Herschel / HIFI observations of CO, H₂O and NH₃ in Mon R2*,**

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Preprint online version: May 1, 2014

ABSTRACT

Context. Mon R2, at a distance of 830 pc, is the only ultracompact H ii region (UCH ii) where the associated photon-dominated region (PDR) can be resolved with Herschel. Owing to its brightness and proximity, it is one of the best-suited sources for investigating the chemistry and physics of highly UV-irradiated PDRs.

Aims. Our goal is to estimate the abundance of H₂O and NH₃ in this region and investigate their origin.

Methods. We present new observations ([C ii], 12CO, 13CO, C₁₈O, o-H₂O, p-H₂O, o-H$_{18}$O and o-NH₃) obtained with the HIFI instrument onboard Herschel and the IRAM-30 m telescope. We investigated the physical conditions in which these lines arise by analyzing their velocity structure and spatial variations. Using a large velocity gradient approach, we modeled the line intensities and derived an average abundance of H₂O and NH₃ across the region. Finally, we modeled the line profiles with a non-local radiative transfer model and compared these results with the abundance predicted by the Meudon PDR code.

Results. The variations of the line profiles and intensities indicate complex geometrical and kinematical patterns. In several tracers ([C ii], CO 9−8 and H₂O) the line profiles vary significantly with position and have broader line widths toward the H ii region. The H₂O lines present strong self-absorption at the ambient velocity and emission in high-velocity wings toward the H ii region. The emission in the o-H$_{18}$O ground state line reaches its maximum value around the H ii region, has smaller linewidths and peaks at the velocity of the ambient cloud. Its spatial distribution shows that the o-H$_{18}$O emission arises in the PDR surrounding the H ii region. By modeling the o-H$_{18}$O emission and assuming the standard [O II]/[O I] = 500, we derive a mean abundance of o-H$_{18}$O of ~10⁻⁸ relative to H₂. The ortho-H₂O abundance, however, is larger (≈1×10⁻⁸) in the high-velocity wings detected toward the H ii region. Possible explanations for this larger abundance include an expanding hot PDR and/or an outflow. Ammonia seems to be present only in the envelope of the core with an average abundance of ~2×10⁻⁹ relative to H₂.

Conclusions. The results in this region and investigate their origin. To explain the water and ammonia abundances in the rest of the cloud, the molecular freeze out and grain surface chemistry would need to be included.

Key words. ISM: structure – ISM: molecules – ISM: individual object: Mon R2 – H II regions – ISM: photon-dominated region (PDR) – Submillimeter

1. Introduction

Although the processes that lead to the formation of massive stars are still not fully understood, it is generally agreed that massive stellar objects are formed by the collapse of a dense molecular cloud into one or multiple self-gravitating pre-stellar objects. Once the star is born, the innermost layers of the molecular cloud are heated and ionized by the strong UV radiation field, producing what is called an ultra compact H ii region (UCH ii). These regions are characterized by extreme UV irradiation and very small physical scales (≪0.1 pc), and are embedded in dense molecular clouds with gas densities often higher than 10⁶ cm⁻³ (Hoare et al. 2007). Whereas the H-ionizing radiation is absorbed in the H ii region, UV radiation carrying energies less than 13.6 eV penetrates deeper into the molecular cloud, producing a so-called photo-dissociation region (PDR). In these regions, the chemistry and the physics are driven by the extreme impinging radiation field (more than 10⁵ times the Habing field.

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* Herschel is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

** Based on observations carried out with the IRAM 30m Telescope. IRAM is supported by INSU/CNRS (France), MPG (Germany) and IGN (Spain).
Table 1. Summary of HIFI and 30m observations

