

Spectroscopy with the Herschel Space Observatory

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Abstract — Submillimeter astronomy from space offers many advantages, due to completely avoiding the attenuations and noise from the Earth’s atmosphere. For spectroscopy in the 60 to 670 micron range, the Herschel Space Observatory offers important new capabilities in terms of angular resolution, sensitivity, and over much of this range, for high spectral resolution observations. Herschel builds on the success of two earlier space missions devoted to submillimeter spectroscopy: SWAS and Odin. In this paper, I briefly highlight the results from those missions. I then discuss the capabilities of the three instruments on the Herschel Space Observatory, known by their acronyms HIFI, SPIRE, and PACS, focusing on spectroscopic observations. I conclude with a short summary of some of the astrophysical highlights that may be anticipated when Herschel is operational, which should be about 6 months after launch, currently scheduled for September 2008.

Index Terms — submillimeter spectroscopy, far-infrared spectroscopy, spectrometers

I. THE EARTH’S ATMOSPHERE

The submillimeter spectral range may be defined as the decade in wavelength shortwards of 1mm, thus covering the range of 1000 μm to 100 μm . This is also referred to by some as the far-infrared, although that term generally includes wavelengths as short as a few tens of microns. The primary impediment to astronomy in the 1000 μm to 100 μm wavelength region, whether referred to as the submillimeter or far-infrared, is the earth’s atmosphere. Both in terms of the absorption, and also due to variability and inhomogeneities, the atmosphere is a real obstacle. Water vapor is the primary culprit, and only at the highest, driest sites is the amount of water low enough to provide reasonable transmission at the most favorable wavelengths. These “atmospheric windows” fall between strong rotational transitions of the water molecule, but at frequencies near the transition frequencies themselves, the atmosphere remains opaque even from airplane altitudes. This situation, shown in Figure 1, means that while good astronomy can be done in submillimeter windows, to get good coverage **throughout** the submillimeter range, one has to go into space.

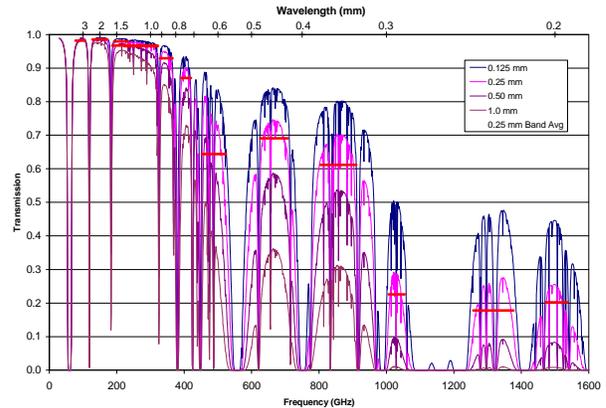


Figure 1 – Atmospheric transmission at millimeter and submillimeter wavelengths for different values of atmospheric precipitable water vapor. The different ALMA bands are indicated by the horizontal lines. The spectral regions with essentially zero transmission coincide with strong rotational transitions of H₂O, with the exception of the ranges blocked by the O₂ lines near 60 GHz and that obscured by the single line near 118 GHz.

Submillimeter astronomy can be done from the ground, but this does require a high altitude site. Until the present, this has primarily meant Mauna Kea, in Hawaii, where the Caltech Submillimeter Observatory (CSO), James Clerk Maxwell Telescope (JCMT), and the Submillimeter Array (SMA) are located. There is a growing movement to utilize the high Chajnantor plateau in northern Chile, where the APEX, RLT, Nanten, and ASTE telescopes are sited, where the Atacama Large Millimeter Array (ALMA) is under construction, and where the Cornell Caltech Atacama Telescope (CCAT) will be located. Getting above most of the water vapor has been possible with airborne telescopes, notably the Kuiper Airborne Observatory (KAO), and the Stratospheric Observatory for Infrared Astronomy (SOFIA) which should be operational in a few years. Many of these instruments are described in other talks in this conference, and the best additional sources of information about their capabilities are their respective web sites.

