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			Removal of band 7 throughout the document, in particular:
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			p. 10 bullet 1 removed
			p. 11 table 1 updated, bullet 4 removed
			p. 12 table 2 updated
			p. 14 figure 1 updated
			p. 15 figure 2 updated
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13 March 2000	issue 1.0		Small updates regarding the science
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TABLE OF CONTENTS

HIFI Science Users Requirements Document

1 EXECUTIVE SUMMARY

This report has been made to show a one to one connection between the main HIFI science drivers and the instrument requirements. It is derived from a report that is an update version of the science case for the HIFI instrument proposal, dated February 1998. (A.G.G.M. Tielens et al., 1999).
It consists of two parts. The first part (Executive Summary), summarises the (unique) HIFI science drivers and the resulting instrument requirements. The second part presents the underlying details for the various drivers.

HIFI, the heterodyne instrument for the ESA cornerstone Far InfraRed Space Telescope (FIRST), is designed to study the universe in one of the last unexplored regions of the electromagnetic spectrum from space. It will do so with an unprecedented spectral resolution and sensitivity. Since it is an observatory-type instrument it needs to be versatile to be able to address many key themes in modern astrophysics.

These themes are for HIFI mainly related to the understanding of the cyclic interrelation of stars and the interstellar medium of galaxies. On the one hand, stars – and planetary systems - are formed through gravitational collapse of interstellar molecular clouds. On the other hand, the interstellar medium is formed from the ashes - enriched by newly synthesised elements - of dying stars. This complex interplay between stars and the ISM drives the evolution and, thus, the observational characteristics of the Milky Way and other galaxies, all the way back to the earliest proto-galaxies at high redshift.

In several areas HIFI has unique capabilities.

- In particular, while some other space-borne instruments will measure or have measured only a few transitions of H_2O, HIFI will cover an unparalleled number of water lines that are sensitive to a wide range of physical conditions at high spectral resolution. From the few existing data, it is already clear that water plays a dominant role in the chemical evolution as well as in the energy balance of a wide variety of objects, including regions of star and planet formation, shocks, Hot Cores, winds from dying stars, diffuse interstellar clouds, toroids around active galactic nuclei, and comets and planetary atmospheres.
- Because of its exceptional spectral coverage, HIFI is eminently suited to study the molecular universe, including large organic molecules, through spectral line surveys. Such studies will provide an unbiased view of the molecular inventory of a wide range of objects. Moreover, the large number of lines of individual molecules present in these spectra will allow detailed study of the physical conditions in the emitting gas.
- HIFI is currently the only instrument which can survey the redshifted [CII] 158 micron line, the dominant cooling line of interstellar gas and a direct probe of massive star formation, through the very important redshift-range of 0.5-3 when galaxy evolution was in full swing.

These HIFI-unique science topics are briefly summarised in 1.1 and 1.2. In section 1.3, we list the other important science areas and related specific instrument requirements. The results in terms of the instrument requirements and their related science drivers are summarised in various forms in Tables 1 and 2.

From the described science drivers and considerations it is concluded that there is no evident area in the instrument capabilities domain (frequency range, sensitivity, spectral resolution) that is not essential for one or more science drivers. The conclusions of the individual instrument requirements can be summarized as follows:

- Frequency coverage: Closure of the frequency-gaps between bands 5 and 6 would provide contiguous coverage of the high frequency range for spectral surveys.
- Sensitivity drivers are observations of isotopic water lines and isotopic fine-structure lines at the higher frequencies, and the [CII] line detection at high redshift.
- High spectral resolution is required for several water studies and [NII] and [CII] studies of the diffuse ISM, for dense cores, for absorption lines, for comet emission lines, and for planetary absorption lines.
- Wide instantaneous bandwidth is needed for efficient line surveys and for extragalactic lines especially the [CII] line at high redshift.

1.1 HIFI Science Drivers

It is important to have, at all times, a clear view of the key scientific objectives that are specific to HIFI and the way these objectives drive the instrument requirements. Here we will re-evaluate that question for the main areas of science for HIFI, including the ones that will make a unique contribution.

HIFI is by nature of its extensive spectral coverage, high spectral resolution, and high sensitivity an instrument that will have an impact on a wide range of key problems in modern astrophysics. The HIFI proposal summarises a diverse set of problems to which HIFI can make important contributions. Here we single out 7 scientific areas where HIFIs contribution will be very important:

A. The water trail
B. The molecular universe
C. CII as a probe of star formation at high redshift
D. The interstellar medium and star formation in galaxies
E. The diffuse ISM in the Milky Way
F. Comets

It should be emphasised that these do not form an exhaustive list of all the important science that HIFI can or will do.

The instrument requirements that are considered here include:

- Frequency coverage
- Spectral resolution and instantaneous bandwidth
- Sensitivity
- Stability and dynamic range
- Calibration accuracy
- Pointing accuracy
- Side-band separation
- Observing modes and strategies including different signal switching schemes

1.2 Unique Science with HIFI

HIFI because of its heterodyne spectral resolution, contiguous spectral coverage and lack of residual atmospheric absorption lines, high accuracy of calibration and the consistency of measurements from space will be able to address key questions in modern astrophysics. Below we summarise three important science areas. These are the study of water in the universe, studies of the molecular universe, and studies of [CII] 158 micron emission as a probe of star formation at high redshift.

1.2.1 The Water Trail

Water is a key ingredient in many environments, including young stellar objects, late type stars, planetary nebulae, dense molecular clouds, interstellar and circumstellar shocks, solar system objects such as comets, planets and satellites, and circum-nuclear disks in Active Galactic Nuclei; essentially in any dense and warm environment. Water is a cornerstone molecule in interstellar chemistry and it can be a dominant reservoir of elemental oxygen in the gas phase. Because of its many levels, water is also an important coolant, which can dominate the energy balance of the gas in such regions. This occurs in a very subtle way through a delicate balance because the radiation field can couple different parts of the cloud, leading to complex line profiles, hence requiring high spectral resolution. Of course, the many

water levels with their different Einstein A-values also provide a powerful diagnostic of the physical conditions in the emitting gas.
Within the broad field of water studies, we single out the "water trail in star-forming regions" as a key project for HIFI. The aim is to follow the origin and evolution of water from dark dense, pre-stellar cloud cores, through the onset of collapse, the formation of the YSO and its circumstellar disk, and the eventual incorporation into planetesimals and eventually planets. Because of atmospheric conditions, studies of interstellar and circumstellar water are unique to space and, particularly to HIFI with its high spectral resolution at sub-millimetre wavelengths where the most important water transitions reside.

1.2.2 The Molecular Universe

The origin and evolution of the molecular universe starts with the injection of material by stars in the later stages of their evolution. After subsequent processing of this material in the interstellar medium by the prevalent ultraviolet radiation fields and strong shocks, its evolution ends with its incorporation into newly formed stars and their budding planetary systems. Understanding this pre-biotic evolution and its relationship to the origin of life on Earth and possibly other planetary systems in the universe is a key problem within astrophysics.

Through spectral surveys, HIFI can measure the molecular inventory of a wide variety of regions associated with star and planet formation, star death, and the ISM in the Milky Way and other galaxies. Over the last decade, it has become increasingly clear that molecules are an important component of the interstellar medium even outside the shielded environments of molecular clouds. The infrared signature of large Polycyclic Aromatic Hydrocarbon molecules (PAHs) dominate the mid-infrared spectra of circumstellar regions, the local diffuse ISM, bright PDRs associated with HII regions and reflection nebulae, nearby normal galaxies, and starburst regions in galactic nuclei. The visible diffuse interstellar bands - long known to be present in the spectra of diffuse interstellar material - are now also generally accepted as electronic fingerprints of molecules and various carbon chains are likely candidates. HIFI will provide a unique opportunity to search for the ro-vibrational transitions associated with low-lying vibration modes of such complex species. These modes are very molecule specific and are a prime tool for identification purposes. Complete line surveys, unhindered by telluric absorption in the sub-millimetre, of a variety of objects ranging from later type stars, to young stellar objects, to comets will form therefore an important cornerstone of HIFI science.

1.2.3 [CII] and the Star Formation History of the Universe

The [CII] 158 μm line is expected to be the dominant cooling line of the gas in dusty star-forming galaxies in the early universe with line luminosity between 0.01 and 1% of the far-infrared continuum luminosity. Because of its high luminosity, this line can be observed to very high redshift and will provide a direct measure of the FUV starlight in dusty galaxies, and this is important for galaxy evolution.
HIFI will be able to detect this line through the important redshift range of 0.5-3 (bands 1-5). SOFIA will be limited by sensitivity and telluric absorption through this redshift-range. Redshifts beyond 1.5 can be studied using ALMA, but not contiguously. There is currently no instrument that covers the $0.35<z<0.5$ range (the gap between bands 5 and 6 in HIFI). The nearby universe ($0<z<0.35$) will be covered by band 6. There is overlap with PACS in this range but HIFI will provide spectrally resolved lines allowing to disentangle emission and absorption, and kinematic components within galaxies. Moreover, HIFI makes it possible to directly compare line profiles of e.g. CO and HI and thus the kinematics. In any case, because the 0.5-3 redshift interval is crucial for the evolution of galaxies, the formation of their disks, and the production of metals, observation of the [CII] line in the redshift range 0.5 to 3 will be a fundamental contribution of HIFI to the field of galaxy evolution.

