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Design Reference Mission Case Study
Stratospheric Observatory for Infrared Astronomy Science Steering Committee

Water in Space: Comets and the Interstellar Medium

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Scientific category:	INTERSTELLAR MEDIUM
Instruments:	EXES, CASIMIR, HAWC
Hours of observation:	253

Abstract

During the past few years our knowledge of the abundance of the astrophysically and biologically important water molecule in the interstellar medium has advanced considerably. However, uncertainties remain in our knowledge of the abundance of water vapor in both cold and hot regions, the interstellar water cycle which traces the form of water during the formation of stars and planets from diffuse gas, and the potential relation between interstellar chemistry and cometary ices. SOFIA has the capability to contribute significantly to our knowledge of the distribution and amount of water vapor in a variety of regions tracing a range of physical processes from shocks to star formation. We outline here a program of SOFIA observations to address these uncertainties using high spectral resolution observations (R $\sim 10^6$) of water vapor tracing the spectrum of star formation activity in the interstellar medium and the evaporation of water in comets.

Observing Summary:

Target	RA	Dec	F_{Jy}	Configuration/mode	Hours
10 GMC CORES	gal. plane	gal. plane	1	CASIMIR	24
10 GMC CORES	gal. plane	gal. plane	100	HAWC	1
10 GMC LOS ABSORPTIONS	gal. plane	gal. plane	100	CASIMIR	36
3 GMC LOS ABSORPTIONS	gal. plane	gal. plane	300	EXES	6
10 SHOCKED REGIONS $0.5' \times 0.5'$ MOSAIC	gal. plane	gal. plane	10	EXES	100
10 COLD POST-SHOCK REGIONS	gal. plane	gal. plane	100	CASIMIR	24
10 HOT CORES	gal. plane	gal. plane	10	CASIMIR	14
2 COMETS	ecl. plane	ecl. plane	1	CASIMIR	48
				Grand total hours	253

Scientific Objectives

Because of its association with biology on Earth, water is one of the most important molecules in the solar system and beyond. Over the past few years observations of water in molecular clouds by NASA's *Submillimeter Wave Astronomy Satellite* (SWAS), ESA's *Infrared Space Observatory* (ISO), and *Odin* (Sweden/Canada/France) have drawn a compelling connection between water in interstellar space and planetary water. These observations have found that water vapor has a surprisingly low abundance in the dense cores of molecular clouds (Snell et al. 2000) and a "normal" abundance in low density diffuse clouds (Neufeld et al. 2000; Moneti, Cernicharo, & Pardo 2001). The most comprehensive solution suggested is one which water vapor freezes onto the surfaces of dust grains in the cold dark interiors of molecular clouds – the very sites of the formation of star and planetary systems (Bergin et al. 2000). These water-ice coated grains will eventually coagulate to form pre-planetary rocks and comets that ultimately become incorporated into the interiors and atmospheres of planetary bodies. Thus the origin of water in interstellar medium (ISM) and the water cycle during star formation is a question with clear astrobiological import.

Water is also a molecule with strong connections to astrophysics. It holds the keys to our understanding of the chemistry of oxygen, the third most abundant element in the Universe. It is also a gas coolant, which, when balanced with cloud heating, controls the thermal balance and stability of cloud cores against collapse. It is the most abundant molecule in the icy mantles covering grains, and its presence on the grain surface is believed to change the optical properties of grains and to aid in the coagulation process that ultimately produces planets (e.g. Ossenkopf & Henning 1994; Dominik & Tielens 1997; Whittet et al. 2001).

Our understanding of the presence and formation of water certainly received a large boost from the observations of ISO, SWAS, and *Odin*; however water abundances are still uncertain and major theoretical questions still exist. (1) *SWAS* and *Odin* were the only instruments capable of detecting water emission from cold gas, primarily through the ground state transition of o-H_2O, which has large optical depth. To obtain abundance information required assumptions with respect to the physical structure of the sources. Herschel will make great strides in alleviating this particular situation. However, the puzzle of the creation of interstellar water cannot be answered by Herschel alone – as we will discuss below the final answer requires a significant contribution that can only be provided by SOFIA. In addition, with the combination of high spectral resolution observations offered by EXES and CASIMIR there is a powerful pairing for providing more information than offered by Herschel instruments.

