In this paper, we discuss the astronomical search for water vapour in order to understand the disposition of water in all its phases throughout the processes of star and planet formation. Our ability to detect and study water vapour has recently received a tremendous boost with the successful launch and operation of the Herschel Space Observatory. Herschel spectroscopic detections of numerous transitions in a variety of astronomical objects, along with previous work by other space-based observatories, will be threaded throughout this paper. In particular, we present observations of water tracing the earliest stage of star birth where it is predominantly frozen as ice. When a star is born, the local energy release by radiation liberates ices in its surrounding envelope and powers energetic outflows that appear to be water factories. In these regions, water plays an important role in the gas physics. Finally, we end with an exploration of water in planet-forming discs surrounding young stars. The availability of accurate molecular data (frequencies, collisional rate coefficients and chemical reaction rates) is crucial to analyse the observations at each of these steps.

**Keywords:** star formation; planet formation; water

### 1. Introduction

Because of its importance for life on Earth, water is one of the most important molecules in the Solar System and beyond. However, the Universe is not filled with water, and thus the creation of H$_2$O from oxygen and hydrogen atoms, along with its disposition within each stage of the formation of stars and planets, are topics clearly associated with our own origins. The search for a greater understanding of this ‘water cycle’ is complicated by the fact that water in the Earth’s atmosphere impedes direct observation of water emissions in star-forming gas, except for some
Review. Water in star and planet forming

Thus, we rely on space-based observatories to gain access to the full spectrum of water vapour. Following water in star and planet formation involves a decrease in size scale of over $10^5$, from parsec (pc) to below an astronomical unit (AU); $1\text{ pc} = 206265\text{ AU} = 3.086 \times 10^{18}\text{ cm}$; $1\text{ AU}$ = distance from Earth to the Sun $= 1.5 \times 10^{13}\text{ cm}$. The gas involved in the gravitational collapse undergoes sharp increases in physical properties spanning many orders of magnitude in density and several in temperature. The water chemistry and its resulting emissions track these changes, leading water to be a true astrophysical probe, and leaving a trail in the water cycle.

In this paper, we will outline some of our basic understanding of the water cycle gleaned through astronomical observations over the past several decades. To a large extent, no single observatory is capable of capturing the entire picture, and much of this understanding is built upon analyses performed by numerous individuals using observations of $\text{H}^{18}\text{O}$ from ground-based observatories and $\text{H}_2\text{O}$ (along with the isotopologues) from space-based platforms such as the Infrared Space Observatory (ISO), the Submillimeter Wave Astronomy Satellite (SWAS), Odin, the Spitzer Space Telescope, and today with the Herschel Space Observatory. The aim of this paper is to elucidate our basic understanding of water vapour in space. However, for completeness, we also refer the reader to additional articles that summarize some of the relevant results from these missions [3–6]. The legacy of Herschel is still unfolding, but initial results are summarized in van Dishoeck et al. [7].

In §2, we briefly discuss star and planet formation, along with the observed gas physical conditions and dominant chemical processes. Section 3 outlines the use of water vapour emission as a probe of astrophysics. We will also discuss the disparate capabilities of the space-based observatories, along with an outline of the chemistry of water in space. In §4, we discuss the observational constraints on water vapour and star formation in relation to our understanding of its formation and destruction and primary phase. Finally, we summarize our high-level understanding in §5.

2. Star formation and properties of molecular gas

Below, we outline a general understanding of star and planet formation. Table 1 lists some of the relevant physical properties associated with each stage outlined. The role and disposition of water will be discussed within this context.

(a) Molecular clouds

Stars are born in molecular clouds with typical densities of a few thousand $\text{H}_2$ molecules per cubic centimetre, gas temperatures of approximately $10–20\text{ K}$ and typical masses of $10^3–10^5\text{ M}_\odot$. The clouds are predominantly gaseous in composition, with a solid-state component labelled as dust grains that are silicate and carbonaceous (graphite and amorphous carbon) in composition [18]. Molecular clouds exist over scales of tens of parsecs, but exhibit definite

\footnote{Water vapour has long been detected from the ground in the atmospheres of cool stars [1,2]. However, the physical conditions in star-forming clouds populate the rotational transitions of colder water ($T < 800\text{ K}$), which are generally blocked by the Earth’s atmosphere.}
Table 1. Estimated physical properties of star- and planet-forming gas. Parameters are provided to illustrate the range of values inferred from emission studies and may not be representative of the extremes.

<table>
<thead>
<tr>
<th>stage</th>
<th>volume density$^a$ (cm$^{-3}$)</th>
<th>$T_{\text{gas}}$ (K)</th>
<th>$\Delta v^b$ (km s$^{-1}$)</th>
<th>references</th>
</tr>
</thead>
<tbody>
<tr>
<td>extended cloud</td>
<td>$\sim 10^3$</td>
<td>10–15</td>
<td>1–3</td>
<td></td>
</tr>
<tr>
<td>pre-stellar core</td>
<td>$10^5$–$10^6$</td>
<td>10–15</td>
<td>0.3–1.5</td>
<td>[8]</td>
</tr>
<tr>
<td>protostar</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>hot core</td>
<td>$&gt;10^6$</td>
<td>100–300</td>
<td>5–15</td>
<td>[9,10]</td>
</tr>
<tr>
<td>extended outflow$^c$</td>
<td>$10^3$–$10^4$</td>
<td>10–100</td>
<td>5–15</td>
<td>[11,12]</td>
</tr>
<tr>
<td>protoplanetary disc$^d$</td>
<td>$10^6$–$10^{15}$</td>
<td>10–2000</td>
<td>1–5</td>
<td>[16,17]</td>
</tr>
</tbody>
</table>

$^a$Density as inferred from the excitation of high-dipole-moment molecules (similar to water vapour).