1.3 Other key science areas

HIFI is an excellent instrument to probe the physics, chemistry, and dynamics of the ISM, near and far, in great detail. It will therefore have an impact on a wide range of astrophysical problems. The science areas highlighted above as unique were selected because no other instrument will be able to address this science with competitive sensitivity. The great strength of HIFI is however in its versatility and therefore it will be equipped to address many newly emerging science issues.

The original HIFI proposal has identified a number of science areas where HIFI can make important contributions. These will be briefly summarized here and their implications for the instrument requirements are discussed in greater depth in the document and summarized in the tables.

- The interstellar medium and star formation in galaxies. HIFI can address the nature of the interstellar medium in galaxies, its role in the evolution of galaxies, and the processes controlling the formation of stars on a global scale. Such studies will also provide the templates required to understand observations of the era of galaxy formation at high redshift.

- The diffuse ISM in the Milky Way. The structure and dynamics of the diffuse ISM in the Milky Way is central to studies of galactic evolution driven by star formation. HIFI will measure the pressure of the interstellar gas throughout the Milky Way, isotope abundance gradients, and the molecular inventory of diffuse interstellar gas.

- Comets. Comets are among the most pristine objects preserved in the solar system. HIFI can measure directly the outgassing rate of comets, and derive clues to their origin.

1.4 Summary

The conclusions of this report are summarised in Table 1 in terms of the instrument requirements and the science that is driving them. In Table 2, this is rearranged to list the science projects that specifically drive the instrument requirements for each HIFI band.

These tables serve to give a quick and accurate overview of the relation between instrument requirements and science drivers. However, many programs will use more bands, different spectral resolutions, observing modes etc. Here the most demanding science with respect to the requirements is presented. The complete rationale for the tables is found in part 2 and summarized below the tables.

Table 1 HIFI Science Drivers for Frequency coverage

		HIFI Bands					
	Science Drivers:	**1**	**2**	**3**	**4**	**5**	**6**
	Frequency range (GHz)	**480-640**	**640-800**	**800-960**	**960-1120**	**1120-1250**	**1410-1910**
UNIQUE + CORE	(A) Water	**X-H-S**			**X-H-S**	**X-S**	**X-S**
	(B) Molec. Universe	**X**	**X**	**X**	**X**	**X**	**X**
	(C)[C II] at high z	**X-S**	**X-S**	**X-S**	**X-S**	**X-S**	
	(D) ISM in Galaxies	**X**	**X**	**X**	**X**	**X**	**X**
	(E) Diffuse ISM	**X-H**		**X-H**	**X**		**X-S**
	Star Formation	**X**	**X**	**X**	**X**	**X**	**X**
	Death of Stars	**X**	**X**	**X**	**X**	**X**	**X**
	(F) SSO: Comets	**X-H**		**X-H**	**X-H**		
	SSO: Planets	**X**	**X**		**X**	**X**	**X**

X = Required Band **H** = HRS Required **S** = Goal Sensitivity Required

In Table 1 the unique and core science drivers are listed together with the instrument requirements. In the table **X** denotes the bands needed to achieve all the science goals of that particular science driver.

- In the case of water as a science driver, bands 1, 4 and 6 contain the frequencies of the lines ending in the rotational ground states. These are particularly important in cold clouds and absorption studies, but will also be observed in warm/hot regions. Many other lines fall in band 5, whereas bands 2 and 3 only contain one water line. The latter ones therefore are not considered drivers for bands 2 and 3. In order to study water in comets the HRS is needed in the lowest water lines, marked in the table with a **H**. In band 6 the required resolution is reached by the WBS. The goal sensitivities, marked with **S,** are generally directed at observing the much weaker lines of water-isotopomers, although the goal sensitivity may be needed for very cold sources as well.
- For the molecular universe driver the principal requirement is the availability of an as wide as possible frequency coverage.
- The C$^+$ at high redshift is only planned for bands 1-5, because PACS will be able to cover the lower redshifts. A high (goal) sensitivity is required for these observations.
- Each HIFI band contains frequencies of important lines for the studies of ISM in galaxies. For the observations of nearby galaxies, the knowledge of the error beam pattern at all frequencies is mandatory.
- The diffuse ISM science driver requires observations of [C I], [N II] and [C II] in bands 1, 3 and 6. Important absorption features are expected in bands 1, 3, and 4. High spectral resolution, obtained with the HRS, is required for bands 1 and 3. Goal sensitivities are needed for the [N II] line and the [^{13}C II] line in band 6. The knowledge of the error beam pattern is also mandatory for the out-of-plane observations.
- The cometary science requires high spectral resolution for the ground state H_2O and HDO lines.

Table 2 Science and instrument Requirements

		HIFI Bands					
Instrument Requirements		**1**	**2**	**3**	**4**	**5**	**6**
Frequency range (GHz)		**480-640**	**640-800**	**800-960**	**960-1120**	**1120-1250**	**1410-1910**
Frequency Coverage		**A, B, C, D, E, F**	**B, C, D, F**	**B, C, D, E, F**	**A, B, C, F**	**A, B, C, D**	**A, B, D, E, F**
Goal Sensitivity needed		**A, C, E**	**C**	**C**	**A, C**	**A, C**	**A, E**
Baseline Stability1)		**C**	**C**	**C**	**C**	**C**	**F**
Spectral Resolution		**A, E, F**	**F**	**E, F,**	**A, F**		
Pointing/Tracking Accuracy2)		**F**	**F**	**F**	**F**		**A, B, D, F**
Instantaneous Bandwidth3)		**B, C, D**	**B, C, D**	**B, C, D**	**B, C, D**	**B, C, E**	**B, E**
Beam Pattern		**D, E**	**D, E**	**D, E**	**D, E**	**D, E**	**D, E**
Obs. Mode4)	FreqSwitch	**A, E, F**	**F**	**E, F**	**A, F**	**A**	**A, E, F**
	Chopper	**A, B, C**	**B, C**	**B, C**	**A, B, C**	**A B , C**	**A, B**
	PosSwitch	**A, D, E**	**D**	**D, E**	**A, D**	**A, D**	**A, D, E**
	OTF Map	**A, E**		**E**	**A**	**A**	**AE**
	Absorption studies	**A, B**	**B**	**B**	**A, B**	**A, B**	**A, B**

In band 6 the WBS also reaches the required resolution of 0.1 km/s

Table 2: The six science drivers from Section 1.1 (labeled A through F) are listed as a function of their demand for instrumentation requirements. Frequency coverage, need for goal sensitivities or spectral resolution from table 1 are repeated here for completeness.

1) Top drivers for good baseline stability over all HIFI bands are the [C II] at high redshift and the diffuse ISM. However, all programs require stable baselines.

2) The pointing/tracking accuracy may be demanding for comet observations and for the small beams at the highest frequencies.

3) Because of the large line widths [C II] at high redshift and the ISM in galaxies require a large instantaneous band width. Efficient line surveys also require the large instantaneous bandwidths.

4) The observation modes list the most important ways of observing with HIFI for each of the seven science drivers.

Throughout the document, a calibration accuracy of 10% baseline and 3% goal as given in the Instrument Specification Document is assumed. The science team also assumes a TBD MHz frequency switching and three arcminutes chopper throw as listed in the Instrument Specification Document.

2 HIFI SCIENCE DRIVERS AND RELATED INSTRUMENT REQUIREMENTS: DETAILED DISCUSSION

2.1 Water

2.1.1 Scientific Background

The science of water will form the core of many HIFI observing programs. Presently, the lowest transition of ortho-water is being probed by SWAS. ISO has observed many rotational water lines in the 200-80 micron spectral range (1.5-3.8THz) at low resolution in a wide range of objects mainly with the Long Wavelength Spectrometer. Ro-vibrational transitions of water around 6 micron have been observed by the Short Wavelength Spectrometer on ISO in a limited number of objects. The KAO has observed a number of water lines of the ^{18}O isotope which are shifted out of the completely blocked core of the telluric band. H_2O maser emission has been observed from the ground in many star forming regions, late type giants, and AGNs. It is clear that water is widespread and a key species in the universe. Nevertheless, all these studies of water could not fully address the fundamental questions on the role of water in the ISM, because of the limited coverage of lines, and the lack of spectral and spatial resolution. Here we will concentrate on observations of water itself. However, it should be understood that in order to understand the role of water in interstellar chemistry HIFI will also have to be able to measure key molecular intermediaries in its formation and destruction, including OH, OH^+, H_2O^+, H_3O^+ and HDO and its associated radicals and ions. Frequencies for those species are listed in the appendix A of part IV of the HIFI proposal