SOFIA can make major contributions towards answering these issues. In the following we will make a detailed science case for a series of SOFIA observations that will answer the following questions:

- How does water form in the cold dense component of the ISM?
- How much water is created in interstellar shocks. How does this compare to the cold quiescent gas and do shocks affect the water cycle?

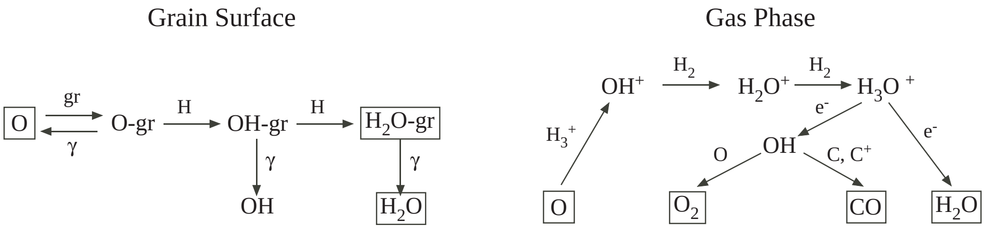

Figure 1: Key elements of the oxygen chemistry believed to occur on grain surfaces and in the cold gas phase. Photodesorption is denoted by γ. The boxed species are the most abundant and are of greatest interest in our study. O-gr, OH-gr, and H_2O-gr denote O, OH, H_2O, respectively, on grains.

- What is the nature of the ISM–Cometary Connection?

SOFIA and the Formation of Water in the Cold Interstellar Medium

Fig. 1 shows a schematic of the oxygen chemistry that is believed to power water formation in interstellar space. Chemical models (see Elitzur & de Jong 1978, Neufeld et al. 1995) show that for T >300 K, water vapor will account for most of the gas-phase oxygen that is not bound as CO, as a result of the neutral-neutral reactions: $H_2 + O \rightarrow OH + H$ and $H_2 + OH \rightarrow H_2O + H$. At temperatures less than 300 K, however, these reactions are negligibly slow because they possess significant activation energy barriers. Gas-phase water is then produced either by means of reactions of atomic oxygen with hydrogen on grain surfaces with subsequent sublimation or via cosmic-ray driven ion-neutral chemistry, as shown in Fig. 1. Water formed on grains will remain frozen on the grain until either the grain temperature exceeds $\sim$110 K or the water molecule is photodesorbed by a UV photon.

SWAS and Odin observations have determined that the water vapor abundance in cold gas is several orders of magnitude below theoretical expectations (see, e.g. Bergin et al. 2001). The primary solution provided as an answer to this question is that the formation of water ice on grains results in a depletion of atomic oxygen from the gas. In this model the fuel for the chemistry, oxygen atoms, is frozen onto grains in the form of water ice. This ice will not evaporate unless temperatures exceed 110 K (Fraser et al. 2001) and hence most oxygen is essentially unavailable to make water vapor or molecular oxygen in the gas. Thus the low abundance of water vapor hints at a lack of gaseous atomic oxygen in the densest regions of molecular cloud cores. Even a little amount of oxygen in the gas would create water vapor that could be detected by SWAS and ODIN.

Herschel has a key program that focuses exclusively on water, Water in Star-Forming Regions with Herschel (WISH; PI: E. van Dishoeck). This program will survey the spectrum of activity in both low and high mass star forming regions. With access to multiple transitions of both ortho and para forms of water, and higher angular resolution than SWAS/Odin, Herschel will determine accurate water vapor abundances and thereby challenge these theories.