$^b$Full width at half-maximum of spectrally resolved molecular emission lines, usually representative of turbulent or dynamical motions.

$^c$Referring to the swept-up molecular outflow with the properties summarized.

$^d$If line broadening is dominated by Keplerian rotation, as generally assumed, then line widths should increase if the molecular emission originates from closer to the star. Values reported are for unresolved (or barely resolved) discs.

substructure, with stars being born in denser ($n > 10^5$ cm$^{-3}$) cores with typical sizes of 0.1 pc. The boundaries of the parsec-sized clouds are generally defined by the extent of CO emission, which is the primary observable gas-phase molecular constituent at large scales.

(b) Pre-stellar cores

Dense cores (0.1 pc) have been primarily characterized as clumps of concentrated sub-millimetre dust emission or infrared absorption [19–21] and through transitions of simple molecules with high dipole moments (e.g. NH$_3$, N$_2$H$^+$, CS [8,22–24]). For the most part, these molecules are formed via ion–molecule chemistry in the gaseous state (e.g. CS, N$_2$H$^+$). However, prior to stellar birth, the condensation of the core increases the central density by two to three orders of magnitude, while still remaining quite cold ($T \sim 10$ K). Because the density increase leads to more frequent collisions with cold dust grains ($T_d \sim 10$ K), the central regions of the core are dominated by the freeze-out of atoms and molecules from the gas onto dust grains (see [8], and references therein), forming an ice mantle coating on the solid silicate grains [25,26]. There is also the possibility of subsequent reactions within the ice mantle, which leads to greater complexity [26–29]. This is provided the dust temperature is below the relevant sublimation temperature for a given atom or molecule.

(c) Protostars and outflows

Molecular cloud cores are rotating and, upon gravitational collapse, the infalling envelope flattens to a disc and a central source (see [30,31], for more discussion). At this time, the central source releases gravitational energy and
heats its surrounding envelope. The central region is characterized by gas-phase emissions at high temperature (greater than or equal to 100 K) and it is called the ‘hot core’. The hot core exhibits a diverse chemistry powered by evaporation of the ice mantle along with subsequent gas-phase reactions [32–34]. During the protostellar stage, the forming star begins to eject material, the envelope is disrupted along the poles and the star begins the process of destroying its natal envelope. This mass ejection powers what are known as bipolar molecular outflows, which are characterized by two extremes (that probably span a continuous range of physical properties). At one extreme is a more extended (sub-parsec to parsec scale) molecular outflow of entrained gas with temperatures somewhat elevated above the natal cloud (table 1). At the other extreme are smaller regions of emission where faster-moving material has impacted slower-moving gas, leading to a shock. Shocked gas is characterized by temperatures in excess of several hundred kelvins; crucially, this can power reactions with barriers that were inactive in the cold ($T \sim 10–20$ K) gas and the release of ice mantles and more refractory material into the gas.

(d) Protoplanetary discs

As the envelope dissipates, the gas-rich disc becomes exposed. The disc surface is directly irradiated by energetic ultraviolet (UV) and X-ray photons from the star, but also by the external (interstellar/local) radiation field. Observational systems in this stage are often called T Tauri stars. Discs have strong radial and vertical gradients in physical properties, with most of the mass residing in the middle of the disc, labelled as the midplane [35–38]. It is the midplane that is the site of planet formation. The density of the midplane significantly exceeds that of the dense natal core, by many orders of magnitude. The midplane is, in general, colder than the disc upper layers, which can also be called the disc atmosphere. Finally, the outer part of the disc ($r > 10$ AU) has reduced pressure and temperature, but contains most of the mass. Molecular observations are only beginning to probe this stage but a general picture has emerged. At large radii ($r > 10–30$ AU), molecules are destroyed on the exposed disc surface as a result of photodissociation. In the midplane, the temperatures are below the sublimation temperature and most molecules are frozen as ices. In between are warm molecule-rich ($T \sim 50$ K) layers where some ices are able to evaporate (e.g. CO [39,40]). Inside of 30 AU, the midplane temperature progressively increases and a so-called ‘snow-line’ is believed to exist. Inside the snow-line, a given species would exist in the gas phase and beyond as ice. This line might be species-specific.

