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WATER IN SPACE

Water is a key molecule in the cosmos, from distant galaxies and star-forming regions in the Milky Way to the Solar System and our own blue planet. The Herschel Space Observatory, launched in 2009 by the European Space Agency, provides astronomers with a unique opportunity to observe water throughout the Universe unhampered by the Earth's moist atmosphere. Initial results show that water emission elucidates key episodes in the process of stellar birth.

The space between the stars forms a gigantic physical-chemical laboratory with conditions that cannot be readily simulated in an experiment on Earth. It is filled with a very dilute gas, of which the denser concentrations are called 'interstellar clouds'. These clouds are present throughout our galaxy and can sometimes be seen as dark regions on optical images of the sky (Figure 1). They appear dark against a light background because of the presence of small solid particles which absorb and scatter the visible radiation. New generations of stars like our Sun and planets like Jupiter or Earth are born inside these dense clouds [1].

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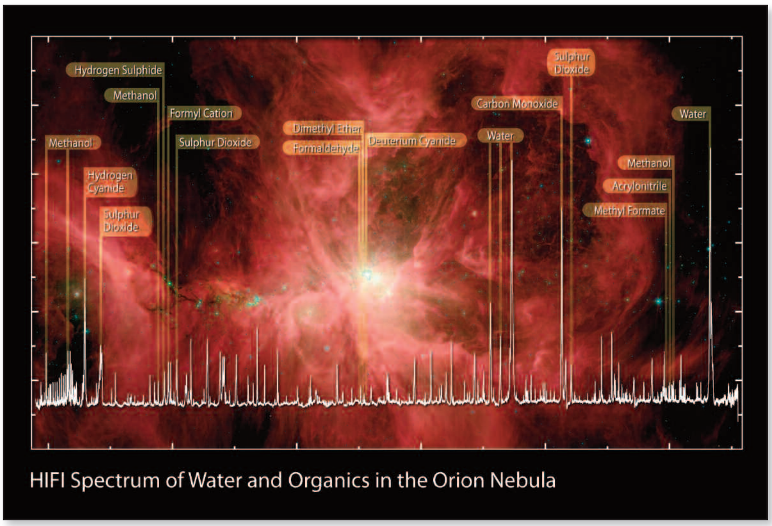
With typical densities of only 10^4 particles per cm^3 and temperatures down to 10 K, traditional chemistry would predict that virtually no molecules can form under these extremely low temperature and density conditions. Yet it has become clear over the last 40 years that interstellar space has a very rich chemistry, with more than 150 different molecular species detected (not counting isotopes) (Figure 2). Main questions in the field of astrochemistry include: how are these molecules produced? How far does this chemical complexity go? Can they become part of new planetary systems where they may form the building blocks for life?

Water is undoubtedly one of the most important of molecules found in space. As a dominant form of oxygen, the most abundant element in the universe after H and He, it controls the chemistry of many other species, whether in gaseous or solid phase. It is a unique diagnostic of the warmer gas and the energetic processes that take place close to forming stars, as will be shown below. Water is also partly responsible for keeping the gas at low temperatures because the cloud cools whenever line radiation escapes. These low temperatures, in turn, allow clouds to collapse to form stars. In cold regions, water is primarily in solid form, and its presence as an ice may help the ▸

▲ **FIG. 1:** Hubble Space Telescope optical image of the Carina nebula. The dark regions are dusty clouds which contain a wealth of molecules and in which new stars are born. (Credit: NASA/ESA)



▲ **FIG. 2: HIFI spectrum of the Orion nebula around 1 THz (300 µm wavelength) showing lines of water and complex organic molecules, superimposed on a Spitzer Space Telescope mid-infrared image of Orion [2]. This figure illustrates the spectral richness of regions of star and planet formation. (Credit: ESA, HEXOS and the HIFI consortium; Background image: NASA/JPL-Caltech)**