II. SUBMILLIMETER ASTRONOMY FROM SPACE – THE PATHFINDER MISSIONS: SWAS & ODIN

Submillimeter astronomy from space offers the following important advantages:

- access to the full spectral range, which is essential to obtain an unbiased inventory of molecules in astronomical sources and to determine the spectral energy distribution (SED) of dust in cool molecular clouds;
- ability to observe key species totally blocked by the earth's atmosphere, notably H_2O and O_2 ;
- superior calibration accuracy due to the absence of large and variable atmospheric attenuation;
- lower noise due to absence of short-term atmospheric fluctuations, particularly important for broadband (continuum) observations;
- better system stability due to the absence of atmosphere and also diurnal local temperature variations.

The above considerations were key factors in the decision to develop two previous missions dedicated to high resolution submillimeter spectroscopy. Other space missions, including the Infrared Space Observatory (ISO) and the Infrared Astronomy Satellite (IRAS) observed in the short wavelength portion of the submillimeter. ISO had moderate resolution spectrometers, while IRAS did not carry out spectroscopic observations. The Submillimeter Wave Astronomy Satellite – SWAS (NASA) and the Odin satellite (Swedish space agency together with other European space agencies) utilized heterodyne receivers with phase locked local oscillators and mixers, an IF amplifier chain, and acousto-optical and digital spectrometers for spectral analysis. As such, the signal path is very similar to that found in ground-based radio astronomy systems [1].

SWAS was a relatively simple system with few tuning adjustments. The front end had an ambient temperature calibration load, and a nutating secondary for rapid beam switching on the sky. However, most observations were carried out by position switching, that is, by repointing the entire spacecraft at 30s intervals, alternating between the “source” and “reference” positions. This was efficient due to the very rapid slewing and acquisition (using a star tracker) of the satellite resulting from its relatively large gyros and good control system (see Figure 2). The system stability was excellent, due to careful thermal design, and a number of very long integrations were carried out which achieved noise levels consistent with those expected from the radiometer equation and the noise temperature.

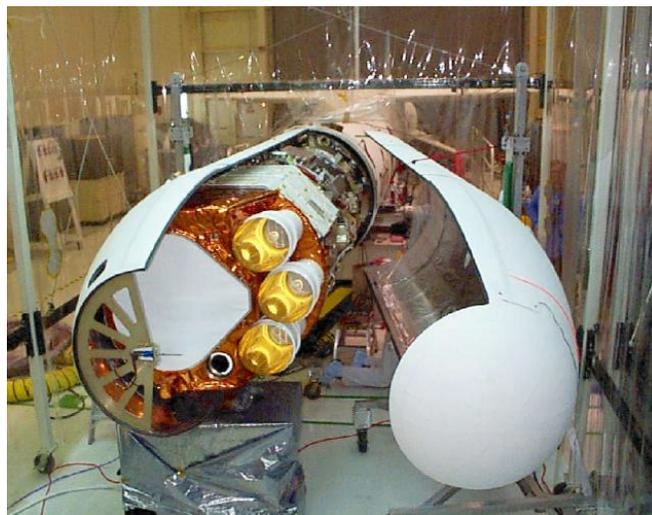


Figure 2 – SWAS spacecraft being readied for launch by Pegasus XL rocket. The woven teflon film covers the elliptical aperture on the left. Three Winston cone radiators which passively cool the front end to ~ 170 K are on the right, and the star tracker aperture is visible at lower middle.

