO) and hence low angular resolution, whereas comparabel HI and CO observations tell us, that there is structure down to the smallest scales, and that structure is relevant for understanding the physics and exciation
(ii) except for one set of pioneering [CII] KAO observations, all with spectral resolution of 30 km/s or poorer, i.e. only integrated line intensities w/r to the issues discussed below.

However, a global description of the structure of the ISM is missing and the overall structure of the ISM remains elusive, in particular the volume filling factor of the various phases, the amount of small scale structure present in each of them, the density contrasts and perhaps most importantly the thermal pressure of each of these phases, and its variation with the distance z to the galactic plane, and at various distances from the Galactic center. The link between the various phases (e.g. are they in thermal pressure balance?) is likely to be related to their formation mechanism and has to be established. Is the hierarchy of structures observed in the coldest component (that of molecular clouds) a fossil of thermal/gravitational instabilities developed initially in a placental warm medium at 10^4 K? The structure of the diffuse ISM may thetrefore be related to that of the coldest self-gravitating components, and thus ultimately to the process of star formation.

The structure and physics of the diffuse ISM has also important bearings to (i) understanding the gaseous structure of one of the many screens between the Cosmic Background (CBG) and the Sun, and therefore that of the dust distribution which affects the continuum measurements of the CBG, (iii) the large observed porosity of the neutral medium to UV photons and (iv) understanding the first steps of interstellar chemistry.

The capabilities of HIFI will allow new important steps in the study of the ISM thanks to its high angular resolution, its sensitivty, but most important, its high spectral resolution: HIFI will for the first time allow to obtain fully velocity resolved spectra across the FIR spectral range, It will thus provide for the first time for the many important trace lines of the ISM in its different phases the velocity information that is fully comparable to the rich information in the extensive HI- and CO-surveys of the denses phase of the ISM.

Within the core science program we focus on the the most important contributions expected trough HIFI:

1.1.1 Thermal pressure determination from [CI] fine structure lines

Thermal pressure determinations as derived from [CI] fine structure lines and molecular line observations vary from tracer to tracer. The thermal pressure derived from [CI] absorption lines in the general **JST: what is "general" here? which of the phases discussed above? I guess,it is the diffuse component.** ISM is $P_{th}/k \sim 3 \times 10^3$ K cm^{-3} (Jenkins & Shaya 1979, Jenkins & Tripp 2001) with large excursions above this value, while recent observations of molecules in absorption against extragalactic sources provide $P_{th}/k \sim 2 \times 10^4$ K cm^{-3} (Lucas & Liszt 1994). If large pressure differences exist, shocks propagating into the coldest phases should be present. Small scale density structures are also prominent in the spectra of nearby lines of sights (Pan et al. 2001, Andrews et al. 2001).

JSt: what we completely lack here, is an argument that says why HIFI CI observations are better than other possibilities in deriving the pressure, and thus, why it is worthwhile to spend precious HIFI time on integration on pretty damned weak CI lines! HIFI will extend the present observations of the [CI] fine structure lines to low column densities HI clouds. In such clouds most of the gas carbon is ionised and C is only a minor constituent. However carbon abundances derived from UV absorption studies (Jenkins & Tripp 2001) show that the [CI] fine structure emission lines can be measured with HIFI. Thanks to the high spectral resolution of HIFI we can use the information on the level population **JST: what does the high spectral resolution have to do with being able to use the info on the level pop? rearrange!** , and from the line profiles to determine the gas pressure **: how dow we get the pressure from the line profiles?** for each of the velocity components of the clouds which is a fundamental information to understand the origin of clouds structure.

JST: I suggest to restructure and move the details of the proposed observations into the individual sections, i.e. right after the following paragraph and have the present subsection "proposed observations" as a summary only; this avoids some hopping back and forth

Proposed observations:

An illustration of a possible target field is shown in Figure from Miville-Deschênes et al. (2002). The HI emission there reveals conspicuous small scale filaments, the width of which has not been quite resolved by the instrument (DRAO interferometer, resolution 1'). Such a small scale structure in the

HI emission seems to be found in many directions.

JST: we lack a quantitative estimate of the line intensities for such clouds (note: we might use the high latitude cloud observations from AST/RO and the recent KOSMA observations from Heithausen's group as a guideline).

1.1.2 [CII]: separate the contribution from WIM and CNM

JST: we lack a section on why it is important to separate the WIN and CNM contribution to the [CII] emission; who from the broader astrophysics community is interested in this, and why? Or is it just the [CII] specialist, who would like to know? High spectral resolution observations of the [CII] fine structure line will allow the separation of the contribution of the cloud phase from that of the warm ionized medium (WIM) and, together with Hα and HI emission spectra, the thermal and non-thermal contributions to the observed line widths. The narrowest velocity components in HI clouds have velocity widths of 3 kms^{-1} (FWHM) which are close to the expected thermal width for gas at a few 100 K. For the corresponding [CII] emission components we expect to see a narrowing of the lines due to the higher mass of carbon. **JST: what does it imply, if we in fact find this narrowing? What, if not? How about similar attemps in the optical/UV absorption work? What are their results?** Maps in the [CII] line will also help in understanding the small scale structure of the WIM. **JST again: why is this important? What does it tell us about the ISM, that we need to know? The mere fact that maps help to understand structure is somewhat week, I guess!** Warm components are presumably more smoothly distributed, but CaII absorption lines against binary stars (Meyer and Blades 1996; Watson and Meyer 1996) suggest that small scale structure also exists in the WIM.

proposed observations: JST: note: here we actually give estimated line intensities, which we presently do not in the [CI] section; this has to be made coherent

[CII] line emission for an HI cloud with a column density of N(H) $\sim 5\times10^{20}$cm^{-2} is estimated to be I(CII) $\sim 10^{-6}$ erg cm^{-2} s^{-1} sr^{-1} (Matsuhara et al. 1997), **JST: compare with Timmerman et al. 1998 results on L1457** while the WIM contribution is I_{WIM}(CII) $= 4\times10^{-7}$ erg cm^{-2} s^{-1}sr^{-1} assuming I(CII)/N(H) $= 3\times10^{-26}$ erg s^{-1} H^{-1} (Gry et al. 1992) and all the carbon in the gas phase. **JST: drop, repeats above: The velocity information will be a critical input to disentangle the relative contributions of the CNM and WIM to the line intensity.**

1.1.3 [NII]: exclusive tracer for the WIM

The [NII] line at 205 μm is expected to be 0.06 times weaker than the [CII] line in the WIM and will therefore be detectable by HIFI only up to a few degrees from the plane. It is an excellent tracer of ionized gas, with no contamination from any other phase of the ISM. The comparison of [NII], [CII] and HI emission spectra will permit the investigation of the degree of association between the so-called cold (or cloud)(T$<$ a few 100 K) and warm intercloud (T$\sim$ 8000 K) neutral phases of the interstellar medium and the role of thermal instability in the formation of small scale density structure within the diffuse ISM (Hennebelle & Pérault 2000). **JST: this is much too vague, at least for my taste! How does the comparison of spectra allow to do all to investigate all this? Which feature of the spectra are the crucial ones?** The warm neutral gas does not contribute to the [CII] emission while both the cold and warm neutral phases contribute to the HI emission. The [NII] observations allow subtraction of the fraction of [CII] from ionized gas. **JST: reading the last sentence, I get completely confused! We introduce new termini: cold neutral (or cloud) phase, warm intercloud neutral medium; and then list various lines associated with various components, but not given a clear clue of what finally comes**

from what; plus: how is the subtraction of the fraction of [CII] from ionized gas going to work? Simply by identifying it through the line profile? Or by scaling it with some reasonable assumptions from the [NII]??