| Line               | ν [GHz] | HPBM ['"] | η \textsuperscript{a} | Telescope |
|--------------------|---------|------------|------------------------|-----------|
| \(^{12}\text{CO} (9\rightarrow8)\) | 1036.912 | 20.4 | 0.77 | Herschel |
| \(^{13}\text{CO} (2\rightarrow1)\) | 220.398 | 10.0 | 0.67 | IRAM     |
| \(^{13}\text{CO} (5\rightarrow4)\) | 550.926 | 38.5 | 0.79 | Herschel |
| \(^{13}\text{CO} (10\rightarrow9)\)| 1101.349 | 19.3 | 0.77 | Herschel |
| \(^{13}\text{O} (2\rightarrow1)\) | 219.560 | 10.0 | 0.67 | IRAM     |
| \(^{13}\text{CO} (5\rightarrow4)\) | 548.830 | 38.6 | 0.79 | IRAM     |
| \(\text{o-H}_2\text{O} (10_0 \rightarrow 10_1)\) | 556.936 | 38.1 | 0.79 | Herschel |
| \(\text{p-H}_2\text{O} (11_1 \rightarrow 00_0)\) | 1113.343 | 19.3 | 0.77 | Herschel |
| \(\text{o-H}_2\text{O} (11_{10} \rightarrow 12_{00})\) | 547.676 | 38.0 | 0.79 | Herschel |
| \(\text{o-NH}_3 (1_0 \rightarrow 0_0)\) | 572.498 | 37.0 | 0.79 | Herschel |
| \(\text{H} (42\alpha)\) | 85.688 | 29 | 0.63 | IRAM     |

\[^{(a)}\) \eta = B_{\text{eff}} / F_{\text{eff}}.\]

Mon R2 has been targeted as part of the Herschel guaranteed-time key program “Warm and Dense Interstellar Medium” (WADI, PI: V. Ossenkopf) as prototype of UC H\textsc{ii} regions. The first Herschel observations of this source were presented by Fuente et al. (2010), who reported the detection of several far-IR/sub-mm lines, including \(^{12}\text{CO} ( \rightarrow8)\) 1,1→0,0, toward the so-called molecular peak (hereafter MP, see Fig. 1). On the basis of these observations they estimated an average water abundance across the PDR of \(\sim 2 \times 10^{-9}\) relative to H\(_2\). This value is slightly higher than that obtained by Snell et al. (2000), which was based on lower angular resolution observations of the o-H\(_2\)O ground state line with SWAS \((\sim 2 \times 10^{-9}\) relative to H\(_2\)).

In this paper we present new Herschel observations and complementary mm data obtained at the IRAM-30m telescope to improve our knowledge of the molecular gas surrounding the H\textsc{ii} region, and investigate the origin of the CO, H\(_2\)O and NH\(_3\) emission in more details.

2. Observations

Table 1 summarizes the observed transitions with the corresponding frequencies, beam sizes, and beam efficiencies\(^1\). In this paper, the intensity scale is main beam temperature \((T_{\text{mb}})\), and offsets were calculated relative to the ionization front (hereafter IF: RA\(_{2000}\)=06\(^{h}\)07\(^{m}\)46.2\(^{s}\); DEC\(_{2000}\)=06\(^{\circ}\)23\(''\)08.3\(''').

2.1. Herschel observations

The Herschel (Pilbratt et al. 2010) observations presented here were obtained with the heterodyne instrument for the far infrared HIFI (de Graauw et al. 2010) as part of the WADI guaranteed-time key program (Ossenkopf et al. 2011). A single local oscillator (LO) configuration allowed us to simultaneously observe the o-H\(_2\)O (10→9) and \(^{13}\text{CO} (10→9)\) lines. A third LO setting allowed us to observe the o-H\(_2\)O (10→9) line as well as the \(^{13}\text{CO} (5→4)\) and C\(^{18}\)O (5→4) lines. Finally, dedicated setups were used for the \(^{12}\text{CO} (9→8)\) line and the [C\(_{\text{ii}}\)] line. All lines were observed in one strip across the region, oriented 4\(^{5}\) (east of north). The [C\(_{\text{ii}}\)], o-H\(_2\)O, p-H\(_2\)O and \(^{13}\text{CO}\) strips extend 2\(''\) in each direction relative to the IF (see Fig. 1). To achieve a better signal-to-noise ratio (S/N) in the o-H\(_2\)O (10→9) line, this strip extended for only \(\sim 1''\) on each side of the IF. The strips were obtained using the on-the-fly (OTF) observing mode using Nyquist sampling and with the reference position at the offset (+10'; 0''), which is free of emission.