The SWAS front end included two Schottky diode second harmonic mixer receivers operating in opposite linear polarizations. The local oscillator, which was essentially fixed tuned, was provided by frequency-tripled Gunn oscillators. The choice of IF and LO frequencies resulted in the 487.25 GHz $3_1 - 3_2$ transition of O_2 being in the lower sideband of receiver 1, and the $^3\text{P}_1 - ^3\text{P}_0$ 492.16 GHz transition of CI being in the upper sideband. For receiver 2, the 550.93 GHz transition of ^{13}CO was in the lower sideband, and the 556.94 GHz $1_{10} - 1_{01}$ transition of H_2O was in the upper sideband. The outputs from both receivers were frequency diplexed into an acousto-optical spectrometer which devoted 350 MHz bandwidth to each spectral line. By retuning the Gunn oscillator, receiver 2 could be configured to observe the H_2^{18}O isotopologue of water. The front end was passively cooled to ~ 170 K and system noise temperatures were 2200 – 2500 K DSB for the four primary lines of interest.

The SWAS satellite operated extremely well from its launch in December 1998 through July 2004 when it was put into hibernation. SWAS carried out large-scale surveys of neutral carbon (CI) and the $J = 5 - 4$ transition of ^{13}CO in many giant molecular clouds. These provided a great deal of information on their structure and density. But the greatest effort was spent observing the ground state transition of water, which of course cannot be observed from the ground. While H_2O can readily be detected in warm regions, its abundance relative to H_2 was found to be typically a factor of 100 below that predicted by models of interstellar chemistry. A collection of

the early scientific results from SWAS can be found in [2]. Along with this, the O_2 line was not detected, and the limits in a wide range of sources [3] showed that this species, which was anticipated to be a major reservoir of oxygen in dense interstellar clouds, was again a factor ~ 100 less abundant relative to H_2 than had been anticipated.

These SWAS results indicated that our ideas about chemistry in dense clouds would have to be modified. Naturally, there was some surprise and controversy about the low abundance of water and molecular oxygen. However, not long after SWAS results were published, the Odin satellite was launched. Odin was considerably more complex than SWAS having several different receivers, widely tunable local oscillators, and a digital autocorrelation spectrometer as well as an acousto-optical spectrometer [4]. Also, Odin's primary reflector was 1.1m in size compared to the 0.54×0.68 m elliptical primary mirror employed by SWAS, giving a smaller beam. The Odin satellite was designed to carry out observations of the earth's atmosphere as well as astronomy, and thus could look "down" as well as "up". The front end was cooled by a mechanical cooling system rather than by passive radiators as was SWAS. The latter system could thus not look towards the earth without dramatically upsetting the thermal balance of the receiver system.

Odin's results on water and molecular oxygen were largely consistent with those of SWAS. In particular, water lines were again found to be very weak, and the abundance of this species low. Odin confirmed this by observing the rare $H_2^{18}O$ isotopologue of water (Figure 3), and from this astronomers concluded that the fractional abundance of H_2O relative to H_2 is only $1-8 \times 10^{-8}$ [5]. One of the possible explanations is that oxygen atoms stick to dust grains, are then hydrogenated to water, which remains on the grain surfaces as water ice. The result is a deficiency of oxygen in the gas phase, and that which remains tends to be in the form of carbon monoxide, leading to much reduced abundances for other oxygen-containing species, notably water and molecular oxygen [6]. There are other competing theories including circulation of material between cloud edges and well-shielded interior. This is just one of the areas that will be addressed by the Herschel Space Observatory.

III. THE HERSCHEL SPACE OBSERVATORY

The Herschel Space Observatory (HSO) can be considered to be a second-generation submillimeter spectroscopy facility for astronomy. This does not mean that it can only do spectroscopy. In fact, two of its instruments together cover the entire $60 \mu\text{m}$ to $500 \mu\text{m}$ range for broadband photometry, using imaging arrays of detectors. The purpose of this paper is, however, to focus on the spectroscopic capabilities of

Herschel. General information about the satellite, as well as the capabilities of the three focal plane instruments can best be found on the web, at <http://herschel.esac.esa.int/> and <http://www.ipac.caltech.edu/Herschel/>.

