Preparatory work for the Herschel Space Observatory

Chapter 1

Executive summary

The Herschel mission will open up the universe to high spatial and spectral resolution studies at far-infrared and submillimeter wavelengths. Herschel will be the premier observatory to study the cool and dark universe and, hence, all objects deeply enshrouded in dust and gas. Among the key science drivers for Herschel are thus probing the formation process of stars and planets in the near universe, tracing the life cycle of the elements and the evolution of the Milky Way and other galaxies like it, measuring the star formation history of the universe, and providing an inventory of the molecular universe and the chemical processes shaping it. To meet the objectives of Herschel and to make its findings accessible to the wide public in clear understandable terms, a wide ranging and coherent preparatory science program has to be started, combining astronomical observations with laboratory studies, quantum mechanical calculations, and astronomical modelling.

This white paper provides a summary of a workshop held at the Leiden Lorentz Center, October 22 - 24, 2001 on preparatory science studies for the Herschel Space Observatory. A list of the scientific program and the participants of this meeting are provided in Appendix D and C, respectively. Among the wide range of scientific topics, this workshop put special emphasis on:

- Description of the instruments and their expected preparatory science needs.
- Laboratory studies of the spectral characteristics of astrophysically relevant atoms and molecules in the far-infrared and submillimeter.
- Modeling of spectral line data in astrophysical settings.
- Laboratory studies on the spectral characteristics of interstellar dust analogs.
- Modeling of the spectral energy distribution of dusty objects.
- Theoretical studies on the excitation of astrophysically relevant molecules, including collisional cross sections, dipole moments, and transition frequencies.
- Preparatory astronomical observations.

The recommendations of this workshop are as follows:

The interpretation and analysis of observations on the spectral energy distribution of all dust enshrouded objects in terms of the mass of the object as well as the temperature and composition of the dust requires a major laboratory effort on the wavelength-dependence of the opacity in the far-infrared and sub-millimeter spectral region and its dependence on the characteristics of the dust, including composition, structure, size, shape, and temperature of astrophysically relevant materials. This laboratory effort has to be suplemented by the development of 2-D radiative transfer codes which can handle the complex geometries expected for astronomical objects and which include the absorption and emission by transiently heated nano-particles.

Observations with the Herschel Space Observatory can be expected to lead to the detection of thousands and thousands of new spectral features due to a variety of simple and complex molecules. Identification, analysis and interpretation of these features in terms of the physical and chemical characteristics of the astronomical sources will require detailed astronomical modeling tools as well as supporting laboratory measurements and theoretical line strength and collisional excitation studies on species of astrophysical relevance. Of particular importance is H_2O because of its expected widespread presence in space, because of its unique diagnostic value for the physical conditions in astronomical environments, and because Herschel will be the only observatory which will be able to probe the ‘water universe’ in such great detail.

Finally, this data and the relevant analysis tools will have to made easily accessible to the scientific community through web-based data archives.

Chapter 2

The Herschel Space Observatory

The 'Herschel Space Observatory' (formerly known as the 'Far InfraRed and Submillimetre Telescope' – FIRST) is the fourth cornerstone mission in the European Space Agency (ESA) science programme. It will perform imaging photometry and spectroscopy in the far infrared and submillimetre part of the spectrum, covering approximately the $57-670$ μm range.

The key science objectives emphasize current questions connected to the formation of galaxies and stars, however, having unique capabilities in several ways, Herschel will be a facility available to the entire astronomical community. Because Herschel to some extent will be its own pathfinder, the issue of instrument calibration and data processing timescales has special importance.

Herschel will carry a 3.5 metre diameter passively cooled telescope. The science payload complement – two cameras/medium resolution spectrometers (PACS and SPIRE) and a very high resolution heterodyne spectrometer (HIFI) – will be housed in a superfluid helium cryostat. Herschel will be placed in a transfer trajectory towards its operational orbit around the Earth-Sun L2 point by an Ariane 5 (shared with the ESA cosmic background mapping mission Planck) in early 2007.

Once operational Herschel will offer a minimum of 3 years of routine observations; roughly 2/3 of the available observing time is open to the general astronomical community through a competitive proposal procedure.

The exiting science which will be possible with Herschel has recently been summarized in the proceedings of the Symposium: "The promise of the Herschel Space Observatory", ESA-SP 460.

Chapter 3

Preparatory Science and the PACS Instrument

3.1 The PACS Instrument in a Nutshell

The Photodetector Array Camera and Spectrometer (PACS) is the short-wave instrument of the Herschel mission. It employs two Ge:Ga photoconductor arrays (stressed and unstressed) with 16×25 pixels, each, and two filled Si bolometer arrays with 16×32 and 32×64 pixels, respectively, to perform imaging line spectroscopy and imaging photometry in the $60 - 210\mu$m wavelength band. In photometry mode, it will simultaneously image two bands, $60-90$ or $90-130\mu$m and $130-210\mu$m, over a field of view of $\sim 1.75' \times 3.5'$, with full beam sampling in each band. In spectroscopy mode, it will image a field of $\sim$ $50'' \times 50''$, resolved into 5×5 pixels, with an instantaneous spectral coverage of $\sim$ 1500km/s and a spectral resolution of $\sim$ 175km/s. In both modes background-noise limited peformance is expected, with sensitivities (5σ in 1h) of $\sim$ 3 mJy or $2 - 8 \times 10^{-18}$W/m^2, respectively.

3.2 PACS Observing Modes

The observing modes supported by PACS are combinations of *instrument modes* and *satellite pointing modes*. All satellite pointing modes – stare, raster, and line scan (with or without nodding) – are foreseen to be used for PACS observations. The following section describes the PACS instrument modes.

3.2.1 Dual-band Photometry

In this mode, both bolometer arrays are operating, providing full spatial sampling in each band. The long-wave array images the $130 - 210\mu$m band while the short-wave array images either the $60 - 90$ or the $90 - 130\mu$m band. The respective sub-band is selected by a filter. This mode is the standard mode for PACS as prime instrument. Observing parameters are the chopper mode (off/on; waveform, throw), pointing parameters (stare/raster/scan;nod), and the integration time per pointing.

3.2.2 Single-band Photometry

In this mode, only one bolometer array is operating such that either the long-wave array images the $130 - 210\mu$m band or short-wave array images the $60 - 90$ or the $90 - 130\mu$m band. This mode serves as a test mode for PACS as prime instrument, but it is also foreseen as standard mode for PACS/SPIRE parallel observations. Observing parameters are the chopper mode (off/on; waveform, throw), pointing parameters (stare/raster/scan;nod), and the integration time per pointing.

3.2.3 Line Spectroscopy

In this mode, one or two photoconductor arrays are operating for observations of individual lines. The long-wave array will observe in the $105 - 210\mu$m band while the short-wave array observes in the $57 - 72$

or $72 - 105\mu$m band. The wavelength in the primary band automatically determines the wavelength in secondary band; therefore, for most practical purposes, one can assume that only one line can be observed at a time, and only one array needs to be read out. This will help to reduce the integrated data rate. Observing parameters are the scan width (default 0), the chopper mode (off/on; waveform, throw), pointing parameters (stare/raster/scan;nod), and the integration time per pointing.

3.2.4 Range Spectroscopy

In this mode, both photoconductor arrays are operating for effective observations of extended wavelength ranges. Such observations can be continuous scans with full spectral resolution or steps for a coarser sampling of, e.g., SEDs. The long-wave array will observe in the $105-210\mu$m band while the short-wave array observes in the $57-72$ or $72-105\mu$m band. Observing parameters are the start- and end wavelength, the resolution mode, the chopper mode (off/on; waveform, throw), pointing parameters (stare/raster/scan;nod), and the integration time per pointing.

3.3 System Performance

Based on the present knowledge of the components of PACS and of the Herschel satellite, the performance of the entire system can be estimated in terms of what the observer is concerned with, i.e., an assessment of what kind of observations will be feasible with Herschel/PACS, and how much observing time they will require.

3.3.1 Image Quality and Beam Sampling

The photometer optics delivers diffraction-limited image quality (Strehl ratio $\geq$95%). We therefore assume that the instrument optics will only contribute in a neglible way to the dilution of the central peak of the telescope PSF.

The concept of approximately full beam sampling with our (filled) array will distribute the flux of a point source over several pixels. An equivalent dilution applies to the background received by the pixel. To recover the total flux (in the central peak of the PSF) several pixels have to be co-added. For the calculation of the system sensitivity this is taken into account through a pixel efficiency factor, which is defined as the fraction of the pixel area to the PSF area.

The spectrometer, and in particular its image slicer, is used over a large wavelength range. The (spatial) pixel scale is a compromise between resolution at short wavelengths and observing efficiency (mapped area) at long wavelengths. Full spatial sampling will require a fine raster with the satellite, for spectral line maps with full spatial resolution. For the sensitivity calculation this is neglected as the line flux will always be collected with the filled detector array. Therefore, for the plain detection of a line source, one pointing is sufficient. Fully resolved maps will require between 2 and 8 raster pointings, between the long and short wavelength end of the spectrometer range, with correspondingly longer integration time.

The spectral sampling also varies within each grating order; detection to the instantaneous resolution as given by the convolution of the diffraction-limited resolution with the pixel function is the default for the sensitivity estimates.

3.3.2 System Sensitivity

For the calculation of the system sensitivity we have included our present best knowledge of all components in the detection path as described above. The following tables summarise the pertinent performance data for photometry and spectroscopy.

Table 3.1: PACS Photometer Mode Specifications

Pixel size	$3.3''$	$6.6''$
FOV	$3.5' \times 1.75'$	$3.5' \times 1.75'$
Wavelength range	$60-90/90-130\mu$m	$130-210\mu$m
Point source detection limit (5 σ, 1 hour)	3.1/3.0 (2.2/2.1)* mJy	3.2 (2.3)* mJy

*) with on-array chopping

Table 3.2: PACS Spectrometer Mode Specifications

Pixel size		$9.4''$
FOV (5 ×5 pixel)		$47'' \times 47''$
Wavelength range		57μm–210μm
Resolution ($c\Delta\lambda/\lambda$)		100 – 250 km/s *
Instantaneous spectral coverage		1300 – 3000 km/s *
Point source detection limit (5 σ, 1 hour)	$\lambda = 60\mu$m	$7.8(5.5)^{**} \times 10^{-18}$W/m^2
	$\lambda = 90\mu$m	$4.0(2.8)^{**} \times 10^{-18}$W/m^2
	$\lambda = 130\mu$m	$2.8(2.0)^{**} \times 10^{-18}$W/m^2
	$\lambda = 180\mu$m	$2.5(1.8)^{**} \times 10^{-18}$W/m^2

*) varies with wavelength
**) with on-array chopping

3.4 Major Science Topics for PACS

The PACS consortium has identified a number of science topics which may be taken as examples of the kind of observations that will become possible with PACS, but also demonstrating what may be required in terms of preparatory work in advance of the mission.

3.4.1 Deep Extragalactic Surveys

These observations – in conjunction with SPIRE observations – are aimed at characterizing the obscured part of high-redshift star and galaxy formation and at resolving the cosmic FIR background. Multi-waveband information is essential for starburst vs. AGN discrimination and for photometric redshift determination. PACS will provide the highest spatial resolution which is crucial to beat confusion as well as for source identification with potential optical/NIR counterparts. Position accuracy to ∼arcsec is essential in this case. Example: A 1000 hour dual-band PACS survey to 5σ depths of 10mJy at 110μm and 170μm will cover ∼15 square degrees and detect tens of thousands of galaxies. Combined with a matching SPIRE survey, this will result in a catalog of low-resolution SEDs for most of these objects.

3.4.2 Spectroscopy of Galaxies

Extragalactic spectroscopy will include detailed maps of the brightest atomic and ionic fine structure lines of nearby galaxies which will give detailed insight in the heating an cooling of the ISM and the formation of stars on the scale of entire galaxies, yet with sufficient spatial resolution to study the mechanisms that trigger local star formation or global star bursts. The superior sensitivity of PACS as compared to e.g. ISO will allow observations of a large sample of (U)LIRGs in a number of atomic, ionic, and molecular lines to better understand the origin of their extraordinary luminosity and to ”sharpen our tools” for the interpretation of observations of more distant, high-extinction objects.