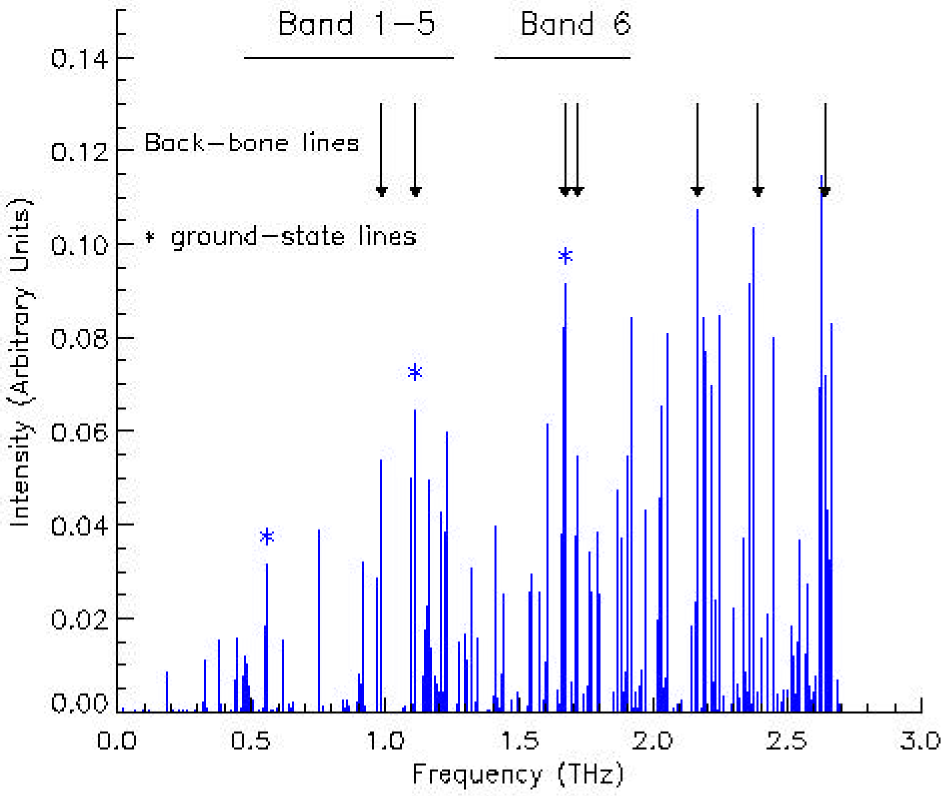

Figure 1 Thermal water spectrum calculated for a temperature of 800 K. P and R ($\Delta J = \pm 1$) backbone levels are indicated by black arrows. HIFIs frequency ranges are indicated by horizontal bars at the top of the figure.

2.1.2 Frequency coverage

Ground state lines

The water lines covered by HIFI are summarised in Figure 2 and in the appendix. Lines ending in the ground states are identified in Appendix 3.1 Table 1. These lines are essential for absorption studies of cold water. They fall in bands 1 (557 GHz), 4 (1.11 THz), and 6 (1.67 THz). These frequencies will be essential for all our water studies.

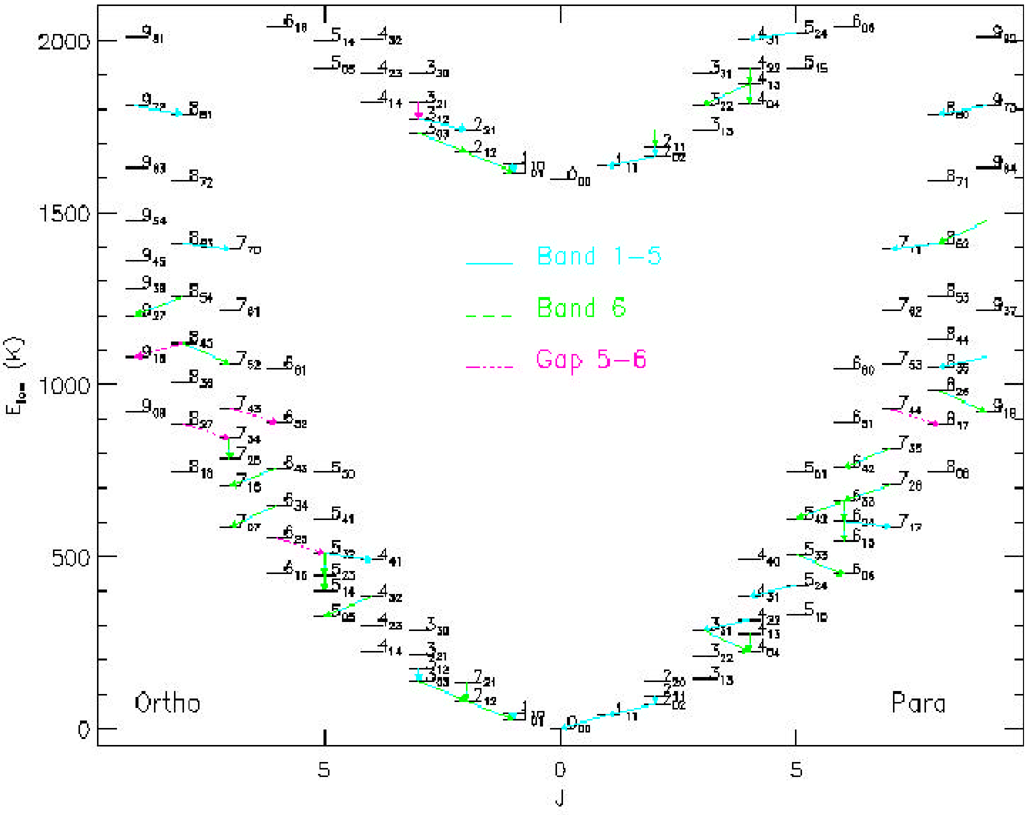

Figure 2. Energy-level diagram of water in the ground state and the ν_2=1 bending state. Transitions covered by HIFI are indicated by lines. The colour coding indicates the HIFI band.

Backbone transitions

The backbone transitions (J_{0J} $(J-1)_{1,J-1}$ or J_{1J} $(J-1)_{0,J-1}$) form the “artery” through which excitation is channelled down. These backbone lines will be highly optically thick and this optical trapping will set the population distribution over all the other levels. In order to estimate the optical depth, the corresponding ^{18}O isotope lines will have to be probed as well. These are close in frequency (within 10's of GHz). It is clear that it will be of prime importance to cover these backbone levels in any investigations of interstellar and circumstellar water.

For para-water, the lowest two backbone lines will be covered by band 4, and the next one will fall beyond band 6). In ortho-water, the lowest two backbone levels are covered by band 6 and the next ones fall beyond band 6. The present HIFI frequency range is ill-matched to the water backbone levels.

The water skeleton

As the kid-song goes, the backbone is only important as long as it is connected to the rest of the skeleton. Hence, it will be essential to cover also a large number of other H_2O transitions to accurately determine the water abundance and excitation in space. At present, it has not completely been settled how many of these transitions have to be observed to attain our science goals. Nevertheless, a few points can already be made. First, there is only 1 transition in each of bands 2 and 3 with E below 1000

K. Possibly, these might be “replaced” by equivalent lines in other bands with minimal impact on the science. Second, the coverage of water lines by HIFI separates into three groups (Fig. 1) a low energy group (J_{upper}=1-3, E_{upper} 200 K; 11 lines), 2) a medium energy group (J_{upper}=4-5 , 200 E_{upper} 700 K; 8 lines), and, 3) a somewhat more spottily covered, high energy group (J_{upper} > 6, 500 < E_{upper}< 1400 K; 19 lines). Because of the different excitation energies, these lines will be probing different types of regions, or different zones in a thermally stratified region. Adequate coverage for the lowest energy group requires bands 1 (1 [back bone] line), 4 (3 lines), 5 (3 lines), and 6 (3 lines. The lines of the second group are more concentrated in band 6; band 1 (1 line), 3 (1 line), 4 (1 line), 5 (1 line), and 6 (6 lines). Group 3 is isolated and spottily covered because of the high frequency limit of band 6. Most lines are in band 6 (10 lines).

The two lower line groups are not connected. Lines in the gap between bands 5 and 6 are not essential in connecting these groups and also seem at first sight not to add much to water studies. Overall, the gap between these line groups will limit the understanding of the excitation of water in warmish regions (T>200 K; i.e., YSOs). This will adversely affect our water science goals.

2.1.3 Sensitivity

Because of the high abundance and large dipole moment of H_2O many water lines will be optically thick. As long as the source has a size comparable to the beam, these lines should be bright (except perhaps in dark clouds). As an example, consider the $3_{0,3}$-$2_{1,2}$ line at 1.72 THz which has a measured flux of 10^{-12} erg cm^{-2} s^{-1} (ISO/LWS) in the spectrum of the low mass proto-star IRAS-16293 (total luminosity 30 L_{sun}). Assuming that this flux originates from a region with a size of 10″, T_A 20 K, which is readily observable.