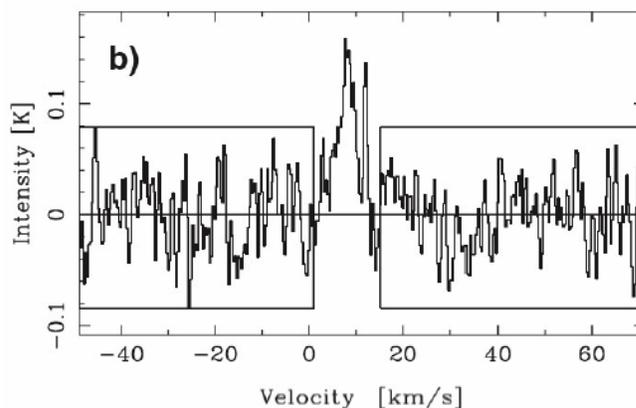


Figure 3 – Odin detection of $H_2^{18}O$ in Orion [5]. This very weak line confirms the low abundance of gas phase water in quiescent molecular clouds.

The HSO has a 3.5 m diameter primary reflector, which is passively cooled to ~ 70 K. This low temperature is made possible by the HSO's orbit – it will be near the L2 Lagrange point, 1.5 million km farther away from the sun than is the earth, along the line from the sun to the earth. This orbit gives good thermal stability as well as low thermal pickup from the earth. The instruments in the Herschel focal plane are cooled to 2 K by liquid helium, and some of the detectors are cooled to sub-Kelvin temperatures by additional refrigeration stages. Herschel is scheduled to be launched in September 2008 by an Ariane V rocket, which in a dual launch, will also take the Planck spacecraft into orbit.

Herschel has three focal plane instruments which operate as spectrometers. They are

HIFI: Heterodyne Instrument for the Far Infrared, a high resolution heterodyne spectrometer covering $157 \mu\text{m}$ to $212 \mu\text{m}$ and $240 \mu\text{m}$ to $625 \mu\text{m}$;

SPIRE: Spectral and Photometric Imaging Receiver, an imaging Fourier Transform spectrometer covering $200 \mu\text{m}$ to $670 \mu\text{m}$;

PACS: Photoconductive Array Camera and Spectrometer; grating spectrometer with image slicer covering $60 \mu\text{m}$ to $210 \mu\text{m}$.

This set of instruments is particularly interesting purely from the point of view of technology as they cover almost the complete gamut of existing technology in terms of detectors

and achieving spectral resolution. In the next sections, I will briefly discuss each of the three Herschel instruments.

A. HIFI

HIFI uses two mixers operating in orthogonal linear polarizations at each frequency. To cover the very large frequency range, there are 7 bands, and for each the local oscillator is divided into a high frequency and low frequency unit. The mixers in the five lowest frequency bands (480 – 1250 GHz) are Superconductor Insulator Superconductor (SIS) mixers and in the two highest frequency bands (1410 – 1910 GHz) are Hot Electron Bolometer (HEB) mixers. Providing a broadly tunable local oscillator was a major technical challenge for HIFI. It is realized by a chain starting with a relatively conventional frequency synthesizer at K-band, which is then frequency tripled to W-band. From there, different combinations of frequency doublers and frequency triplers multiply the frequency by factors between 6 and 24 to obtain the power required to pump the pair of mixers operating at the desired submillimeter frequency.

The IF from the SIS mixers is in the range 4 to 8 GHz, and that from the HEB mixers covers 2.4 to 4.8 GHz. The HIFI mixers are cooled to 2 K, and each mixer is followed by a low noise amplifier at a temperature of 15 K. Further amplification is followed by frequency conversion for the HEB channels, and the signals from the selected band are sent to the ambient temperature spectrometer subsystem.

