

Herschel and the Molecular Universe

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ABSTRACT

Over the next decade, space-based missions will open up the universe to high spatial and spectral resolution studies at infrared and submillimeter wavelengths. This will allow us to study, in much greater detail, the composition and the origin and evolution of molecules in space. Moreover, molecular transitions in these spectral ranges provide a sensitive probe of the dynamics and the physical and chemical conditions in a wide range of objects at scales ranging from budding planetary systems to galactic and extragalactic sizes. Hence, these missions provide us with the tools to study key astrophysical and astrochemical processes involved in the formation and evolution of planets, stars, and galaxies. These new missions can be expected to lead to the detection of many thousands of new spectral features. 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 supported by laboratory measurements and theoretical studies of chemical reactions and collisional excitation rates on species of astrophysical relevance. These data will have to be made easily accessible to the scientific community through web-based data archives. In this paper, we will review the Herschel mission and its expected impact on our understanding of the molecular universe.

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Europe has recognized the challenge in analyzing and interpreting the multitude of data that will become available and has started a closely knit but wide ranging scientific network in the area of molecular astrophysics. This “Molecular Universe” network combines 21 institutes in 9 countries and is funded through the Marie Curie program of the European Union. The network will support training of some 15-20 young graduate students and postdocs. The scientific emphasis of the network will be on a deeply interwoven research program on molecular complexity in space and chemistry in regions of star formation. The results of this network will be made widely available through data bases and web interfaces. This network will be described in some detail and the challenges of research in this highly interdisciplinary research area will be discussed.

1. Herschel

The Herschel Space Observatory (Originally called Far InfraRed and Submillimeter Telescope (FIRST)), the European Space Agency’s 4th cornerstone mission, is designed for observations in the far-infrared/sub-millimeter wavelength region. Herschel is equipped with a 3.5 meter diameter reflecting telescope and instruments cooled to close to absolute zero. Herschel will be launched together with Planck on an Ariane 5 with an expected launch date of mid-2008. After a four-month journey from Earth, Herschel will spend a nominal mission lifetime of three years in orbit around the second Lagrange point of the Sun-Earth system (L2). The ESA Science Center is located at ESTEC Noordwijk, The Netherlands (<http://www.rssd.esa.int/herschel>). NASA is a minor partner providing hardware for HIFI (mixers and local oscillator chains for bands 5 and 6) and SPIRE (spider web detectors) as well as software support. The US Herschel Science Center is located at IPAC, Caltech (<http://www.ipac.caltech.edu/Herschel/>). Details on the Herschel mission are provided in Pilbratt (2004).

Herschel has three instruments, HIFI, PACS and SPIRE, which cover the $\sim 60-600 \mu\text{m}$ with imaging and medium-to-high resolution spectroscopy capabilities. These instruments are optimized to address key questions in astronomy: “the origin and evolution of galaxies in the early universe”, “the origin and evolution of stars and their interaction with the interstellar medium”, and “the composition and evolution of the molecular universe”. Many of the key objects and evolutionary stages of the universe – including protostars, protoplanetary systems, dying stars and their ejecta, and starburst and massive black hole activity in the centers of galactic nuclei – are hidden from view by copious amounts of cold dust and gas. Most of the energy emitted by these objects escapes therefore in the far-infrared and sub-millimeter spectral windows. Conversely, this implies that Herschel will provide a unique handle on the physical and chemical conditions and the processes taking place in these environments.

1.1. HIFI

The Heterodyne Instrument for the Far-Infrared (HIFI) is a high resolution heterodyne spectrometer with 6 bands covering almost completely the 150 to 600 μm range. The mixer bands use SIS (Superconductor-Insulator-Superconductor) mixers in bands 1-5 and HEB (Hot Electron Bolometer) mixers in band 6. Instantaneous Intermediate Frequency bandwidth is 4 GHz in Bands 1-5 and 2.4 GHz in Band 6. The resolving power can be as high as $\nu/\Delta\nu = 10^7$ or 0.3 km/s. Specifically, two available backends, the wide band spectrometer (dual acousto-optical) and the high resolution spectrometer (autocorrelator), provide frequency resolutions of 140 kHz, 280 kHz, and 1 MHz. HIFI is being designed by a large consortium spread over 13 countries led by Thijs de Graauw, SRON Groningen, The Netherlands. Details on HIFI and its science program can be found in de Graauw et al. (2004).