3. Molecular astrophysics and the chemistry of water

(a) $H_2O$ emission and observations

Water is a highly asymmetric molecule with its energy levels labelled by a set of three quantum numbers, $J_{K_A,K_C}$. Water comprises two identical hydrogen nuclei, each with nuclear spin. As such, owing to Fermi–Dirac statistics, it exists in two forms or spin isotopomers. The one with a total spin of unity is ortho-$H_2O$, while the other with a total spin of zero is para-$H_2O$. The energy levels are different for each, with ortho-$H_2O$ having $K_A + K_C =$ odd, and para-$H_2O$ characterized by $K_A + K_C =$ even. Transitions across ortho and para levels are
strictly forbidden [41], and conversion among the spin isotopomers occurs via reactions that transfer an H atom. In the high-temperature limit, the ratio of these two species is set by the ratios of the spin statistical weights, resulting in an ortho-to-para ratio (OPR) of 3:1. The ground state of para-H$_2$O is 34.3 K below that of ortho-H$_2$O. Thus it is possible, if water forms at temperatures below this value, that para-H$_2$O can dominate. Comets are known to have an OPR below three, possibly coincident with formation at approximately 30 K. However, the mechanisms for ortho-to-para conversion in the gas phase and on the grain surface are not well characterized (see Lis et al. [42] for a discussion).

H$_2$O, as a light hydride, has large energy-level spacings when compared with heavier molecules (e.g. CO), and its main transitions lie in the sub-millimetre to far-infrared wavelengths. In addition, with a high dipole moment of 1.85 D and large line frequencies, it has rapid spontaneous decay coefficients. This can lead to large line opacities for small columns. To elucidate this point, the lower state column ($N_l$) of ortho-H$_2$O $1_{10} \rightarrow 1_{01}$ is related to the line centre optical depth ($\tau_0$) by $N_l$(o-H$_2$O) = 4.89 \times 10^{12} \tau_0 \Delta v$ [43]. In this formula, $\Delta v$ (km s$^{-1}$) is the full width at half-maximum of the line; $N_l$ represents the total ortho-H$_2$O column, provided the gas density does not exceed $n_{H_2} > 10^7$ cm$^{-3}$ (assuming $\Delta v = 1$ km s$^{-1}$). Thus, $\tau_0 = 1$ for a $N$(o-H$_2$O) $\sim 5 \times 10^{12}$ cm$^{-2}$. To place this in perspective, a typical cloud would have regions with a total H$_2$ column of $10^{22}$ cm$^{-2}$. Thus, water emission is optically thick in a representative cloud (again assuming $\Delta v = 1$ km s$^{-1}$) even at very low abundances of $n$(o-H$_2$O)/$n$(H$_2$) $\sim 5 \times 10^{-10}$. The solar elemental oxygen abundance is $9.8 \times 10^{-4}$ (relative to H$_2$ [44]), while the average oxygen abundance is approximately solar in a large sample of F, G and K stars [45]. Thus, this amount of water traps only a tiny fraction of the available oxygen.

Water has long been observed in star- and planet-forming regions via its masing emissions at centimetre wavelengths [46]. In this paper, we will focus on observations of thermal water vapour emission and in particular its rotational transitions, which are attuned to the physical conditions of star-forming regions. Figure 1 shows the optically thin local thermodynamic equilibrium (LTE) emission spectrum of water from 30 to 600 $\mu$m ($\sim$500 GHz–10 THz) for gas temperatures of 30, 250 and 1000 K. It is clear that the spectral shape, or emission envelope, exhibits a strong temperature dependence. Lower-temperature gas emits primarily in the sub-millimetre, where the ground-state lines lie (557 GHz for ortho-H$_2$O, and 1113 GHz for para-H$_2$O), while at $T \sim 250$ K, the emission peaks in the far-infrared. Finally, very hot gas has numerous emission lines that extend to mid-infrared wavelengths and beyond the right-hand edge of the plot. This clearly demonstrates that water has numerous emission lines and the relative intensities bear information on the gas temperature. Of course, that is not the complete story, as water emission will also depend on density and column density. For water emission to truly reach LTE, it requires very high densities (at 1000 K it will be greater than $10^{13}$ cm$^{-3}$). Thus, this spectrum shows the maximum number of emission lines for water over this spectral range, and the true number of lines for typical conditions will be well below this level.

Another aspect is the relative utility of a given observatory to trace water vapour emission. Essentially, the different platforms are capable of probing a specific range of physical conditions and thus explore specific aspects of star formation physics (table 2). The top of figure 1 presents the spectral grasp of
Figure 1. Optically thin emission spectrum of water vapour in LTE at 30, 250 and 1000 K. Intensities for each temperature are normalized to emphasize the range of spectral lines as a function of wavelength as opposed to the overall intensity. To create this model spectrum, we made use of the myXCLASS program (http://www.astro.uni-koeln.de/projects/schilke/XCLASS), which accesses the JPL [47] (http://spec.jpl.nasa.gov) molecular database for water vapour line assignment. (Online version in colour.)

each of the respective space-based observatories. The wavelength coverage and moderate spectral resolution of *Spitzer* enabled the detection of very hot gas that is found in outflows [55] and also in the innermost regions of protoplanetary
Table 2. Main space-based platforms for observations of rotationally excited H$_2$O.