Spectral analysis is carried out by two different subsystems. Each is doubled to provide independent analysis for each linear polarization. The wideband system (WBS), based on an acousto-optical spectrometer, first divides the signal into 4 1GHz-wide sub bands. These are sent to four Bragg cell transducers in a collimated laser beam. The diffracted energy is collected by a CCD readout which has 4 lines of detectors - one for each of the 4 sub bands. Each linear array provides 1000 pixels with 1 MHz nominal channel separation, and noise bandwidth slightly greater than 1 MHz. Thus, there is a total of 8000 spectral channels in the two polarizations from the wideband spectrometer system. At the highest HIFI frequency, the 2.4 GHz IF bandwidth corresponds to a velocity range of 380 km/s and the channel width corresponds to a velocity range of 0.16 km/s. At the lowest frequency, the 4 GHz IF bandwidth corresponds to 2500 km/s, and the resolution is 0.6 km/s. HIFI thus has a maximum fractional frequency coverage of 0.008, which is adequate for individual lines even in active galaxies. For line surveys, numerous

observations with different local oscillator settings will be required.

The velocity resolution of the wideband spectrometer is not quite adequate for observations of quiescent regions in the interstellar medium. To enable this science a high resolution narrow band system (NBS) based on a digital autocorrelation spectrometer, is included. The NBS can provide resolutions as fine as 0.125 MHz, corresponding to a maximum velocity resolution of 0.08 km/s. This high resolution data covers up to 235 MHz of frequency, which can be moved within the bandpass of the WBS, to examine a particular spectral line in more detail, for example. The NBS can also provide somewhat lower frequency resolution over bandwidths up to 500 MHz.

HIFI noise temperatures represent impressive progress, especially given that this is in a space-qualified system which has had to undergo rigorous testing and is capable of nearly autonomous operation. The double sideband (DSB) noise temperature for the SIS systems increases approximately linearly from 50 K at 480 GHz to 1000 K at 1250 GHz. These values are the average over the 4 GHz IF band. For the HEB mixers, noise temperatures are somewhat higher, but the primary variation is as a function of IF frequency rather than RF frequency: typical values are 1000 K and 2.4 GHz and 2000 K at 4.8 GHz IF frequency.

The HIFI system optics includes a chopper which can make the operating receiver look at one of two temperature-controlled absorbing loads for calibration. It can also switch the beam between two positions in the focal plane, which has the effect of introducing an angular offset of 3' for the beam on the sky. Each of the 7 HIFI bands points to a different position on the sky, and that only one band can be used at any one time. Thus, the telescope pointing must correct for the band that has been selected, while the data can be taken by moving the entire telescope between the "source" and "reference" position at a relatively slow rate, by rapid beam switching using the focal plane chopper, or by frequency switching. The actual performance of these various observing modes will be proven only during the verification phase once the satellite is on orbit. Additional HIFI information can be found in [7].

B SPIRE

The SPIRE instrument has largely separate sections for photometry and spectrometry. The most complete and up to date information can be found at <http://www.spire.rl.ac.uk/> and in [8]. SPIRE spectroscopy is based on the Fourier Transform Spectrometer (FTS). An input wavelength range is determined by an input filter, and power within this range is processed by a dual-beam interferometer, with the interferogram being taken over a selected path length difference. An off-line Fourier Transform of the interferogram yields the power spectrum of the input signal. This basic system has been used in many astronomical (and other) spectrometers, and has the advantage that the entire frequency range is analyzed simultaneously. Thus, at low resolution, this can be used to measure the spectral energy distribution (SED) of continuum emission from dust grains. At higher resolution, individual spectral lines can be observed.

A limitation of the FTS in the submillimeter is that the restricted path length difference (in cm) that can be achieved implies a maximum spectral resolution (in cm^{-1}). For SPIRE, the highest resolution of 0.04 cm^{-1} corresponds to a modest fractional resolution, as indicated in Figure 4. This resolution is adequate to obtain the integrated intensity in spectral lines, but only for external galaxies with relatively large line widths will any lines be resolved. Nevertheless, the fact that the entire bandpass is analyzed simultaneously makes SPIRE a powerful tool for diagnostics of galaxies, as well as for objects such as the giant planets in our solar system which have pressure broadened spectral lines.