With the gas temperature and pressure estimates deduced from the neutral carbon lines, it might be possible to derive the carbon abundance from the [CII] line intensity. **JST: I regard this and the following as highly speculative, i.e. I agree with the "might". I guess, what is meant here, is that the temperature and/or pressure from [CI] can help to estimate the level population in [CII]? But his assumes that they come from the same gas. What if not? How do we tell?** We will be able to correlate variations in the carbon depletion with local physical conditions and dust extinction and emission properties including observations of the dust emission spectrum with PACS and SPIRE. Such measurements will open a completely new perspective on the cycling of carbon between dust grains, small aromatic hydrocarbon particules, CO and atomic carbon. Indeed, Miville-Deschênes et al. (2002) show evidences for correlation between the abundance of the very small dust particles responsible for the mid-IR emission, and the gas velocity structure.

JST: shouldn't this go to section 1.3? Observations of the emission lines of the ISM as described above should be also performed in fields surrounding the lines of sight studied in absorption in the UV by the HST and FUSE. The absorption studies give access to abundances and Doppler broadening for many atomic and ionic species but they are limited to a spectral resolution of about 3 km s^{-1} (HST) and the spatial information is almost non existent. However they provide unique information on the abundances and ionization state of numerous IS 'components' i.e. defined by a common absorption velocity. Some of the components are neutral and clearly associated with the WNM, and some are at least partially ionized, the origin of the ionization being not always clear. Some of these components in the lines of sight to halo stars should correspond to the extended Hα emitting layer in the Galaxy but its identification is not straightforward, especially because of the lack of spatial information of UV observations and the lack of spectral resolution of Hα observations. **JST: what exactly are the HIFI observations going to contribute to this? How do we handle the difference between the pencil and 15-30 arcsec beam? What observations in detail do we propose? How much time do we need?**

1.2 proposed observations

For each source **JST: which sources are we talking about? Wrap up from previous discussion!** we propose to map small fields using the OTF mode in order to have a description of the small scale structure, and to have global information to compare with previous large scale observations (IRAS, ISO **JST add: BICE**). For [CII] and [NII], we use a system temperature of 1800 K and adapt the frequency resolution to the expected line width. **JST: I am not so sure that we want to use a frequ resolution adapted to the line width; the purpose is, to really see the detailed line profile structure, so that we need some other constraint on the resolution aimed at: thermal width, turbulent width of individual components?** The expected [CII] line strength is 10^{-6} erg $cm^{-2}s^{-1}sr^{-1}$ for high latitude clouds, and 4×10^{-4} erg $cm^{-2}s^{-1}sr^{-1}$ for a line of sight across the Galactic Plane at $b = 0.5°$. This corresponds to line integrated intensities of 0.14 K kms^{-1} ($\delta v = 2$ km s^{-1}) and 60 K kms^{-1} ($\delta v = 30$ km s^{-1}) respectively. The ionised nitrogen line at 205 μm is about 10 times weaker than [CII], but has broader features.

Adopting a velocity resolution of 1 kms^{-1} for [CII] and 4 kms^{-1} for [NII], a single pixel is detected at the 3σ level in 900s (high latitude), 30s (Galaxy, [CII] and [NII]). **JST: is the resolution of 1 km/s really sufficient for the [CII] observations? We argue above, that CII should be narrower than HI by sqrt(mass) and quote 3 km/s as the thermal width of HI. Thus, 1km/s resolution is only a single resolution element for the whole, thermal [CII] line,**

certainly not sufficient, and definitely not at a S/N of 3!

We need to observe both [CI] lines as well, covering the same area in the 492 GHz line, and observing a few positions in the 809 GHz line. The estimated line strength is 0.1 $Kkms^{-1}$ for the 492 GHz line in a high latitude cloud and 6 $Kkms^{-1}$ across the Galaxy. The 809 GHz line is very sensitive to the gas pressure. In diffuse clouds, it is weaker than the 492 GHz line, by a factor of 10 approximatively.

We adopt use a system temperature of 233 K for 492 GHz and 454 K for 809 GHz, and select a frequency resolution of 1 MHz (or 0.6 km s^{-1}) at 492 GHz. For the high latitude fields, the requested integration time per pixel is 120 s for the 492 GHz [CI] line. The 809 GHz lines requires 4 hours integration per position.

For the Galaxy fields, the signal is expected to be stronger over a larger velocity coverage than for the HLCs and we plan to decrease the integration time by a factor of two in the plane. Since the lines, if they follow the latitude dependence of the emission measure, decrease by a factor 3 between $b = 0$ and $b = 2°$, the integration time for fields at larger latitude will be similar than for HLCs.

To cover a 4'×4' field in the [CII] line, a map of 40 × 40 positions with a sampling of 6" is required. For the high latitude clouds, the spatial resolution will be degraded to 30" to be comparable to the [CI] data. We give the integration time for a total of 64 points. For the lines of sight through the Galaxy, we compute the integration time for a spatial resolution of 20 arcsec (144 independant points)

We list below the requested integration times to observe one field of size $M \times N$ in arcminutes, with a resolution δv and a final rms σ once the angular resolution has been smoothed to 30" for the HLCs and 20" for the galaxy at $b = 0$. Frequency switching is used for the HLC fields.

- High latitude [CII] : 16 hours $(M \times N/4' \times 4')(14\text{mK}/\sigma)^2(3\text{kms}^{-1}/\delta v)^2$
- High latitude [CI] : 5 hours $(M \times N/4' \times 4')(12\text{mK}/\sigma)^2(3\text{kms}^{-1}/\delta v)^2$
- Galaxy [CII] : 1.2 hour $(M \times N/4' \times 4')(60\text{mK}/\sigma)^2(4\text{kms}^{-1}/\delta v)^2$
- Galaxy [NII]: 1.2 hour $(M \times N/4' \times 4')(60\text{mK}/\sigma)^2(4\text{kms}^{-1}/\delta v)^2$
- Galaxy [CI] : 2.5 hours $(M \times N/4' \times 4')(17\text{mK}/\sigma)^2(3\text{kms}^{-1}/\delta v)^2$

Adding at least one 809 GHz [CI] point, the total time per field is thus 25 hours (high latitude) and 9 hours (Galaxy, $b = 0$). The total satellite time will be at least a factor of two larger due to various overheads.

We have selected the two fields in the Ursa Major cirrus which have been observed with ISOCAM (Miville-Deschênes et al. 2002). The first one, where no CO is detected, bears the signatures in the mid-IR of large abundances of small dust grains, the second is located at a transition region between atomic and molecular gas. The spectral dust properties and gas kinematics in these two fields are different.

In the Galaxy, we propose to observe 4 fields at increasing Galactic latitude to measure the scale heights of the different phases. The position has been chosen at the tangent point, to minimize the spread in velocity. The physical conditions have been studied using ISO data (Verstraete et al. 1999). We shall observe in the OTF mode for all lines of sight. We can use the frequency switching mode for the high latitude cloud observations where we expect narrow lines. We will investigate further the best observing mode for the fields through the Galaxy, depending on the instrument performances as revaled by the coming instrument tests. The overheads will likely be larger than for the high latitude cloud observation, and we applied a factor of 2.5.