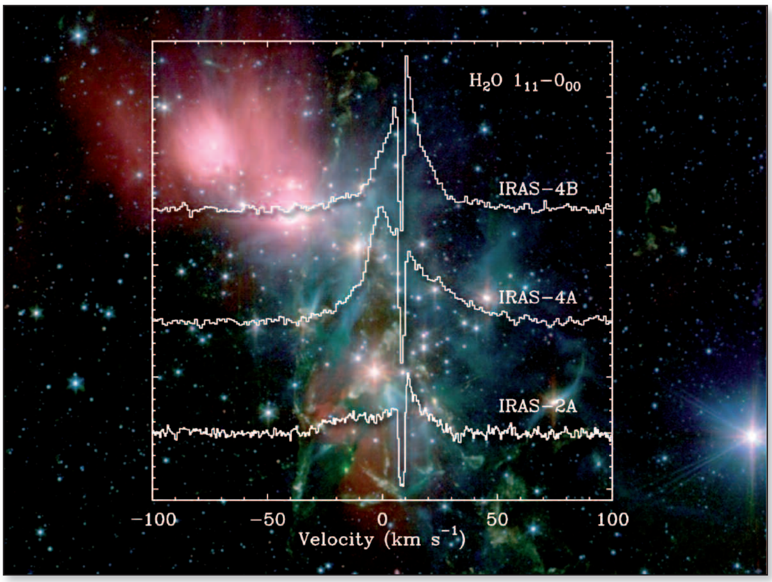
▶ coagulation process of dust grains that ultimately produces planets. Asteroids and comets containing ice have likely delivered most of the water to our oceans on Earth, where water is directly associated with the emergence of life. The distribution of water vapor and ice during the entire star and planet formation phase is therefore a fundamental process relevant to our own origins.

How to observe water?

Most interstellar molecules are observed through their pure rotational lines at millimeter wavelengths, excited by collisions with H_2. Radio telescopes situated at high dry sites on Earth operating at wavelengths around 1 millimeter can readily detect many species. However, because of its high abundance in our own atmosphere, lines from interstellar water generally do not reach the Earth's surface. Thus, space observatories equipped with state-of-the-art instruments are essential to detect the bulk of the interstellar water.

On May 14 2009, the European Space Agency successfully launched the long-awaited Herschel Space Observatory from French Guyana (see box). Herschel is the largest space telescope ever built, with a single mirror measuring 3.5m in diameter, even exceeding the Hubble Space Telescope mirror in size. Its three instruments provide imaging and spectroscopic capabilities in the 50-500 µm wavelength range, one of the last unexplored regions of the electromagnetic spectrum. This wavelength range is particularly rich in rotational transitions of H_2O and related hydrides such as OH. Indeed, observing water in space was one of the main drivers for the design of Herschel.

▼ **FIG. 3: HIFI spectra of the p-H_2O ground-state 1_{11}-0_{00} line at 1.1 THz (270 µm) toward three low-mass protostars in the NGC 1333 star-forming region [5]. (Credit: ESA, WISH and the HIFI consortium; Background Spitzer image: NASA/JPL-Caltech)**



A WISH comes true

The Heterodyne Instrument for the Far-Infrared (HIFI) is one of the three instruments onboard Herschel. It was built by an international consortium under the leadership of the Netherlands Institute for Space Research (SRON) [3], and its very high spectral resolution is particularly well suited for studying water vapour. As a reward for its investments, the HIFI consortium was awarded guaranteed observing time to carry out a number of key programs. The largest of these programs is 'Water In Star-forming regions with Herschel' (WISH), which uses 425 hr to observe ~80 sources throughout the galaxy which are currently in the process of forming stars [4]. A wide range of stellar masses and luminosities are covered, from the lowest to the highest mass protostars, and a large range of evolutionary stages, from the first stages represented by dense cores that have not yet collapsed to form stars to the last stages where the cloud surrounding the young star has been dissipated.