An important advantage of the FTS is that a number of beams corresponding to different directions on the sky can propagate through the spectrometer simultaneously. In the case of the SPIRE FTS there are two detector arrays. For the short wavelength band covering $200 \mu\text{m}$ to $325 \mu\text{m}$, there are 37 detectors in a hexagonal close packed array. For the long wavelength band covering $315 \mu\text{m}$ to $670 \mu\text{m}$ there are 19 detectors. Each detector, which is a germanium spider web bolometer, is coupled to the telescope with an individual feed horn. The result is that the array samples essentially every other diffraction limited beam on the sky. The long wavelength horns are larger than those for the shorter wavelength band, and the two are arranged so that 13 of the beams look at the same direction in the sky in each band. This imaging capability obviously speeds up mapping of extended objects dramatically. Special techniques using the beam steering mirror included in SPIRE will be available to make fully Nyquist-sampled maps of modest size. Larger regions will be mapped by a combination of telescope pointing and scan mirror motion. Several of the projects already proposed for SPIRE involve spectral maps of extended regions in the Milky Way and other galaxies.

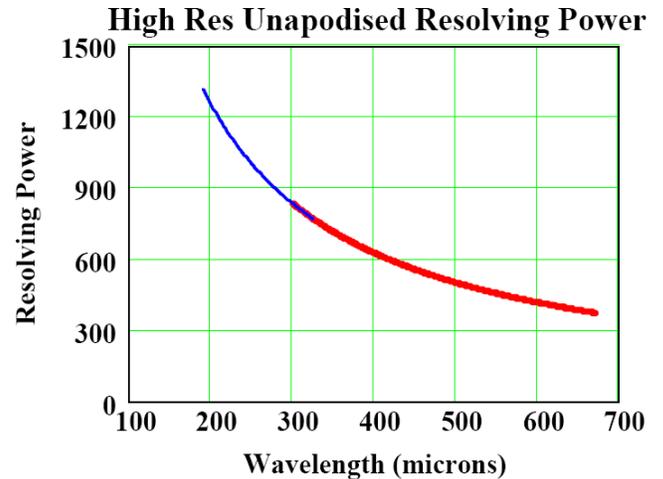


Figure 4. SPIRE resolving power ($\lambda/\Delta\lambda$) as a function of wavelength with highest spectral resolution.

The sensitivity of the SPIRE spectrometer system is fairly uniform as a function of wavelength. For an integration time of 1 hr, a 5σ limit is $\sim 3 \times 10^{-17} \text{ W m}^{-2}$ in units of integrated flux density.