It sums to a total of **50 hours** for the two fields in the Ursa cirrus, and **36 hours** for the 4 lines of sight through the Galaxy which corresponds to a total of about **200 hours** including the overheads. **JST: what about the FUSE lines-of-sight?**

JST: we have to make sure, that prep observations give us HI, CO etc. data at similar specral and spatial resolution for those fields

Table 1: Position for Maps

Name	RA(2000)	DEC (2000)	Comment
Ursa Major	9:45:00	70:25:00	Cirrus, 2 $4' \times 4'$ fields
Galaxy	18:39:16.3	-05:42:58	4 $4' \times 4'$ fields with different b starting at $(l, b) = (26.86, 0.09)$

PDRs in diffuse gas

JST: I suggest to change this subsection title. This is not at all specifically on PDRs, but on the chemistry of diffuse gas; hence:

1.3 Chemistry in diffuse gas

The chemical properties of diffuse clouds such as those lying along the line of sight to the bright O9 star ζ Oph are well known from a continuous effort on visible and UV spectroscopy during the past 40 years. Using the same technique in the radio domain, with distant radio sources as background objects, Liszt and Lucas (1996 to 2001) have measured the abundance of other molecules, not easily studied in the UV/visible wavelength range. There is little overlap so far. By observing a few lines HIFI can bring critical information on these two types of lines of sight (bright stars and continuum sources). As described above, the combination of the fine structure lines of C and C^+ with the H and H_2 column densities (available from FUV data) gives access to the gas pressure and carbon abundance. Since the sources are extended, observations will be performed in frequency switching. We shall use PACS for mapping one field of view in C^+ to assess the structure of the ISM in the vicinity of these particular lines of sight. **JST: (I) time estimate for the PACS observations! (ii) is the PACS data really sufficient, i.e. can we get sufficient structure information form integraetd profiles? Why don't we include such a field as one of the ones to measured in the preceeding section?**

In addition to the special direction towards ζOph, it is interesting to study a few more points where the CO emission gets stronger to sample the transition from atomic to molecular gas. Information on the line profile is important for performing a meaningful comparison with models since the behaviour different velocity components, detected in e.g. sodium lines, is expected to be different.

The selected lines of sight are listed below.

We expect a line intensity of ~ 0.1 K for the 1-0 [CI] line and ~ 1 K for [CII], similar as for the diffuse HI clouds. **JST: not true: we quote above 0.14 K km/s for a 2 km/s wide line from a high latitude cloud! Needs to be consistent. IN any case: based on what assumption are these intensities estimated?** The program therefore requires ~ 15 min integration time for [CI] and ~ 10 minutes for [CII] per line of sight. **JST: for what velocity resolution is this estimated?** Stronger [CI] lines are expected towards the additional positions in ζ oph, so we plan to spend 5 minutes only for those positions for both [CII] and [CI].

This sums to a total of $10 \times 0.25) + (5 \times 0.1) + (10 \times 0.2) + (5 \times 0.1) = 5.5$ hours of integration, hence a total of **11 hours** of telescope time including overheads.

Table 2: Single lines of sight from FUSE and/or IRAM

Name	RA	DEC	Comment
ζ Oph	16 37 09.5378	-10 34 01.524	Star + 5 positions ?
B0212+735	02 17 30.8134	+73 49 32.622	BL lac
B055+508	03 59 29.7473	+50 57 50.162	QSO
B2013+370	20 15 28.7	+37 10 59	Radio source
B2037+511	20 38 37.12	+51 19 12.7	QSO
PG0804+761	08 10 58.55	+76 02 41.8	FUSE QSO, radio quiet
HD73882	08 39 09.5344	-40 25 09.262	FUSE HD
HD34078	05 16 18.1497	+34 18 44.341	FUSE warm H_2
HD185418	19 38 27.4827	+17 15 26.052	FUSE, double system
HD102065	11 43 36.9487	-80 29 00.521	

XXXXXXXXXXXXXXX (JST: presently edited until here) XXXXXXXXXXXXXXXXXX

2 Physical and Chemical processes in the Warm and dense ISM

2.1 PDRs as probes of the Photoelectric heating in the ISM

The interstellar gas is efficiently heated by the photoelectric effect on dust grains (visible-UV photons from stars eject energetic electrons from dust grains which heat the gas while thermalizing). As a consequence, the gas temperature - which controls the chemical and thermal evolution of the interstellar medium - depends on the photoelectric heating rate. Recent theoretical (Bakes & Tielens 1994, Wolfire et al. 1995, Weingartner & Draine 2001) and observational (Habart et al. 2001) studies have shown that the photoelectric heating of the gas is dominated by the contribution of *small carbonaceous dust grains* (nanoparticles of radius less than 150 Å, conversely the so-called *big grains* have larger sizes). In addition, the photoelectric heating rate depends on the local physical conditions (radiation field intensity, gas density: Weingartner & Draine 2001).

At thermal balance (heating and cooling rates are equal), the gas heat budget can be determined from observations of the major cooling lines. Moreover, in regions of low excitation, the gas heating is mostly due to the photoelectric effect on dust grains. This implies that abundance variations of the small carbonaceous grains should be reflected in the gas heat budget as well as variations of the local physical conditions (see Habart et al. 2001).

We propose to study the heat budget of interstellar gas across a number of low-excitation photodissociated interfaces in relationship to the carbon abundance. The goal is to follow the carbon cycle between the gas phase and the small carbonaceous dust particles and its impact on the gas heating.

The HIFI instrument – because of its high spectral resolution and sensitivity – will detect the main gas cooling lines from C^0, C^+ and CO without contamination from the background emission. Physical conditions of the gas (pressure, density and radiation field intensity) will be obtained through observations and theoretical modelling of the carbon cooling lines. The hydrogen column density at each position will be constrained from ancillary observations of the HI-21cm line (Penticton, VLA) and also from the emission of the big grains.

To carry out this project, we will observe the major gas cooling lines (HIFI: $[C^+]158\ \mu$m, $[C^0]370,609\ \mu$m and CO(J=8-7 and up), PACS: $[O^0]63\mu$m) and compare it to the emission of small

Table 3: Target list and physical conditions

Target	Position (J2000)	χ [a]	n_H [b] (cm^{-3})	$T_\star$ [c] (10^4 K)
L1721[1]	16h14m30s, -19°5'	5	$3(3)^\dagger$	2.2
Octopus[2]	16h52m30s, -25°45'	5	4(3)¶	2.5
Ced 201[3]	22h13m25s, 70°15'	10	2(3)¶	1.0
ρ Oph. Fil.[4]	16h25m55s, -24°21'	400	$4(4)^\dagger$	2.2
L1630[5]	5h41m45s, -2°15'	1000	1(4)¶	2.3
Horsehead[5]	5h40m55s, -2°28'	100	$2(4)^\dagger$	3.3
California Neb.[6]	4h03m17s, 36°28'	6	1(3)¶	3.7
Ursa Major[7]	9h45m45s, 70°22'	1	100¶	2.2

[a] Intensity of the UV radiation field in units of the Habing flux at 1000 Å, $\lambda u_\lambda = 1.2\ 10^{-3}$ erg/s/cm^2.
[b] The hydrogen density of the region as derived from modelling (†, Habart et al. 2001, 2002) and roughly estimated (¶). Notation: $1(4) = 10^4$.
[c] Effective temperature of the illuminating star.

References: [1] Habart et al. 2001, [2] Bernard et al. 1998, [3] Cesarsky et al. 2000, [4] Habart et al 2002*a*, [5] Habart et al 2002*b*, [6] Boulanger et al. 1990, [7] Miville-Deschênes et al. 2002.

grains as traced by ISOCAM. The emission of bigger grains will be measured by PACS and SPIRE. We will perform these observations towards regions where the emission of small and big grains are contrasted indicating dust abundance variations. Our target list is given below as well as the integration times. In each case, the 5×5 pixels field of PACS will be centered on the photodissociated interface (one side of the field parallel to the interface) and five HIFI spectra will be taken along a cut in the central part of the PACS field and perpendicular to the interface. For the case of the diffuse ISM (Ursa Major), we took the C^+ line flux of Gry et al. (1992). The other line fluxes were estimated from the model results of Wolfire et al. (1995). The Ced 201 and Octopus lines of sight will sample regions with a grain size distribution significantly different from that of the general ISM (as described, e.g., in Désert et al. 1990).