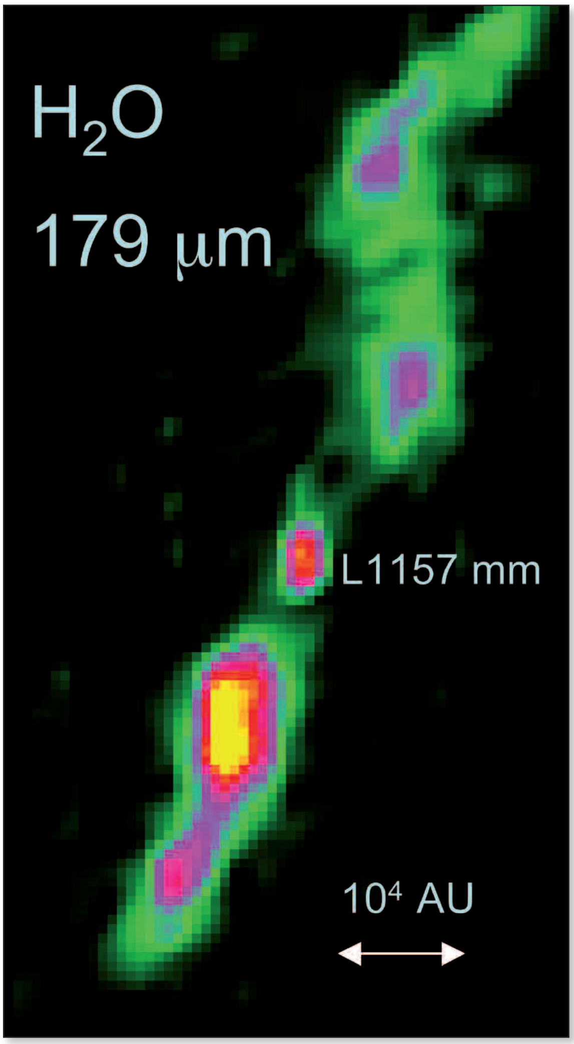
Various lines of water originating from a range of energy levels are targeted to probe both cold and warm water. In addition, deep integrations on lines from $^{18}OH_2$ and $^{17}OH_2$ are performed. Because their lower abundances by factors of ~500 and ~2500, respectively, the lines from these isotopologues suffer less saturation and are thus easier to analyze than those of $^{16}OH_2$. This plethora of water lines provides anything but redundant information: it actually helps to overcome one of the natural drawbacks of astronomical observations, which yield only two-dimensional images due to the projection on the sky. Since each line arises in a slightly different volume in an interstellar cloud, all the information put together provides a three-dimensional view. Thus, the HIFI data provide a natural tomography of these regions.

Figure 3 presents recent HIFI spectra of H_2O in three low-mass star-forming regions [5].

The quality of the data is excellent and the line profiles are fully resolved (resolution 0.07 km/s at 1 THz). The profiles are surprisingly complex, revealing both broad emission and narrow absorption components. The narrow absorption lines (few km/s width) originate in quiescent cold gas in the outer envelope surrounding the protostar. The broad lines (widths up to 50 km/s) arise in fast-moving gas caused by shocks associated with the jets and winds from the young stars.

These characteristics are seen for all lines, arising from energy levels up to several hundred K above ground, and for all isotopologues. Thus, it can be concluded immediately that the bulk of the water emission originates from hot shocked gas rather than cold quiescent material. A quantitative analysis of the data shows that the abundance of water with respect to the basic molecule H_2 is about 10^{-4} - 10^{-5} in the hot gas, but only 10^{-8}-10^{-9} for the cold gas. Since the overall abundance of oxygen with respect to hydrogen is about 3.10^{-4}, this means that most of the available oxygen is driven into water in hot gas, whereas most water is frozen out on grains in cold clouds.

The importance of water as a physical diagnostic stems precisely from these gas phase abundance variations by an order of magnitude between warm and cold regions. Water vapour acts like a 'switch' that turns on whenever energy is deposited in molecular clouds in the processes accompanying stellar birth. This fact is beautifully illustrated in the first water map of a forming star (Figure 4): The water emission 'lights up' close to the protostar and in hot spots where the jet interacts with the surrounding cloud [6].



◀ **FIG. 4:** PACS image of the water 179 μm (1.7 THz) line toward L 1157 (a low-mass protostar comparable to our Sun when it was a toddler), lighting up the two-sided outflow of gas [6]. The scale is indicated in Astronomical Units, with 1 AU = distance Sun-Earth = $1.5\ 10^{13}$ cm.

Water formation routes

How is this water produced and why are its abundance variations so large? Under interstellar conditions water gas is mainly formed through reactions between ions and neutral species, starting with the $O + H_3^+ \rightarrow OH^+ + H_2$ reaction. However, in cold and dense clouds H_2O is formed more efficiently on the small solid particles (0.1 μm-sized silicates and carbonaceous material) which act as a sink on which gaseous species can freeze out (Figure 5). Although the details how O and H combine on a solid surface to form H_2O are not yet fully understood, there is ample observational evidence that the H_2O ice abundances in protostellar envelopes can be as high as 10^{-4}, locking up most of the available oxygen.