3.4.3 Initial Mass Function in Cores and Clusters

Photometric multi-band surveys of a number of star forming regions / molecular clouds over large areas will give good statistics on the mass distribution of condensations within molecular clouds down to equivalent brown dwarf masses. This may answer the question whether/how the mass distribution of stars relates to the fragmentation of the gas and dust in molecular clouds. An observing program of ∼500 h will cover a large area (12 sq.deg) in all 3 PACS bands to a 5σ detection limit of 0.08 $M_\odot$. The photometric surveys will be complemented by targeted, spectroscopic studies of molecular and atomic lines of embedded sources, including those found in the photometric surveys.

3.4.4 HD

PACS will offer a unique opportunity to observe the 112 μm rotational line of HD in many sources, from the Solar System to external galaxies. The abundance ratio of the (primordial) D/H ratio allows one to estimate the baryon density in the universe; once that ratio is known, the local value of this ratio in the ISM is a measure for the level of stellar processing the gas has undergone and, therefore, of star formation history.

3.5 Preparatory Efforts

Preparatory efforts for PACS observations include the establishment of celestial calibration standards as well as preparatory scientific work.

3.5.1 Celestial Calibration Sources

Operation of the PACS instrument requires in-orbit photometric and spectroscopic calibration.

For *photometric calibration*, continuum sources with accurately known flux levels are needed. For the spectrometer channels the outer planets provide convenient standards while for the photometer channels with their highly non-linear bolometric detectors a range of celestial calibrators is required. This will require preparatory photometric observations of bright, normal stars in regions with low cirrus at submm to mm wavelengths. Modelling/interpolation with photometric measurements in the visible/NIR will then lead to a sufficiently accurate knowledge of the FIR fluxes. For the full flux range to be covered by PACS, characterization of a few more asteroids will be needed to a high level of accuracy.

For *spectroscopic (wavelength) calibration*, PACS will use well-characterized, bright emission line sources, like planetary nebulae and PDRs or H_2O lines from late type stars. Dedicated preparatory observations are probably not necessary as rest-frame wavelengths and source radial velocities are known to sufficient precision, and preparatory work will be limited to literature search and estimates of line fluxes.

For *positional calibration*, suitable sources could be the outer planets or asteroids, with the drawback that they are moving sources. Stars with well-known astrometric positions could be better sources provided they are bright enough in the FIR to give high signal-to-noise ratios after short integration times and point-like at both optical and FIR wavelengths. Ideally, one would request an "FIR cluster" to also map imaging distortions without repointing of the satellite which will introduce errors of the same scale as these distortions. To find and astrometrically characterize such a cluster would be a highly desirable project.

3.5.2 Properties of Interstellar Dust

For most of the scientific targets of PACS, dust plays a key role through emission as well as through extinction.

FIR dust emission is used to derive quantities like luminosity, mass, temperature, or photometric redshift of objects. In-depth knowledge of the dependence of the spectral energy distribution (SED) on physical and chemical conditions is essential to derive any of these parameters. Dust composition may vary, and the abundance of large particles becomes increasingly important in the FIR. Dust "features" like water ice at the short wavelength end of PACS and bands from hydrated silicates or carbon-rich compounds can make noticeable contributions within the (broad) photometric bands of PACS. Laboratory studies on dust of various chemical composition and grain size distribution are still far from sufficient for a good modelling of the SEDs we will observe in space.

Dust extinction influences the "excitation profile" of the interstellar medium around luminous sources, while at the same time physical conditions, like radiation field and density, may influence parameters like size distribution or clumping. The extinction enters into the radiative transfer, both for continuum radiation and for spectral lines. Dust extinction is likely to vary as a function of parameters such as metallicity. Again, laboratory studies as well as modelling will comprise major efforts.

3.5.3 Radiative Transfer in Complex Sources

A representative treatment of radiative transfer for complex/unknown geometries is a notorious problem. While existing models mostly address "simple" geometries, their validity for "real" sources is often doubtful. "Real" sources have complex morphologies, with multiple/complex excitation, non-simple source geometry, and a mix of foreground extinction and self-absorption within the emitting region, both by dust and by line transitions. Models must combine dust and gas radiative transfer. How can we get "robust" models for the interpretation of observations of maybe just a few FIR line (in the case of more distant objects) from highly complex sources?

3.5.4 Conclusion

It is very clear that the points which have been barely touched here represent major efforts which need to be tackled for a successful interpretation of the data we are looking forward to collect with Herschel. Any such effort is in the interest of the entire community.

Chapter 4

Preparatory Science Needs for SPIRE (Spectral and Photometric Imaging REceiver)

The SPIRE instrument is designed to undertake rapid mapping of large areas of sky with the aim of detecting faint point sources in three bands between 200 and 600 μm. An additional scientific programme is low to medium resolution spectroscopy on point sources between at least 200 and 400 μm, extending to 670 μm. To maximise the scientific gain the instrument is designed to have simultaneous mapping in the three photometric bands and have an imaging spectroscopic capability with variable resolution of at least 1 cm^{-1} to 0.4 cm^{-1} with a goal of 2 to 0.04 cm^{-1}. The instrument is also designed to have an ability to chop a large portion of the FOV and have the ability to jiggle or micro-step the FOV across the detection plane.

To address these separate capabilities, the SPIRE instrument consists of two sub-instruments with a common optical feed. A three channel imaging photometer uses single feed horn NTD bolometer arrays with channels centred on 250, 350 and 500 μm ($R \sim 3$). Simultaneous spatial/spectral coverage is achieved through the use of dichroic beam splitters and the optics design has been customised to give the largest possible field of view through the instrument (4x8 arcmin). A beam steering mirror (BSM) within instrument enables chopping, micro-stepping, scanning and peak up. The optics are designed to give a pupil image on BSM and second pupil stop close to the detectors for straylight control.

The imaging spectroscopy capability is provided by an imaging Mach-Zehnder Fourier Transform Spectrometer (FTS). This novel design uses intensity beam splitters rather than polarising beam splitters allowing maximum throughput and the use of all four ports. The mirror mechanism is designed to give $R \sim 1000$ at 250 μm (0.04 cm^{-1}) at least for an on axis source and $R \sim 100$ (0.4 cm^{-1}) is guaranteed across the 2.6 arcmin diameter FOV. Two channels are needed to cover the 200-670 μm range, hence the necessity for a second output port. Also, the telescope background needs to be nulled therefore a source representative of the telescope background signal is placed at the second input port.

4.0.5 Requirements for the photometer

The SPIRE photometer is required to have an absolute accuracy of 15% or better at all wavelengths with a goal of 10% and a relative photometric accuracy better that 10% with a goal of 5% over a dynamic range of 4000 for astronomical signals (confusion limit $\sim$ 15 mJy - $\sim$ few 10's Jy). We expect to achieve a highly stable calibration and this will tie in with the international temperature standard (ITS 90) on the ground and will be a significant improvement on the 10-20% currently achieved by ground-based facilities. The photometer will use a set of well known sources as primary calibrators, then a set of secondary calibrators will be established. For calibration we need:

- point-like objects in the $18''$ beam
- sources within the SPIRE dynamic range
- non-variable sources

- a set of secondary sources fitting the above requirements distributed throughout the sky.
- primary source(s) which must have well modelled spectral energy distributions with in-band absolute accuracies greater than the SPIRE requirement

It is likely that the primary calibrator will be the planet Neptune (as Uranus is too bright) plus possibly stars or asteroids. However in order to achieve the calibration requirements for the photometer the following preparatory activities need to take place:

- observations of calibration sources with ground-based facilities e.g. SCUBA
- modelling of Neptune in the SPIRE wavelength range
- selection and modelling in the SPIRE wavelength range of asteroids
- selection and modelling in the SPIRE wavelength range of stars
- selection of secondary calibrators e.g. from the SCUBA archive
- modelling of galaxy SEDs for science verification

4.0.6 Requirements for the FTS

The SPIRE FTS will not need sources to establish the wavelength calibration but will require sources for photometric calibration and scientific verification. As SPIRE is working in a largely unexplored region accurate predictions of the line fluxes observed must be made from model extrapolations for a clearly defined set of sources. The sources chosen must meet the following requirements:

- They must have a low continuum, as the SPIRE FTS is unable to observe continua brighter than about 200 Jy.
- The line fluxes must either be accurately known or accurately predicted.
- They must be point-like to prevent any optical effects being folded into the calibration.
- They must be non-variable as adding time dependency to the model is adding complexity and introducing error.
- They must have several observable lines to minimise observing time for calibration purposes.
- They must explore the FTS dynamic range as the FTS detectors are non-linear and this non-linearity needs to be calibrated.
- They must be well distributed around the sky in order to allow sources to always be available within the Herschel visibility.
- The lines studied must well isolated from other species.

Once the sources have been identified the models can be enhanced by ground based observations using existing facilities, airborne observations from SOFIA and space observations from SWAS. If accurate models can not be produced, then SPIRE will rely on published data from these observatories although only SOFIA will be capable of observing in the 200-350 μm part of the 200-670 μm FTS range.

Chapter 5

The Heterodyne Instrument for the Far-Infrared (HIFI)

5.1 Short description of HIFI

HIFI is the heterodyne instrument on the Herschel Space Observatory (HSO). As its name states it employes the heterodyne technique to provide the very high spectral resolution (upto $R = 10^7$ necessary to resolve the atomic, ionic and molecular rotational lines in the submillimeter and far-infrared region and being able to probe dynamics, temperatures, densities and abundances within a variety of astrophysically interesting sources.

Direct detection in a high resolution spectrometer is very difficult within the submm and far-IR regime. Therefore HIFI employs the heterodyne technique where the sky signal is mixed with an external signal close to the frequency of interest coming from a Local Oscillator. If the mixing is done in a non-linear device, the result is a signal at much lower frequency, but still containing *all* spectral information. This lower frequency signal is easier amplified and read-out.

In order to achieve a as high as possible sensitivity, HIFI uses cryogenic mixers at a temperature less than 4 K. In the lowest 5 bands, so-called SIS (superconductor-insulator-superconductor) mixers are used, whereas in its highest bands Hot Electron Bolometer (HEB) mixers are favoured.

Amplification takes place right after detection in two steps, whereafter the intermediate frequency (double side-band) signal is detected in a 4 GHz wide-band spectrometer (WBS) (employing a Acousto-Optical (Array) Spectrometer (AOS)) and in a high resolution autocorrelation spectrometer (HRS) in subbands within the same 4 GHz.

The state-of-the-art mixing devices and its location outside the atmosphere will put Herschel-HIFI among the most sensitive single-dish submillimeter instruments ever employed. It can not only observe in the submm atmospheric windows between the telluric water lines but will also cover these water-line frequencies and explore the water content of the (local) Universe in unprecedented detail. HIFI will provide a continuous coverage between 480 and 1250 GHz and between 1410 and 1910 GHz. The instrument will operate in double-side band mode and has an instantaneous frequency coverage of 4 GHz. HIFI is optimized for very deep integration single pointing observations, complete spectral scans and for mapping in single lines. It provides access to the complete suite of ionic lines , like [C II] and [N II], atomic lines, like [C I], and almost every molecular line possible.

Observations with HIFI will thus provide us with important data on the the heating and cooling of the ISM. It will provide important clues to the structure of the ISM; probe deeply into molecular clouds and trace the star-formation dynamics; trace the AGB winds and shells; and outline the molecular inventory and chemical evolution of the ISM and CSM. Moreover the composition of the ISM in other galaxies will be an important target for HIFI.

An overview of the instrumental parameters is given in the table. The science is discussed in a separate section below.

Table 5.1: HIFI instrumental parameters and performance

Band	1	2	3	4	5	6
Freq. range (GHz)	480-640	640-800	800-960	960-1120	1120-1250	1410-1910
Beamwidth ($''$)	39	30	25	21	19	13
DSB Rec. noise (K)	90	130	160	210	370	650
Noise level in 180s integration (mK)	5.0	7.4	10	12	23	48

Noise level is given for 1 MHz channels in the 4 GHz bandwidth. Observing mode is double beam-switch.

5.2 Performance

HIFI is a simple instrument in the sense that it is a single pixel (one beam), single bandwidth (4 GHz) spectrometer. The applicable beam sizes are given in Table (5.1) just as the sensitivities within 1 MHz channels in 180 seconds integration. HIFI will observe in dual side-band mode. So, not only the frequency of interest in the signal side-band, but also the frequencies from the image side band. This may cause blending of lines of interest, with unwanted lines. The treatment of these cases is still topic of study.