Towards most of the lines of sight, the cooling by H_2 may be important: it will estimated from near-IR observations of rovibrational lines and theoretical modelling. Observations of H_2 and low-J CO emission are already available for the ρ Oph filament and for the Horsehead nebula.

We require a total Herschel time of **20 hours** for this section amongst which **6 hours** of the HIFI instrument.

2.2 chemical tracers of PDRs and XDRs

In addition to CH^+ is there any other molecule to search for ?

Table 4: Integration time estimates for the heating budget section

Target	C^+ [a] (158μm)	C^0 [a] (370μm)	C^0 [a] (609μm)	O^0 [a] (63μm)	PACS [b] (2 bands)	SPIRE [c] (3 bands)	Time [d] (mn)
L1721	6(-3)[e]	7(-3)	6(-3)	60[e]	0.3	1.7	40
Octopus[f]	-	-	-	-	-	-	40
Ced 201[f]	-	-	-	-	-	-	40
ρ Oph. Fil.	0[e]	7(-3)	6(-3)	1.5[e]	0.3	1.7	3.5
L1630[f]	-	-	-	-	-	-	3.5
Horsehead	0.2	0.1	5(-2)	25	5	25	55
California Neb.	0.1	1.8	0.9	$*$	3	14	20
Ursa Major	12	$*$	60	$*$	12	$*$	84

All integration times are given in minutes and for a 5σ-detection.
[a] The integration time in minutes. All values are given for a 5σ detection within a resolution element of 0.3 km/s. The integration time for the [O^0]63 μm line with PACS is also given (175 km/s resolution element).
[b] The integration time at 100μm for the PACS photometric mode.
[c] The integration time at 500μm for the SPIRE photometric mode.
[d] Total integration time for one line of sight. Five positions will be observed in each region except for Ursa Major where only 3 positions will be observed.
[e] The line fluxes have been measured by the gratting mode of ISO-LWS.
[f] Ced 201 and Octopus as well as L1630 and the ρ Oph Filament have been assumed to have similar fluxes.

The asterisk (*) indicates observations which can not be performed because they require a too large integration time.

2.3 Emission lines, Photodissociation regions and shocks

In high density warm regions, such as bright photo-dissociation regions, the hydride lines may appear in emission. For example, CH^+ rotational lines have been detected in emission in the young planetary nebula NGC7027 (Cernicharo et al. 1997).

Most models of photo-dissociation regions (PDRs) are static, and use a pure gas phase chemistry, but other physical effects could play a role in these regions. Gerin et al. (1998) and Lemaire et al. (1999) have measured the line profile of the [CII] 158 μm and H_2 v=1-0 S(1) 2.12 μm lines respectively, in NGC 7023. There is a clear velocity gradient through the PDR which is not taken into account by models. Photodissociation and evaporation of molecular gas from the molecular cloud could explain this gradient. Since this example is likely not to be unique (see e.g. Habart et al., 2001), the static description of PDRs should not be valid anymore, and should be replaced by dynamical models including advection of cold molecular into the PDR and evaporation of gas. PDR are good regions to probe how kinetic energy can be fed into dense interstellar clouds : from observations of the carbon recombination lines, combined with [CII] and [CI] data, a low level of turbulence is found in the C^+ region, which contrasts with the larger velocity dispersion in the molecular gas (Wyrowski et al. 2000).

The impact of such dynamical phenomenon on the structure and chemistry of interstellar gas is not well understood as most models focus on either the chemistry or the dynamics separately. With the possibility of measuring detailed line profiles for all species dominating the gas cooling, a quantitative assessment of the role of gas dynamics will become possible. Conclusions based on bright photo-dissociation regions will be valid for the diffuse interstellar gas as a whole. For instance, the dissipation of turbulence is an additional heating source, highly localised in specific regions of a turbulent flow (Pety & Falgarone 2000). Measurements of the main cooling lines, either from the ground (see below) or with Herschel will help to quantify the impact of this additional heating source on the properties of diffuse interstellar gas. In addition, advection of cold gas into the PDR is likely to affect the chemistry. The ice mantles are expected to be destroyed by the combined influence of the enganced temperature and UV radiation. Since water is the main constituent of grain mantles, HIFI is ideally suited to reveal the presence and measure the magnitude of advection processes in PDRs.

The target list includes potential sources covering a range of physical conditions (density, radiation field, shocks) to search for emission lines as well. Lines as weak as 1 K can be mapped with OTF maps using circa 60sec integration time per position. Since the velocity dispersion is small, all lines can be observed in FSW mode, with no loss of efficiency due to telescope slewing. The extension of all sources is a few minutes. For a $2' \times 2'$ map at 15 arcsec sampling, the total number of points is 64, so the total integration time is 3840s. Such a map can be performed in less than two hours including overheads.

We shall search for a restricted number of lines since the physical conditions for emission are more restrictive than for absorption. The sources have been selected as dense PDRs with different illumination conditions $G_0 = 100 - 10^5$, with and without ionisation fronts. We propose to search for CH and CH^+ as tracers of the first steps of the chemistry. Water and H_3O^+ are interesting for two reasons described above : i) as H_2O cooling is important in dense regions, and ii) as water is the main constituent of the grain mantles, we want to search for evidences of the photodesorption of grain mantles. Both the spatial and spectral information are needed for this purpose. Finally, ammonia will trace the dense well shielded molecular gas and help us to separate the emission from the PDR from that of the bulk of the molecular cloud.

Note that the reactive ion CO^+ has been detected in two sources, the Orion Bar and NGC 7023 (Black 1998 and references therein), which is a good eveidence for dynamical processes at least for these two sources. We have also included the young supernova remnant IC443 as a prototype of shocked region in the ISM.

For 6 sources and 9 maps per source ([CII], CH, CH^+, H_2O (2 ground state lines, ortho species at 1.7 THz and para species at 1.1 THz) and $H_2^{18}O$ (same 2 lines), H_3O^+, NH_3) it sums to a total of **$6 \times 7 \times 2$ = 94 hours** of telescope time.

Ground based data on the spatial distribution of the submillimeter C and CO lines should be obtained in the coming years to set the optimum size an position of the regions to be mapped with Herschel, and provide the necessary information on the warm molecular gas. There is no need to perform these observations with Herschel as the C and CO lines are bright and accessible from the ground.

Table 5: Photo dissociation regions and shocks

Name	RA(2000)	DEC(2000)	Comment
PDRs			
NGC 7023	21 01 36.92	+68 09 47.8	Origin on HD 200775
Orion-Bar	05 35 22.90	-05 24 57.8	Origin on θ_2 Ori (HD 37041)
NGC 7027	21 07 01.7	+42 14 10	Young PNe
Horsehead nebula	05 40 59.0	-02 27 30	
IC 63	00 59 01.37	+60 53 17.8	
Shocks			
IC 443-G	06 16 43.0	22 32 38.0	

Complementary data Finally, the spatial structure of the continuum sources must be known to interpret properly the absorption data. Since the sources are bright, they can be observed almost instantaneously. We have chosen an integration time of 5 minutes for each instrument. For a total number of 8 sources, the required time for photometry is $7 \times 0.12 \times 2 =$ **2 hours**.