Table 1: HIFI characteristics

Band	1	2	3	4	5	6
Frequency coverage	480-640	640-800	800-960	960-1120	1120-1250	1410-1910
FWHM [arcsec]	41	29	25	21	18.5	14.5, 12.5
Sensitivity ^a [10^{-18} W m ⁻²]	1.3	2.9	4.9	8.1	24	34

^a[5σ in 1 hr at $R = 10^4$]

1.2. PACS

The Photodetector Array Camera and Spectrometer (PACS) is a bolometer array photometer and a photoconductor array imaging spectrometer operating at a wavelength range between 60 and 210 μm . The characteristics of the three band imaging photometer are summarized in Table 2. Observations are made simultaneously in two bands: the 170 μm band and either the 75 or 110 μm band. The two filled bolometer arrays consist of 32×16 (red) and 64×32 (blue) pixels covering the same field of view (1.75×3.5 arc minutes). The point source detection limit is approximately 3 mJy (5σ in 1 hr).

In addition, PACS has an integral field spectrometer which covers simultaneously the spectral bands from 57 to 105 and 105 to 210 μm . The $47'' \times 47''$ field of view (5×5 pixel array) is rearranged via an image slicer on two 16×25 stressed Ge:Ga detector arrays. The spectral resolution is ~ 1500 and the line sensitivity is $\sim 5 \times 10^{-18}$ W m⁻² 5σ in 1 hr. PACS is being designed and built by a consortium of institutes and university departments from across Europe under the leadership of Principal Investigator Albrecht Poglitsch located at

Table 2: PACS imaging characteristics

Central wavelength [μm]	75	110	170
Band range [μm]	60-85	85-130	130-210
FWHM [arcsec]	6	8	12
Spectral resolution, $\lambda/\Delta\lambda$	2.5	2.8	2.1

Note. — Observations are simultaneously in two bands: the red band (170 μm) and either of the two blue bands (75/110 μm).

Max-Planck-Institute for Extraterrestrial Physics (MPE), Garching, Germany. Details on PACS and its science program can be found in Poglitsch et al. (2004).

1.3. SPIRE

The Spectral and Photometric Imaging Receiver (SPIRE) consists of a 3-band imaging photometer and a Imaging Fourier Transform Spectrometer and will operate at wavelengths between 200 and 670 μm . The imaging photometer array on SPIRE consists of hexagonally packed spider-web bolometer arrays, which observe simultaneously in three bands (Table 3). The field of view is 4×8 arc minutes but requires jiggling or scanning for full spatial coverage. The point source sensitivity is ~ 3.5 mJy 5σ in 1 hr.

Table 3: SPIRE imaging characteristics

Central wavelength [μm]	250	360	520
FWHM [arcsec]	18	25	36
Spectral resolution, $\lambda/\Delta\lambda$	~ 3	~ 3.2	~ 3

Note. — Observations are simultaneously in three bands.

The Fourier Transform Spectrometer has a field of view of 2.6 arc minutes diameter. The two bolometer arrays cover 200-325 and 315-670 μm with 37 and 19 hexagonally close-packed detector arrays, respectively. The FWHM will vary between approximately 20 to 25 and 30 to 50 " in the short wavelength and long wavelength band, respectively. The spectral resolution can be adjusted between 0.04 and 2 cm^{-1} , corresponding to a resolution of 1000 to 20 at 200 μm . SPIRE is being developed by a consortium of European and American institutes, led by Matt Griffin at the Physics and Astronomy Department of Cardiff University. Details on

SPIRE and its science program can be found in Griffin et al. (2004).