5.3 Observing modes

HIFI is designed to have essentially three different observational strategies: Deep integration at a single position; A spectral scan over the whole frequency range available to HIFI at a single position; and mapping in selected spectra lines. This can be achieved in several observing modes, where one uses frequency or spatial modulation to remove instrumental and background contributions.

In single-pixel mode the frequency-switch modulation is likely to be preferred, with the double beam-switch mode, known from ground-based observatories, providing a reliable modulation alternative. The spectral scans, are likely to be performed through double beam-switch, especially when many spectral lines are present. For mapping the On-The-Fly (OTF) mapping technique will be mostly used. In this techniques the telescope moves over the map in a regular pattern, during the integrations. Extensive use on ground-based observatories have shown this technique to be superior over conventional raster maps.

HIFI will be able to detect continuum radiation, if present, with a high accuracy, however the high spectral resolution makes HIFI to be best tailored to spectral line observations.

5.4 HIFI Core Science

HIFI will be able to make large contributions to many aspects of astrophysics, and the most important ones are likely still unknown to us now. However, the instrument capabilities make this instrument especially well suitable for detecting and resolving spectral lines from sources that exhibit line widths between 1 and a few hundred km/s.

From all the possible topics we have singled out 2 core science topics for which HIFI will make unique contributions: The water trail and the molecular universe. Other important science topics worth mentioning include the ISM in our and other galaxies, star-formation and the death of stars. More science topics are described on http://www.sron.rug.nl/hifiscience.

While the Infrared Space Observatory (ISO) and the Submillimeter Wave Astronomical Satellite have shown beyond any doubt the presence of water in the Universe, these satellites were severy hindered by their low spatial and/or spectral resolution or the availability of only a small number of lines. With Herschel-HIFI, with its small beam, we will be able to study the spatial scales of water much better. Its high spectral resolution enables studies of the dynamics of the regions under study, whereas the broad frequency range available, allows for studies of many water lines, isotopes and related species such as OH and H_3O^+, within the same object, probing a large range of temperatures and densities and chemical conditions. Finally, the spectral capabilities of PACS allow a continuation of the spectral studies to higher frequencies, albeit at a reduced spectral resolution, constraining the excitation of all the water lines.

The submm range is full of rotational lines of many molecular species. Millimeter and submillimeter observations have been the most important tools to detect many exotic species in the interstellar medium for the first time. The exceptional frequency coverage of HIFI makes it possible to extend the exploration space to these higher frequencies. Here we expect hydride-molecules to be present and to be detected, but also complex molecules known from biology, like e.g. glycine. Many of the frequencies for these species are not well known, therefore discovery has to be preceeded by studies in the lab, assisted by surveys in the telluric windows. Future Herschel spectral surveys will provide us with all lines within the HIFI frequency range and thus assures the measurement of all the lines of a single species instead of only a small number. Furthermore, it provides us with data from which molecules can be serendipitously found and identified.

5.5 Summary of preparatory efforts

It is clear that in order to go from HIFI data to physical models, many parameters have to be known before hand. Observations generally require a good knowledge of line-frequencies and line-strengths. The excitation can only be determined when accurate collisional excitation parameters are known from either calculation or measurement. Chemical reaction rates have to be known to link different species together in a comprehensive frame work and last not but not least detailed understanding of radiative transport in lines and accurate modelling tools have to established. In addition, HIFI would benefit from preparatory spectral surveys in the telluric windows of template objects. In this report these areas are addressed in detail. It is clear that HIFI would benefit tremendously from advancements in the fields mentioned. It should be noted that HIFI is not alone in this respect. The heterodyne instruments on SOFIA and ALMA could benefit just as much.

Chapter 6

Preparatory efforts for modeling of spectral lines

The dramatic increase in the sensitivity of submillimeter receivers and the quality of ground-based submillimeter telescopes on high, dry sites have resulted in orders of magnitude improvement in the speed and quality of submillimeter ground-based data obtained over the last decade. However, the analysis of such data has shown little evolution over this period: much of the data are still interpreted using a single excitation temperature with some correction for optical depth, or equivalently, in the case of line surveys in which many lines of a single species are available, the rotation-diagram method. Non-LTE statistical equilibrium excitation calculations are largely limited to homogeneous clouds with a constant temperature and density. While such analyses are useful in zeroth order, the inferred abundances and physical conditions can be in error by an order of magnitude or more if source structure is not taken into account.

In the last few years, several groups have started to develop radiative transfer and physical models which go beyond the simple traditional analysis sketched above. In these cases, the analysis starts from a physical source model in which the excitation and radiative transfer of a molecule is calculated and the resulting emission convolved with the beam of the observations. The abundance and/or physical structure is subsequently adjusted to obtain agreement with observations. Such models have now been developed in 1-D and 2-D and are being expanded to 3-D. The two methods are illustrated in Figure 1. The next step is to couple the physical model with a chemical network and test the model by comparing the resulting abundance profiles with observations. This model philosophy has already been sucessfully applied to some types of regions, e.g. PDRs, photoionized regions and shocks, but in many other situations there is much room for improvement. Also, with the rapid development of hydrodynamic codes of various types of sources, a set of generic model tools is needed to couple the physical mdels with chemistry and radiative transfer.

The type of data provided by Herschel will resemble those from ground-based submillimeter telescopes, in the sense that they are single-dish submillimeter data in beams comparable to those of large ground-based telescopes. These beams usually do not resolve the sources. In order to make a leap forward not just in technology but also in our astrophysical understanding, the Herschel teams need to raise the analysis to a new level of sophistication. This requires state-of-the-art computer programs in at least 3 areas:

- Radiative Transfer
- Chemical Models
- Physical Models

In the following, a brief and probably incomplete inventory of existing modeling programs is presented.

6.1 Inventory of Modeling Programs

6.1.1 Radiative transfer

1. Expertise:

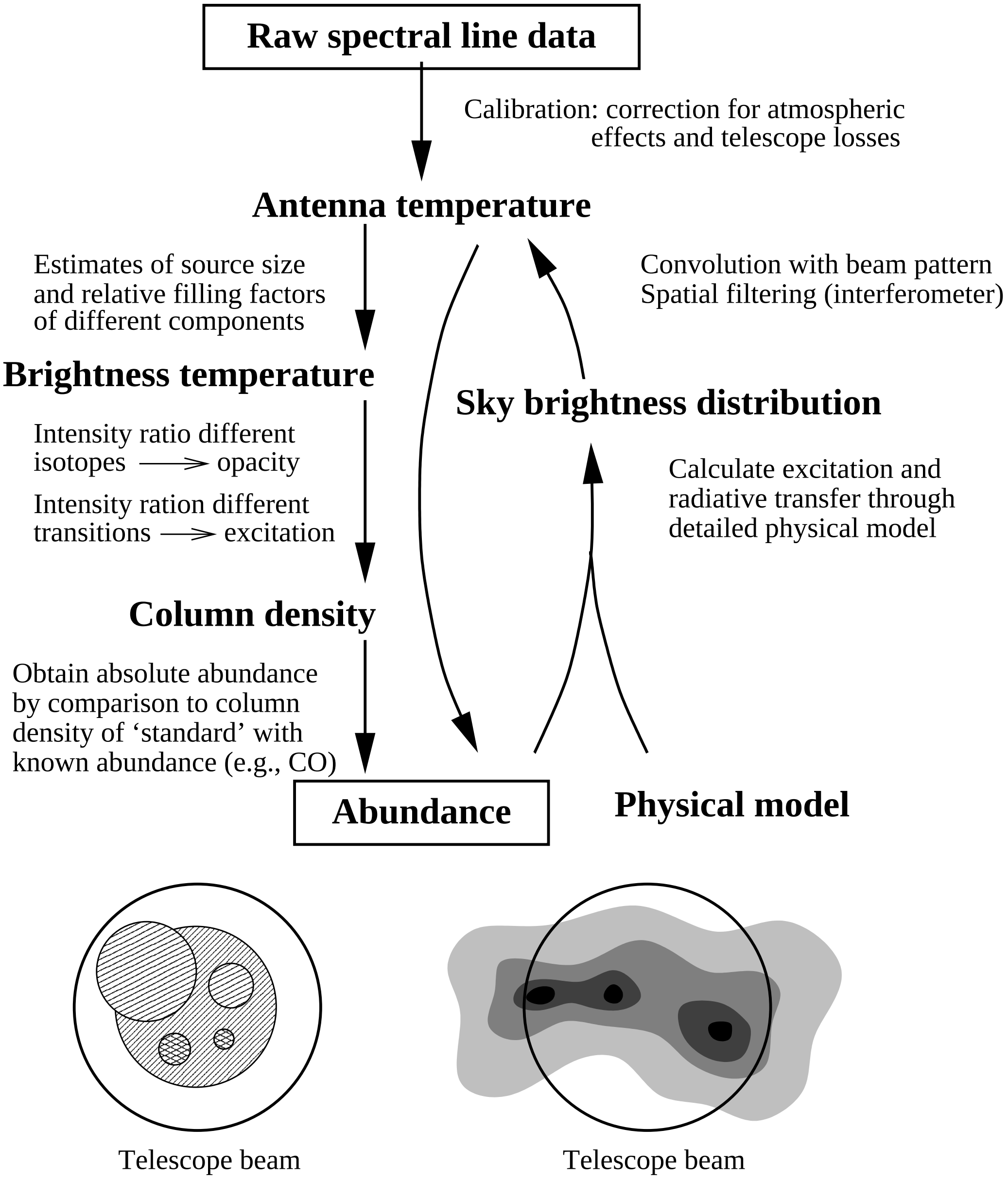

Figure 6.1: Steps involved in deriving molecular abundances from spectral line data. The left-hand side shows the traditional 'homogeneous' approach, the right-hand side the recent 'detailed' approach (from: van Dishoeck & Hogerheijde 1999, in Origins of Stars and Planetary Systems).

Various numerical methods for non-LTE line radiative transfer have been developed over the years. These codes have been compared to each other and the results are presented on the website: http://www.strw.leidenuniv.nl/˜radtrans, where further details can be found. Continuum radiative transfer codes are discussed in depth in Chapter 7.

2. Needs: the radiative transfer models need molecular data as input, in particular:

   - optical constants dust (see Chapter 9)
   - energy levels molecules (see Chapter 8)
   - Einstein-A coefficients (see Chapter 8 and 10)
   - collisional rate coefficients, both pure rotational and ro-vibrational (see Chapter 10)

   An inventory of molecules for which these data are lacking or are incomplete needs to be made.

6.1.2 Chemical models

1. Expertize:

   Reaction rates among astrophysically relevant species are summarized on the website (http://saturn.phy.umist.ac.uk:8000/) where references to the original literature can be found as well.

2. Needs:

   - basic set of chemical reactions for various n, T regimes to be used as benchmarks
   - sensitivity analysis tools to check important reactions and select optimized (small) chemical networks to be coupled with physical models
   - gas-grain and gas-PAH interactions; Monte-Carlo vs rate equations approach

6.1.3 Physical–chemical models

1. Needs:

   Models for the following astronomical objects will have to be developed: low and high mass YSO envelopes, hot cores, giant molecular clouds, photodissociation regions, ionized gas, diffuse interstellar gas, shocks (C and J-type), disks, planetary nebulae, extragalactic objects, Planetary atmospheres, and comets.

6.2 Models for H_2O emission

Water studies have been identified as an important science driver for Herschel because it is a key ingredient in many environments, because it is a key chemical species, because it can be an important gas coolant, and because it provides a powerful diagnostic of the physical conditions of the emitting gas. It is therefore essential to develop a sufficiently detailed model for H_2O emission in various environments.

6.2.1 Predicting observables

Recently, a number of numerical radiative transfer codes of water emission have been developed. These can provide us with calculated line intensities and profiles of water lines for a variety of astrophysically relevant conditions. Initially, simple, homogenous slabs of various densities, temperatures, and column densities can be considered. The results of these calculations can be used as numerical "observations" to identify the best analysis techniques for real astronomical data; which are the key lines? What lines ratios probe physical conditions best? What spectral resolution is required ? How do measurement errors propagate? Can low frequency, high spectral resolution data (e.g., HIFI) on H_2O effectively be combined with high frequency, low spectral resolution data (e.g., PACS) ?