Even if the previous results are confirmed by WISH, there is one area where there is a direct conflict with current theories that strikes at the heart of our understanding of water formation. This arises from ISO observations of atomic oxygen which find large atomic oxygen columns towards several sources (Caux et al. 1999; Lis et al. 2001 and references therein). To account for the low abundances of water and molecular oxygen, this [O I] emission/absorption must be probing the outer, low density, layers of the cloud. However, analysis in these papers suggest that some oxygen is found in the denser gas (which has greater column). Discriminating between these potential possibilities requires knowledge of the line width as denser gas has lower velocity widths than the more extended cloud (especially when compared to the possibility that [O I] should trace both atomic and molecular layers). However, this is impossible with current data as the [O I] lines were not resolved by ISO (and will also not be resolved by PACS on Herschel). To answer this question, and obtain the final piece of our understanding of water formation, therefore requires high spectral resolution observations at 63 μ and 145 μ which will be obtained using the GREAT instrument on SOFIA.

Water in Absorption

Observation of lines in absorption are subject to much less uncertainty than emission lines. If the observations can measure true continuum and zero level, the optical depth of a weakly excited absorption line is straightforward to determine. Assuming that the absorption seen is confined to a column defined by the angular size of the background source, it is possible to compare with other observations even if made using other beam sizes, with a reasonable accuracy. This includes such species as OH, which is intimately related to water in the chemical reaction networks. For this study, the EXES instrument can be used to provide a view of water that is complementary to that offered by Herschel.

Herschel has several programs to detect water in absorption from extended cold gas components (and follow-up can be anticipated using CASIMIR). EXES will be sensitive to the warmer more abundant water that exists in close proximity to deeply embedded young stars. In this regard, the capabilities of EXES are a significant improvement when compared to ISO detections of water vapor in absorption at 6μm. With EXES one can observe essentially any rotational level of the main isotope, including the ground rotational state. A single frequency setting will provide information on the water abundance and gas temperature in warm gas local to young massive stars (Richter et al 2001). The spectral resolution offered by EXES is also significantly larger than the more sensitive JWST/MIRI and therefore probes a different range of parameter space. This will prove to be a useful counterpoint to the studies of water in emission with Herschel/HIFI, providing a powerful tool to examine the line of sight water abundance structure in several key sources (e.g. Boonman et al. 2002).

Water in Shocked Gas

Water formation in shocked gas is strongly favored either via the rapid production from gas phase atomic oxygen (via a series of neutral-neutral reactions that are inactive in the cold ambient gas) or by the removal of grain mantle material by ablation. Thus shocks in the interstellar medium are water factories and this signature will exist for a considerable period of time. Despite the detection of water in numerous shocks (Neufeld et al. 2000; Nisini 2003) there are lingering questions regarding the true water vapor abundance inside the shock and its spatial distribution when compared to other shock tracers such as vibrationally excited H_2. This is primarily due to the low spatial resolution of instruments capable of observing cold post-shock water (e.g. SWAS and *Odin*) and the low spectral resolution of instruments capable of detecting hot shocked water (e.g. ISO and *Spitzer*). For a discussion see Snell et al. (2005).

Herschel has a strong effort directed towards the study of water in shocks using both heterodyne (HIFI) and direct detection (PACS) instruments. Because of this issue the study of shocked water with CASIMIR will lie predominantly in terms of follow-up. However, the EXES instrument offers two things not available with Herschel or JWST. (1) The ability to spectrally resolve emission lines. Studies of SWAS emission suggest a sharp (2 order of magnitude) increase in water abundance as a function of velocity in the line wings (Franklin et al. 2008). This will be an excellent tool for comparison to HIFI data and should greatly extend the capability to distinguish between different emitting clumps along the line of sight. (2) The ability to detect the primary gas constituent, H_2. Any study of water chemistry requires knowledge of the gas temperature, density, and total column. The gas temperature/density can be estimated via observation of many water transitions. However, the total column requires observation of either H_2 or CO. With the EXES instrument we will be able to spectrally resolve the emission of molecular hydrogen in shocks and provide a direct measurement of the total gas column in the shock (as a function of velocity). This will be a unique contribution to studies of shocked gas.