1.4. The Herschel science program

About 7000 hours of science time will be available per year. About one-third of the total observing time is reserved for the consortia which build the three instruments. The other two-third is open to the world-wide science community. While Herschel builds upon the legacy of the Infrared Astronomical Satellite (IRAS), the Infrared Space Observatory (ISO) and the Spitzer Space Telescope in the far-infrared, the sub-millimeter sky is largely unexplored and hence Herschel is often called *its own precursor mission*. To accommodate this sub-millimeter survey aspect, a considerable portion of the total science time ($> 50\%$) on Herschel is envisioned to be part of large scale coherent programs, so-called Key Programs. These Key Programs should exploit unique Herschel capabilities to address (an) important scientific issue(s) in a comprehensive manner, require a large amount of observing time to be used in a uniform and coherent fashion, and produce a resulting, well-characterized dataset of high archival value. Indeed, much of the instrument teams guaranteed time is expected to be devoted to Key Programs. The large format arrays of PACS and SPIRE are designed for sensitive large scale mapping programs and the PACS and SPIRE guaranteed time Key Programs are centered on large scale, unbiased surveys of the high redshift universe and of star forming regions. For HIFI, the guaranteed time Key Programs focus on unbiased spectral surveys of the molecular universe and on studies of the many rotational transitions of water. In addition, many open time Key Programs are also expected. These Key programs will be selected before launch – first, the guaranteed time and then the open time. After launch and the science verification phase, a call for normal (guaranteed time followed by open time) programs will be issued.

2. HIFI preparatory science

Interpretation and analysis of the data obtained by the Herschel instruments will require careful science preparation. Requirements for preparatory science are summarized in the Herschel preparatory science white paper available at the links section of <http://www.sron.nl/hifiscience/>. Here, we will focus on the data required for HIFI. The unbiased spectral surveys – central to the HIFI Key Program – will return 1000's of spectral lines for selected sources while the water studies will bring line intensities of rotational transitions in broad samples of sources. The goal of these observations are to understand the physics and chemistry of these regions, including the physical conditions, dynamics, the molecular inventory, and the underlying chemical processes.

Molecular astrophysics is a highly interdisciplinary field of research as schematically illustrated in figure 1. The identification of species in space requires direct comparison of

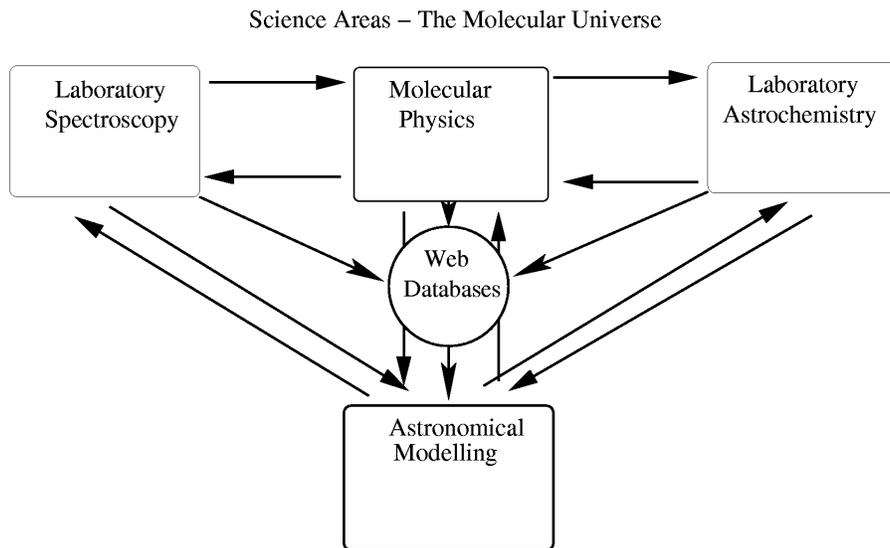


Fig. 1.— Schematic figure illustrating the multidisciplinary aspect of the field of molecular astrophysics. The four different science areas involved in molecular astrophysics are characterized by the use of different techniques and methods. In addition, the results of studies will have to be made available to the whole science community through data bases accessible through special webportals.