<table>
<thead>
<tr>
<th>Observatory</th>
<th>Spectral Range (µm)</th>
<th>Angular Resolution</th>
<th>$R$ $(\lambda/\Delta\lambda)$</th>
<th>$(\text{km} \cdot \text{s}^{-1})$</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>ISO</td>
<td>SWS 2.4–45.2</td>
<td>$14'' \times 20'' - 20'' \times 33''$</td>
<td>1500 200</td>
<td>[48]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SWS 11.4–44.5</td>
<td>$10'' \times 39'' - 17'' \times 40''$</td>
<td>30000 10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SWAS</td>
<td>538.6</td>
<td>$3.3'' \times 4.5''$</td>
<td>$5 \times 10^5$ 0.5</td>
<td>[49]</td>
<td></td>
</tr>
<tr>
<td>Odin$^b$</td>
<td>517–617</td>
<td>2.1'</td>
<td>$&gt;5 \times 10^5$ 0.05–0.5</td>
<td>[50]</td>
<td></td>
</tr>
<tr>
<td>Spitzer</td>
<td>IRS SH/LH</td>
<td>5'–10''</td>
<td>600 5000</td>
<td>[51]</td>
<td></td>
</tr>
<tr>
<td>Herschel</td>
<td>SPIRE 194–671</td>
<td>17''–41''</td>
<td>370–1300 230–810</td>
<td>[52]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PACS 53–260</td>
<td>9.4'</td>
<td>1000–4000 75–300</td>
<td>[53]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>HIFI 157–625</td>
<td>10''–40''</td>
<td>$&gt;5 \times 10^5$ 0.15–0.6</td>
<td>[54]</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ISO, operated primarily by the European Space Agency (ESA), was in operation from 1995 to 1998. SWAS was a National Aeronautics and Space Administration (NASA) mission that observed from 1998 to 2004, while Odin is primarily operated by the Swedish Space Corporation and was launched in 2001. The Spitzer Space Telescope (NASA) performed spectroscopy during its cooled mission from 2003 through 2009. The Herschel Space Observatory is an ESA satellite with NASA participation that was launched in 2009 and is expected to operate for approximately 3.5 years. $^b$Odin also had the capability to observe at 118.75 GHz.

discs [56]. ISO was best suited for the detection of warm and hot water in shocks and also in the hot cores around massive stars (see [4,57] and references therein). In the case of Spitzer and ISO, the lines are generally not velocity-resolved. SWAS and Odin both were tuned to the ground-state line of ortho-H$_2$O, which is approximately 26.7 K above the ground state. This line was sensitive to the cold ($T \sim 10–40$ K) and warm ($T \sim 100$ K) gas that can be present in outflows, hot cores and quiescent gas [3,5]. These observatories used heterodyne techniques allowing for enough spectral resolution to resolve the emission lines, even in the extended cloud. However, both SWAS and Odin had moderate angular resolution and were not sensitive enough to detect water in pre-stellar cores or discs. In addition, the analysis was hampered by observing only one emission line (supplemented by the ground state of ortho-H$_2^{18}$O). Finally, Herschel has tremendous capability to explore all the components of star formation with the greatest angular resolution to date through instruments that offer both high and low spectral resolution; it also has receivers that have noise temperature only just above the quantum limit. There is a dedicated Key Programme on the topic of water: ‘Water in Star-forming Regions with the Herschel Space Observatory’ (WISH; E. van Dishoeck, PI). A summary of the initial WISH results is given by van Dishoeck et al. [7] and some results are further discussed below.

(b) Chemical perspective

Oxygen is the third most abundant element in the Universe, and its gas-phase chemistry is linked to products of cosmic ray ionization of H$_2$ and the eventual formation of the trihydrogen ion (H$_3^+$). H$_3^+$ will react with O and a sequence
of rapid reactions produces $\text{H}_3\text{O}^+$. The next step involves the dissociative recombination of $\text{H}_3\text{O}^+$ with electrons:

$$\text{H}_3\text{O}^+ + e^- \rightarrow \text{H} + \text{H}_2\text{O} \quad f_1$$
$$\quad \rightarrow \text{OH} + \text{H}_2 \quad f_2$$
$$\quad \rightarrow \text{OH} + 2\text{H} \quad f_3$$
$$\quad \rightarrow \text{O} + \text{H} + \text{H}_2 \quad f_4$$

(3.1)

where $f_{1-4}$ are the branching ratios.\(^2\) Via this sequence of reactions, water vapour is then created. The primary \textit{gas-phase} destruction pathway in shielded gas is via a reaction with $\text{He}^+$ (another ionization product); at the disc surface photodissociation also plays a key role. These reactions for pure gas-phase chemistry result in an abundance (relative to $\text{H}_2$) of a few times $10^{-6}$. It should be stated that the example above provides only the primary formation and destruction pathways under typical conditions (i.e. where ionizing agents are available). In addition, water participates in numerous other reactions as both reactant and product and some water can be created via other pathways, albeit at reduced levels [61].

A critical factor in cold gas is the likelihood that water is created \textit{in situ} on grain surfaces via a series of reactions starting with atomic O and H and forming water ice [62,63]. In fact, water ice is observed with abundances close to approximately $10^{-4}$ (relative to $\text{H}_2$) along several lines of sight [64,65]. The evaporation temperature of water ice at interstellar pressures is approximately 100K [66]. Thus, water will probably remain frozen for any evolutionary stage characterized by temperatures below 100K. This can have a direct impact on the abundance of water vapour, as the fuel for the gas-phase chemistry is oxygen atoms. When oxygen atoms are mostly trapped on grain surfaces as water ice, the gas-phase chemistry is incapable of maintaining abundances of approximately $10^{-6}$ and the predicted abundance is much lower [61,67,68]. Since a large fraction of the mass in star-forming cores will be below the sublimation temperature, it has been proposed that non-thermal desorption mechanisms may be needed to release water from the ice mantle coating the grain surface. In particular, UV photodesorption is found to be efficient in laboratory experiments [69,70]. Given the prevalence of UV photons above the Lyman limit in the vicinity of star-forming regions and protoplanetary discs, it is possible that this mechanism would play an important role [71,72].