The basic data reduction was performed using the standard pipeline provided with the version 7.0 of HIPE\(^3\) (Ott 2010) and then exported to GILDAS/CLASS (Pety 2005) for a more detailed analysis. For the \(^{13}\text{CO} (10→9)\) and p-H\(_2\)O (11→10) lines we subtracted a secondary OFF spectrum obtained at a position located at the NE end of the strip that is free of emission. Typical noise rms values are \(\sim 20\) mK (o-H\(_2\)O and o-NH\(_3\)), \(\sim 0.2\) K \(^{13}\text{CO}\), \(\sim 20\) mK \(^{13}\text{CO} 10→9\) and p-H\(_2\)O), \(7\) mK (o-H\(_2\)O), \(^{13}\text{CO} 5→4\) and C\(^{18}\)O 5→4) and 1 K ([C\(_{\text{ii}}\)]), all calculated at the resolution of 0.7 km s\(^{-1}\).

\(^1\) http://herschel.esac.esa.int/Docs/TechnicalNotes/HIFI_Beam_Efficiencies_17Nov2010.pdf
\(^2\) http://www.iram.es/IRAMES/mainWiki/Iram30mEfficiencies
\(^3\) HIPE is a joint development by the Herschel Science Ground Segment Consortium, consisting of ESA, the NASA Herschel Science Center, and the HIFI, PACS and SPIRE consortia.
Because HIFI is a double-sideband receiver, but all our spectra are calibrated to the single-sideband scale, the continuum levels need to be corrected for the contribution from the image sideband. For all our spectra, we can assume a sideband gain ratio of unity (Roelfsema et al. 2012), so that the continuum level needs to be divided by a factor two. After this correction, the continuum levels toward the IF are 0.25 and 0.5 K at 550 GHz and 1110 GHz, respectively. The \([\text{C}^{18}\text{O} 2\rightarrow 1]\) lines present an arclike structure opened in steps of 2 K km s\(^{-1}\), tracing the H\(^{\text{ii}}\) region. Squares represent the positions of the ionization front (IF) and the molecular peak (MP), whereas the triangles represent the points of the observed strip (dashed line) for \(13\text{CO} (9\rightarrow 8)\), H\(_2\)O and NH\(_3\) that are studied in this work. The infrared sources are indicated with black stars.

### 2.2. IRAM-30m telescope observations

The observations of the \(^{13}\text{CO} (2\rightarrow 1)\) and \(^{18}\text{O} (2\rightarrow 1)\) were performed in February and March 2009 using the HERA 3x3 1 mm receiver array at the IRAM-30m telescope located at Pico de Veleta (Granada, Spain). The observations were performed in OTF mode with the same OFF position as above. The spectrometer was the VESPA autocorrelator, configured to provide a spectral resolution of 40 kHz. Typical noise \(\text{rms}\) values are 0.2 K for both the \(^{13}\text{CO}\) and \(^{18}\text{O}\) lines. The integrated intensity maps are shown in Fig. 1. In a different observing run, in July 2009, we observed the H\({}\alpha\) recombination line at 85.688 GHz. The spectrometer was the WILMA autocorrelator, which provides a fixed spectral resolution of 2 MHz, ~7 km s\(^{-1}\) at this frequency. The noise \(\text{rms}\) value of these observations is ~0.05 K.

### 3. Results

Figure 1 displays the integrated emission of the \(^{13}\text{CO}\) and \(^{18}\text{O}\) 2\(\rightarrow\)1 lines in a 160\(^\prime\)\(\times\)160\(^\prime\) field centered at the IF. The emission of the \(^{18}\text{O}\) 2\(\rightarrow\)1 line presents an arclike structure opened to the NW, with several peaks that correspond to regions of enhanced gas density as evidenced by other high-density tracers (Choi et al. 2000; Rizzo et al. 2003). The shape of the integrated intensity of the \(^{13}\text{CO} 2\rightarrow1\) line is similar, although the emission is somewhat more extended and less sensitive to individual clumps. Although it shows some symmetry, the gas detected in \(^{18}\text{O}\) shows an elongated structure extending northeast of the IF. The HIFI strips follows this structure so that individual clumps are likely to influence the emission of far-IR lines in this direction rather than toward the SW, where the molecular emission is more compact.

In the same figure, we present the integrated intensity of the H\({}\alpha\) recombination line, which traces the H\(^{\text{ii}}\) region. The large beam (~29\(^\prime\) half-power beam width, HPBW) of the 30m telescope at this frequency hinders the detection of the small-scale morphology of this UC H\(^{\text{ii}}\) region. The peak intensity of the H\({}\alpha\) line is located \(\approx 3\)\(^\prime\) northwest of the IF and the emission extends in a radius of about 20\(^\prime\). Taking into account the large beam of the 30m telescope at this frequency and typical pointing errors of 1\(^\prime\)–2\(^\prime\), we do not consider that this shift is significant.