the particular frequencies of emission or absorption lines observed in interstellar space with spectroscopic measurements of known species in a controlled laboratory experiment. In order to interpret the measured laboratory spectra in terms of the properties of the molecule (ie., assign lines to specific transitions), supporting molecular physics quantum chemical calculations are required. The intensities of lines observed in space depend directly on the collisional excitation rates of the molecules with the predominant collision partners, atomic or molecular hydrogen and helium. These rates will have to be calculated using quantum chemical methods or measured in the laboratory by molecular physicists. Such rates can then be used by astronomers to determine the physical conditions and the abundances of the molecules involved in the interstellar regions where the emission or absorption arises. The abundances of interstellar molecules are the result of a balance between formation and destruction reactions. The rate coefficients and products of relevant reactions will have to be measured under astrophysically relevant conditions (eg., low temperature, low pressure) or quantum chemically calculated. These rates can then be used by astronomical modelers to calculate the abundances of interstellar species. For example, when specific reaction routes have been proposed and the relevant reaction rate coefficients measured, abundances of new species can be predicted. Laboratory spectroscopists can then measure their transition frequencies while molecular physicists can calculate their excitation rate coefficients. All of these data together can then be used by astronomical modelers to predict the expected line intensities of new species which can then be targeted in specific searches.

It is clear that action in all of these four science areas has to be strongly interwoven in studies of the molecular universe. However, in general, no single group, institute, or often even nation has expertise or experience in all relevant areas. Thus, support for the analysis and interpretation of space-based data requires large scale, global efforts involving many scientists at different institutes and in different countries collaborating together on interdisciplinary projects, each contributing only a subset of the solution. This requires a new structure for astronomy, resembling the structure in science areas such as particle physics where much of the research effort has, for decades, been organized in large scale projects connected to, for example, CERN.

The other challenging aspect is that, while these areas serve great needs for the astronomical community, research on frequencies or oscillator strength of molecular transitions is not forefront science within molecular physics. Likewise, chemical reactions involving astronomically relevant species is not central to modern chemistry. Funding support for activities in these areas is therefore not high priority within these communities. As a result, national space agencies will have to take the lead in organizing, coordinating, and funding these scientific activities.

2.1. The Molecular Universe

In Europe, the importance of a proper preparation for Herschel and ALMA in this area is well recognized and a consortium “The Molecular Universe” has been formed, consisting of 21 institutes in 9 European countries all active in various aspects of molecular astrophysics. The coordinator and co-coordinator of this consortium are Xander Tielens and Marie-Lise Dubernet. This consortium has been funded by the European Union as a Marie Curie Research and Training Network through the 6th Frame Work Program (FP6). More details on the network can be found at <http://molecular-universe.obspm.fr/>.

One main activity of the Molecular Universe network is to train the next generation of researchers in this field. The Marie Curie program provides specific support for this and the network has obligated itself to provide 444 person months of training. This will include training of 9 Early Stage Researcher (ESR; eg., graduate students) and 5 (joint) Experienced Researchers (ER; eg., postdocs). These researchers are spread over the different institutes involved in the network. In addition, through the liberal use of secondments, all students and postdocs will spend part of their training at other institutes where they will acquire complementary skills required for productive research in this field. The training is also supplemented by a yearly summerschool where the different science aspects of the field of molecular astrophysics are covered at a level suitable for such an interdisciplinary mix of young researchers. Finally, the students and postdocs are offered an opportunity to present their scientific research at network meetings and workshops.

The other main activity of the network centers on an active and deeply interwoven

research program. These are focussed in the area of molecular complexity in space – comprising studies on water in the universe, carbon chemistry, and deuterium chemistry – and of chemistry in regions of star formation – including ionization along the star formation trail, nitrogen chemistry as tracer of protostellar condensations, and molecular tracers of shocks. We will highlight two topics here. 1) Within the “water in the Universe” theme, a wide range of studies are coordinated on the physics and chemistry of H₂O in astrophysical environments, including spectroscopy of high excitation levels, theoretical ro-vibrational excitation cross sections, experimental excitation cross sections, the astrochemistry of H₂O, and radiative transfer models of H₂O in astrophysical environments. 2) Similarly, the “carbon chemistry” theme organizes a range of investigations on the physics and chemistry of hydrocarbons in astrophysical environments such as experimental studies of reaction rate coefficients of hydrocarbons, spectroscopy of PAHs and carbon chains, excitation models for PAHs and carbon chains, and astrochemistry of PAHs and carbon chains.