At temperatures below a few hundred kelvins, ion–neutral chemistry dominates. Above this temperature, two neutral–neutral reactions rapidly transform all elemental oxygen in the molecular gas into water vapour [73,74]:

$$\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H} \quad (E_a = 3160 \text{ K})$$

(3.2)

and

$$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H} \quad (E_a = 1660 \text{ K}).$$

(3.3)

\(^2\)Two measurements using a storage ring give roughly consistent results [58,59]. We provide here the latest measurement: $f_1 = 0.25$, $f_2 = 0.14$, $f_3 = 0.60$ and $f_4 = 0.01$. Using a different technique (flowing afterglow), Williams \textit{et al.} [60] find $f_1 = 0.05$, $f_2 = 0.36$, $f_3 = 0.29$ and $f_4 = 0.30$.

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This mechanism (along with evaporation of water ice) will keep water vapour as the dominant oxygen component when the gas temperature exceeds approximately 300 K [75].

4. H$_2$O in star and planet formation

Prior to Herschel the observational perspective of water vapour pointed to some intriguing issues with respect both to its disposition as solid or vapour and to its destruction. ISO found clear evidence for hot water associated with shocks but also perhaps isolated in the hot cores of both low- and high-mass stars (see the reviews of van Dishoeck [4] and Nisini et al. [57]). SWAS and Odin discovered that cold water vapour is less abundant than expected from pure gas-phase chemistry, hinting at a role of freeze-out and ice formation [3,76]. Spitzer was readily suited to search for water emission in young protoplanetary discs [56]; while all of the above was supplemented by ground-based observations using masing transitions in open atmospheric windows or by observing isotopologues that have lower abundance. In the following, we attempt to note the important contributions from the various space-based platforms. However, in general, we will highlight more recent results. Thus, we will focus in large part on the advantages of Herschel to probe hot, warm and cold water, but also the ability to spectrally resolve the line profiles with sensitivity. In the following, we will trace our knowledge of water from the large parsec-sized cloud scale down to an astronomical unit within the terrestrial planet-forming regions of circumstellar discs.

(a) Clouds

Molecular clouds are extended on large, degree-sized, spatial scales, which makes it difficult to probe the full extent of water emission. The largest water maps in existence are the maps of Orion obtained using weak masers observed from the ground [77,78] and the o-H$_2$O ground state by SWAS [79] and Odin [80]. An additional map was made of M17 [81]. These maps demonstrate that water emission is present on approximately 1 pc size scales. However, this does not correspond to the cloud as traced by $^{12}$CO, but rather on scales more representative of the denser star-forming cores traced by C$^{18}$O. Based on analysis of these data, the average water abundance is found to be rather low (approx. $10^{-8}$ [76]) and consistent with models that include the formation of water ice mantles and the freeze-out of water [61,67,68]. Analysis of the masing transitions hinted at higher abundances [77,78], suggesting that there might be an abundance gradient along the line of sight.

Detailed comparisons of the water emission distribution and other gas-phase tracers suggest that water is not tracing the volume of the cloud, but rather is present mainly on the surface [79]. Since the dust temperatures on the surface are still below that of the sublimation temperature of water ice, this has brought the focus onto the potential impact of non-thermal methods to desorb the frozen water molecules. Recent modelling efforts have focused on whether photodesorption might be responsible for the observed water vapour. Such models have been found to be consistent with earlier SWAS results [72]. Thus, water vapour is photodissociated on the exposed surface of the core, but as the radiation field decays deeper in the cloud, water vapour is found within a layer
where photodesorption of ice is balanced by photodissociation of gas. Deeper into the cold \((T \sim 10–20\,\text{K})\) core, the water is predominantly found as ice. It is this type of model that will be directly tested by additional \textit{Herschel} observations that hint at the link between the grain physics and the chemistry (figure 2).

\subsection*{(b) Pre-stellar cores}

Lacking the presence of a central stellar source that releases radiative and kinetic energy, low-mass pre-stellar dense cores provide excellent laboratories to test the basic gas/solid-state physics and chemistry prior to stellar birth. This is strengthened by the fact that the physical structure (density and temperature) is fairly well constrained from observations of dust thermal continuum emission \cite{19,82}, which readily allows for exploration of molecular abundances. Since temperatures are approximately 10K, there is the general expectation that freeze-out will dominate the chemistry. Indeed, these sources exhibit wide-spread evidence for gas-phase abundance depletions of species less volatile than water, such as CO, which confirms this interpretation (see \cite{8,24}, and references therein). Previous observations by \textit{SWAS} and \textit{Odin} had set very low abundance limits in agreement with the dominance of freeze-out \cite{83,84}, and a large amount of water present as ice \cite{85}.