#### 3.1. Kinematics

Figure 2 shows the HIFI spectra observed at different offsets along the strip and Fig. 3 displays their position-velocity (PV) diagrams. Several lines ([\text{C}^{18}]), \(^{13}\text{CO} 9\rightarrow8\), o-H\(_2\)O and o-NH\(_3\)) are detected across the entire strip up to a distance of \(\approx 100\)\(^\prime\). The intensity and velocity structures show systematic variations along the strip, which can be summarized as follows:

1. The [\text{C}^{18}] line is most intense and broader toward the UC H\(^{\text{ii}}\) region, where it covers the velocity range from 0 to 20 km s\(^{-1}\). Outside the UC H\(^{\text{ii}}\) region, the [\text{C}^{18}] emission remains detected but in a narrower velocity range, between 7 and 15 km s\(^{-1}\). A probable origin of the high-velocity gas around the UC H\(^{\text{ii}}\) region is a dense PDR layer, accelerated by the radiative pressure from the central source, where carbon is ionized. The extended and narrower emission is likely related to the first quiescent layers of the molecular cloud or to layers in the external envelope.
2. The \(^{13}\text{CO}\) and o-H\(_2\)O lines peak toward the UC H\(^{\text{ii}}\) region and high-velocity wings are detected in the direction of the
Fig. 2. Raw spectra of the HIFI observations along the cut indicated in Fig. 1. The continuum has not been subtracted so that the off-set in the intensity scale represent the observed continuum. This needs to be divided by two because of the double sideband observations.

ionized gas. Emission in the line wings is also detected at larger offsets toward the southwest (see offset [-40″, -40″]) in Figs. 2 and 3). The origin of this highly accelerated gas is difficult to determine: at small offsets it may be associated to the same expanding layer that emits in [C ii], whereas the wings toward the southwest are more likely related with the molecular outflow mapped by Xu et al. (2006). Yet the outflow may also contribute to the broad emission toward the H ii region.

3. The C^{18}O and H$_2^{18}$O and NH$_3$ lines have relatively narrow line widths (between 2.5 and 3.1 km s$^{-1}$) all along the strip. The $^{13}$CO, C$^{18}$O and H$_2^{18}$O lines peak a few arcsec northeast of the IF, whereas the NH$_3$ emission presents a dip toward the IF and peaks southwest. This extended emission is consistent with the overall structure of the cloud traced by the $^{13}$CO and C$^{18}$O (2 → 1) lines, which present an elongated structure in the NE-SW direction. The dip in the NH$_3$ emission corresponds to a valley in the molecular bar traced by C$^{18}$O (2 → 1).

4. An absorption feature is detected in H$_2$O at the velocity of the molecular cloud, ≈ 11.5 km s$^{-1}$, toward the UC H ii region, which likely originates in the same quiescent gas that is emitting for instance in NH$_3$ and C$^{18}$O. The [C ii] spectra also show a self-absorption feature centered at ≈ 12 km s$^{-1}$ but its origin is more doubtful. In other cases we do not detect the self-absorption feature.

5. All CO and NH$_3$ lines show a systematic shift of their peak velocities, which suggests that the expansion is not isotropic, and/or that a slow rotation (v$_{rot}$ ≈ 0.5 km s$^{-1}$, Loren 1977) of the cloud may be ongoing.

Summarizing, these observations suggest that the high-velocity wings are coming from a gas that is pushed away from the H ii region. This gas could be associated either to the innermost layers of the expanding PDR, the outflow, or both. On the other hand, the emission and the absorption at central velocities of H$_2$O and H$_2^{18}$O, as well as the NH$_3$ and the low-J (J$_{up}$ ≤ 5) CO emission are more likely related to the interface of the PDR with the molecular cloud and to the bulk of the molecular cloud, respectively. In the following sections, we model the emission from CO and isotopologues, H$_2$O and NH$_3$ with different degrees of approximation to derive the physical conditions.
at which they arise and derive an estimate of their abundances. The detailed analysis of the \[\text{CII}\] line is postponed for a more detailed study that includes the \[\text{[CII]}\] observations (Pilleri et al., in prep.).