2.2. Data bases and web interfaces

A wide dissemination of the fundamental data acquired within this field to the wider astronomical community is of key importance to the success of the planned space missions. The best tool for this is provided by data bases made accessible through special web-interfaces. Data bases exist in all relevant areas. For spectroscopy there is the JPL data base (<http://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.html>), the Cologne data base (<http://www.ph1.unikoeln.de/vorhersagen/>), and the HITRAN data base at Harvard (<http://www.cfa.harvard.edu/HITRAN/>). In molecular physics, there are the data bases at Meudon (<http://amdpo.obspm.fr/basecol/>) and Goddard (<http://data.giss.nasa.gov/mcrates/>). Several astrochemistry databases exist, including UMIST (<http://www.udfa.net>), Ohio State (<http://www.physics.ohio-state.edu/~eric/research.html>), and SWRI (<http://amop.space.swri.edu>). The cassis group in Toulouse has developed special tools for fitting pure rotational spectra (http://www.cesr.fr/~walters/web_cassis/).

Despite this wide array of data bases, access by the community is still of great concern. First, the data that is included in these data bases require careful and critical evaluation and validation. Preferably, this validation should be delegated to a small board of experts in the field who are qualified to carefully balance any conflicting experimental measurements and/or calculations. Such evaluation structures have been set up already in related fields such as combustion chemistry research community (eg., the PrIme network). However, this requires man power and support and validation of data is presently generally not standard in these data bases. Second, many of these data base activities are performed as unheralded services to the community driven by personal conviction and commitment and are hardly or not supported by funding agencies. For example, the JPL spectroscopy data base has not been funded for several years, the Cologne data base has just lost its funding from the German equivalent of the national science foundation, the Goddard data base on molecular physics

has not been maintained since the untimely death of Sheldon Greene, and the astrochemistry data base at SWRI is no longer maintained after the retirement of Walter Huebner. Third, maintenance of data bases is not an area of growth – scientific growth, personal growth, or funding growth – and young scientists are not steered in this direction – and rightfully so ! The absence of funding, the loss of key scientists, and the lack of young influx threatens these endeavors right at the time when they are needed the most.

3. Conclusion

Analysis and interpretation of space missions require fundamental data on atomic, ionic and molecular species. Specifically, Spitzer, Herschel and SOFIA, as well as JWST need experimental and theoretical data on frequencies and oscillator strength of transitions of astrophysical relevance. This is a highly interdisciplinary field where physics and chemistry meet astronomy. The US has many researchers who are at the forefronts of these disciplines. However, typically, no single group or institute has the required expertise and experience to address all the relevant aspects and instead progress will have to come from large scale consortia where multiple partners bridge this gap. Astronomy will have to organize itself much like other branches of physics and chemistry have done earlier. NASA as well as other space agencies will have to take the lead in supporting such endeavors. Such funding support will also go a long way to convince young researchers to step into this field and provide these essential support studies. In addition, NASA and other agencies will have to start supporting efforts in the area of data bases and web interfaces. These will be key to make the results of such studies widely available to the astronomical “customer”. Only when these challenges are met, will we be able to reap the full science benefit of the large money and manpower investments in space projects.

Europe has recognized the importance of organization and collaboration in this multidisciplinary field and has started such a concerted effort funded by the European Union. The US has to quickly follow suit if its science community does not want to lag behind in this effort. Initial steps have been taken by a group centered around Ben McCall (University of Illinois, Urbana) and Eric Herbst (The Ohio State University) with additional centers at, among others, the University of Colorado, Boulder (V. Bierbaum), the University of Georgia (N. Adams), and the University of Toledo (S. Federman). Additional centers of expertise in the area of molecular astrophysics are located at University of Arizona (L. Ziurys), Caltech (G. Blake), and Harvard (P. Thaddeus). There are also very active groups at NASA Centers including NASA Ames Research Center (L. Allamandola; F. Salama), JPL (J. Pearson), and Goddard Space Flight Center (J. Nuth). Together, these groups cover all the relevant expertise in molecular astrophysics. Compared to the total costs of NASA science missions, a modest investment of funding by NASA – covering joint students and postdocs as well as the networking aspects – will be able to crosslink the scientific efforts of these different groups and mold an integrated science area to the benefit of space sciences. This is a clear

case where the whole will be more than the sum of the parts.

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