The luminous proto-stellar regions in Orion and Sgr B2 showed strong H_2O lines in their LWS spectra and these can be readily observed with HIFI. In contrast, other luminous proto-stars showed little evidence for H_2O in their LWS spectra. Probably, this reflects the large beam size (80″) and low spectral resolution of these observations: Hot cores around such objects have sizes of a few ″ and, hence, are much better matched to HIFI's beam. SWAS in its large beam (3.2 x 4.5′) typically observed T_A = 0.05-0.4 K for the ground state 557 GHz line with a line width of 4-10 km s^{-1} in GMC cores such as S140, Cep A, and NGC 2071. Again, beam dilution was probably important and HIFI should be able to observe these sources readily.

Total time estimates will be determined by the weakest lines which can be measured in a reasonable amount of time, where reasonable in the context of water is of course meant to be fluid. Measuring weak lines will however be a key step in the analysis. An important point in this case is the fact that the backbone lines of the isotope will have a column density down by a factor 500. Probably this will translate into optical depths of the order of 0.01-0.1 and, for warm gas, these lines should still be readily observable. In Orion, the KAO observed a 0.6 K $1_{1,0}$-$1_{0,1}$ $H_2^{18}O$ line in a 150" beam. Of equal importance will be the measurement of (main isotope) lines originating from the same upper level but with very different Einstein A's. As an example, consider the level $3_{1,2}$, which connects to the $2_{2,1}$ level and $3_{0,3}$ level through transitions with an Einstein A ratio of 6. For low-mass protostars, these lines are calculated to be in absorption at the 0.2 K level. Even more extreme are the $5_{3,2}$ $4_{4,1}$ and $5_{3,2}$ $5_{2,3}$ transitions with a Einstein A ratio of 10^3 . Because these lines are so high in excitation, they might not be observable for low-mass YSOs and even for a massive proto-star these lines may be beyond us.

2.1.4 Spectral resolution

Most studies will be performed at a resolution of 0.5 km s^{-1}. Studies of dark cloud cores and the onset of collapse will be performed at 0.1 km s^{-1}. Studies of the release of water by comets will need high resolution (0.1 km s^{-1}) at 557 and 1113 GHz.

2.1.5 Pointing

Water emission is expected to come from spatially complex regions with a number of emission/absorption components closely packed. Particularly, the high frequency lines will therefore require accurate pointing.

2.1.6 Observing modes and strategies

We can expect that a large sample (hundreds) of sources will be surveyed in the water lines; both in the guaranteed time and in the open time. We envision that, initially, a few sources will be studied fully and the results will be used to guide (i.e., select most promising lines) in the remainder of the sample.

As a rule of thumb, in order to reap the most benefit from water observations, in terms of deriving the physical conditions of the gas, as many lines as feasible have to be observed. Studies of the dynamics and abundances might be sufficient with fewer lines but these goals are unlikely to be studied in isolation. It should also be kept in mind that nobody else will be able to measure all these water lines again in the foreseeable future. So, it is better to err on the side of “more is better”. As an example, consider various stages in the star formation process

- Cold dark clouds (T ~10 K): Only the lowest levels are populated and including isotope lines makes 6 lines.
- Low mass proto-stars (T ~100 K): some ten $H_2^{16}O$ lines plus 4 back bone lines of the ^{18}O isotope.
- Massive proto-stars (T ~400 K): some tens of lines.
- Shocked gas (T ~1000 K): The full slew (32 lines).

Given the spatial complexity, it is obvious that it would be best to observe all lines in one pointing. A comprehensive water sample might contain some 200 sources taken from low mass (50, spread over class 0, I and II) and high mass proto-stars (25), solar system objects (5), late type giants (25), super-giants (10), dark clouds/GMCs (25), AGNs (25), and ULIRGs (25).

Many of the stronger lines in star forming regions will be spatially extended and should be mapped. The best lines to be mapped will be determined from the line surveys or the multi-line H_2O surveys of selected regions. Spatial studies of H_2O would require on the fly mapping. Mapping of cold dark clouds will be most demanding for cases in which the predicted and observed line intensities of the 557 GHz line are in the range of 0.05-0.1 K. For a 0.1 K line, the mapping speed will be approx. 20 square arc minutes per hour for a 5 sigma detection per point (baseline performance). Thus, a dark cloud core such as TMC 1 (100 square arc minutes) can be mapped in some 5 hours. Mapping of the 557 GHz line in warmer, active star forming regions will be easy. For a low mass YSO, we would also want to map the $2_{1,2}$-$1_{0,1}$ back bone line line at 1670 GHz. Theoretical analysis of LWS observations of IRAS-16293 yields peak intensities of some 14 K in the HIFI beam (13″) and emission at the 10% level will be extended on a 2’ scale. HIFI (baseline) can map 2 square arc minutes in 1 hour at 1670 GHz for 5 sigma detection of this extended emission (i.e., an assumed noise level at 0.02 of the peak intensity). For extended shock emission in regions of massive star formation, we would, for example, want to map the $3_{0,3}$-$2_{1,2}$ back bone line at 1716 GHz. Theoretical studies predict a peak flux of 0.06 erg s^{-1} cm^{-2} for a 30 km/s shock travelling into 10^5 cm^{-3} density gas, reasonably consistent with the ISO observations of (other H_2O lines in) the shock in

Orion. With an assumed line width of 30 km s^{-1} (T_A 30 K) and demanding 5 sigma, HIFI can map an area of approximately 10^4 square arc minutes in one hour (baseline) in this line. Mapping of lower lines would be quite easy. In all these mapping studies, system stability is required on these timescales.

In terms of switching procedure, YSOs will be most demanding. In those regions, the strong water lines are likely to be very extended and hence require frequency switching. Weaker lines could use beam switching but probably all lines will be treated in the same way. In the proto-stellar outflow in Orion, the H_2O linewidths are measured to be approximately equal to 60 km s^{-1}. This is probably a somewhat extreme case but nevertheless a line width of 30 km s^{-1} can be expected in proto-stellar outflow sources.

In total, a comprehensive water survey may well take some 500 hours.

2.1.7 Absorption studies

Calculations have long predicted that many H_2O lines will be in absorption. Because of the strongly increasing dust continuum, this will be particularly important at the higher frequencies. In the diffuse ISM, a cloud with a H column of 2×10^{21} cm^{-2} will have an optical depth larger than unity in the ground state H_2O transitions if the water abundance is larger than 10^{-8}.
The ISO LWS and SWS FP observations of the Orion Star forming region show complex P Cygni profiles. SWAS studies of the 557 GHz line in absorption have typical continuum levels of 0.1-0.5 K and absorption depth below the continuum of 50-100%. The observed widths vary from as narrow as 2 km s^{-1} to as wide as 12 km s^{-1}. A 50 sigma measurement of 0.1 K at 557 GHz would take less than 5 minutes. The continuum level needs to be measured to an accuracy of a few percent. In many cases (isolated background sources), position switching can be done. In more complex regions, such as YSOs particularly those with outflows, frequency switching will be required.

2.2 The Molecular Universe

2.2.1 Scientific Background

Spectral line surveys are a superior way to measure the molecular inventory of a variety of regions and hence characterise the origin and evolution of the molecular universe. Moreover, there are some species which have not yet been found, and which are hoped to be seen by HIFI. These species partially drive the frequency ranges for the HIFI receivers (a list of those lines is in Appendix 3.2 and in Appendix 1 of the HIFI proposal Part IV), but those are targeted observations, since the frequencies are known.

For the discovery of unknown species, the most promising candidates seem to be ro-vibrational transitions associated with vibrational, torsional or puckering motions of long chain or ring molecules including PAHs. Not much is known at present about the frequencies of those, except that one expects them to be in the 1-3 THz regime rather than below. PAHs and carbon chains will show low-lying ro-vibrational bands in emission in regions which show the UIR bands (i.e., PDRs associated with bright HII regions, reflection nebulae, and, Planetary Nebulae). Because of the strong FUV field, those regions will not show emission by simple (abundant) molecules in these spectral regions. Absorption line spectroscopy toward bright submm/FIR background sources is one promising technique for finding these molecules in the diffuse ISM and in dark clouds. Finally, hot cores around YSO's might show low-lying ro-vibrational lines in emission in this same spectral region. In this case, confusion may be more of an issue since even simple molecules such as HCN and CH_3CN will show such emission lines.

One clear advantage of HIFI for such studies is the complete coverage of the spectral window unhindered by telluric absorption. Besides the atmosphere, a systematic study of this kind with SOFIA would also be impossible because of the large amount of observing time involved (typically 24 hrs).

Finally, spectral line surveys constitute the ideal probe of the physical conditions in the emitting gas.

2.2.2 Frequency coverage

Since a priori not much is known about these lines, the requirement for finding them is not so much a specific frequency range, but large bandwidths to maximise the chances. The THz region seems particularly promising. Getting contiguous coverage at high frequencies from 1 through 1.9 THz is therefore of the highest priority (i.e., closing the gap between bands 5 and 6). It will also be desirable to have coverage of those lower frequency regions which are unobservable due to telluric absorption.
The atmospheric windows can in principle be left to ground-based telescopes. However, for calibration purposes it will be desirable to cover these as well. That will facilitate intercomparison of line strength, which is very important for the determination of physical conditions and chemical abundances from these surveys.