6.2.2 H_2O radiative transfer

It will be very important for Herschel to have access to a number of numerical radiative transfer codes which solve simultaneously the statistical equilibrium equations and the line transfer of water in the comoving frame. This is a numerically very demanding task because of the intricate radiative coupling between the various rotational levels, the large variations in optical depth between different lines, the coupling with the far-infrared continuum, and the occurrence of masering action in some lines, but recently developed numerical schemes (ie., accelerated lambda iteration methods and accelerated monte carlo methods) have provided a breakthrough in this area of research. Such codes will have to include temperature, density and velocity gradients appropriate for star forming regions and stellar outflows (following various theoretical and observational analyses already developed). The results of such codes can be used to re-evaluate the instrument requirements for Herschel and optimize observing strategies.

6.2.3 Existing data

The numerical radiative transfer code optimized for H_2O modeling can be used to analyze the limited existing data on H_2O emission in star forming regions. Presently, the lowest level of water has been probed by SWAS. LWS, and to a lesser extent SWS, on ISO have observed many water lines in the 200–80 μm spectral range (1.5–3.8 THz) at low resolution in a wide range of objects. The KAO and ISO have observed a number of water lines of the ^{18}O isotope which are shifted out of the completely blocked core of the telluric bands. H_2O maser emission has also been observed from the ground in many star forming regions. Besides an important test bed for these codes and the analysis techniques developed, it is expected that this will lead to new insight in the role of water in star forming regions.

6.3 Future steps

An inventory of the available modeling expertise within the Herschel community is only a first step toward preparation. The proposed next steps are:

1. Devise realistic test problems for different types of sources
2. Compare existing codes with each other through test problems and make results available to community
3. Test analysis methods and codes on existing ground-based and ISO/SOFIA/SIRTF data
4. Identify new developments, enhancements and upgrades needed for various codes before Herschel data become available, both for 1-D and multi-D codes
5. Improve user-friendliness of codes so that they can be used by other groups within the community and eventually become availabile through the WWW
6. Prepare preliminary source models for Herschel guaranteed time sources based on existing data and make predictions for lines to be observed within the Herschel core program

The most effective way to carry out these steps is through a series of specialized, well-focused workshops on these topics. With respect to needs for radiative transfer codes, the community should focus on improving the accuracy and speed of 1-D codes at very high optical depth (especially for H_2O models) further development and improvements (including speed) of 2-D codes (especially for circumstellar disks) and self-consistent coupling of radiative transfer with physical-chemical and/or hydrodynamical codes.

Chapter 7

Continuum Radiative Transfer Models - Preparing for the Herschel Science

A major goal of PACS and SPIRE will be the measurement of spectral energy distributions of dust-enshrouded objects. Without a detailed radiative transfer modeling, an adequate interpretation of the data will not be possible. Furthermore, HIFI line measurements very often require the knowledge of the continuum radiation field in order to analyze the data by line transfer models. The goal of analyzing spectral energy distributions is to derive physical source parameters (luminosity, mass, density and temperature distributions), to determine the geometrical structure of the source (envelopes vs. disks, hidden AGN, distributed starbursts), or to characterize the evolutionary state of the objects (change of SED with evolutionary state of disks).

The solution of the radiative transfer equation is often more complicated than the solution of the hydrodynamical problem for the same configuration. The reason is the directional and frequency dependence of the radiation field which introduces additional dimensions: for the time-independent 1-D case (slab or spherical symmetry) the specific intensity $I_\nu(r, \theta)$ is a function of three variable (frequency ν, vertical/radial distance r, direction θ). In the general 3-D case, we have to consider $I_\nu(x, y, z, \theta, \phi)$ with the three spatial coordinates x, y, z and the directional variables θ and ϕ. An additional complication is the coupling between the different wavelengths and the need to calculate the scattering of light correctly. This usually leads to an iterative solution procedure.

Despite these difficulties, reliable and fast 1-D models are available which even treat the difficult case of high optical thickness correctly (see the paper by Ivezic & Elitzur 1997 for test results (MNRAS 287, 799)). Even for higher spatial dimensions, numerical radiative transfer calculations are possible due to increased computer speed and storage capacity, the parallelizing of codes, and new numerical algorithms (e.g., adaptive/nested grids, energy cells, domain decomposition, accelerated convergence). Meanwhile a number of 2-D codes are available and a benchmark project for this case, led by the Jena group, is presently going on. First results, based on self-consistent 3-D radiative transfer simulations, were recently published. They are mainly based on the Monte-Carlo-method, although a few grid-based codes exist. It is necessary to note that most of the available 2/3D codes are very difficult to use by non-experts in the field.

The treatment of radiative transfer is always a combination of the chosen structure of the configuration (heat sources, density distribution, clumpiness) and the microphysical properties of the medium. For continuum calculations, we need the absorption and scattering efficiencies of the grains as a function of frequency. These quantities depend on the material, shape/size, and temperature of the grains.

Continuum radiative transfer solutions very often include only one dust component and consider only particles of a certain size. This is clearly insufficient because any individual grain component will have their own temperature. Averaging over material properties is a dangerous approximation. In addition, many spectra of circumstellar disks and envelopes around young and evolved stars as well as of starburst galaxies show evidence for emission from very small grains and PAHs. This requires the treatment of temperature fluctuations and practically leads to an NLTE treatment of the continuum transfer. There are only very few codes available which include such non-equlibrium heating.

The message, we learned from ISO, is the fact that we need an equally good knowledge of the radiative transfer and the underlying optical properties of the dust particles (cf., Chapter 9). This implies that radiative transfer models and optical databases are equally important. In addition, we have to stress that spectral energy distributions contain limited geometrical informationand just fitting these curves can lead to non-unique models.Therefore, one has to add knowledge from theoretical considerations (e.g. hydrodynamical models) or other high-resolution data (intensity and polarization maps whenever possible). One has also to keep in mind that too simple models may violate basic physics (e.g. energy conservation).

For the analysis of Herschel data 1-D models are widely available and can be used via the web (http://www.pa.uky.edu/˜moshe/dusty/ for the DUSTY code). Note that Elitzur's latest models, although spherical symmetric, provide a self-consistent approach to both radiative transfer and dynamics.. Support is definitely needed to offer such a tool for 2-D calculations which should include the option to treat PAH emisssion and the emission of very small grains. In addition, databases of optical grain properties need the necessary attention.

Chapter 8

Preparatory studies in the laboratory for gas-phase species

The high resultion povided by the heterodyne technique requires extensive spectroscopic preparation in the laboratory.

The spectral range covered by HIFI (480-1910 GHz) and Herschel in general (480–5000 GHz) includes:

- fine structure transitions of atoms and atomic ions
- pure rotational transitions in the ground state as well as in the excited vibrational states of small molecules and radicals, including in particular of hydrides: H_2O, H_3O^+, CH^+, OH, NH, CH, SH, LiH, HCN, CH_2, HCO^+, NH_2, C_2H, HF,...
- rotational-torsional spectra of small internal rotors: H_2CO, CH_3OH, CH_3CN, CH_3SH, CH_3COOH, C_2H_5CN, C_2H_5OH, CH_3OCH_3,...
- rotational-vibrational transitions such as the low-frequency bending modes of carbon chains and the flopping modes of polycyclic aromatic hydrocarbons (PAHs).

8.1 Laboratory studies

Which laboratory measurements?

- Laboratory work at the Herschel frequencies is quite sparse.
- Measurements of frequencies and dipole moments (oscillator strengths) are needed. Theoretical values for rotational dipole moments are often employed. This is reasonable for rigid molecules but much more difficult in the case of floppy molecules. Other data are important as well such as cross-sections for rotationally inelastic collisions that govern excitations in non-thermal regions and reaction rates that are needed to predict the chemical abundance of the considered species. In particular, much work has to be done on neutral-neutral reactions.
- Measurements of frequencies and dipole moments should not be limited to the Herschel spectral range. Indeed some important complementary transitions could fall in the far-IR covered by the ISO spectrometer LWS or could be observable with ground-based (radio) telescopes. Furthermore, for each species, the most abundant isotopomers have to be considered.
- It is important to mention that the detection of non-polar carbon chains and of complex molecules such as PAHs through their low-frequency rotational-vibrational transitions could be the unique way to identify these species. It is therefore a real challenge for Herschel.

8.2 Laboratory groups

Preliminary list of research groups / contacts for laboratory measurements

1. Spectral studies
    - John Pearson (JPL, CA):
        - JPL catalogue
        - unpublished results mostly on small internal rotors (NH_3, C_2H_5-OH, HC=CCH_2OH, CH_2=CH-CH_2-OH, CH_3CH_2CN, CH_2DOH)
        - Laboratory capabilities: FTS 0.0015 cm^{-1} resolution, microwave spectrometer 0-600 GHz, diode laser photomixer, spectrometer 300-1600 GHz, laser sideband system.
    - Gisbert Winnewisser / Thomas Giesen (KOSMA - Cologne University - Germany)
        - Laboratory capabilities: very high resolution spectrometers (e.g. $\sim$10 kHz at 1 THz) from the IR (15–100 THz) using an IR-tunable diode laser to the far-IR, sub-millimeter and millimeter ranges (53–2000 GHz) using Backward Wave Oscillators and a CO-sideband laser with very high resolution ($\sim$10 kHz at 1 THz). Studies in absorption cells (77–300K) and in supersonic jets (1–20K). With the latter technique, possibility to study carbon-chains (C_nH_m) and clusters (C_n, C_nSi_m).
        - Recently published spectra of molecules in the 200-2000 GHz:
            - Hydrides: CH, NH, OH, PH, SH, NH_2, SH_2, PH_2, NH_3
            - Carbon containing molecules: ^{12}C, ^{13}C, many isotopes of CO, H_2CO, HCN, HC_3N, HC_5N, c-C_2H_4NH
            - Ions: $^{12}C^{16}O^+$, $^{13}C^{16}O^+$
        - Cologne Database for Molecular Spectroscopy
    - Geoff Blake (CalTech - USA)
        - Laboratory capabilities:
          a THz photomixer spectrometer (developed with JPL); a Balle-Flygare FT microwave instrument; resonance ionization instruments that operate from the near-IR to the vacuum UV (5 microns to 109 nm)
        - Interest: Spectroscopy of large carbonaceous species that may be pursued for the first time with FIRST, improvement of the JPL catalog for light species and internal rotors.
    - Richard Saykally (University of California - Berkeley - USA)
        - Laboratory capabilities: tunable far-IR laser sideband spectrometer; a diode laser spectrometer optimized for the 10-30 micron range; cavity ring down instruments from the near-UV to 5 microns; jet expansion and discharge sources; a 3-20 micron emission specrometer based on the Rockwell SSPM photon counting devices
    - Shuji Saito (Fukui University - Japan)
        - Laboratory capabilities:
          high sensitivity millimeter- and submillimeter-wave spectrometer (10 - 850 GHz) combined with a free-space absorption cell (77-300 K) for observations of free radicals and molecular ions and a parallel plate Stark cell for measurements of dipole moments.
        - Studied species: HNO, DNO, HCO, DCO, CCS, C_3S, CH_2CN, CH_2, CD_2, ND, PH, PD, NH_2, ND_2, NHD, PH_2, PD_2, PHD, D_3O^+, H_2Cl^+, $HDCl^+$, and about 100 simple free radicals and molecular ions including interstellar molecules and potential candidates.
        - Interest: Interstellar deuterium fractionation and dark cloud core evolution.
    - Shozo Tsunekawa (Toyama University - Japan)
        - Laboratory capabilities: tunable Far Infrared Spectrometer (300–6000 GHz) and microwave spectrometer (8–200 GHz)
        - Previous studies: CH_3OH, H_2O, NH_3,...
    - Marcel Bogey, Jean Demaison, Georges Wlodarckzak (Lille University, France)

  - Laboratory capabilities: tunable far infrared laser spectrometer (500-2600 GHz), microwave Fourier transform spectrometer (5-20 GHz), millimeterwave and submillimeterwave spectrometers (50-700 GHz)
  - Species of interest: stable species (also with internal rotors), molecular ions, free radicals, carbon chains, PAH's
- Michel Vervloet (LPPM and LURE - Orsay - France), Pascale Roy (LURE - Orsay - France)
  - Laboratory capabilities: FTS 0.005 cm^{-1} resolution using the synchrotron radiation of LURE as the absorption continuum source, measurements possible from far-IR down to 5 cm^{-1} FTS 0.002 cm-1 resolution in the spectral ranges covered by the PACS, SPIRE, and HIFI instruments.
  - Activity: High resolution spectroscopy of stable molecules and unstable species produced in discharges.
- Guy Guelachvili (LPPM - Orsay - France)
  - Laboratory capabilities: FTS 0.005 and 0.002 cm^{-1} resolution, IR studies down to ~500 cm^{-1} with possibility of extension in the far-IR
  - Determination of rotational constants from IR rotational-vibrational transitions, dipolar moments derived by time-resolved spectroscopy
- Peter Bernath (University of Waterloo - Canada)
  - Laboratory capabilities: FTS 0.0015 cm^{-1} resolution, possibility to use far-IR synchrotron radiation in the coming years
  - Special interest in the bending modes of carbon chains
- Gerard Meijer & Gert von Helden - FOM Institute (NL)
  - Laboratory capabilities: tunable IR and far-IR laser, FELIX, from 40 cm^{-1} upwards
  - Experience, interests: IR-laser induced depletion of van der Waals complexes, IR spectra of gas-phase PAHs,...
- Louis d'Hendecourt (IAS - Orsay - France)
- Louis Allamandola (NASA Ames, CA, USA)
- Willem Schutte (Sackler Laboratory, Leiden)
  - Laboratory capabilities: These groups have an FTS IR-FIR spectrometer and use rare-gas matrix isolation spectroscopy for studies at low temperatures.
  - Experience, interests: spectroscopy of PAHs and ices.
- Dieter Gerlich (Chemnitz, Germany) http://www.tu-chemnitz.de/physik/ION/

2. Cross sections for rotationally inelastic collisions

   - Frank De Lucia (Ohio State University - USA)
     - Laboratory capabilities: collisional cooling cell, millimeter wave pump/probe set-up for time resolved measurements of inelastic cross-sections at very low temperatures.