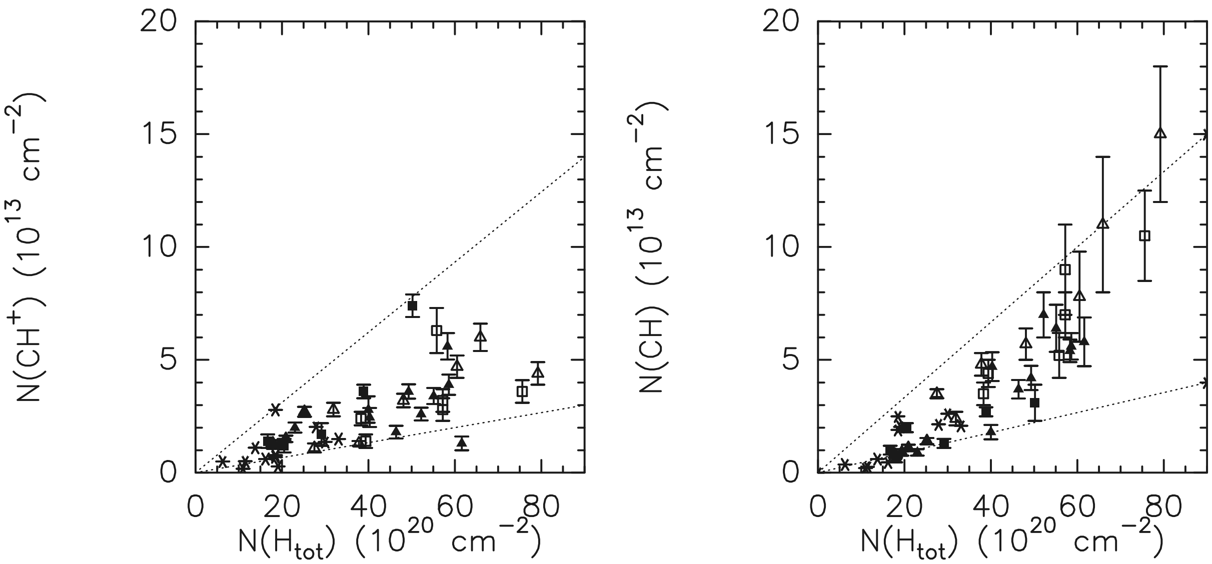

Figure 1: The column densities of CH^+ (left) and CH(right) as a function of the total hydrogen column densities. Data points are taken from (Crane et al. 1995, Gredel 1997).

3 Transition from atomic to molecular gas

Due to the large opacity of earth atmosphere to far infrared and submillimeter radiation, light interstellar molecules, with rotational transitions below 1mm, are less well known than heavier molecules, radiating in the millimeter region. Though hydrides such as OH, CH, CH^+ have been known as interstellar molecules since the 1940's and 1950's, their production is not yet completely understood. In fact, the abundance has been measured over a much smaller range of physical conditions than for e.g. CO or HCN. Also the kinematic properties which provide very important information concerning the physical conditions, are poorly known for species observed through their electronic transitions. In some exceptional cases, data with very high spectral resolution have been obtained, in which CN, CH and CH^+ present different line profiles : while CN electronic transitions have a similar velocity structure than the ground state rotational line of carbon monoxide seen in emission, the CH^+ line is broader, and has a different velocity structure.

Chemical models describe the production of interstellar molecules through a series of two-body chemical reactions in the gas phase, coupled with solid phase reactions on dust grains. Molecular hydrogen is the most important molecule formed on the dust grain surfaces, but similar processes are efficient to produce hyrogenated species. In the interstellar chemistry framework, molecules are formed gradually from atoms and ions. Small light molecules convey very important chemical information since they are formed in the first steps of chemical networks, and are therefore sensitive to a small number of chemical reactions. Models of interstellar sources have been devised in the past twenty years, which describe the interstellar medium with an increasing degree of complexity, but are still far simpler than the structure revealed by the data. The simplest models are steady state, with a single density and temperature. More sophisticated models deal with time dependent effects, density structure, solve the thermal balance etc., but still fail to reproduce the observed abundance of important species unless they introduce a coupling between the chemistry and the gas dynamics.

The likely reason for this failure is the still incomplete description of the structure and kinematics of the ISM in these models, leading to an incomplete coverage of the relevant physical and chemical processes. In fact, diffuse interstellar clouds appear more active chemically than anticipated, given their low gas density and average temperature (Lucas & Liszt 2000, 2001). This unexpected chemical activity has been known for years, after the detection of large amounts of CH^+ and CH in absorption against nearby stars. Large abundances of molecules like HCO^+ and OH have been observed recently in regions with no CO emission nor absorption (see Figure 2 from Lucas & Liszt 1996). Contrary to CH, which shows a tight correlation with the gas column density, CH^+ is less tightly correlated with total gas column density, as shown in Fig. 3. The observed level of CH^+ column densities (10^{12} to 10^{14} cm^{-2} are difficult to explain because the formation paths of molecules such as CH^+ require triggering of endothermic reactions or overcoming activation barriers. Their formation therefore requires the presence of energetic events and, whatever these events are, HIFI is ideally suited to detect lines in this highly excited, probably small scale, component of the interstellar medium. Magneto-hydrodynamical shocks (Draine 1980, Flower & Pineau de Forêts 1998) fulfill these criteria, but predict a velocity shift between neutral and ions (~ 2 kms^{-1} in the recent comprehensive models by Flower & Pineau des Forêts 1998). An alternative would be that these reactive species form in regions in atomic clouds where bursts of turbulent dissipation locally heat the gas to temperatures as large as 10^3K (Falgarone et al. 1995; Joulain et al. 1998 A&A 340 241). In that case all species would form with the same centroid velocity, as observed in most lines of sight.

CH^+, as other reactive molecules (H_2^+, CO^+, OH^+, H_2O^+etc.), is particularly interesting as a potential diagnostic for the interstellar medium, since this molecular ion is destroyed rapidly (by collision with H, H_2 and other neutrals), and may keep a memory of its formation process in its velocity distribution and rotational excitation (Flower & Pineau des Forêts 1998, Black 1998).

HIFI is ideally suited for such studies since it gives access to the ground state rotational lines of most interstellar hydrides, and most importantly, provides the critically needed high spectral resolution. The sensitivity is such that we shall be able to probe the abundance of interstellar hydrides in a large range of physical conditions, which overlaps the domain probed by electronic transitions for e.g. CH and CH^+. Studying hydrides, HIFI will be able to investigate the role of chemistry on dust grains and small aromatic hydrocarbons as well. Dust observations from mid-IR to sub-mm wavelengths (IRAS, COBE and ISO) show that significant dust growth by gas accretion and/or coagulation occurs even within translucent clouds where ices are not observed. The accretion of gas atoms on grains may be followed by the formation of simple molecules such as hydrides on grains in the same way as H_2. Such a formation process has been proposed to explain the detection of NH in the diffuse medium (Crawford & Williams 1997, Goiecochea et al. 2000).

3.1 Proposed observations : survey for absorption lines

In the diffuse ISM, HIFI is able to search for absorption features due to hydrides. The selection criteria for the sources should be the availability of a strong far infrared continuum and the presence of interstellar clouds along the line of sight of the continuum source. The sample is built with targets already studied by ISO and SWAS (SgrB2 Neufeld et al. (1997), W49N Caux et al. (2002)) as well as HII regions studied at mm wavelenghs. In addition, we searched for a few specific lines of sight bright in the visible and the far infrared to allow a meaningful comparison with previous work. The selected sources are located at different galacto-centric distances and have different properties to allow us to sample a wide variety of physical conditions.

¿From published ground based and space data, we expect continuum intensities of hundreds of janskies in the HIFI domain. High spectral resolution data (1 MHz) can be obtained with a S/N ratio for the continuum larger than 10 in a few minutes of integration for most sources. The average time spent on each source is estimated to be 15 minutes per tuning. The most intense lines for interstellar hyrides are listed in Table 7. The third column gives an estimation of the line opacity for a total column density of 10^{13}cm^{-2} and a line width of 1 kms^{-1}. The most promising lines are the ground state lines of CH (2 tunings), CH^+ (1), NH (1), NH_2 (1), NH_3 (1), NH_2D (1), H_2O (8 lines for ^{16}O, ^{18}O and ^{17}O isotopes) HDO (1), D_2O (1) H_3O^+ (1), HF (1) and DF (1), HCl (1).