The ISM-Cometary Connection

Much of the interstellar–cometary connection is drawn through the similarity of the D/H ratio of water ices in the ISM with that seen towards the three Oort cloud comets (Halley, Hale-Bopp, Hyakutake) with HDO detections (Ehrenfreund & Charnley 2000). In addition, the ortho-to-para ratio which is estimated to be $\sim 2 - 2.5$ in comets (Dello Russo et al. 2005) will be characterized by Herschel in the ISM to probe that as a direct link. Finally the $^{16}O/^{18}O$ ratio is emerging as another potential link (Lee et al. 2008) - SOFIA is unique in its capability to explore this particular aspect.

The CASIMIR instrument on SOFIA is also capable of detecting $H_2^{18}O$ in out-gassing cometary coma provided the water production rate exceeds 10^{29} molecules/sec (Bensch & Bergin 2004). In Figure 2 we show a sample of the predicted lines that can be observed by SOFIA in comets with different water production rates. SOFIA will provide a direct measurement of the water production rate and a measurement of the ortho/para ratio of water, which can be compared to ISM values estimated by Herschel extending the ISM-cometary comparison towards new ground. It is important to note that water can be observed from the ground in the so-called "hot-bands" (Dello Russo et al. 2005). However, submm observations couple more directly to the coma and can be used to explore spatial variations and have the capability to search for temporal variations such as seen in comet Temple 1 (Bensch et al. 2007).

An exciting emerging area is the suggestion that CO self-shielding in the ISM or Solar

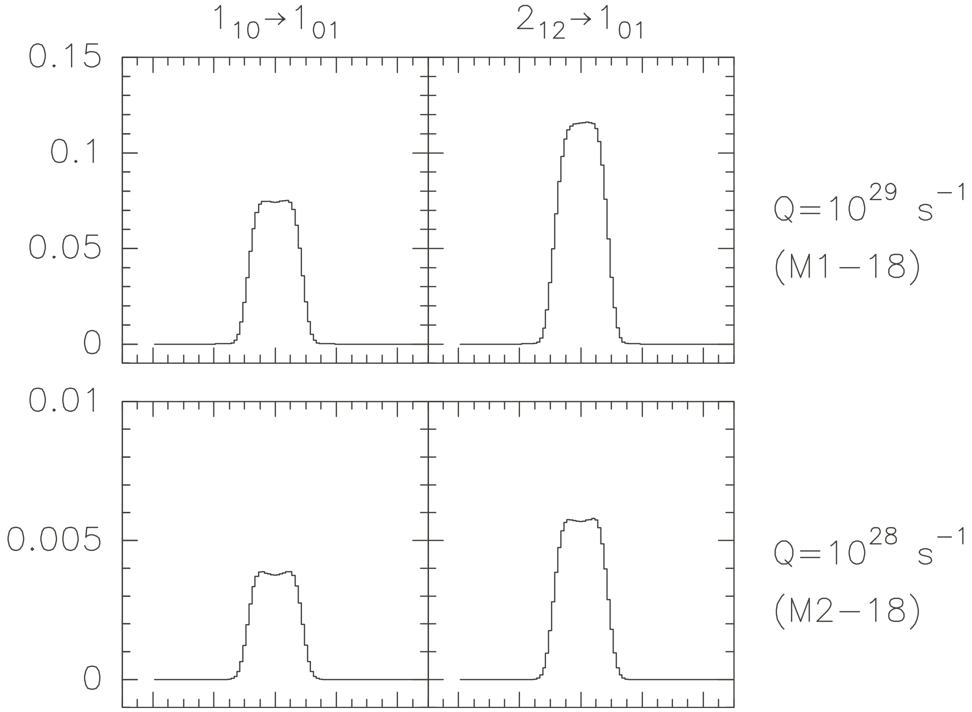

Figure 2: Model predictions for SOFIA CASIMIR observations of ortho-$H_2^{18}O$ (Bensch & Bergin 2004). The ground-state transitions, indicated at the top of the top panels, are shown for the a comet model with a water production rate as listed to the right in the figure. The double-peaked profile is typical for optically thin emission from an expanding shell.