3. Reactive cross sections

   - Bertrand Rowe, Christiane Rebrion-Rowe (Rennes University, France)
   - Ian Smith, Ian Sims (Birmingham University, UK)
     - Both groups use the CRESU method to measure the rates of neutral-neutral reactions, ion-molecule reactions, electron attachment and energy transfer (in particular in collisions) at very low temperatures.
   - Mats Larsson (Manne Siegbahn Laboratory, Stockholm, Sweden)
     - Laboratory capabilities: storage rings, studies of dissociative recombination at very low temperatures involving molecular ions of mass 2-75 a.m.u.

- Christine Joblin (CESR - Toulouse - France), Pierre Boissel (LCP - Orsay - France)
  - Laboratory capabilities: Ionic Cyclotronic Resonance cells to study the photophysics and chemistry of ionized large molecules, molecular complexes, agregates,... in physical conditions that approach those of the interstellar medium: ultra-high vacuum and very low temperatures.
  - Possible studies: photostability of the trapped species, radiative recombination, gas-grains interactions, ...
  - Special interest in large carbonaceous molecules and in particular in PAHs.

8.3 Catalogues

- JPL spectral line catalogue http://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html
- NIST database (F. Lovas compilation) http://physics.nist.gov
- Compilation by J. Crovisier http://wwwusr.obspm.fr/˜crovisie/basemole/
- ”Microwave Catalog” Universitat Ulm, Germany (annual compilation of spectroscopic data starts 1945)
- Microwave Spectroscopy Information Letter rbohn@uconnvm.uconn.edu
- Cologne Database for Molecular Spectroscopy
  http://www.ph1.uni-koeln.de/vorhersagen/index.html
- HITRAN (atmospheric IR CD ROM Commercial) 1996 Edition
- GEISA, ATMOS (atmospheric IR data)

8.4 Plans and difficulties

Planning of laboratory studies: For spectral surveys, laboratory data can come after the observations for a precise identification of the observed lines. When dedicated line studies are performed, spectroscopic laboratory data are required to prepare the observations. In any case, laboratory experimentalists will require detailed guidelines from the astronomical community on, for example, the molecules of interest.

Funding difficulties: laboratory experiments will require at least operating budgets but also may required new equipment. This is also true for catalogues and databases (cf. difficulties experienced by the JPL catalogue). Funding solutions should be found. For the French commmunity, there is a Research National Programme called PCMI: Physique et Chimie du Milieu Interstellaire for physics and chemistry of the interstellar medium. This programme has supported preparatory work for the ISO mission and is likely to do the same for the Herschel mission. Other possibilities have to be explored.

Chapter 9

Laboratory studies on cosmic dust

The main goal of laboratory experiments focused on the simulation of cosmic dust is to investigate the relations between intrinsic (i.e., structure, morphology, chemistry) and observable (e.g., optical behaviour) properties of materials. The experiments are targeted to produce, by different techniques, samples which may represent cosmic dust. Furthermore, in order to properly determine the properties of materials in different space environments, laboratory activities are also dedicated to explore the efficiency of various processes to modify the nature and optical characteristics of samples. Coherent programs are, therefore, based on iterative sequences in which dust is analysed both as-produced and after processing.

9.1 Experimental techniques

9.1.1 Materials

According to a variety of astronomical observations, typical materials of interest are:

- Carbons, in different forms (pure or hydrogenated, crystalline or amorphous)
- Silicates (crystalline or amorphous) of two main classes
  - Olivines: $(\mathrm{Mg}_x, \mathrm{Fe}_{1-x})_2\mathrm{SiO}_4$, where forsterite has $x = 1$ and fayalite $x = 0$.
  - Pyroxenes: $\mathrm{Mg}x,\mathrm{Fe}_{1-x}\mathrm{SiO}_3$, where enstatite has $x = 1$ and ferrosilite $x = 0$.
- Molecular ices consisting of a variety of simple molecules (e.g., H_2O, CO, CO_2, CH_3OH, ...) at low temperatures.

9.1.2 Production techniques

Several production techniques are used in laboratory to synthesise samples useful to simulate cosmic compounds:

- Arc discharge between carbon/graphite electrodes in inert (Ar, He) or H_2 atmosphere, resistive heating of graphite rods coupled with molecular beam extraction, IR laser pyrolysis of gas phase molecular species, quenching of hydrocarbon plasmic gas in vacuum are typical condensation techniques used for carbon-based material production.
- High power laser bombardment of bulk targets in inert or H_2 or O_2 atmosphere is applicable to obtain both carbon- and silicon-based materials.
- Silicate grains are also produced by chemical reactions in gas phase or grinding of natural minerals.
- Molecular ices are generally vapor deposited from pre-mixed or co-deposited bulbs onto sample substrates which are held at a low temperature within a cryostat.

Table 9.1: Astronomically relevant processes

Process	Dose		Units
	Space	Laboratory	
UV irradiation	3×10^{25} diffuse ISM in 10^9 yr 4×10^{20} dense ISM in 10^9 yr	4×10^{22}	eV cm^{-2}
Ion bombardment	3×10^3 diffuse ISM in 10^9 yr 3×10^2 dense ISM in 10^9 yr 1×10^6 pre-comet 6×10^2 comet	660	eV mol^{-1}
H atoms	8×10^{21}	7×10^{19}	cm^{-2}
Thermal	1000 stellar outflows 50-1000 planetary disks depending on location 5-50 ISM	1300	K

9.1.3 Processing

An important step of laboratory experiments is to study the effects produced on the properties of samples by processes which are expected to be active in space. Of course, laboratory experiments become meaningful for space applications when doses and rates applied in laboratory simulations are comparable to those typical of different space environments. The most relevant agents, with typical doses/rates expected in space and levels achieved in laboratory simulations, are reported in Table 9.1.

9.1.4 Sample characterization

At each step of production and/or processing, dust samples must be characterised by different techniques in order to investigate the properties obtained by tuning production parameters and/or applying the processes listed above. The most useful and commonly used techniques are reported in Table 9.2, with the relevant information derived. Spectroscopy, in particular, is a diagnostic method that explores different properties of materials depending on the used wavelength range. In fact: the spectral behaviour/features in the ultraviolet and far-infrared ranges probe characteristics linked to the structure of materials, while the near/medium infrared spectra presents mainly the fingerprints of molecular vibration modes (e.g., C-H bonds in hydrogenated carbon compounds and ices and Si-O stretching and bending modes in silicates). Moreover, various methods can be used for spectroscopic analyses: transmission, absorption, scattering, emission, which probe different characteristics of grains, including size and shape distribution.

Dust produced by the condensation methods mentioned above usually occurs as clumps of grains whose mean size may vary between 10 and 100 nm. The size can be tuned, to some extent, by the gas pressure inside the condensation chamber. Some experimental techniques result in the deposition of films.

9.2 Laboratory groups

As mentioned above, various groups have been very active in the recent years in the field of "laboratory astrophysics", with specific concern to the dust simulations. In the following, some of the most relevant results are reported, also with the aim to give an inventory of teams operating on the subject.

9.2.1 Carbonaceous materials

For carbon-based materials, various efforts have been concentrated to produce grains of different hydrogenation degree, with the aim to reproduce infrared bands observed in different interstellar environments. Much of that was achieved either through the choice of an appropriate parent material from which the grain was formed or through subsequent processing with atomic hydrogen beams often in the presence of FUV photons.

Table 9.2: Laboratory analysis techniques

Technique	Information
Scanning electron microscopy (SEM)	3-D aggregation, surface status, grain shape and size
Transmission electron microscopy (TEM)	2-D grain distribution, internal structure
Electron diffraction	degree of crystallinity
X-ray diffraction	Crystal structure
Energy dispersive X-ray analysis (EDX)	Elemental distribution
UV spectroscopy	Electronic transitions
Visible spectroscopy	Optical band gap
IR spectroscopy	Vibrational modes
Far-IR spectroscopy	Structure
Raman spectroscopy	Structure
Electron energy loss spectroscopy (EELS)	Electronic properties

- The group operating at Saclay (CEA-Saclay, Gif-Sur-Yvette Cedex, France) applied laser pyrolysis of hydrocarbons to produce hydrogenated carbon grains characterised by strong C-H stretching and bending bands in the medium infrared.

- The team of Jena (University of Jena, Astrophysical Institute and University Observatory, Germany) extracted single grains from molecular beams and trapped them in argon matrix for spectroscopic investigation.

- The group at Waterloo in Canada has used laser ablation of graphite in the presence of hydrogen to study hydrogenated amorphous carbon materials.

- The group operating in Naples (Astronomical Observatory of Capodimonte, and Parthenope University, Naples) has focused attention on evolution of carbon materials, produced by arc discharge or laser bombardment of graphite/amorphous carbon targets and subject to different processes: thermal annealing, UV irradiation, and ion bombardment. Recently, the treatments have also included hydrogen atom bombardment of pure carbon grains and UV irradiation of grains coated by different ice mantles, to simulate some of the most important gas-dust interaction processes in the interstellar medium.

These studies demonstrate the extreme sensitivity of characteristics of carbon-based grains to the physical conditions during formation and subsequent processing.

9.2.2 Silicate materials

For silicates, laboratory experiments have reached a high degree of reliability, especially with regard to the production of compounds with desired metal (e.g., Mg, Fe) content. Recent experiments are moving towards the same approach followed for carbonaceous materials, i.e., the study of their evolution due to thermal processing and ion bombardment. Among the groups active in this field are:

- the Astrochemistry Branch, NASA Goddard Space Flight Center

- the Astronomical Observatory of Capodimonte, Naples, Italy

- the University of Jena, Germany

- the Institute d'Astrophysique Spatiale (Orsay), France

- Kyoto Pharmaceutical University, Yamashina-ku, Kyoto, Japan.

Because astronomical observations have shown that the amorphous-to-crystalline transition in silicates is of main interest, laboratory experiments have focused on crystallisation through thermal annealing of amorphous silicates and amorphitization of crystalline silicates through ion-bombardment.

9.2.3 Molecular ices

Studies on molecular ices have concentrated on the IR properties of specific species, either in pure films or in more component mixtures. Generally, spectra are recorded over the relevant temperature range, from about 10 K to the evaporation temperature of the ice to follow the changing interaction between molecules as ices anneal. Processing of ices by FUV photons and by ion-bombardment is considered to be of relevance. Groups in

- Leiden
- NASA Ames
- the Institute d'Astrophysique de Spatiale
- Catania
- NASA Goddard

are active in this field. The former three focus on processing of ices by FUV photons while the latter two concentrate on the effects cause by ion bombardment or a combination of both. The structure of interstellar ices has been probed using transmission electron microscope during the annealing and chlathrate formation processes.