Initial surveys by \textit{Herschel} focused on detecting the ground-state line of o-H$_2$O in two template objects, B68 and L1544 \cite{86}. In the case of B68, no emission was found with a 3\(\sigma\) limit on the abundance \(x(\text{o-H}_2\text{O}) < 1.3 \times 10^{-9}\) (relative to H$_2$). In figure 3, we show the spectrum of L1544 along with objects at different evolutionary stages. As seen in the expanded view of the spectrum, coincident with the source velocity, there is a surprising detection of water in absorption. This absorption is seen at the 5\(\sigma\) level and represents the first detection of water vapour in a cold \((T \sim 10\,\text{K})\) object. Initial analysis suggests that the water abundance peaks 0.1pc away from the core centre, with an abundance approximately \(10^{-8}\), again with water inferred to be present mostly in the form of ice \cite{86}. A deeper observation of this line towards L1544 is planned to confirm this result.

\subsection*{(c) Protostars and outflows}

\subsubsection*{(i) Low-mass star-forming regions}

Low-mass solar-type protostars are important in tracing the stage where the star builds up its mass and the disc forms from the collapsing envelope. An important aspect of water in these regions is the expected large abundance \((\gtrsim 10^{-4}, \text{relative to H}_2)\) of water vapour that might result from evaporating ices or high-temperature reactions. This large abundance would lead water to be an important coolant both in the inner envelope close to the star \cite{88} and also in the outflow \cite{75}. Thus, water can participate in the physics of collapse and mass ejection. Initial studies by \textit{ISO} found evidence for strong water emission and high abundances, with water playing an important role as a gas coolant \cite{89,90}. However, the exact disposition of the water was in doubt. One theory posited the water as tracing molecular outflows \cite{91,92}; other theories favoured the inner collapsing envelope, which is warm enough to evaporate ices \cite{89,93}, or perhaps is due to envelope accretion shocks \cite{94}. High spectral resolution observations...
Figure 2. Integrated intensity map of the Orion molecular ridge in $1_{10}-1_{01}$ 556.9 GHz transition using SWAS and taken from Melnick et al. [79]. The starred numbers within the spectra in the inner square indicate the values by which the antenna temperatures have been divided so that the scaled spectra fit within this plot.
Figure 3. The $^{1}\text{H}_2\text{O}$ emission spectra obtained with *Herschel*/HIFI spanning evolutionary stages that trace the formation of low-mass stars and planets. The pre-stellar core L1544 is shown on top, along with an expanded view of the central regions of a baseline-subtracted spectrum near the system velocity. The middle spectrum illustrates the strong and broad emission seen towards the Serpens SMM1 protostar. The bottom spectrum shows the tentative detection towards the DM Tau protoplanetary disc along with an expanded view near the systemic velocity. In the case of the blow-up region of L1544 and DM Tau, the systemic velocity is given as a dashed line. Each of these spectra has been presented and analysed previously [86,87]. (Online version in colour.)

by SWAS and Odin found evidence for broad line wings in the spectrum of ortho-$\text{H}_2\text{O}$ $^{1}_1\text{H}_2\text{O}$ towards representative protostars [95,96]. This is clearly associated with the outflow, but the low spatial resolution hampered any search for emission associated with the protostar.

A *Herschel* survey of water emission towards protostars reveals that water emission is quite common and dominated by outflows/shocks [97–99]. One sample spectrum of a low-mass protostar as seen by *Herschel* is given in figure 3, where we show the o-$\text{H}_2\text{O}$ $^{1}_1\text{H}_2\text{O}$ transition observed towards Serpens SMM1. This spectrum shows representative features—a broad line profile with full width at half-maximum of greater than 20 km s$^{-1}$ and evidence for a narrow absorption feature at the systemic velocity, both with line widths (at half-maximum) of...
approximately a few km s\(^{-1}\). A survey of over 29 objects in the ground-state line of o-H\(_2\)O finds similarly complex profiles, with broad emission lines and narrow absorption/emission. Higher excitation lines are present, but also are found to have broad (greater than 10 km s\(^{-1}\)) line widths \([97,99]\). Even the lines of H\(_2\)\(^{18}\)O, a factor of \(\sim 500\) less abundant, are still broad.

In all we have learned that water emission in low-mass sources shows a clear dominance of emission from the outflowing gas. This emission is attributed to shocks in the inner envelope, and analysis suggests that the abundance ratio of H\(_2\)O/CO increases with velocity, with water trapping approximately 5–10% of the available oxygen at the highest velocities \([97]\). The narrow emission/absorption components from the envelope are consistent with abundances of approximately \(10^{-8}\) (relative to H\(_2\)). This is comparable to that seen in pre-stellar cores and again points to the importance of water ice and freeze-out. Deep searches for high-\(J\) H\(_2\)\(^{18}\)O have begun to reveal water in the inner envelope, but abundances (approx. \(10^{-5}\), relative to H\(_2\)) appear to be lower than the expected value of \(10^{-4}\) \([100]\).