2.2.3 Sensitivity and time estimates

In an absorption line study, for a continuum of 1 K (250 Jy at 2 THz), a 24 hour line survey would reach 25 sigma at a resolution of 1 MHz in the high frequency bands (adopting goal sensitivities), allowing detection of features 10% of the continuum. From the IRAS data base there are more than 3000 sources with continuum flux densities exceeding this value, including some 600 extragalactic point sources. This also includes heavily embedded YSOs (class 0) which can be used to detect long chain or ring molecules in absorption.

For PAH emission, the whole ro-vibrational envelope, containing some 200 lines, is expected to span 15 GHz for a 50 C-atom species, decreasing to 3.7 GHz for a 200 C-atom species. The intensity of an individual ro-vibrational line of one PAH species (with an abundance of 10^{-2} of the total PAH abundance) is expected to be about 100 mK with a (turbulent) line width of 10 MHz. A 24 hour line survey at a resolution of 1 MHz would reach a 1 sigma of 40 to 70 mK in the baseline (30 to 40 mK goal sensitivities) at the higher frequencies.

2.2.4 Observing modes and strategies

As for target selection, the minimum list should be two or three
proto-typical sources for the following kind of objects:

- high mass YSOs
- low mass YSOs
- dense cores without star formation
- shocked regions: outflows, SNRs
- PDRs
- Stars:
    - carbon stars
    - oxygen stars
    - PN
    - PPN
- absorption line clouds
- galaxies
- the planets
- any bright comet that happens to come by.

A larger target list for complete surveys should contain mostly objects with many lines, i.e. high mass YSOs, stars and absorption line regions. An even larger list should contain targets for partial surveys. The frequency ranges for these surveys will depend on the type of object (e.g. YSOs vs. stars) and should be finalized only after the results from the first surveys are analyzed. This is a very conservative approach and some interesting lines in inconspicuous objects could be missed, but it avoids surveying lots of blank spectra.

The objects on the minimum list should be observed fairly early in the mission and with high priority. The procedure has to be as standardized as possible, but depends on the actual system layout. For example, since the data will be taken in DSB mode and have to be deconvolved, a high redundancy, i.e. many tunings are desirable if the line density is high, i.e. in particular for high mass YSOs. How many tunings depends on factors like overhead (if tuning is quasi-instantaneous, one can afford many tunings, in particular for high mass YSOs, since there the confusion limit due to line confusion will be reached rather quickly). If the overhead is considerable, one wants to minimize the tunings. Likewise, if mechanical tuners exists and one wants to minimize their use. Based on experience, stepping through the frequency ranges with steps of 1/4 of the instantaneous bandwidth is the preferred mode of operation. Tuning is likely to be faster than slewing, so one would observe one source as long as possible with many tunings rather than many sources at one tuning.

2.2.5 Spectral deconvolution

The deconvolution procedure necessary for reconstructing the single sideband spectrum can, if needed, handle different sideband gain ratios and even varying gains across the band, although the reliability will be degraded somewhat. However, it cannot compensate for varying spectra due to different pointings in structured sources (e.g. Orion-KL). This will inevitable produce ghost lines which are very difficult to remove. Thus for sideband deconvolution, the blind pointing accuracy and pointing stability are very important.

2.2.6 Summary of instrument requirements

For unbiased line surveys, the specific frequency ranges are less important than total receiver bandwidths and total IF bandwidths, which should both be maximized. Other science drivers and searches for molecules with known frequencies will define the frequency ranges.

The possibility of finding vibrational modes of complex molecules makes the THz range more interesting than the sub-THz range. Successful sideband deconvolution needs very good and stable pointing. Some template sources should be observed and analyzed early in the mission to define frequency ranges for partial line surveys.

2.3 CII as a probe of star formation at high redshift

2.3.1 Scientific Background

The SIS bands 1-5 of HIFI will give access to [CII] 158 micron emission in the redshift range of approximately 0.5 - 2.8, which covers almost exactly the “gap” between PACS on the low redshift side and ALMA on the high redshift side. ALMA will be able to probe limited redshift ranges corresponding to the small, higher frequency, atmospheric windows (e.g., 670 GHz) but this coverage will not be contiguous. Given that this is a key capability of HIFI, it is important to have the required instrumental performance specified below, uniformly over the entire relevant frequency range.

2.3.2 Baseline Stability

The expected lines will have widths from a few 100 to 1000 km/s (FWZI); we will thus be looking for faint broad lines. Typically spectra will be rebinned to 50-100 km/s velocity resolution, depending on the actual line-width and S/N ratio available. With an expected line-width of 500 km/s, the expected line fluxes translate to antenna temperatures of 0.4 and 0.03 mK at 1.25 THz and 500 GHz, respectively. Base line stability will be very challenging.

2.3.3 Instantaneous Bandwidth

Expected line-widths will be up to 1000 km/s FWZI (see spectra of e.g., Arp220, NGC6240, but also lower-luminosity objects such as NGC3079). It is essential to have enough free baseline on both sides, say 200 km/s, which requires 1400 km/s minimum instantaneous bandwidth. This leads to a high instantaneous required bandwidth at the high frequencies; i.e., at 1 THz, this requirement corresponds to approximately 5 GHz instantaneous bandwidth. This is slightly larger than the expected bandwidth of 4 GHz (nominal). Lower line-widths are expected for less luminous sources. The bandwidth requirement becomes somewhat more favourable at lower frequencies. Presently, sufficiently accurate redshifts are not available. This is because optically-derived red-shifts sample Lyman alpha or high-excitation rest-frame UV lines which can be displaced by 1000 km/s or more from low-excitation lines due to outflows, winds, etc. However, the situation may be expected to improve dramatically in the coming years with near-IR spectrographs on 8m telescopes so that the redshift accuracy may not be a problem by the time FIRST flies.

Note that for these faint broad lines it will be very dangerous to piece the required bandwidth together from several overlapping spectra of smaller bandwidth, so we really need instantaneous frequency coverage. Also, lower instantaneous bandwidth (due to, for example, reduced sensitivities at the band edges because of the use of diplexers) will severely impact this part of the science programme!

2.3.4 Observing Modes and Strategies

Position switching with the focal-plane chopper will suffice. We expect that, when FIRST is launched, there will be extensive catalogues of star forming galaxies at various z-ranges. We might select some 10 galaxies at each of the following redshifts - 0.1, 0.25, 0.5, 1, 2, and 3 - for a total of 60 objects. In this way, the evolution of star formation in the universe could be effectively probed. This would require some 500-1000 hours, depending on the actual [CII] intensity of such systems. Coordination with PACS and SPIRE to measure the IR/Submm luminosity of this sample will be important as well for the interpretation of these results.

2.3.5 Resolution

A few tens of km/s will be the highest resolution that will ever be used here.

2.3.6 Sideband deconvolution

There are no bright lines expected nearby so this does not lead to a special requirement.

2.3.7 Pointing

High redshift [CII] studies are limited to the lower frequency bands where the beam size exceeds 20″ and pointing should not present a problem.

2.3.8 Sensitivity

We will always be S/N-limited here, so more sensitivity always helps. But as a minimum, we should have the sensitivities in the HIFI proposal. The figure in the proposal that shows the detectability in [CII] with HIFI as a function of redshift, is based on these sensitivities. Of course, the most interesting candidates (i.e., near z is 3) are at the low frequency end of the HIFI frequency range and the goal sensitivities are in reach. Poorer sensitivities in any HIFI range will STRONGLY impact this part of the program, and will result in particular red shift ranges being totally inaccessible in [CII]!
Assuming a 10^{11} L_{solar} galaxy and $5x10^{-3}$ of that luminosity in the [C II] line, expected line fluxes range from approximately 70 Jy km/s ($3x10^{-15}$ erg cm^{-2} s^{-1}) in the near universe (at 1.25 THz) to 4 Jy km/s ($7x10^{-17}$ erg cm^{-2} s^{-1}) in the far universe (at 500 GHz). Adopting baseline sensitivities ($R=10^5$), these line fluxes can be detected by HIFI: at the lowest frequencies, integration times of some 10 hrs will be required.
Adopting a 500 km/s line width, the expected line-to-continuum ratio will be approximately 10. ISO-LWS has measured smaller line-to-continuum ratios for the nearby starburst Arp 220 (even after taking the difference in resolution into account). However, because of the low resolution, the LWS was possibly spectrally confused between emission and absorption [C II] components; Arp 220 is known to be anomalous in this respect due to the very large column densities involved.

2.4 The Interstellar Medium and Star Formation in Galaxies

HIFI will provide wide spectral coverage with high spectral resolution in a wavelength regime that is barely or not accessible at all from ground. Therefore HIFI will open new perspectives in various fields of extragalactic astrophysics. Key questions that will be addressed, refer to the understanding of the evolution of galaxies, the nature of the interstellar medium and the processes controlling the formation of stars.