9.3 Far-IR and submillimeter absorption properties of interstellar dust

The study of cosmic dust analogues at wavelengths longer than 50 μm is a specific task, within the program of analysing the properties of materials in laboratory. Generally speaking, two aspects characterise the spectral properties of dust in the far infrared (FIR): discrete absorption bands and general spectral index. At present, this characterisation is incomplete and several questions are still subject of laboratory investigation.

Bands are observed in the FIR for silicates and molecular ices, while carbon materials are generally featureless. Experimental studies on various kinds of silicates have been performed in Italy, Germany, and Japan. Bands above about 50 μm are weak, in general, but still evident. They are mostly due to various kinds of translational modes. The phonon modes of ices occur at long wavelengths. However, at present, there is no systematic study of astrophysically relevant materials.

One of the most important characteristics of grains in the FIR is the featureless spectral trend of the absorption coefficient: $\kappa\,(\nu) = \kappa_o\,\lambda^{-\beta}$. The spectral index, β, may depend on several factors, such as structure (crystalline, amorphous), electronic properties (conductor, dielectric) and morphology (size, particle clustering). Moreover, it is sensitive to temperature.

Specific studies to compare the FIR spectral dependence on crystalline degree of carbon and silicate compounds have been performed by teams in Japan and Italy. The common feature of obtained results is that crystalline materials have a steeper behaviour with respect to amorphous counterparts; e.g., various kinds of amorphous carbons show β in the range $0.6 - 1.3$ (probably depending on detailed micro-crystallinity), while β for graphite ranges from 1.8 to 2.75. Similarly, β increases from $\simeq$1.3 to 2 when going from amorphous to crystalline fayalite. To interpret such behaviour the electronic properties of materials must be accounted for. Without going into details for crystalline silicates the spectral index reflects the tail of the last IR band. For amorphous compounds, selection rules break down, activating a larger number of modes and resulting in flatter spectral indices. For carbons, the spectral index is related to the so-called "aromatic coherence length". Graphite particles are metallic in nature and the behaviour $\sim\,\lambda^{-2}$ is due mainly to the presence of free electrons. Theoretical studies have shown that, besides crystal structure, the far-IR behavior of grains is also influenced by clustering of small grains into larger fractal units. This aspect has not yet been investigated experimentally.

The dependence of the spectral properties on temperature has to be considered when interpreting far-IR astronomical observations. Various groups have studied the temperature dependence of silicate and carbonaceous materials in the laboratory. In all cases the bands falling in the medium-far IR show a shift toward shorter wavelengths, an enhancement of the peak absorption and a decrease of the band width as the temperature varies from room values to 20 - 4 K as a result of the reduction of the interatomic distance and of the damping constant at low temperature. The FIR index, β, generally increases with decreasing temperature. The effect is observed both in silicates and in carbons, and is more marked for crystalline materials. At very low temperatures (< 10 K), the spectral index, β, starts to decrease again.

9.4 Future perspectives

This overview illustrates that laboratories are fully equipped to produce and characterise different kinds of astronomically relevant materials and that great progress has occurred in the recent years. However, the optical characteristics in the far-IR range as a function of the intrinsic dust properties have not been fully explored. Future experiments must address the characteristics (e.g., peak position and band width) of typical features falling at $\lambda > 50$ μm and their dependence on production and processing (thermal annealing, in the first place) conditions. The spectral index, β, of the FIR extinction must also be studied in more detail in order to clarify how intrinsic properties of materials (e.g., crystalline status on macro- and micro-scale, detailed chemical composition, grain agglomeration, size and shape) affect the behaviour. The range of examined materials must be extended to include species and mixtures of materials that have not been studied so far and may have a relevance as cosmic dust analogues.

Very important information is contained in far-IR astronomical observations, such as dust mass and temperature of circumstellar and interstellar regions, dust mass-loss rate from evolved stars surrounded by dusty envelopes, contribution of various phases of the interstellar medium to the total emission from galaxies, and the contribution of diffuse dust emission to the observed cosmic background. To take full advantage of the far-IR observations which will become available with Herschel will require detailed knowledge of the properties of interstellar dust and an intimate interaction with laboratory groups actively involved in this area.

Chapter 10

Molecular excitation studies

One top priority, collisional rates, is essential for the interpretation of excitation conditions and the determination of chemical abundances, which are major goals for Herschel and specifically HIFI studies of the ISM and stars.

What will be needed are high quality experimental or theoretical values of collisional excitation rates of various key molecules by H, He and molecular hydrogen at temperatures ranging from about 10K up to 2,000K or so. This goal requires concerted efforts of the scientific community involved in chemical and collision physics.

10.1 Experimental aspects

Experimentally determined inelastic cross sections mostly cover a limited range of states and transitions and hence have limited use for spectral line modeling. However, the laboratory data is essential to calibrate and validate theoretical cross section calculations. Very few experimental setups are dedicated to direct collisional excitation studies. To my knowledge, some experiments have been performed in Nijmegen on the OH - H_2, NH_3 - H_2 and NH_3 - He systems at room temperatures. There are some recent attemps with the CRESU system to get such information. Results have been obtained in Rennes on fine structure excitation and the Birmingham group intends to work on HCN excitation. Indirect information on collisional excitation is available in line broadening or Raman scattering experiments. Such data are valuable since they allow to test the validity of theoretical treatments (see below). Most recent results concern CO - H_2, NO - He, H_2S - He, HCO^+ - He, and H_2CO-He and H_2 (cf., Table 10.2).

10.2 Theoretical aspects

Close-coupling calculations are the best technique to achieve accurate calculations of excitation studies. The collision theory of non reactive collisions is well established since the first semi-classical studies and quantal theory assessments. A useful summary of the theoretical aspects and achievements performed until 1990 is available in D. Flower's book (Molecular collisions in the Interstellar Medium, Cambridge University Press). The standard technique involves the expansion of the total wave function of the system in the vibrational × rotational basis sets of the colliding species and a partial wave expansion (in sperical harmonics) for the angular part of the collision coordinate. This leads to as set of coupled second order differential equations for the radial functions labelled by the asymptotic basis and the partial waves. The coupling, which vanishes asymptotically, is due to the intermolecular potential. Truncation of the infinite asymptotic basis sets (generally on an energy criterium) leads to the close-coupling method. The S-matrix is obtained by matching the resulting radial functions at large distances to those which would have been obtained in the absence of an electronic potential. It is generally advantageous to transform the asymptotic basis sets to a representation involving the total angular momentum and a definite parity. Experimental observables (differential and integral cross sections, line broadening and shifts, depolarization cross sections) are expressed in terms of S-matrix elements for a particular velocity and relative energy. Once the cross sections are obtained, a Maxwellian average has to be performed to get the excitation (or de-excitation) rate coefficients or line broadening parameters as functions of the kinetic temperature T.

Table 10.1: Intermolecular Potential

System	Reference
H_2, HD - H	Boothroyd A.I., Keogh W.J., Martin P.G. and Peterson M.R., 1996, JCP 104, 7139
H_2, HD - He	Muchnik & Russek 1994, JCP 100, 4336
H_2, HD - H_2	Schwenke 1988, JCP 89, 2076
CO - H	Keller et al. 1996, JCP 105, 4983
CO - He	Heijmen et al. 1997, JCP 107, 9921
CO - H_2	Jankowski & Szalewicz 1998, JCP 108, 3554
OH - He	Degli Esposti, Berning, Werner, 1995, JCP 103, 2067
OH - H_2	Offer & van Hemert, 1993, JCP 99, 3836
O_2 - He	Bohn, 2000, PRA 62, 032701-1
CO_2 - He	Korona et al. 2001, JCP 115, 3074
H_2O - H_2	Phillips T. et al., 1994, JCP 101, 5824
H_2O - H	Wu, G.S., et al. 2000, JCP 113, 3150
C_2H_2 - He	Moszynski et al. 1995, JCP 112, 8385
NH_3 - He	van der Sanden, Wormer & van der Avoird, 1996, JCP 105, 3079
CH_3OH - He	Pottage, Flower & Davis, 2001, J. Phys. B. 34, 1

10.2.1 Intermolecular potentials

The availability of appropriate intermolecular potentials is critical for achieving scattering calculations. Table 10.1 gives the available intermolecular potentials relevant for collisional excitation since 1990.

10.2.2 quantal close coupling calculation

There are a number of programs for collision cross section calculations available from the internet.

- **MOLSCAT** The latest version of the code, which was written by J. Hutson and S. Green (1994) is available on : **http://www.giss.nasa.gov/molscat/** There is a detailed documentation and examples. Different cases may be treated:

  1. Atom - linear rigid rotor scattering
  2. Atom - vibrating diatom scattering
  3. linear rigid rotor - linear rigid rotor scattering
  4. Asymmetric top - linear molecule scattering
  5. Atom - symmetric top scattering
  6. Atom - asymmetric top scattering
  7. Atom - corrugated surface diffractive scattering

  Different levels of approximation may be implemented when close coupling calculations become prohibitive in computing time, such as effective potential approximation, the coupled states (centrifugal sudden) approximation, decoupled l-dominant approximation and infinite order sudden approximation. There are also different algorithms proposed to solve the differential second order coupled equations.

- **MOLCOL**

  This code treats quantum non-reactive scattering of atoms and diatomics and has been written by Flower and collaborators (Flower, Bourhis & Launay, 2000, CPC 131, 187). it is available on : **http://massey.dur.ac.uk/drf/molcol/CPC**

- **HIBRIDON** This code has been written by M. Alexander and coworkers (D. E. Manolopoulos and M. H. Alexander, J. Chem. Phys. 97, 2527 (1992); M. H. Alexander, C. Rist, and D. E. Manolopoulos, J. Chem. Phys. 97, 4836 (1992). Quantum inelastic scattering of open shell diatoms, photodissociation, collisions of atoms and/or molecules with flat surfaces, and bound states of weakly-bound complexes

can be treated. It is available on
http://www.chem.umd.edu/physical/alexander/hibridon

Since the codes are described as "users friendly", it could appear straightforward to derive collisional cross-sections once intermolecular potentials are available. There are, however, some caveats when performing scattering calculations.

- **Interatomic potentials**
  These should be introduced with an analytical expansion obtained from ab-initio results. Particularly critical is the matching between long range expansion and the short range results. It is also worthwhile to care about units and symmetry axis. Note that the MOLSCAT code allows to introduce numerical values of the intermolecular potentials via the so-called VRTP procedure.

- **Dynamic calculations**

  1. It is important to test the convergence of the S matrix elements (number of steps, values of R_{min} and R_{max} for the starting and last point to propagate the wavefunction) for one value of J, the total angular momentum.
  2. Convergence of the cross sections as a function of the total angular momentum
  3. Energy grid of the calculations (resonances)
  4. Convergence of the Maxwellian average for high energies. It is generally necessary to integrate the Maxwellian average up to an energy about 10 times kT where T is the kinetic temperature.

It may be advantageous to combine quantal and semi-classical treatments for the high energy calculations.

10.3 Recent results on collisional calculations of astrophysical interest

Many of the molecular data of interest for modeling of astrophysical line radiation are not easily accessible. The Herschel mission would be a good opportunity to set up a platform, probably in the form of a web page, collecting and comparing the available data. A first step would be to go over the list of interstellar molecules and make an inventory of existing computations & measurements. Table 10.2 of this document could serve as the starting point.

10.3.1 Rotational excitation of dipolar molecules and molecular ions by electrons

The fractional ionization is typically of the order of 10^{-4} in diffuse and translucent clouds and much smaller in dense dark clouds. However, electrons may become efficient in rotationally exciting dipolar molecules, such as CN and molecular ions due to strong electrostatic interactions. Rotational excitation of CN by electrons has been studied by Takayanagi K. and Itikawa Y. , 1968, PASJ 20, 376 and by Crawford O.H., Allison A.D. and Dalgarno A., 1969, A&A 2, 451. Rotational excitation of molecular ions by electrons has been studied by Neufeld D.A. and Dalgarno A.,1989, Ph. Rev. A 40, 633 in the frame of the Coulomb-Born approximation where the rates are dependent on the Einstein A coefficient of the transition. The group of University College London headed by J. Tennyson, has reconsidered the problem via R-matrix calculations. They show that the simple Coulomb-Born approximation should be used with care. The present results concern linear molecular ions only. They intend to extend their methods to other symmetries (H_3^+, ...)