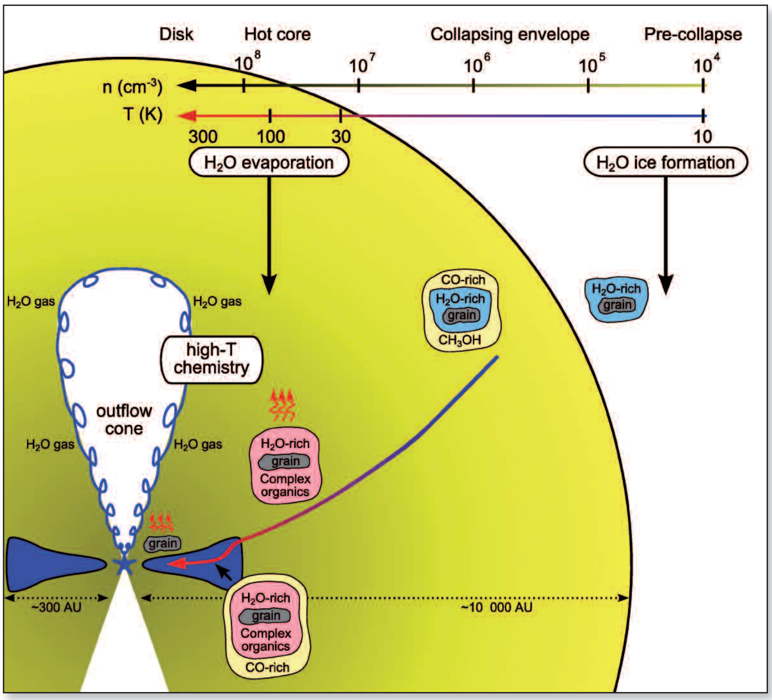
Once the protostars turn on, they heat the surrounding material and the grain temperature can rise above 100 K. As a result, all H_2O ice thermally desorbs, just like the ice in a comet evaporates when its nucleus is heated as it passes close to the Sun. At even higher temperatures, above 230 K, the gas-phase reactions of $O + H_2 \rightarrow OH + H$ and $OH + H_2 \rightarrow H_2O + H$ become significant. The combination of these processes explains why hot gas is literally 'steaming'.

Herschel Space Observatory

Herschel is a 3.5m passively cooled telescope built and launched by the European Space Agency (ESA)
(Figure 7). It contains three instruments built by large international consortia of institutes, housed in a superfluid helium cryostat which provides an operational lifetime for astronomical observations of about 3 yr. From conception to launch, the building of Herschel and its instruments took about 30 years. Herschel is currently in orbit some 1.5 million km from Earth.

The Heterodyne Instrument for the Far Infrared (HIFI) is a very high resolution heterodyne spectrometer covering the 490-1250 GHz (600-240 μm; 16-42 cm^{-1}) and 1410-1910 GHz (210-157 μm; 47-64 cm^{-1}) bands. HIFI observes a single pixel on the sky at a time.

The Photodetector Array Camera and Spectrometer (PACS) consists of a camera and a medium resolution imaging spectrometer for wavelengths in the range 55-210 μm (180-47 cm^{-1}). The spectrometer obtains spectra simultaneously over a limited wavelength range at each pixel of a 5x5 array. The Spectral and Photometric Imaging REceiver (SPIRE) is a camera and a low resolution Fourier Transform Spectrometer complementing PACS for wavelengths in the range 194-672 μm (51-15 cm^{-1}).

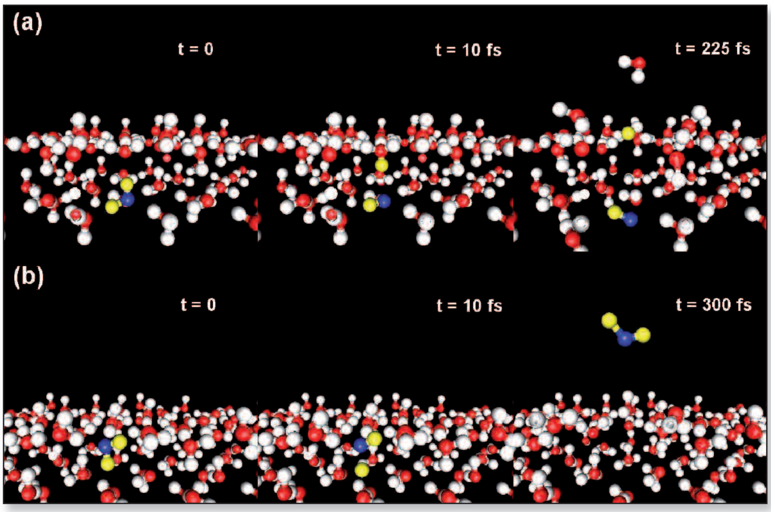


▲ FIG. 5: Evolution of water from a cold core through a collapsing envelope into the planet-forming zones of disks. Water is formed primarily on the surfaces of sub-micron-sized grains (not drawn to scale) and can evaporate back in the gas in the warm regions close to the protostar. Water is also produced in the shocks associated with the outflows [1,4]. Most water is thought to enter the disk as ice.