The total number of lines per source is 20 including deuterated species and isotopes. With 17 sources, the total time is $\mathbf{20{\times}17{\times}0.25 = 85}$ **hours**.

Table 6: Absorption line sources

Name	RA 2000	Dec	F100 (Jy)	F350 (Jy)	Comment
RAFGL2136	18 22 29.1	-13 29 46	5696	100	
RAFGL2591	20 29 24.9	+40 11 21	5721	100	
RAFGL 490	03 27 38.4	+58 47 04	785	45	
W33A	18 14 39.9	-17 51 59	6310	400	
W3-IRS5	02 25 40.7	+62 05 52	42100	200	
W3-H_2O	02 27 04.6	+61 52 25	10600	498	
S140-IRS1	22 19 18.4	+63 18 45	13460	400	
RAFGL7009S	18 34 19.7	-05 59 44	2136	200	
NGC7538-IRS1	23 13 45.38	+61 28 10.7	14100	301	Confused IRS1-IRS9
NGC6334-IRS1	17 20 00.8	-35 57 33	19800	1263	extended emission, IRAS source 1 arcmin
W49N	19 10 13.2	+09 06 12	36200		
W51	19 23 43.90	+14 30 34.8	26800		IRAS 1 arcmin
Sgr B2	17 47 20.4	-28 23 07	66600	3962	SgrB2(M)
Sgr A*	17 45 39.95	-29 00 28.2	23300		
GCS-3	17 46 14.9	-28 49 37	410	Visible data possible	
Cyg OB12	20 32 41.1	+41 14 28	131	Visible data available	
IRAS05389-6908	05 38 36.7	-69 06 29	2490		LMC, 40" from Sk -69 243

Fluxes from IRAS point source catalog, Sandell (1994), van der Tak et al. (2000), Goldsmith et al. (1990)

Complementary data Finally, the spatial structure of the continuum sources must be known to interpret properly the absorption data. Since the sources are bright, they can be observed almost instantaneously. We have chosen an integration time of 5 minutes for each instrument. For a total number of 17 sources, the required time for photometry is $17 \times 0.12 \times 2 = \mathbf{4}$ **hours**.

4 Molecular complexity

The inventory of the molecules present in the interstellar medium is fairly incomplete. For example, the identification of the carriers of most Diffuse Interstellar Bands (DIBs) is still pending. The full opening of the far infrared and sub-millimetre domain with HSO will offer the opportunity to search for many new species in the interstellar medium (e.g the contributions J. Goicochea & J. Cernicharo in the Toledo meeting, present detailed calculations of the expected spectra for some molecules).

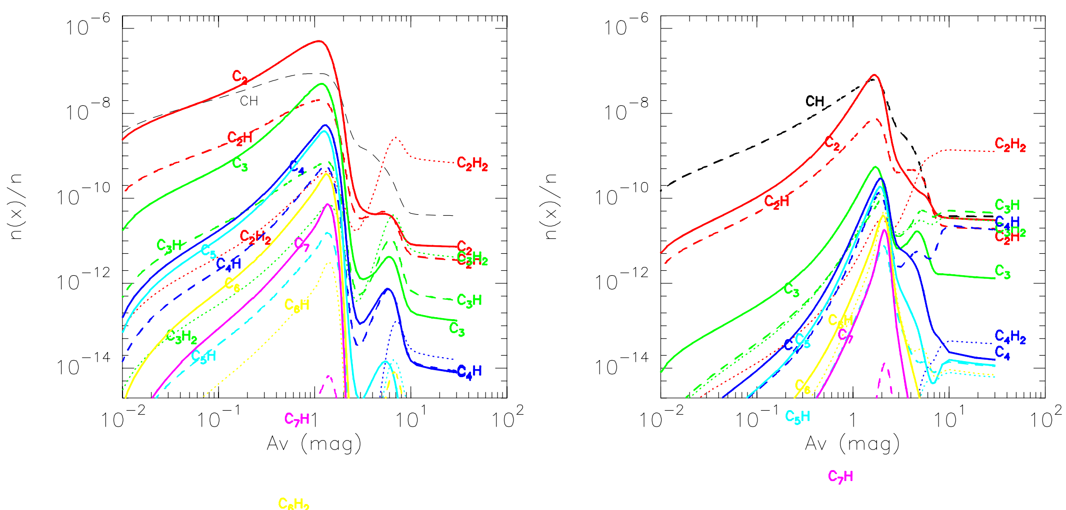

Figure 2: Prediction of the abundance of hydrocarbons having one (black) to seven (purple) carbon atoms using two different chemical networks : the New Neutral Neutral chemical model from E. Herbst and the UMIST95 data rate. The calculations are performed for a moderate gas density ($n_H = 2 \times 10^4$ cm^{-3}), illuminated by a mild UV radiation ($G_0 = 100$). Carbon chains are shown with full lines, C_nH species with dashed lines and C_nH_2 species with dotted lines. There is a clear tendency to have C_n species more abundant than the corresponding C_nH species, more abundant than the corresponding C_nH_2 species. (E. Roueff, private communication).

4.1 carbon chains and cycles

It is expected that some large molecules, bridging the gap between the known gas phase species and the Polycyclic Aromatic Hydrocarbons (PAHs), survive in the diffuse ISM. Large molecules are good candidates for some Diffuse Interstellar Bands, though no definitive identification has been made yet. The strength of these absorption features require quite high abundances for their carriers (Herbig 1995, 2000). Carbon is generally thought to be a major constituent of the DIBs carriers, therefore, carbon chains and other hydrocarbons have been suggested as possible carriers (e.g. Thaddeus et al. 1995). Carbon chains (linear or cyclic) are also very good candidates for Herschel since they have low lying vibrational modes in the far infrared. Hence absorption measurements in the far infrared will allow to detect symmetric species which escape detections in the radio domain. For example, the C_3 radical has been recently detected towards the Galactic Centre by ISO (Cernicharo et al. 2000).

It is possible to use gas phase chemical models to obtain predictions for the abundances of some large molecules. Though the chemical networks have not been as extensively tested for these large species as they are for smaller species, these models provide some inputs to drive the observational effort. For example, we show in Figure 2 predictions for a PDR (Le Bourlot et al. 1993) obtained with two different chemical networks, the "New Neutral Neutral" chemical network from E. Herbst (Terzevia et al. (1998, 2000)) and the UMIST95 network. From this model, as from preliminary observations on small hydrocarbons (Fossé, 2001 and in prep., Liszt and Lucas 2001) hydrocarbons may have a significant abundance in photon dominated regions. There is a clear pattern with C_n species being more abundant than C_nH species, which are themselves more abundant than C_nH_2 species. C_n species cannot be detected in the radio domain as they have no permanent dipole moment, but could be seen in the diffuse ISM with Herschel through their ro-vibrational far infrared spectrum.

As the ro-vibrational frequencies are not accurately known at present, it is difficult to set a particular frequency range and integration time. This search should be combined with the line surveys. The best target is probably one of the strong continuum sources in the SgrB2 molecular clouds, either SgrB2N or SgrB2M, since these lines of sight cross several clouds along the line of sight with different chemical properties. SgrB2 is listed already in the hydrides section. The search for carbon chains and cycles will be part of the line surveys and does not require additional time given the current knowledge.