10.4 Ortho/para conversion

The ortho-para conversion is of great interest, particularly for water and molecular hydrogen. Because the conversion rates are slow, they would make for excellent clocks, if they were well-understood. In particular, if one knew the rate of conversion from a low-temperature ortho-para equilibrium, to a high-temperature equilibrium, one would be able to judge the length of time since the respective materials had been at very

Table 10.2: Collisonal excitation calculations

System	Comment	Reference
H_2 - H	rotational excitation; CC	Flower D.R., 1997, J. Phys. B 30, 3009
H_2 - H	rotational excitation; CC	Forrey et al., 1997, ApJ 489, 1000
H_2 - H	rovibrational excitation; CC	Flower D.R. & Roueff E., 1998, J. Phys. B 31, 1105
HD - H	pure rotational excitation; CC	Roueff E. & Flower D.R., 1999, MNRAS 305, 353
H_2 - He	rovibrational excitation; CC	Flower D.R., Roueff E., Zeippen C.J., 1998 J. Phys. B 31, 1105
H_2 - He	rovibrational excitation; CC CC + quasi-classical trajectories	Balakrishnan et al., 1999, ApJ 524, 1122
HD - He	pure rotational excitation; CC	Roueff E. & Zeippen C.J., 1999, A&A 343, 1005
HD - He	rovibrational excitation; CC	Roueff E. & Zeippen C.J., 2000, A&AS 142, 475
H_2 - H_2	rotational excitation; CC	Flower D.R., 1997, MNRAS 288, 627
H_2 - H_2	vibrational relaxation with rotationally excited H_2; CC	Flower D.R., 2000, J. Phys. B. 33, L193
HD - H and HD - H_2	rovibrational excitation; CC with para-H_2	Flower & Roueff, 1999, MNRAS 309, 833
CO - H		work in progress
CO - He	vibrational quenching	Balakrishnan, Dalgarno, Forrey, 2000, JCP 113, 621
CO - H_2	29 levels for para H_2 and 20 levels for ortho H_2; CC	Flower , 2001, J. Phys. B34, 2731
CO - H_2		Mengel M., De Lucia F.C., Herbst E. 2001 Can. J. Phys. 79, 589
OH - He	CC; only some specific energies considered	Degli Esposti, Berning, Werner, 1995, JCP 103, 2067
OH - H_2	CC with Hyperfine structure	Offer, van Hemert, van Dishoeck 1994, JCP 100, 362
O_2 - He	CC; for ultra cold collisions	Bohn, 2000, PRA 62, 032701-1
HCO^+ - He		Flower, 1999, MNRAS 305, 651
HCO^+ - H_2		Flower, 1999, MNRAS 305, 651
H_2O - He	$20 \text{ K} \leq T \leq 2000 \text{ K}$ CC	Green S., Maluendes S., McLean A.D., 1993, ApJS 85, 181
H_2O - H_2	$20 \text{ K} \leq T \leq 140 \text{K}$ for para and ortho H_2	Phillips T.R., Maluendes S., Green S., 1996, ApJS 107, 467
C_2 - H_2	para and ortho H_2 is considered	Phillips T., 1994, MNRAS 271, 827
OCS - He	rotational excitation at low T; CC	Flower D.R., 2001, MNRAS 328, 147
NH_3 - He	only some transitions	van der Sanden, Wormer & van der Avoird, 1996, JCP 105, 3079
SiC_2 - H_2		Chandra S., Kegel W.H 2000, A&A 142, 113
C_3H_2 - H_2		Chandra S., Kegel W.H 2000, A&A 142, 113
CH_3OH - He	CS approximation, no torsional quantum number	Pottage, Flower & Davis, 2001, J. Phys. B. 34, 1

Table 10.3: Collisional excitation by electrons

System	Comment	Reference
CH^+ - e		Lim, Rabadan & Tennyson, 1999, MNRAS 306, 473
CO^+ - e		Faure & Tennyson, 2001, MNRAS 325, 443
HCO^+ - e		same paper
NO^+ - e		same paper
$H_2{}^+$ - e		same paper
HeH^+ - e^-		Rabadan I., Sarpal B.K., Tennyson J. 1998, MNRAS 299, 171

low temperature. Unfortunately there is very little theoretical work available, and laboratory studies would be particularly welcome, both in the gas phase as well as on solid surfaces and, perhaps with some added paramagnetic impurities, likely to be found in nature.

10.5 priority objectives

10.5.1 Accuracy assessment

The evaluation of the needs in the context of the Herschel mission should concern not only the systems to study but also the temperature range to consider, the particularly important transitions and the required accuracy. This problem is connected with the radiative transfer group. Accuracy tests of the available data for both potential energy surfaces and cross sections can be obtained from spectroscopy studies and depend consequently on the spectroscopy group. Links to available data and the possibility of retrieving them via the web have been evocated.

10.5.2 Choice of systems

The water molecule is the most important target for these calculations because of its critical role as a tracer of ISM conditions and for the unique opportunity Herschel has to observe many transitions of H_2O. Previous calculations focused on the fewest rotational lines of H_2O up to kinetic temperatures of 140K. However, we will require many more J states and kinetic temperatures up to 2,000K or so. M.L. Dubernet has begun to tackle the problem and P. Valiron and colleagues are willing to test the accuracy of the corresponding potential surface and to compute its vibrational dependance. Other potentially interesting systems are HCN laser transitions at high J and vibrational states, methanol, formaldehyde, HC_3N, CH , and OH (this list is not intended to be complete).

Finally, we should not neglect the potential importance of torsionally excited species (expected in hot cores).

Collisional excitation of complex deuterated molecules is often assumed to be identical to the main species. This is certainly not true since some symmetry properties may become broken. Then it would also be highly desirable to consider such cases which do not require supplementary ab-initio quantum mechanical studies.

Chapter 11

Preparatory observations

11.1 Inventory of observational opportunities

We live in the best of times when observational opportunities abound. This is particularly true for the infrared and submillimeter where a number of telescopes and missions are nearing completion while ever more ambitious projects are on the drawing boards. These include:

11.1.1 Space-based and Airborne missions

- The Submillimeter Wave Astronomy Satellite (SWAS) is the first submillimeter telescope -(about 60 cm mirror) in space observing the galaxy in five spectral lines of CI, H_2O, CO, and O_2.

- ODIN is a 1.1 m telescope which was recently launched by the Swedish Space Corporation. Odin has five heterodyne receivers on board which for part of the time observe the heavens in various atomic and molecular transitions of astrophysical interest including CI, $H_2^{18}O$, H_2O, O_2, CS, ^{13}CO, H_2CO, SO, and SO_2.

- The Space InfraRed Telescope Facility (SIRTF) will fly three instruments - a mid IR camera (3.6, 4.5, 5.8, and 8.0 μm), a far-IR camera (24, 70, and 160 μm) with low resolution spectroscopic capabilities, and a spectrometer (5-40 μm $R = 150$ and 10–38 μm $R = 600$). SIRTF is projected to be launched in January 2003.

- The Stratospheric Observatory for Infrared Astronomy (SOFIA) is a USA-German mission to fly a 2.5 m telescope on board of a Boeing 747-SP operating at some 40000 feet with a varied complement of instruments spanning the full infrared and submillimeter range. First flights are expected in 2005.

- ASTRO-F (Also known as IRIS, InfraRed Imaging Surveyor) is dedicated to infrared sky survey with a much better sensitivity than IRAS. It has a 70cm telescope cooled to 6 K, and carries two focal plane instruments. The Far Infrared Surveyor (FIS) will survey the entire sky in the wavelength range from 50 to 200 μm with angular resolution of $30 - 50$ arcsec. The InfraRed Camera (IRC) will take deep images of selected sky regions in the near and mid infrared range. The field of view is 10 arcmin with a spatial resolution of approximately 2 arcsec. This mission is scheduled to be launched in February 2004. http://www.ir.isas.ac.jp/ASTRO-F/index-e.html

- Next Generation Space Telescope (NGST) is a 6 m class passively cooled telescope with near– and mid–infrared cameras and spectrometers. This NASA project with contributions from ESA is slotted to fly in 2010.

- H2ex A proposed space mission dedicated to study the mid infrared lines of molecular hydrogen. The mission is not approved yet but more data on H_2 would be very useful for different aspects of Herschel science.

- The Russian space project on the ISS : Submillimetron The schedule is uncertain but this project will probably come after Herschel.

- There are also a number of balloon borne experiments. BLAST, a long duration balloon experiment, will fly a 2m-class mirror with large format bolometer arrays at 350, 450 and 750 microns, taking advantage of the (SPIRE) technology being developed for Herschel. Flying an upgraded Development Model of HIFI before the launch of Herschel is also a possibility. ELISA from CESR and Archeops from IAS/Grenoble (http://archeops01.free.fr/main_archeops/) are still under study, but are planned to be launched before Herschel. These Balloon experiments are supposed to test the technology and to help planning Planck and Herschel.

SWAS was designed to study the chemical composition of interstellar gas clouds. It discovered the ubiquitous presence of water in regions of star-formation. However, in contrast to theoretical predictions H_2O is not very abundant in dark clouds. Likewise, SWAS has put stringent upper limits on the abundance of O_2 in the ISM.

Odin will be able to address the issue of the gaseous oxygen budget in the ISM further. A full-scale attack on this problem will, however, have to await the high sensitivity and small beam of Herschel.

The observational plans for SIRTF are of much relevance for Herschel. In particular, besides guaranteed time observations, a large fraction of the time is allocated to six legacy programs. These programs are designed to maximize the scientific utility of SIRTF by yielding an early and long-lasting scientific heritage. The raw and pipeline-processed SIRTF data will enter the public domain immediately following processing and validation at the SSC. Among the legacy programs are deep extragalactic surveys, surveys of nearby galaxies, and studies of star and planet formation - all subjects which are at the core of Herschel science.

SOFIA will be very complementary to and, in some ways, competitive with Herschel. In the far infrared and submillimeter, the instrumentation is similar. Of course, Herschel has the advantage of the stability of a space-based facility and at airborne altitudes SOFIA observations still suffers from telluric absorption which completely blocks portions of the spectrum. Because it is passively-cooled and has a slightly larger mirror, Herschel will win sensitivity-wise and has the advantage of higher observing efficiency (some 7000 hours versus 900 hours per year) during its operational phase. Of course SOFIA has a larger operational life time (20 years versus 3 years) and it is more versatile and has a wider wavelength coverage. Moreover, several generations of new instrumentation can be developed and flown over SOFIA's lifetime. Both of these points make it an ideal follow-up observatory where new Herschel results can be further interrogated. Herschel holds of course the advantage for deep surveys in the spectral or spatial domain.

11.1.2 Ground–based observatories

The following ground-based observatories are also very relevant,

- Ground-based observations in the near-IR and optical windows have really opened up with the new class of 6–8 m telescopes (Keck, VLT, Gemini, Magellan, Subaru, ...).

- Ground-based observations in the submillimeter are possible using a variety of single dish telescopes (JCMT, CSO, IRAM 30 m, SEST, FCRAO, KOSMA, Mt Fuji, Nanten, Nobeyama, HHT). Many of these have heterodyne instruments and bolometer arrays for the telluric windows.

- Ground-based observations in the submillimeter can use existing interferometers. These include BIMA (10 6-m dishes), NMA (6 10-m dishes), OVRO (6 10-m dishes), PdBI (6 15-m dishes), and the SMA (8 6-m dishes).

- Future single dish telescopes include the Large Millimeter Telescope (LMT), the German Atacama Pathfinder EXperiment (APEX) and the Japanese Atacama Submillimeter Telescope (ASTE) which are precursor facilities designed to test telescopes and instrumentation at the ALMA Chajnantor site in Chili.

- ALMA – an interferometer consisting of 64 telescopes on a high, dry site in the Andes – will become operational over the timeframe 2007-2010. This interferometer will revolutionize the field of submillimeter astronomy in terms of sensitivity and spatial resolution at submillimeter wavelengths.

The BIMA and OVRO (sub)millimeter interferometers will be combined with the SZ Array (8 3.5-m dishes) into one array, CARMA, at Juniper Flat, California. OVRO will move in 2003, BIMA in 2004, and full operations will start in 2005.

11.2 Preparatory observational needs

Because the far-IR/sub-millimeter sky has never been truly surveyed, Herschel will be in some sense its own discovery mission. From that perspective, the Herschel mission can really benefit from preparatory ground-based or space based studies in related windows. Pathfinder and ancillary programs for Herschel still have to be prioritized but a number of key preparatory observations can be identified.