Surprise: ionized water

An early surprise from Herschel is the detection of widespread ionized water, H_2O^+, in a variety of galactic and even extragalactic sources. Although this ion was predicted to be detectable in regions exposed to energetic radiation, its ubiquitous presence was unexpected since H_2O^+ is readily transformed into H_3O^+ through reactions with H_2. Its relatively high abundance implies that the radiation driving its formation is even more widespread throughout interstellar clouds than thought before.

▲ FIG. 6: Snapshots of trajectories of mechanisms of H_2O desorption for a crystalline ice model exposed to UV radiation. The blue + yellow O and H atoms denote the water molecule that is (randomly) chosen to bephotodissociated by UV radiation at t=0. Top: kick-out mechanism; Bottom: H + OH recombine and desorb [11].



Molecular physics and water

To use water as a physical and chemical probe of star-forming regions, many basic molecular processes need to be understood. Often, these astronomical needs drive further molecular physics studies, thus leading to a fruitful synergy between astronomy and physics. A prime example of this interaction are the cross sections for collisions of H_2O with the main collision partner in clouds, H_2, which are needed to translate the observed line intensities into abundances. Discrepancies between experiment and theory have recently been resolved thanks to intense discussions in the physics community, allowing astronomers to quantitatively analyze their data [8].

Accurate line frequencies are crucial for identification of new molecules in space. Those for water are well known to better than 1 part in 10^7, but frequencies of ions such as H_2O^+ and OH^+ are still uncertain by tens of MHz [7]. Since (hyper)fine-structure can aid in making a firm identification, astronomical spectroscopy is in this case ahead of laboratory work.

Photodissociation plays a key role in the destruction of water. The absorption of a UV photon by gaseous H_2O leads directly to dissociation into OH and H. The interstellar radiation field contains photons with energies up to 13.6 eV (the Lyman limit of the H atom). Very little is known, however, what happens inside a water ice exposed to this UV radiation. Our group in Leiden has for the first time simulated outcomes of this process in the computer [9]. In most cases, H escapes from the ice, but about 0.05% of the dissociations result in desorption of a H_2O molecule, either following reformation of H + OH or through a process in which the energetic H 'kicks-out' a neighboring H_2O molecule (Figure 6). These results agree well with recent experiments [10]. Astronomically, ice photodesorption turns out to be a key process in explaining the presence of a low abundance of molecules in cold gas at temperatures where they should all have been frozen out onto the dust grains.

The formation of water ice itself from O and H atoms was postulated 25 years ago but never tested in the laboratory until recently, when a number of groups started building ultra-high-vacuum surface science experiments dedicated to simulating the interstellar conditions. Key steps in the ice formation process have now been elucidated in this exciting new field [11].

Outlook

Although less than 10% of the WISH data have been analyzed, the observations obtained so far indicate that Herschel will indeed be able to follow the water trail from the most diffuse gas to dense collapsing clouds, and eventually comets and planets in our own

▲ **FIG. 7:** Artist impression of the Herschel Space Observatory superimposed on an image of the Rosette nebula taken by Herschel. (Credit: ESA)

Solar system (Figure 5). Initial surprises include the absence of gaseous water in cold clouds at levels even lower than predicted, the dominance of shocks in controlling the bright water emission from protostars, and the ubiquitous presence of some ions. In turn, the Herschel data raise new questions on molecular spectroscopy, collision cross sections and basic processes involving water and related species, both in the gas and in the solid state. Herschel will surely strengthen the stimulating interactions between astronomy and physics in the coming years. It is fascinating to realize that the water molecules that constitute the bulk of our bodies and that we drink every day were produced on the dust grains in the cloud from which our Solar system formed some 4.5 billion years ago. ■

About the author

E.F. van Dishoeck studied chemistry in Leiden (the Netherlands), obtained her PhD in astronomy in Leiden, was postdoc and (visiting) professor at Harvard, Princeton and Caltech (all USA), before moving back to Leiden in 1990, where she holds a professorship in molecular astrophysics. She is also an external scientific member at the Max Planck Institute for Extraterrestrial Physics in Garching (Germany). She first became involved in Herschel in 1982 and has actively promoted Herschel and HIFI over the last 30 years. She is the principal investigator of the WISH key program.

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Further information about WISH, including outreach and educational material: www.strw.leidenuniv.nl/WISH. Further information about Herschel: http://herschel.esac.esa.int

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