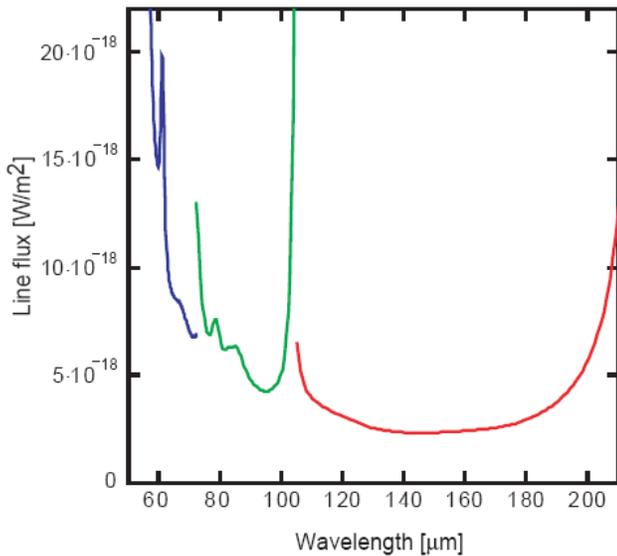
C. PACS

PACS, like SPIRE, has independent units for photometry and spectroscopy. They cover approximately the same wavelength range but use different types of detectors. Additional information about PACS can be found in [9] and at http://www.mpia.de/PACS/index_B.html. The PACS spectrometer is based on a diffraction grating. In this instrument, an image slicer takes a 5×5 array of $9.4''$ pixels on the sky and reimages them onto a 25 element line, which is effectively the input slit to the grating. The grating sends light in different directions according to wavelength, but it does this for each of the 25 spatial elements along the slit. The detector arrays have 16 spectral elements by 25 spatial elements. Each detector is a Ge:Ga bolometer, unstressed for shorter wavelengths and stressed for longer wavelengths. Since different wavelength ranges can be diffracted in different orders, one can observe in two wavelength ranges simultaneously. These are $65 - 85 \mu\text{m}$ and $130 \mu\text{m} - 210 \mu\text{m}$, or $85 \mu\text{m} - 130 \mu\text{m}$ and $130 \mu\text{m} - 210 \mu\text{m}$.

The resolution of the PACS spectrometer depends on wavelength (in part due to different orders being used in different ranges), varying from 3000-4000 at the short wavelength end to 1000-2000 at the longest wavelengths. These are high enough that some spectral lines in active regions, such as the Galactic Center, may be resolved, and

emission lines from nearby galaxies almost certainly will mostly be spectrally resolved.

PACS sensitivity varies considerably as a function of wavelength as shown in Figure 5. As is the case for SPIRE, PACS gains an impressive advantage in spectroscopy of



extended sources since 25 spatial pixels are observed

Figure 5. PACS sensitivity in terms of 5σ integrated line flux limit achievable in 1 hr integration. From [9].

simultaneously. At the relatively short PACS wavelengths, even though the spectrometer detector pixels correspond to a beam size larger than determined by diffraction, the $9.4''$ beams are quite small, and many interesting sources will definitely be spatially extended. Thus there are a number of mapping modes for exploiting PACS.

IV. HERSCHEL SCIENCE

Due to the large wavelength coverage, the greatly improved sensitivity compared to past submm missions, and the great variety of frequency resolution and types of observation that can be carried out, it is impossible to give fair treatment to all the astronomy that has already been proposed to be done with Herschel, and that likely will be carried out. I here give only a few selected highlights, focusing on the types of observations that can be carried out in the general category of “Herschel Spectroscopy.”

One of the key goals of Herschel spectroscopy is to study molecules in the interstellar medium, as well as in solar system objects and the atmospheres of evolved stars. Many

molecules have their rotational transitions in the millimeter and submillimeter regions. The most abundant of these is carbon monoxide, and the lowest rotational transitions are shown in Figure 6. While the lower transitions can be well studied from the ground at millimeter wavelengths, at the temperatures characteristic of star forming regions in the Milky Way and other galaxies, as well as in protoplanetary disks and the solar system, the strongest transitions will be in the submillimeter/far infrared, exactly the region covered by Herschel. As seen in Figure 6, the different Herschel instruments together cover CO transitions with upper level quantum number between 4 and 43. This wide range will allow extremely good use of CO as a diagnostic of physical conditions in a very wide range of environments, as well as being optimal to trace gas in regions with very different physical conditions.

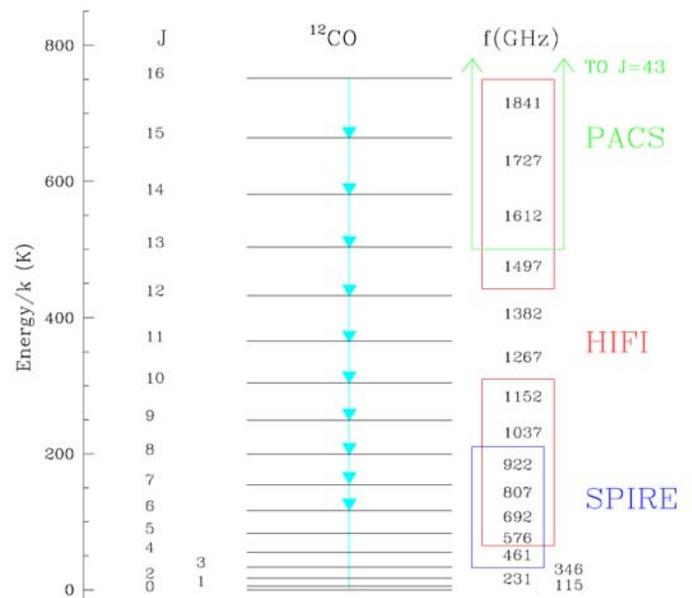


Figure 6. Lower rotational energy levels and transitions of the carbon monoxide molecule, with indication of which can be observed with which Herschel instrument.