In particular, three classes of prepatory observations will be extremely important both in guiding the mission planning and optimum observing strategies as well as in preparing the expected science: 1) Spatial surveys of classes of objects whether they be dark cloud cores and embedded protostars or high-z extragalactic objects. The SIRTF legacy programs may be of particular relevance for this; 2) Spectral surveys in telluric windows with single dish telescopes of a number of key objects to estimate the expected level of spectral detail and the level at which the spectral confusion limit is reached. In this respect, the high frequency windows are largely unexplored; and 3) Detailed studies of template sources, ranging from individual protostars to whole galaxies.

It may prove to be difficult to convince Time Allocation Committees to approve proposals with a heavy Herschel preparatory science angle. Time is generally of the essence in the discussions of TACs, including observing time as well as publication time. The long term aspects of timely preparation for space missions is of secondary importance. It may well be very advantageous for the three instruments to cooperate on convincing observatory directors to make observing time available to Herschel preparatory survey projects. This worked well for SIRTF which convinced NOAO to allocate supporting observing time to successfull legacy teams.

In general, Herschel will have to make aggressive use of SIRTF and SOFIA and of ground based sub-millimeter telescopes on Mauna Kea and in Chili for preparatory observations. Here cooperation between the different instruments may prove to be valuable as well. For follow up observations on Herschel scientific discoveries, ALMA, NGST, and SOFIA will be indispensable.

11.2.1 Preparatory studies for line surveys

Molecular line surveys will be a key tool for HIFI.

Molecular line surveys are performed by very few people, consequently there are very few specific resources available. Fortunately, there is very little which is line survey specific, many of the things needed however do overlap with other study areas, in particular the model/analysis tools and laboratory studies areas. In the following we make a short inventory of what is needed, and what the current status is.

<u>DSB deconvolution</u>: A MEM algorithm exists and has successfully been employed on the CSO 650 and 850 GHz surveys. In its current implementation (as part of the XCLASS program, a superset of CLASS) it is actively further developed at the MPIfR in Bonn. It is unclear if it will ever be used in its present form for HIFI data reduction, but the principle could easily be ported to another software package. This hinges on what kind of data reduction is envisioned for HIFI.

To have a quantitative idea of the potential problems (ghosts, accuracy of reconstruction), and of the optimum observing strategy (i.e. how many tunings per bandwidth) simulations are necessary, including simulations of observations of extended sources with chemical inhomogeneities and pointing errors. Such simulations are planned in the framework of a PhD thesis in Bonn (Claudia Comito).

The algorithm will also be tested with real world data, such as the existing CSO surveys. It would also be advisible to take a few dedicated data sets with varying parameters (frequency spacings) to check on the simulations. This could be done e.g. at the CSO, since it possesses DSB receivers.

<u>Model Fitting</u>: An LTE fitting code linked to the JPL catalog does exist in XCLASS, it is being worked on and improved in Bonn. We are not aware of similar activities elsewhere. This fitting takes care of line blendings and, under certain conditions, can deal with optical depth problems. A whole line survey is fitted at once, which is the only way to deal with the flood of line survey data HIFI will produce. A logical next step will be to link it to data cubes of LVG models for specific molecules, in order to get first order NLTE corrections in, and to determine densities and temperatures. This also will be part of Claudia Comitos PhD thesis in Bonn. Ideally, one would then go on and link it to more sophisticated Monte Carlo or ALI models to determine the structure. This would have to be looked at once a ”standard” sophisticated radiative transfer model is available. These efforts might be severely limited by the non-availability of collision rates for many molecules, particularly complex ones.

We want to stress again that a good molecular data base (frequencies, line strengths, collision rates) is mandatory for this enterprise.

Appendix A

Various Databases and websites

A.1 Herschel and its instruments

http://sci.esa.int/home/herschel/index.cfm
http://pacs.mpe-garching.mpg.de/
http://www.astro.cf.ac.uk/groups/instrumentation/projects/spire/index.html
http://www.sron.nl/divisions/lea/hifi/index.html

A.2 Radiative Transfer

http://www.strw.leidenuniv.nl/~radtrans
http://www.mpifr-bonn.mpg.de/staff/fvandertak/ratran/frames.html

A.3 Collisional cross-sections

http://BASECOL.obs-besancon.fr/BASECOL (preliminary)
http://www.giss.nasa.gov/data/mcrates/
http://www.giss.nasa.gov/molscat/
http://massey.dur.ac.uk/drf/molcol/CPC
http://www.chem.umd.edu/physical/alexander/hibridon

A.4 Photo-cross sections and rate-coefficients

http://www.space.swri.edu/amop/
Hübner, Link & Mukherjee (SWRI)
Hübner et al. 1992, Astrophys. Space Science 195, 1

A.5 Ion reactions data base

http://astrochem.jpl.nasa.gov/asch/
Anicich 1993, APJS 84, 215

A.6 Line catalogues

http://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html
http://physics.nist.gov
http://wwwusr.obspm.fr/~crovisie/basemole/
http://www.ph1.uni-koeln.de/vorhersagen/index.html

A.7 Dust radiative transfer

http://www.pa.uky.edu/~moshe/dusty/
http://www.astro.uni-jena.de/Group/Subgroups/Theory/theo.html
http://www.strw.leidenuniv.nl/~lab/

A.8 NIST

http://www.nist.gov/srd/thermo.htm
Thermochemical Databases

- NIST Critically Selected Stability Constants of Metal Complexes PC product
- NIST Molten Salts PC product
- NIST Chemistry WebBook Free online system
- Polycyclic Aromatic Hydrocarbon Structure Index Free online system
- Electron Interactions with Plasma Processing Gases Free online system
- NIST/TRC Table Database PC product
- NIST/TRC Vapor Pressure Database PC product
- http://physics.nist.gov/PhysRefData/micro/html/contents.html
  NIST Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1991 Revision
- http://physics.nist.gov/Pubs/Mono115/contents.html
  The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules
  Jon T. Hougen
- http://kinetics.nist.gov/index.php
  Kinetic database on line
- http://www.nist.gov/srd/nist17.htm

A.9 Center for Astrophysics (CfA)

http://cfa-www.harvard.edu/amdata/ampdata/amdata.shtml
Databases maintained by CfA:

- Kurucz Atomic Linelist: data from Kurucz CD-ROM 23
- European Server (Click on #5 Kurucz-Data) Kurucz CD-ROM 18
- other Kurucz data (maintained by R. L. Kurucz)
- R.L. Kelly: Atomic and Ionic UV/VUV Linelist
- CfA Molecular Data: VUV cross sections, energy levels and wavelengths (ASCII files)
- HITRAN molecular spectroscopy database
- SAO Molecular Line Database for Aeronomy 10 cm^{-1} to 800 cm^{-1}

A.10 Varia

http://www.uni-ulm.de/strudo/mogadoc/index.html
MOGADOC (Molecular Gasphase Documentation) Vogt et al. 1999, J. Mol. Struct. 485, 249
http://diref.uwaterloo.ca/
P.F. Bernath and S. McLeod, “DiRef, A Database of References Associated with the Spectra of Diatomic Molecules”, J. Mol. Spectrosc., 207, 287 (2001)

A.11 Chemistry

UMIST database: http://saturn.phy.umist.ac.uk:8000/

Other chemistry links:

- http://chemfinder.cambridgesoft.com/
- http://www.chemieonline.de/
- http://www.liv.ac.uk/Chemistry/Links/links.html
- http://www.webelements.com/
- http://www.liv.ac.uk/Chemistry/Links/verti_fr.html
- http://www.liv.ac.uk/Chemistry/Links/softwarecomp.html

Appendix B

Acknowledgments

The workshop on "Preparatory science for the Herschel Space Observatory" was held at the Leiden Lorentz Center, October 22-24, 2001. This workshop was organized in order to reap the full benefits of the Herschel mission and to guide development efforts and instrument characteristics. It had a dual purpose: first, to bring the needs of the Herschel mission to the attention of a wide (interested) science community and, second, to arrive at a "workplan" to address the most important of these needs/issues. This white paper contains the recommendations of this workshop. We want to express our deep gratitude to Göran Pilbratt, Albrecht Poglitz, Tanya Lim, Ewine van Dishoeck, Thomas Henning, Christine Joblin, Luigi Colangeli, Peter Schilke and Evelyne Roueff who wrote chapters for this white paper and to all the participants for the critical discussion during the workshop and their comments on an earlier version of this draft.

There were 52 participants representing 10 countries. The format was informal with ample time for discussion. Summaries of all the talks are available through the web at the Lorentz site (http://www.lc.leidenuniv.nl). Overall, this was a very successfull meeting, largely because of the setting at the Lorentz center which with its multiple meeting rooms and separate offices allows a variety of simultaneous splinter meetings ranging in size from 10's of people to one-on-one.

This workshop has been made possible through generous travel grants by ESA and NASA and through financial support by the Dutch Space Agency, SRON, the Dutch Astronomy organization, NOVA, and the Lorentz Center. Last but not least, we want to take this opportunity to thank the Lorentz center for their dedicated and professionel effort in organizing this workshop. Over the years, we have organized some dozen workshops. It has never been as easy as at the Lorentz center.

Frank Helmich
Xander Tielens

Appendix C

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Appendix D

Scientific Program

Time	Speaker	Title
	MONDAY 22 October 2001	
Session I	THE HERSCHEL MISSION	
09:00–09:30		Coffee and Registration
09:30–09:40		Welcome and logistics
09:40–10:00	Goeran Pilbratt	The Herschel mission
10:00–10:30	Thijs de Graauw	Prepatory science and the HIFI instrument
10:30–11:00	COFFEE	
11:00–11:30	Albrecht Poglitsch	Prepatory science and the PACS instrument
11:30–12:00	Tanya Lim	Prepatory science and the SPIRE instrument
12:00–12:30		General discussion
12:30–01:30	LUNCH	
Session II	LABORATORY SPECTROSCOPY	
01:30–02:00	Christine Joblin	Overview of laboratory spectroscopy opportunities
02:00–02:20	John Pearson	Spectral catalogues
02:20–02:40	Thomas Giesen	High resolution spectroscopy in the Terahertz region
02:40–03:10	TEA	
03:10–03:30	Dieter Gerlich	Laser induced reactions in low temperature traps: Spectroscopy and collision dynamics
03:30–03:50	Michel vervloet	THz Spectroscopy
03:50–04:30		General discussion

The times listed include time for discussion.

Time	Speaker	Title
	TUESDAY	
Session III	OBSERVATIONAL STUDIES	
09:00–09:30	Geoff Blake	Overview of observational opportunities
09:30-9:50	Juergen Stutzki	SOFIA
09:50–10:10	Martin Harwit	Prepatory studies: the SWAS experience
10:10–10:40	COFFEE	
10:40–11:00	Dieter Lutz	Extragalactic prepatory studies
11:00–11:20	Maryvonne Gerin	Calibration and prepatory science
11:20-12:00		Discussion
12:00–01:30	LUNCH	
Session IV	DUST STUDIES	
01:30–02:00	Luigi Colangeli	Overview of laboratory dust studies
02:00–02:20	Gert von Helden	Cluster studies
02:20–02:50		Discussion
02:50–03:20	TEA	
03:20–03:50	Thomas Henning	Overview of SED studies
03:50–04:10	Rens Waters	Disk models
04:10–04:40		Discussion
Session V	MOLECULAR EXCITATION STUDIES	
04:40–05:10	Evelyne Roueff	Overview of molecular excitation studies
05:10–05:30	Pierre Valiron	Floppy molecules
05:30–05:45	Marie-Lise Dubernet	Excitation of H_2O
05:30–06:00		Discussion
07:00		DINNER at Anuk Bandung

The times listed include time for discussion.

Time	Speaker	Title
	WEDNESDAY	
Session VI	SPECTRAL LINE MODELLING STUDIES	
09:00–09:30	Ewine van Dishoeck	Overview of spectral line modeling
09:30–09:50	Jeremy Yates	ALI radiative transfer methods
09:50–10:10	Marco Spaans	Monte Carlo methods
10:10–10:30		Discussion
10:30–11:00	COFFEE	
Session VII	SUMMARY	
11:00–11:30	Martin Harwit	Road map
11:30–12:00		Discussion and reports
12:30–01:30	LUNCH	

The times listed include time for discussion.