For starburst or active galaxies as well as nuclei of nearby “normal” galaxies, the large number of molecular and atomic transitions that should be detectable with FIRST will for the first time enable a detailed analysis of the physical properties (and structure) of the star forming ISM in these galaxies. Excitation studies in CO (like those done in the past towards the nearby starbursts M 82, NGC253 and others) and H_2O can be extended to distances beyond the Virgo Cluster. Complementary observations of key atomic fine-structure lines will independently trace the gas density and the associated interstellar UV-radiation field, thereby providing insight into the underlying activity processes (starburst versus accretion onto a central engine). In particular, the brightness of the main cooling line of the interstellar medium, [CII], will serve as indicator for the high-mass star formation rate.

How unique will be the science that can be performed with HIFI? Potentially the important carbon lines can also be observed from ground or aboard SOFIA, but the range of accessible source velocities is limited. With the exception of nearby galaxies (V < 500 km/s), limited atmospheric transmission will restrict ground-based observations of the two [CI] fine-structure lines at 492 & 809 GHz to well separated velocity windows. Similarly, observations of [CII] with SOFIA will be limited to various windows and V < 3000 km/s. Because many of the sources will be unresolved, FIRST/HIFI will gain a factor 3 in sensitivity compared to SOFIA. HIFI will complement observations with PACS, providing the spectral resolution that will be needed to discriminate between emission and absorption processes along the same line-of-sight (see the complex spectra with absorption superposed on broader emission lines detected by ISO LWS towards e.g. Arp 220 and prominent molecular clouds in the Galactic Center (Sgr B2)).

While IRAS and ISO have revealed the often huge enhancement of IR-luminosity of interacting galaxy systems, only FIRST will provide sufficient spatial and spectral resolution to study the nature of the interaction in detail in the main spectroscopic tracers of the warm ISM. Science programs will target at the dynamics of the merging process and at the physics of the interstellar medium in the interaction zone, at conditions in the associated nuclei, on the nature and the trigger of the enhanced star formation rate.

In comparison with far-IR continuum, CO and HI measurements, studies of the atomic fine-structure lines of [CI], [CII] and [NII] will unravel the physics and distribution of the various phases of the interstellar medium in normal galaxies. The different tracers couple to different phases of the ISM (diffuse and molecular clouds, the warm inter-cloud medium), therefore will characterize the global properties of the ISM in galaxies. Studies of the [NII] transitions will uniquely be done by HIFI. However, for [CII] studies of “local” spatially extended galaxies (with velocities matching the atmospheric transmission windows) competition with SOFIA will be strong, due to the spatial multiplexing benefit of the [CII] array-detectors that are under development for SOFIA.

2.4.1 Frequency coverage

Table 3. Spectral lines for ISM and star formation in galaxies

Transition	Frequency	Band	Notes
	(THz)		
CO	Jx0.115	1-5	Multi-transition CO excitation studies
H_2O		1,4-6	Multi-line water excitation studies
SiO		1-5	Shock tracing molecule, excitation studies
[CI]	0.49	1	not observable from ground for 1200 < V < 4750 km/s 1)
[CI]	0.81	2&3	not observable from ground for 480 < V < 850 & V > 5000 km/s
[CII]	1.90	6	Observation with SOFIA limited to various windows
[NII]	1.47	6	Shifts into band gap 5/6 for z > 0.05

1) The edge of band 1 is set to include slightly redshifted [C I] (490 GHz) in nearby galaxies (V < 4750 km/s).

There is clearly a niche for [CI] and [CII] studies with HIFI towards galaxies with systemic velocities not accessible with ground-based or airborne observations

2.4.2 Sensitivity

For e.g. observations of the [CII] line at 1.9 THz we should reach a 3 sigma detection limit of 1 mK after approximately 1 hour of integration. This will make all ULIRGs, starbursts and AGN, seen with ISO, easy targets for high-resolution spectroscopy with HIFI, and will allow studies on a much larger sample.

The sensitivity and resolution of HIFI will allow us to spatially resolve the interaction region of e.g. NGC4038/39 (the “Antennae”). The [C II] flux for this archetype of a merging system is $4x10^{-12}$ erg cm^{-2} s^{-1} (about 500 mK for a line width of 300 km/s) and therefore detectable within minutes of integration with HIFI. A fully sampled map in [CII] with a dynamic range of 1/10th the ISO-fluxes can be done in hours (size: 2′x2′). Similarly, molecular transitions like mid-J CO rotational lines are easily detectable. Extending the sample of interacting systems to larger distances will be limited by the sensitivity of the HIFI-detectors. For example, “antennae”-like mergers will be detectable up to redshifts z ~ 0.1.

Extrapolating the results from COBE for the Milky Way, HIFI will detect the [CII] emission from spiral galaxies like NGC891 to the distance of the Coma cluster, and from dwarf galaxies like IC10 out to 60 Mpc.

2.4.3 Spectral Resolution

For AGNs, an as wide as possible velocity coverage would be desirable; for most objects, however, the 4 GHz IF-bandwidth will be sufficient. A spectral resolution of approx. 10 km/s per channel is required. Using NGC4038/39 as an example again, the velocity coverage required is approx. 400-600 km/s, with strong local velocity gradients in the interaction layers that require a spectral resolution of a few 10 km/s. For normal galaxies, a velocity coverage of a few hundred km/s, with a resolution of order 10 km/s per channel, will be fine.

2.4.4 Pointing, Stability and Calibration

For all excitation studies a calibration accuracy for the individual line of a few percent is required. The major contributions to this error budget derive from uncertainties in establishing the correct temperature scale and from pointing errors (most nuclei will be un- or barely resolved only).

2.4.5 Observing Strategies

Most AGNs will be point-like and observed in beam-switching mode. For interacting galaxies we require OTF and line raster maps for stronger lines, beam-switched otherwise. For optimal OTF scanning, chopping should be done in scanning direction. No frequency-switching mode is required.
We will need OTF and line raster for extended normal galaxies beam-switched otherwise.

2.4.6 Absorption Studies

Extra-galactic absorption line studies are a unique niche for HIFI to probe the physical conditions of e.g. the nuclear gas in AGNs - independent of red-shift and limited only by the availability of a suitably luminous background source. Absorption line studies are an order of magnitude more sensitive to column density than a corresponding emission line measurement, but in order to deduce the physical parameters, the line must be resolved (R approximately 10^5). Absorption at mm wavelengths was first detected in the nearby galaxy Cen A, more recently absorption was measured towards cosmological absorbers (z=0.89 in PKS1830-21). ISO LWS spectra of Arp220 and Mrk231 show numerous unresolved atomic and molecular absorption features, including H_2O, CH and NH_3 .

Given the large number of transitions that potentially will be detectable in a HIFI absorption study, basically all bands will be required. Even for lines that could also be measured with SOFIA, for these point-source experiments HIFI will have a factor 3 higher sensitivity due to FIRST's larger telescope and aperture efficiency.

The sensitivity of an absorption line study is directly proportional to the brightness of the background source. We estimate that a few 100 IR sources of fluxes >35Jy will be available to perform a dedicated absorption study at 1 THz (25% absorption at 5 sigma in 1 hour). While covering a wide range of l-o-s velocities (few 100 km/s), the individual absorption feature may be as narrow as a few km/s only (Cen A). In almost all cases, the background continuum will be unresolved, and the observations will be done in beam-switching mode. For some narrow-line cases, observations may be performed in frequency-switching mode.

2.5 The diffuse ISM

2.5.1 Scientific Background

Observations of the structure and dynamics of the diffuse ISM are of key importance for understanding the galactic evolution driven by star formation. Stars inject matter enriched by their nucleosynthetic products into the ISM. Stars also heat the ISM through their photons and through mechanical action (shocks). This results in a number of phases - various clouds and intercloud phases characterised by their own physical conditions – from which subsequent generations of stars form. The characteristics, origin and relationship of these phases is however poorly understood. HIFI can measure a variety of lines of interstellar gas throughout the Galaxy, and extract information on the densities, pressures, filling factors, porosities, dynamics, ionization sources, cooling processes, and elemental and isotopic abundances of the various phases of the constantly evolving ISM. In particular, the diffuse ISM provides a major contribution to the global emission of entire galaxies in the C^+ and N^+ lines. Studies of this kind are also important for our understanding of the first stages of galaxy formation and templates for such distant objects must be obtained from detailed spectroscopy of our own galaxy and nearby galaxies.

HIFI will observe lines of sight over a range of galactic latitudes in [NII] (probing the warm ionised medium) [CII] (probing the warm ionised medium as well as cold diffuse clouds) and [CI] (probing cold diffuse clouds). These observations can be used to determine the physical conditions in these phases and their galactic distribution (e.g., scale height). Moreover, using the velocity structure and spatial distribution, the interrelationship of the warm ionised medium and cold diffuse clouds can be studied. The combination of [NII] and [CII] can be used to determine the relative importance of the warm ionised medium and cold diffuse clouds for the [CII] emission on a galactic scale, one of the key unresolved galactic questions pointed out by the COBE results. Absorption line studies towards selected background sources such as galactic star forming regions, including Sgr B2, as well as extra-galactic sources will provide a unique opportunity to measure the physical conditions in intervening diffuse clouds. This will also allow the study of the products of the first steps in interstellar chemistry.