The picture of water in low-mass stars is not complete without looking beyond the central pixel associated with the protostar. Low-mass sources are well known to have extended bipolar outflows that have been traced in a variety of species, including H\(_2\)O \([12]\). The direct association of water with molecular outflows is shown in the beautiful emission map of the 179 \(\mu\)m line of o-H\(_2\)O seen towards L1157 \([101]\), which is given in figure 4. Analysis of these data shows that water is closely associated with hot H\(_2\) emission associated with the flow \([102]\), and with other shock tracers such as SiO. The H\(_2\) emission traces shocked gas with temperatures of approximately 300–1300 K, which is clearly capable of powering the neutral–neutral reactions discussed in §3, or perhaps water is formed via sputtering of the ices \([103]\). Regardless, for this source, water is formed in abundance \((x(H_2) \sim 10^{-5}–10^{-4})\) and is a major coolant in the high-velocity gas \([101,104]\). Whether this is representative of all molecular outflows is an outstanding issue and will be answered by additional Herschel WISH observations.

(ii) High-mass star-forming regions

Stars significantly more massive than our Sun are important in astronomy as they dominate the life cycles of galaxies. Moreover, young massive protostars are surrounded by a rich envelope of molecular material and are the chemically richest sources in the Milky Way \([34]\). In fact it has long been known, based on ground-based observations of H\(_2\)\(^{18}\)O, that massive hot cores harbour large amounts of water vapour \([105–107]\): this was further supported by ISO observations \([108–111]\). A sample of the rich ISO data of high-mass stars is shown in figure 5. Here, the 6 \(\mu\)m \(v_2\) band of water is observed in absorption towards Mon R2 IRS3. A comparison of model and data shows that the gas in the inner envelope is clearly hot and rich in water vapour, with abundances approximately \(10^{-5}\) \([112]\). One of the strengths of ISO was the ability to observe both the gas (shown here) and the solids \([64,113]\), and in high-mass sources the gas/solid ratio increases with temperature, hinting at some contribution from grain mantle evaporation \([112]\).

Figure 6 presents Herschel observations of Orion KL and W3 IRS 5, which are representative of massive star-forming cores. This illustrates several facets of these regions. First, because of the high temperatures, high densities \((n_{H_2} > 10^6 \text{ cm}^{-3})\)
and large gas columns ($>10^{23}$ cm$^{-2}$), numerous water lines can be detected. In Orion, the lines are strong enough to observe a suite of isotopologues with over 50 detected transitions \cite{114}. This is shown in figure 6a with detections of the $3_{21}-3_{12}$ transition of H$_2^{16}$O, H$_2^{18}$O, H$_2^{17}$O and HDO. This is even extended to a detection of HD$^{18}$O \cite{87}. Second, the line profiles are very complex, with different transitions having significantly different structures. In W3 IRS5, there is evidence for cold foreground absorbing spectral components (often more than one) superposed on broad (greater than 5–10 km s$^{-1}$) components arising from outflows and also from a zone within the envelope where ices are evaporated \cite{115}.

Models of the line emission use the standard procedure of estimating the physical structure from the overall dust emission and its spectral energy distribution \cite{116,117}. Within the envelope, the water abundance assumes a jump structure. When the dust temperature exceeds the sublimation temperature of water ice of approximately 100K, the abundance is elevated; this traces the hot core. In the colder outer envelope, the abundance is another variable, but is always found to be below that of the hot core. With these assumptions, some

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clear facts are emerging [115,118–120]. (i) The abundance of hot water in the inner hot core is elevated to high values greater than $10^{-5}$–$10^{-4}$ (relative to $H_2$). (ii) The outer envelope has water vapour abundances approximately $10^{-8}$, which is below that expected from pure gas-phase chemistry alone. This is interpreted to be the influence of the freeze-out of water onto the surfaces of dust grains.

Since massive star-forming regions are more distant, even the improved angular resolution of Herschel does not always provide a resolved picture of the bipolar outflows. Moreover, there is often more than one source within the telescope beam, which further complicates the analysis. However, in general, the molecular outflows are clearly associated with water emission as is evidenced by the broad line wings shown in figure 6. Detailed analysis of the Orion spectrum finds an abundance of approximately $10^{-4}$ [111,114], which confirms the important role that water plays as a major coolant in shocked molecular gas [75].

\(d\) Protoplanetary discs

What we have learned from our study of dense cores is that water is provided to the planet-forming disc primarily as ice. Within the disc itself, there is the potential for complex motions that could alter the water ice reservoir that originated from the parent cloud [121,122]. However, there is a general expectation for water vapour to exist inside the radius where the temperatures rise above the sublimation temperature. This is the so-called ‘snow-line’. Inside this radius, water is found in the gas phase and beyond the snow-line water resides predominantly as ice [123,124]. Despite the observational challenge of observing systems with small angular size (<1–2\′′), the distribution of water vapour in protoplanetary discs is now becoming clear.