4.2 Search for low energy bending modes of PAHS

Polycyclic aromatic hydrocarbons (PAHs) have been proposed as the carriers of the Aromatic IR (AIR) bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μm since about twenty years. Interstellar PAHs absorb UV photons and they cool down by emitting in their vibrational modes (Léger et al. 1989, Allamandola et al. 1989). The identification of interstellar PAHs has motivated a lot of observational, laboratory, quantum chemical and modelling studies. Although progress has been made, identification of a specific PAH has remained elusive. Part of the difficulty is due to the fact that all PAHs have aromatic CC and CH bonds which give IR modes close to the AIR bands. One idea to circumvent these difficulties is to look for the rotational structure of the low-frequency IR bands of PAHs. Indeed, PAHs are known to have flopping modes which involve the deformation of the whole skeleton, some of them being located in the THz domain. Detecting such a rovibrational structure would help a lot in identifying the carriers. For a symmetric rotor, the rotational constants are inversely proportional to N_C^2 and the spacing between the 2 rotational lines would therefore gives an immediate idea on the size of the rotor. The position of the whole band (the Q branch) is on the other hand specific of the molecule itself. Finally, another interest is the characterisation of the rotational temperature of PAHs which would have strong impact in the models (cf. Rouan et al. 1992).

HIFI can have a very unique role in these studies regarding the identification of "large" carbonaceous molecules such as PAHs (but also carbon chains), through the rovibrational structure of their low frequency bending modes. This programme requires both I) a large spectral coverage, and II) a good sensitivity.

- I) The extend of the rovibrational structure depends on the rotational constants (i.e. the molecular size) as well as on the rotational temperature. For instance, this extend is 105 and 26 GHz with a line spacing of 667 and 42 MHz for $C_{24}H_{12}$ and $C_{96}H_{24}$ respectively. Note that the line spacing assumes no anharmonic effects (no vibration-rotation coupling). Whereas the rotational structure depends mostly on the molecular size, the position of the band (Q branch) is very specific of the identity of the molecule.

- II) the low-frequency bending bands have weak Einstein coefficients (A = 10^{-4} s^{-1} $N_C{}^{-1}$ or lower) and the best strategy is to search for them in emission where the UV/visible radiation field is sufficiently high to pump them. Indeed, the bands are involved quite efficiently during the last steps of the cooling of the molecules.

Two observation strategies can then be proposed :
1- We have a precise idea on the molecule we want to look for and its spectrum is well characterised in the laboratory. 2- We are ready for something new and certainly we do not want to miss anything important (and for very long!). The identification of these large carbonaceous molecules would really help us a lot in our understanding of interstellar chemistry.

Though the first strategy requires a more limited spectral coverage and therefore allows a deeper integration, it is clear that HIFI is a unique instrument to make decisive progress given its ability to cover a broad spectral range with high sensitivity but also because the the low frequency bending modes are expected to be more frequent and more intense in the high frequency range (THz). The intensity of these bending modes can be estimated as follows. The emission in the AIR bands is estimated to be $I_{IR} = 1.8 \times 10^{-21} G_O \, \mathrm{Wcm}^{-2}$ in the Herschel beam. According to recent calculations (Joblin et al. 2002), the emission in the flopping modes ν_f of PAHs can represent 0.1% of the total IR emission (in the best cases). This lead to a total emission of $I(\nu_f) = 9.0 \times 10^{-19} \, \mathrm{Wcm}^{-2}$ for the Orion Bar ($G_O = 5 \times 10^4$). Assuming a PAH with 1/30 of the total abundance of PAHs, this leads to an intensity of 3.0×10^{-21} Wcm^{-2} emitted in the low frequency IR band of this specific PAH. Now there are about 400 lines per rotational structure (Trot=100K) and the width of the individual lines is assumed to be 3 MHz. This leads at 1 THz to an intensity of 1.46 10-20 W cm^{-2} micron^{-1}, i.e. 3.1 Jy or 6 mK per line. This estimation also does not take into account the effects of anharmonicity that have to be included since the emission in ν_f arises from several v levels. The numbers provided here should be used with caution till more laboratory data are available.

To estimate the required observing time, we performed two calculations :
– For the SIS mixers, we assume a typical system temperature of 500K and a frequency resolution of 2.5 MHz. Then individual lines are detected at the 3σ level after 5 hours integration time. The observations shall be performed in position switching, and cover about 24 GHz, or 4 contiguous tuning.
– For band 6, we use a system temperature of 1800 K and a frequency resolution of 6 MHz. Then 10 hours are needed for a single 4 GHz band. As a whole, this program requires $\sim$ 60 hours of telescope time to reach the required S/N in two or three sources. The sources will be selected from the list of bright PDRs, chosing the position expected to maximise the PAH signal, and the efficiency of observation.

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A Line frequencies for the ISM program

Total number of lines for a complete survey : 27
Total number of lines for the most abundant species with H, C, N or O : 14

Other lines outside HIFI range :
H_2D^+ 1.370146 THz
OH & ^{18}OH 2.5099 THz, 2.494695 2.494734 2.498994 2.499031
CH 2.00679 THz
OD 1.390613 THz, 1.391994

Missing species with no frequencies yet :

- OH^+
- H_2O^+
- H_2DO^+, HD_2O^+ and D_3O^+
- NH_3D^+ and other NH_4^+ isotopes
- $^{13}CH^+$ and CD^+
- ^{13}CH and CD
- NH^+ and ND^+
- ND
- CH_2D^+ and otherCH_3^+ isotopes
- D_2H^+
- CH_2^+
- $H_2O_2^+$
- Carbon chains and PAHs, including the positive ions and radicals (e.g. C_4H)
- What else ?

Table 7: List of lines

Name	Frequency (GHz)	$\tau/1$ kms^{-1} 10^{13}cm^{-2}	Comment
C	492.161		
NH_2D	494.454	0.62	
NH_2D	494.455	1.04	
NH_2D	494.457	0.21	
CH	532.724	0.25	small difference JPL/Cologne
	532.793	0.10	
	536.761	0.27	
	536.796	0.11	
$H_2{}^{18}O$-ortho	547.676	1.80	
$H_2{}^{17}O$-ortho	552.021	1.80	
H_2O-ortho	556.936	1.78	
$^{15}NH_3$	572.113	2.43	
NH_3	572.498	2.46	
D_2O	607.3496	4.03	
$H^{37}Cl$	624.964	0.48	
	624.978	0.72	
	624.988	0.24	
$H^{35}Cl$	625.901	0.48	
	625.919	0.72	
	625.932	0.24	
DF	651.099	3.88	
H_2S-ortho	736.034	0.49	
C	809.342		
CH^+	835.071	1.17	ν not accurate
$HD^{18}O$	883.189	3.49	
HDO	893.639	3.54	
D_2O	897.947	1.89	
NH_2	952.542	0.27	many weaker lines
	952.550	0.10	
	952.562	0.17	
	952.572	0.20	
	952.573	0.10	
	952.577	0.33	
	952.578	0.57	
	952.628	0.13	
	959.426	0.16	
	959.512	0.20	
	959.526	0.12	
	959.562	0.16	

B Deuterated hydrides

The presence of deuterium in the universe is an anomaly that can only be explained by Big Bang theories. It cannot be created any more, but can only burn inside stars causing a drop of its abundance

Table 7 continued

NH	974.462	0.12	Many weaker lines
	974.470	0.21	
	974.479	0.63	Strongest multiplet
	999.973	0.17	many weaker lines
H_3O^+	984.697	0.09	
$H_2{}^{18}O$-para	1101.698	4.00	
$H_2{}^{17}O$-para	1107.167	4.00	
H_2O-para	1113.343	4.00	
HF	1232.476	3.91	
N^+	1470		
H_3O^+	1655.813	1.10	
$H_2{}^{18}O$-ortho	1655.868	1.80	
$H_2{}^{17}O$-ortho	1662.464	1.80	
CH^+	1669.59		uncertain ν
H_2O-ortho	1669.905	1.78	
C^+	1902.346		

with respect to hydrogen as function of time. The measurement of the deuterium abundance relative to hydrogen is an important constraint on primordial nucleosynthesis. Due to its high spectral resolution and sensitivity, HIFI can measure accurately the deuterium fractionation for interstellar hydrides. Deuterated hydrides are chemically important in the early stages of star formation, whereas the deuterated form of some hydrides play a unique role in cosmology. In cold dense prestellar cores, the abundances of deuterated species are enhanced over the gas phase D abundance by chemical processes. This large deuterium fractionation may be kept through the cycle of star- and planet formation, and is in fact used to confirm the primordial origin of some meteorites.