The high frequency resolution of a heterodyne instrument makes HIFI an ideal instrument for this purpose. Moreover, for nearby objects many key lines are blocked by the Earth’s atmosphere. The [CII] and [NII] lines cannot be done from the ground. The [NII] lines, particularly the 2.46 THz line, from the warm ionised medium and from very diffuse HII regions will only be marginally detectable from SOFIA due to poor atmospheric transmission. SOFIA will have a considerable advantage for the study of extended [CII] from bright Photo-Dissociation Regions because of the multiplexing advantage of arrays which are expected to fly by the time FIRST is launched. HIFI has a niche for those studies which require long integration (≥3 hr) or large coherent programs (>> 100 hours) or programs where beam filling is important (i.e., absorption against compact continuum sources and studies of the smallest scale structure). Observations of [CII] with HIFI in support of other studies (i.e., [NII], absorption line studies) are also important.

2.5.2 Frequency coverage

Emission : [NII] 1.47 THz, [CII] 1.90 THz, [CI] 492 GHz and 809 GHz.
Absorption : CH^+ 835 GHz, H_2O 557 GHz, and NH 974 GHz.

Discovery of lines from new species will be done through a spectral absorption survey. The [CII] and [NII] lines have been used to define the upper and lower boundaries of band 6. The (mildly red-shifted) [CI] 492 GHz line defines the lower end of band 1.

Phases of the ISM:

Studies of the phases of the ISM would concentrate on a few selected regions. From ISO data along lines of sight at b =0.5° towards minima of molecular emission (20 mag of total H column density, dominated by CNM), we expect intensities of 5×10^{-5} ([NII]) and 4×10^{-4} ([CII]) erg s^{-1} cm^{-2} sr^{-1}. This emission will be spread out in several emission components over a velocity range of 30 km s^{-1} and this corresponds to T_A is 0.5 ([NII]) and 1.9 ([CII]) K. The expected [CI] intensity at 492 GHz is 0.2 K. Twenty sigma detections take seconds with HIFI. Mapping is therefore feasible. Adopting baseline sensitivities, an area of 0.2 square arc minutes can be mapped to 10 sigma in 1 hour in the [NII] line. For [CII] and [CI], the equivalent areas are 2 and 20 square arc minutes, respectively. Mapping a few judiciously chosen areas, a few arc minutes on a side (10 square arc minutes), takes some 60 hours per area.

HIFI studies of the [NII], [CII], and [CI] towards high latitude regions, where HST and FUSE have measured UV absorption lines, will provide especially useful insight into the nature of the ISM. From COBE and BICE, we expect intensities of 10^{-7} ([NII]) and 10^{-6} ([CII]) erg s^{-1} cm^{-2} sr $^{-1}$ at high latitudes. With expected line widths of 3 km s^{-1}, this corresponds to T_A of 10 and 70 mK for [NII] and [CII]. It would take 9 hours/15 minutes to get a 5 sigma detection of these lines respectively at a resolution of 10^5 (baseline). The [N II] study will be particularly challenging since the emission will be spatially very extended and more than one velocity component may be present within a 50-200 km/s bandwidth. The best here, would be to measure [N II] towards expected bright spots within the large COBE beam (7 degrees).

Absorption Spectroscopy:

Observations of CH^+, CH, H_2O, NH absorption lines for a sample of radio sources. The proposed water absorption lines out of the ground state levels should provide measurements of the ortho/para ratio. For $N(CH^+)= 10^{13}$ cm^{-2} (typical value detected against nearby stars) τ(835 GHz)=1 . Such a column density is typically spread over 2 km s^{-1}. Similar values are expected for other hydrides (similar dipole moments and abundances; for water). For a continuum flux of 250 Jy at 1 THz, an absorption line of 25% requires an integration time of 15 minutes at a resolution of 0.2 km s^{-1} (Narrow lines expected).This provides a unique inventory of the molecular composition of the diffuse ISM: a prime laboratory for interstellar chemistry.

$^{13}C/^{12}C$ abundance gradient:

Measure the hyperfine components of the $^{13}C^+$ fine-structure line at 158 micron in the direction of galactic star forming regions at different galacto-centric radii. C^+ is the main C-reservoir and hence this measures directly the isotope abundance. For Orion, the main $^{12}C^+$ line has a peak intensity of 100 K, while the F=2-1 hyperfine line of $^{13}C^+$, perched on the wing of the $^{12}C^+$ line, has an intensity of 1.5 K. For a good definition of the continuum provided by the $^{12}C^+$ line a noise better than 0.1 K will be required. The F=1-0 hyperfine line of $^{13}C^+$ occurs somewhat further away from the $^{12}C^+$ line (approximately -60 km s^{-1}) and has a similar intensity. For comparison, the 5 sigma line detection limit at a resolution of 10^6 (line-width is some 3 km s^{-1}) is 10 mK in 1 hour. A large sample of sources across the galaxy might be sampled in a reasonable amount of time. Similar observations of the $^{13}C^+$ hyperfine lines from gas in the diffuse ISM will be very challenging because of overlapping velocity components.

2.5.3 Resolution

The emission in the diffuse ISM will be concentrated in a number of components with a typical width of some 3 km s^{-1} spread over some 30 km s^{-1}. A resolution of $3x10^5$ will be required. Because of the extended character of the emission in the diffuse ISM, frequency switching over 400 MHz at 2 THz would be required. Absorption line studies will require higher spectral resolution, $3x10^6$ corresponding to 0.1 km s^{-1}.

2.6 Solar System studies

2.6.1 Planets

2.6.1.1 Scientific background

While HIFI can address a variety of planetary science objectives, we have identified three areas for which the the HIFI spectral resolution will be uniquely suited: (i) water in the Giant Planets and Titan (ii) deuterium in the Giant Planets (iii) the chemistry of the martian atmosphere. The science objectives will be (i) the determination of the vertical profile (and on Jupiter, the search for horizontal variations) of H_2O in the outer planets (ii) the search for new minor species in the martian atmosphere. The instrumental requirements described below aim at filling these goals.

2.6.1.2 Instrumental requirements: frequency range, resolution, bandwidth, sensitivity, calibration.

2.6.1.2.1 Frequency range

The continuous spectrum of the planets is best studied by a combination of low-resolution (100 MHz) and high-resolution (1 MHz) observations. Indeed, depending on the pressure of the formation region, the lines may have typical widths ranging from several GHz - for lines formed in the tropospheres of the Giant Planets - to only a few MHz, for stratospheric lines in the Giant Planets and weak lines on Mars. In some cases, a broad absorption and a narrow core (absorption or emission) may be superimposed.

The target molecules will non-exhaustively include: H_2O, CO, O_2, O_3, H_2O_2, OH, HCl, H_2CO and HDO. The following table lists some of the important frequencies we want to observe:

Table 4: Spectral Lines for Planetary Atmospheres

Bands	Freq. range	Selected observing frequencies
	(GHz)	(GHz)
1	480-640	557 (H_2O)
2	640-800	752 (H_2O), 774 (O_2), 753 (HDO)
3	800-960	
4	960-1120	1121 (O_2), H_2O (1097)
5	1120-1250	
6	1410-1910	1835-1838 (OH), 1876 (HCl), 1625 (HDO), 1716 H_20

Notes:

1. No specific frequencies or bands are required for O_3, H_2O_2, H_2CO, CO which have many lines of generally increasing strengths with frequency; therefore lines can be selected in any available band.

2.6.1.2.2 Spectral Resolution

A spectral resolution of 1 MHz is adequate. Line cores are generally at least several MHz broad (exceptions may include upper atmosphere martian lines). In the high frequency band, the corresponding 200 m/s resolution may be just sufficient to measure winds on Jupiter from the H_2O and transition mapped on the (at most 48”) disk, with the 13” beam of HIFI.

2.6.1.2.3 Bandwidth

Due to the very different linewidths encountered in planetary atmosphere, a 3 GHz instantaneous bandwidth would be adequate for most situations (except the case of the multiplets of PH_3, NH_3... in the Giant Planet tropospheres).

2.6.1.2.4 Sensitivity

Some of the main goals are "first-detection" observations, particularly on Mars. Thus the highest sensitivity is desirable. Typically, a detection limit of 1 mK should be adequate.

One specific problem for the planetary observations is the existence of the strong continuum, which tends to induce artificial baseline ripples. This problem must be taken with the highest care. In most current observations of strong continuum sources (Mars, Jupiter, Saturn), even on a spaceborne telescope like SWAS, the limitation is not due to channel-to-channel noise but to the uncertain continuum and linewings shape.

2.6.1.2.5 Calibration accuracy

If the instrumental baselines are flat as wished, the absolute calibration is not a too serious issue the lines can be analyzed and modelled in line/continuum ratios.

2.6.1.2.6 Observing strategies

Beamswitching can be used as the general mode. For narrow line searches, one may consider frequency switching to improve telescope efficiency. However, even if this produces good spectra (which needs to be tested...), this eliminates the continuum, so in this case an accurate absolute calibration becomes critical.