Another target for Herschel spectroscopy will be fine structure lines – the transitions which arise from interaction of spin and orbital angular momentum in atoms. Two of the most important atomic species with submillimeter fine structure lines are carbon and oxygen. The term schemes along with key spectroscopic information are shown in Figure 7. Neutral carbon has been observed with some difficulty from the ground, but has also been studied using telescopes in stratospheric aircraft, and with the SWAS and Odin satellites. However, almost all of this work has been done on the lower frequency (492 GHz) transition, but both fine structure lines

will be observable with Herschel/HIFI. Observing the two transitions together will greatly increase our ability to disentangle optical depth and excitation effects, making possible a much more accurate determination of the CI abundance, which is a very important issue for modeling of molecular cloud structure.

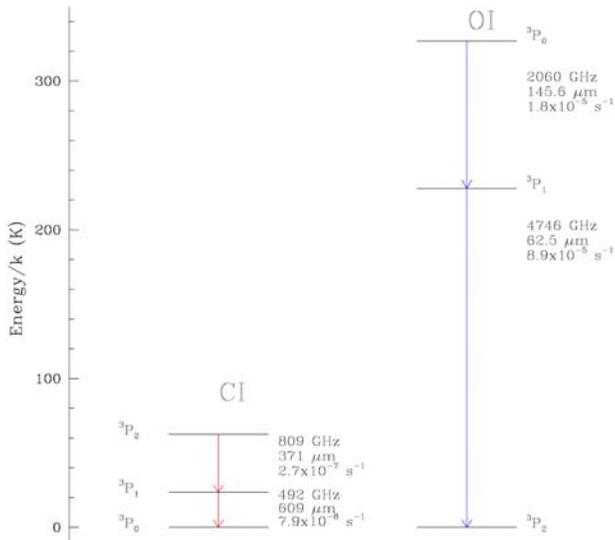


Figure 7. Fine structure transitions of atomic carbon and atomic oxygen.

Atomic oxygen has been observed using the ISO satellite. It is one of the most important cooling lines in photon dominated regions, and is seen throughout the Milky Way and other galaxies. The PACS system will give astronomers dramatically enhanced capability to observe OI, although emission and absorption features in the Milky Way will not be spectrally resolved.

Other important spectral lines for Herschel include fine structure transitions of ionized species, particularly carbon and nitrogen. Again in the PACS range, these lines are crucial for understanding the thermal balance in regions around massive young stars. Herschel projects will be targeting CII and NII lines in a variety of regions ranging from nearby ionized regions to distant galaxies.

V. CONCLUSIONS

The first generation of space missions for submillimeter spectroscopy, SWAS and Odin, had a great impact on our ideas about interstellar chemistry and the structure of

molecular clouds. Herschel, with a far larger primary reflector, and instruments with far greater sensitivity and frequency coverage, will certainly produce many more surprises, as well as filling in our knowledge about the solar system, molecular clouds and star formation, and galaxies near and far. The three instruments, considered as spectrometers, are so different from one another that they make almost a textbook on different ways to build a spectrometer. HIFI has only a single spatial pixel, but extremely broad coverage combined with high frequency resolution. SPIRE and PACS are both imaging spectrometers, but operate very differently. SPIRE covers a large frequency range with modest resolution, while PACS observes a narrow wavelength range at any moment, but offers moderate frequency resolution, sufficient to resolve spectral lines in some situations. HIFI and SPIRE can observe many lines simultaneously, while PACS observes a single line. We certainly anticipate that these disparate spectrometers will together have a great impact on astrophysics starting about two years from now.

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