Nebula imparted oxygen isotopic anomalies into meteorites (Clayton 2002, Yurimoto et al. 2007). The GREAT instrument can be used to observe comets in the lines of ^{16}OH and ^{18}OH. Since OH is the primary photo-product of water in cometary coma this observation is a direct measurement of the water oxygen isotope ratio in the outer nebula. This observation is SOFIA unique and has direct implications for our understanding of meteorites and planet formation.

Here the longevity of SOFIA when compared to Herschel will provide for improved statistics. Based on models of distribution, magnitude, and flux of long period comets (Hughes 2001) and a fit to the relation between cometary visual magnitude and water production rate (Jorda et al. 1991) it is estimated that ~ 1 comet per year brighter than 10^{29} molecules/sec will enter the solar system within 2 AU of the Sun and a fraction of these will be observable with Herschel and SOFIA. In addition, 2 comets brighter than 5×10^{29} mol/sec can be expected in the lifetime of SOFIA. Thus we have the hope of extending the sample to an additional $\sim 7 - 10$ comets beyond what Herschel can accomplish in 3 years. Moreover the observation of comets with $Q_{H_2O} > 2 \times 10^{29}$ mol/sec can be used to determine the oxygen isotopic ratio using OH – a truly unique SOFIA contribution.

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SOFIA Uniqueness/Relationship to Other Facilities

In addressing the issue of water in interstellar space SOFIA has clear overlap with the capabilities of *Spitzer* (for EXES) and *Herschel* (for CASIMIR). With a cooled telescope *Spitzer* and JWST have greater sensitivity than SOFIA, however the resolving power of the IRS spectrometer is only 600 or 3000 for MIRI, when compared to 10^5 for EXES. The higher spectral resolution is crucial for observations of narrow interstellar lines in the presence of strong thermal dust continuum emission. For instance, observations of the shock in Orion are impossible for *Spitzer* due to saturation limits and low line to continuum contrast.

Herschel-HIFI has direct overlap in frequency coverage and sensitivity with CASIMIR. With no atmospheric constraints *Herschel* will also be capable of probing the stronger emission of $H_2^{16}O$ along with $H_2^{18}O$. This program is directed assuming that much of the planned Herschel key programs will be completed and CASIMIR observations will be limited to regions where Herschel observations have not been completed. *Herschel* has a ∼3-5 year mission lifetime and at its end SOFIA will have the only capability to directly observe water in the ISM. In addition, as a cooled mission *Herschel* science will have to be clearly directed towards immediate science return which will limit its ability to survey all sources of interest. Thus, targeted studies with SOFIA during *Herschel* operations can be expected to yield important scientific results with the possibility for long-term followup.

For those comets with sufficient line strengths, SOFIA can effectively complement the capabilities of Herschel in several ways. First, due to the absence of stringent thermal constraints, SOFIA can view comets at significantly smaller angular separations to the Sun than Herschel - e.g., ~30 degrees for SOFIA versus ~90 degrees for Herschel. This will permit SOFIA to monitor comets at much closer approach to the Sun than Herschel. Second, SOFIA is able to continuously observe a comet for up to 2–3 hours per flight. While in principle Herschel can do the same, severe scheduling demands make such a time commitment unlikely except in rare circumstances. The ability to observe fluctuations in the emission of key species, such as water, on short timescales could yield unique information about the rotation and surface properties of the comet nucleus.

Observing Strategy

TBD

Special Requirements

CASIMIR/GREAT observations of bright comets will require target-of-opportunity observations.

Minimum Spectral Resolution:	10^5; $\geq 10^5$ at 5-30;250-600 μm
Maximum water:	low
Minimum tracking rate:	100 mas/sec
RMS pointing jitter:	2.0 as

Precursor/Supporting Observations

ISO, SWAS, *Odin*, and *Spitzer* observations will be useful in leveraging the full scientific return from these data. Coordinated plans with *Herschel* will also be valuable, especially for cometary research.