2.6.2 Comets

2.6.2.1 Scientific background

Water dominates the composition of cometary ices and their evaporation is the driver of the dynamics of cometary outgassing at small ($R_{helio} < 4$ AU) heliocentric distances. The high sensitivity of HIFI will allow to look for the 557 GHz water line even in weak comets, in distant comets, and to search for low levels of activity in extinct comets or in asteroid-related bodies. The recent detection of this water line in comet 1999 H1 (Lee) by SWAS has demonstrated the interest of such observations for comet science.

Water plays an important role in the thermal balance of cometary atmospheres, which in turn mostly governs the excitation of cometary molecules. Significant progress in our understanding of these physical conditions could arise from the observation of a comprehensive series of water rotational lines with HIFI.

The D/H ratio has only been measured in three comets, all coming from the Oort cloud. One can expect that D/H in comets depends upon their formation site. It is therefore important to measure D/H in cometary water in a sample of comets with different origins and evolution, in order to constrain models of Solar System formation. The measurement of D/H in Jupiter-family comets, believed to have formed in the Kuiper belt and likely to be different from Oort-cloud comets, is especially required. Search for new cometary species should be attempted in the brightest objects. Several molecular species, like light hydrides, can only be searched for at submillimetric wavelengths. This should complete our investigation of the cometary chemistry.

2.6.2.2 Instrumental requirements

2.6.2.2.1 Frequency coverage

The fundamental 1_{10}-1_{01} water line at 557 GHz is to be searched for and monitored in a large sample of comets.

A comprehensive series of rotational lines of water will be observed in medium-bright to bright comets, for investigating the physical conditions in the coma. This can be limited to low-energy lines, since water is expected to be cold in cometary environment:

1_{10}-1_{01}	556.9 GHz
2_{11}-2_{02}	752.0
2_{02}-1_{11}	987.9
1_{11}-0_{00}	1113.3
2_{21}-2_{12}	1661.0
2_{12}-1_{01}	1669.9
3_{03}-2_{12}	1716.8

The HDO lines are to be searched for in medium-bright to bright comets for assessing the D/H ratio. The challenge is to measure D/H in Jupiter-family comets, which are not bright. The fundamental 1_{01}-0_{00} line at 465 GHz is not covered by HIFI; priority is given to the 1_{11}-0_{00} line at 894 GHz for which a good sensitivity is required.

If a really bright comet shows up, a spectral survey will search for new cometary molecules (hydrides...); molecules such as CH, OH, H_2O^+, whose rotational lines are in the submillimeter domain and are still unobserved in comets, will also be looked for. The full frequency coverage of HIFI will be used for this purpose. No exhaustive list of lines to be observed can be provided at the present time.

2.6.2.2.2 Spectral resolution

Cometary lines are narrow: 0.2 to 3 km/s. Cometary line shapes contain much information on the kinetics of the cometary atmosphere and the outgassing pattern of the cometary nucleus. The velocity offset of the lines, typically 0.1-0.2 km/s, provides a direct probe of the jet forces that cause non-gravitational perturbations to cometary orbits. Therefore, a high spectral resolution is desirable (hopefully, corresponding to 0.05 km/s) as well as an accurate frequency calibration.

High-resolution observations will be performed on dedicated, strong lines such as the water lines. It is important to observe several lines of water at high resolution because different lines show different levels of saturation and their shapes inform us on their excitation conditions. For other observations such as spectral surveys or observations of several lines in parallel, a medium resolution (e.g., 0.5 km/s) could be used, provided it resolves the line and therefore does not degrade the S/N.

Because of sensitivity frequency switching by a few MHz is the preferred observing mode. Since the lines are narrow and at low frequencies this will pose no problem.

2.6.2.2.3 Tracking and observing strategy

This is not specific to HIFI, rather to FIRST in general, but perhaps it is good to recall here the idiosyncrasies of cometary observations.

The solar elongation constrain of FIRST: This is a strong constrain which will hamper the observations of many comets, especially at the moment they are brighter (close to the Sun).

Ephemeris issues: Like for other Solar System objects, the observations of comets require a specific tracking based upon an ephemeris. For comets, the ephemeris may have to be updated shortly before the observations.

Scheduling issues: Besides already known short-period comets which can be scheduled well in advance, it is desirable to observe unexpected new comets. Most of the bright comets are unexpected (c.f. comets Hyakutake and Hale-Bopp). This is only possible by organizing flexible target-of-opportunity scheduling procedures. Usually, there is a notice of several weeks between the discovery of a new comet and effective spectroscopic observations .

3 APPENDIX Water and Hydrides Spectroscopy

3.1 Selected HIFI Water Line List

Originating from levels with J < 8 and energies lower than approximately 1000 K

Transition	Frequency (GHz)	Band	BackBone / Ground State
6_{24}-7_{17}	488.5	1	
1_{10}-1_{01}	556.9	1	G
5_{32}-4_{41}	620.7	1	
2_{11}-2_{02}	752.0	2	
4_{22}-3_{31}	916.2	3	
5_{24}-4_{31}	970.3	4	
2_{02}-1_{11}	987.9	4	BB
3_{12}-3_{03}	1097.4	4	
1_{11}-0_{00}	1113.3	4	GBB
3_{12}-2_{21}	1153.1	5	
6_{34}-5_{41}	1158.3	5	
3_{21}-3_{12}	1162.9	5	
7_{44}-6_{51}	1172.5	5	
4_{22}-4_{13}	1207.6	5	
2_{20}-2_{11}	1228.8	5	
$7_{4,3}$-$6_{5,2}$	1278.3	Gap 5/6	
$6_{2,5}$-$5_{3,2}$	1322.0	Gap 5/6	
5_{23}-5_{14}	1410.6	6	
7_{26}-6_{33}	1440.8	6	
6_{33}-5_{42}	1542.0	6	
6_{43}-7_{16}	1574.2	6	
4_{13}-4_{04}	1601.2	6	
2_{21}-2_{12}	1661.0	6	
2_{12}-1_{01}	1669.9	6	GBB
4_{32}-5_{05}	1713.9	6	
3_{03}-2_{12}	1716.8	6	BB
5_{33}-6_{06}	1716.9	6	
6_{33}-6_{24}	1762.0	6	
7_{35}-6_{42}	1766.2	6	
6_{24}-6_{15}	1794.8	6	
7_{34}-7_{25}	1797.2	6	
5_{32}-5_{23}	1867.7	6	
6_{34}-7_{07}	1880.7	6	
3_{31}-4_{04}	1893.7	6	

The H_2O back bone lines

Transition	Frequency (GHz)	Band
2_{02}-1_{11}	987.9	4
1_{11}-0_{00}	1113.3	4
2_{12}-1_{01}	1669.9	6
3_{03}-2_{12}	1716.8	6

3.2 Hydrides

Hydride	Transition	Frequency (GHz)	Wavelength (μm)
PH	$^3\Sigma^-$, N=1-0	498.0	602.0

HBr	J=1-0	500.6	598.9
CH	$^2\Pi_{3/2},J=3/2-{}^2\Pi_{1/2},J=1/2$	532.7	562.8
o-H_2O	$J_{KaKc}=1_{10}-1_{01}$	556.9	538.3
NH_3	$J_K=1_0-0_0$	572.5	523.7
HCl	J=1-0	625.9	479.0
SiH	$^2\Pi_{1/2}$, J=3/2-1/2	660.0?	454.2?
CH^+	J=1-0	835.1	359.0
p-NH_2	$J_{KaKc}=1_{11}-0_{00}$	917.9	326.6
NH	$^3\Sigma^-$ N=1-0	974.6	307.6
OH^+	J=1-0	984.5	304.5
p-H_3O^+	$J_K=1_0-0_0$	984.6	304.5
NH^+	$^2\Pi_{1/2},J=3/2-1/2$	1038.1	288.8
HF	J=1-0	1232.7	243.2
SH	$^2\Pi_{3/2},J=5/2-3/2$	1382.9	216.8
HFe		1411.	212.4
o-H_3O^+	$J_K=1_1^+-1_1^-$	1655.8	181.1
OH	$^2\Pi_{1/2},J=3/2-1/2$	1837.8	163.1

3.3 Deuterated Hydrides

Hydride	**Transition**	**Frequency (GHz)**	**Wavelength (μm)**
HDO	$J_{KaKc}=1_{01}-0_{00}$	464.9	644.9
CH_3D	$J_K=2_1-1_1$ E	465.2	644.4
NH_2D	$J_{KaKc}=1_{10}-0_{00}$	470.3	637.4
NH_3D^+	$J_K=2_1-1_1$ E	788.3	380.3
HDO	$J_{KaKc}=1_{11}-0_{00}$	893.6	335.3
OD	$^2\Pi_{1/2}$ J=3/2-1/2	941.6	318.4
p-H_2D^+	$J_{KaKc}=1_{11}-0_{00}$	1373.9	218.2
OD	$^2\Pi_{3/2}$ J=5/2-3/2	1390.6	215.6