Here we propose to observe the fundamental transitions of the following (deuterated-) hydrides by means of their ground state transitions: NH_3, NH_2D, HF, DF, H_2O, $H_2{}^{18}O$, HDO, $HD^{18}O$, D_2O, OD, H_2D^+ (the latter two transitions lie currently in the gap between HIFI Band V and band VI).

This program consists of three parts:

- I)**Is the HDO abundance conserved in the formation process of low-mass, solar-like, stars ?**
  The [HDO]/[H_2O] abundance ratio is rather similar for different stages in the star formation cycle from molecular clouds via YSOs to planets. Observations yield: 3.0×10^{-4} in comets (Hale-Bopp, Haley, Hyakutake), 2.4×10^{-4} in hot cores and high-mass YSOs, 8×10^{-4} in low-mass YSOs (Stark et al. 2002) and 1.6×10^{-4} in the Earth's oceans. These values lie all closely together and suggest that the ratio may be constant in the cycle of star formation. The fundamental question is then where and when is the HDO/H_2O ratio determined? There are two favoured scenarii (Aikawa & Herbst, 1999, 2001): 1) Deuteration from ion-molecule chemistry in the protoplanetary disk; 2) The deuteration is determined by gas phase and/or solid phase chemistry in the parent molecular cloud before star formation sets in, i.e. in the dense ISM. The deuterium enrichment is propagated in e.g. HDO through ion-molecule and neutral-neutral reactions in the gas-phase as well as solid state reactions with atomic deuterium on grains. To investigate these scenarii, we propose to study the fundamental transitions of HDO and $H_2{}^{18}O$ in objects spanning the full range of star formation : ranging from dark cores without star formation, in absorption against background continuum sources, in Class 0, I, II, III YSOs, in the solar system (planets, comets). Since (deuterated) water is already the subject

of many studies with HIFI we do not propose any integration time yet. The project should be coordinated later with the star formation and comet projects. It is important to ensure that a sufficient integration time is spent on these lines so that a uniform sensitivity is reached for all objects.

The main lines for this search are the ground state lines of HDO , H_2O (2 lines, ortho and para) and $H_2{}^{18}O$(2 lines ortho and para)

- II) **Determining the galactic D/H gradient by means of observations of the ground state transitions of HF and DF**.
  The J=2-1 rotational transition of HF has been discovered with ISO-LWS in absorption toward SgrB2N by Neufeld et al. (1997). As for the other hydrides, we most likely will detect lines in absorption in cold regions against a background submillimeter continuum e.g. in the dense warm envelopes around YSOs. The simple chemistry presented by Neufeld et al. (1997) predicts that HF is formed by neutral-neutral reactions between fluorine and H_2 or H_2O. Since HF is a very stable molecule, not easily destroyed in the ISM, it is the main fluorine reservoirs. Reactions with deuterium have not been studied but the [DF]/[HF] fractionation ratio is expected to depend o a very limited set of chemicalreactions. Since the fractionation for molecular hydrogen and water is very low, the deuterium fractionation for HF is expected to be very low also, hence to track accurately the elemental Deuterium abundance. By measuring the [DF]/[HF] ratio we will have a new tool to determine the D/H ratio in the galaxy to be combined with HD measurements on the same sources. *This program should be coordinated with PACS to ensure a good wavelength coverage of the most interesting sources.*

- II)**Studying the basics of HDO and D_2O chemistry** by means of observations of the fundamental lines of HDO, D_2O, $H_2{}^{18}O$ fundamental lines toward high mass star forming regions, combined with H_3O^+ and H_2DO^+.

The integration time for the sections relevant to the interstellar mediun has been included in the main hydrides section.

The following sources should be looked at in the deuterium lines. Most are well known low mass star forming regions, to be checked with the low mass star proposal : IRAS16293-2422, VLA1623, NGC1333IRAS2, NGC1333IR4A, NGC1333IR4B, L1157, L1551-IR5, L1489, TMR1, L483, L1527.

C The $^{12}C/^{13}$ abundance gradient in the Galaxy

The fine structure line of $^{13}C^+$ can be observed simultaneously with the $^{12}C^+$ line at 1.9 THz. Since little fractionation of ^{13}C is expected in regions where the carbon is ionized (Keene et al. 1998), the detection of the faint $^{13}C^+$ lines simulatneaously with the strong $^{12}C^+$ line permits to obtain a good measurement of the elemental $^{12}C/^{13}C$ abundance ratio. The weak $^{13}C^+$ features appear at velocity offsets of -63, 11, and 65 km s^{-1} relative to the velocity of the $^{12}C^+$ line. Signal to noise ratios in the C^+ line will be large (> 100) in the bright star forming regions, providing a good signal-to-noise ratio in the $^{13}C^+$ lines as well.

In the Galaxy, previous work using molecules have found a smooth gradient from the Galactic Center to the solar neighborhood. Using HIFI, a more accurate and less biased determination of this abundance gradient can be obtained. About fifteen sources sampling the Galactic plane have been selected in the list of bright HII regions osberved with the ISO spectrometers (Peeters et al. 2002). For all sources the [CII] line flux as seen by ISO-LWS is larger than 10^{-17}Wcm^{-2} and the source is not spatially resolved by the instrument. So we expect to detect a line intensity larger than 100 Kkms^{-1} for the $^{12}C^+$ line. The $^{13}C^+$ features are expected at the $\sim$ 1Kkms^{-1} level with a line width of a few kms^{-1}, and can be detected after a few hours of integration. The exact figure depends largely on the observing mode since the sources are located in fairly crowed regions of the sky. Assuming a maximum of 4 hours per source, it sums to a total of $\mathbf{4 \times 15 = 60}$ **hours** of HIFI time for this section.

Table 8: Compact HII regions for the $^{12}C/^{13}C$ Galactic gradient

Source	RA(2000)	DEC(2000)	Distance	[CII]
SgrC	17 44 35.6	-29 27 29.3	0.3	31.6
IR01420	01 4 39.6	64 12 02.1	9.5	23.5
IR10589	11 00 59.8	-60 50 27.1	8.0	14.3
IR12073	12 10 00.3	-62 49 56.5	10.8	24.3
IR15502	15 54 06.0	-53 11 36.4	4.6	13.7
IR16128	16 16 39.3	-51 16 58.3	5.5	19.4
IR17160	17 19 26.1	-37 10 53.8	3.0	16.3
IR17455	17 48 41.5	-28 01 38.3	0.2	12.8
IR18116	18 14 35.2	-16 45 20.6	4.3	19.0
IR18317	18 34 24.9	-07 54 47.9	4.5	18.4
IR19442	19 46 20.1	24 35 29.4	7.6	17.9
IR19598	20 01 45.6	33 32 43.7	9.8	14.2
DR21	20 39 00.9	42 19 41.9	8.6	12.8
IR23030	23 05 10.6	60 14 40.6	11.4	12.0
IR23133	23 15 31.4	61 07 08.5	11.7	12.9

The Distance is given relative to the Galactic Center in kpc.
The [CII] flux is given in 10^{-18}Wcm^{-2} (Peeters et al. 2002)