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Figure 6. (a) Sample of the $3_{21}-3_{12}$ emission lines of water and its isotopologues around 1 THz detected towards Orion KL (from Melnick et al. [114]). (b) Selection of water lines observed towards W3 IRS5 (from Chavarría et al. [115]). (Online version in colour.)
Surveys of water vapour emission at near- to mid-infrared wavelengths using *Spitzer* ground-based telescopes have revealed that water is common around Sun-like stars [56,125,126]. A sample of the rich spectrum of emission lines seen towards the AA Tau protoplanetary disc is given in figure 7. These studies have shown that the emission arises from within 0.1–10 AU tracing gas temperatures of approximately 500–1000 K and with abundances that approach that of carbon monoxide. Because the disc surface is heated by stellar irradiation, it is likely that the emission arises from warm surface layers where water is produced *in situ* by the high-temperature reactions discussed in §3 [127,128]. Models of the emission suggest that it is truncated at radii in excess of 1 AU and that there is a lack of water vapour in the upper layers at larger radii [129]. As demonstrated in figure 1, the *Spitzer* wavelength range is optimized towards the detection of warm/hot water (\( T > 200 \) K) emission lines that will probe the terrestrial planet-forming region. *Herschel* observations will sample colder gas at larger radii and eventually will delineate the location of the water snow-line in a variety of systems. It is also worth noting that water vapour emission is generally lacking in the inner discs near young massive stars [126,130,131].

Beyond the snow-line, the disc temperature is below the sublimation point for water ice. However, theory predicts that photodesorption can provide a tenuous layer of water vapour on the disc surface [71]. Since UV photons are plentiful in young stars that are still accreting from the circumstellar disc [132], this provides for the possibility to find water at large distances from the star. Results from a detailed model of the chemistry are shown in figure 8. This model shows

![observed AA Tauri spectrum](image)

*Figure 7. Infrared spectrum of the classical T Tauri star AA Tau taken by the *Spitzer Space Telescope*. Vibrational modes of C$_2$H$_2$, HCN and CO$_2$ along with a transition of [Ne II] are labelled. Diamonds mark detections OH rotational transitions. Numerous rotational transitions of water vapour (not marked) are spread throughout the spectrum. Figure and discussion published by Carr & Najita [56].*
the layer of photodesorbed water that exists above the water-ice-rich (water-vapour-depleted) midplane. Given that the gas temperatures are below 100 K, the strongest emission lines lie in the far-infrared wavelengths (figure 1). A search for this emission was reported by Bergin et al. [133]. A very tentative detection was reported in the o-H$_2$O (1$_{10}$–1$_{01}$) ground-state transition, which is shown in figure 3. The interesting aspect from these observation was that the models shown in figure 8 predict emission lines in excess of the observational limits. A possible answer to this issue is if the upper layers that are exposed to UV have, over time, become depleted in the water-ice-coated grains. A detection of water vapour in this cold layer will be reported by Hogerheijde [135]. Regardless, these observations support the picture of the outer discs being dominated by ice.

5. Summary

This high-level overview overlooks many of the numerous details or unknowns that are still present. For example, we are only now grappling with the full distribution of water along the line of sight and what types of shocks (and where) the water is forming. Moreover, the role of radiation is clearly important as a mechanism to release frozen water via photodesorption, but models need to be more directly confronted with observations in a range of environments. Radiation is also important for the destruction of water and limiting its abundance, but peering close to heavily embedded objects or in the interiors of protoplanetary systems is difficult. More observations and theory will be needed to tease out the exact ways water forms and is destroyed. Nonetheless, it is fair to state that, over the past 20 years, we have undergone a revolution in our understanding of water in star-forming regions and portions of the water cycle have been revealed. The early evolutionary stages are dominated by the formation of a water-ice mantle that traps a significant ($\gtrsim 10\%$) amount of the available oxygen. Thus, the gas-to-solid
ratio prior to stellar birth is low, $\frac{H_2O_{\text{gas}}}{H_2O_{\text{ice}}} \sim 10^{-4} - 10^{-3}$. When a star is born, several things happen: (i) The water in the inner envelope evaporates, but may be limited by stellar radiation. (ii) Water is clearly formed and associated with gas that is in motion. Put another way, water is associated with shocks in the outflowing gas—both close to the star and in the bipolar flow at greater distances. This dominates the water vapour emission profile. (iii) Water is provided to the planet-forming disc predominantly as ice. Within the disc itself, water is clearly present and a snow-line or evaporation front on the disc surface is inferred to be present, but the exact location of the snow-line in the disc midplane is yet to be constrained. Ice again dominates the disc mass and it is possible that it originated in the pre-stellar core before the star was born.

This work summarizes the current state of the art regarding our knowledge of water beyond the Solar System. This summary would not have been possible without the fantastic work of the instrument builders of the various space missions outlined above and we are exceedingly grateful for their efforts. Similarly we are grateful to chemical physicists for providing a wide array of grounding data (collision rates, frequencies, line strengths, solid-state properties, etc.) that are needed for proper interpretation. We are also grateful for the excellent work of the Herschel HEXOS, WISH and CHESS teams, whose initial results are given above. The authors thank L. Kristensen for providing reduced Herschel data as needed for display. The work of E.A.B. is supported by funding from NASA through an award issued by JPL/Caltech (Herschel GTO). E.v.D. is supported by NOVA, by a Spinoza grant and grant 614.001.008 from NWO, and by EU FP7 grant 238258.

References


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120 Marseille, M. G. et al. 2010 Water abundances in high-mass protostellar envelopes: Herschel observations with HIFI. *Astron. Astrophys.* 521, L32. (doi:10.1051/0004-6361/201015103)