4. LVG modeling
In this section, we present local radiative transfer calculations to determine the water and ammonia abundance toward Mon R2, by assuming a uniform density and temperature layer. This approach is somewhat simplistic because different phases of gas are mixed along the line of sight, but gives a first rough estimate of the water and ammonia abundance as a function of the physical conditions in the beam.

For the sake of simplicity, we separated the line profiles into three velocity intervals, and analyzed each of them independently. This allowed us to separate the optically thick and self-absorbed part of the line profiles from the optically thin wings. The velocity intervals are defined as follows:

- $\Delta v_b = [4.5\text{-}8.5] \text{ km s}^{-1}$,
- $\Delta v_c = [8.5\text{-}12.5] \text{ km s}^{-1}$,
- $\Delta v_r = [12.3\text{-}20.5] \text{ km s}^{-1}$.

For each of the velocity intervals, we used a large velocity gradients (LVG) code to fit the line intensities and estimate the column densities and abundances of H$_2$O (MADEX, Cernicharo 2012) and NH$_3$ (RADEX, van der Tak et al. 2007). Table 2 shows the averaged main beam temperature measured per velocity interval ($< T_b > = \frac{1}{\Delta v} \int T_{mb} \, dv$) observed toward the IF. The gas column densities toward the IF were obtained by fitting the intensity of the optically thin C$^{18}$O (2→1) and (5→4) lines as well as their ratio. Gas densities and kinetic temperatures were varied in a reasonable range for this region ($n_H = 10^4\text{-}10^7$ cm$^{-3}$, $T_k = 40\text{-}500$ K) and the grid was repeated for different values of the beam filling factor and abundance.

4.1. H$_2^{18}$O emission
We modeled the intensity of the optically thin line o-H$_2^{18}$O (1$_{1,0}\text{-}0_{1,1}$) to obtain a first estimate of the water abundance in $\Delta v_c$. We fit the intensities of the C$^{18}$O (5→4) and o-H$_2^{18}$O (1$_{1,0}\text{-}0_{1,1}$) lines and their ratio, assuming a standard isotopic ratio $^{16}$O/$^{18}$O=500 and a $^{12}$CO abundance relative to H$_2$ of $X(^{12}$CO) = $1 \times 10^{-4}$. We used the new collisional rate coefficients by Daniel et al. (2011) for o-H$_2$O and Yang et al. (2010).
for CO. We also assumed an H$_2$ ortho-to-para ratio (OTP) of 3. Since the collisional coefficients of H$_2$O with ortho- and para-H$_2$ species are asymmetric, the results depend on the assumed OTP ratio. In particular, assuming a lower OTP ratio would result in the need of higher densities to excite H$_2$O.

Figure 4 shows the results of the LVG modeling. The intensities of the lines and their ratio can be reproduced reasonably well assuming a beam filling factor ($\eta_B$) of 0.1 or lower. Several solutions can be found with this $\eta_B$, corresponding to different density-abundance pairs. The line intensities can be fitted with several combinations of these two parameters, which reflects a degeneracy between the gas density and the water abundance. Considering the range of densities that are expected to be found in Mon R2, the solutions correspond to a water abundance between few $10^5$ cm$^{-3}$ and temperatures to be excited. We modeled the intensity of the o-NH$_3$ emission does not come from the innermost part of the PDR, but from the bulk of the molecular cloud.

To assume a beam filling factor of 1, however, is a limiting case, since the high-velocity wings are concentrated in the PDR around the UC H$\alpha$ region. A beam filling factor $\eta_B=0.1$ would correspond to the case of an emission region extending only in the plane of the sky with a thickness of $\sim2''$ and a diameter of $20''$, which is consistent with the size of the PDR traced by PAH emission around this region (Berné et al. 2009). Assuming these lower values of $\eta_B$, we found a water abundance $X$(o-H$_2$O) in the range $[10^{-6} - 10^{-7}]$ for reasonable physical conditions in this region ($\eta_B$, of several $10^3 - 10^4$ cm$^{-3}$ and $T_\text{K}$ between 50 and 100 K). These values of molecular hydrogen density are consistent with the physical conditions derived by Berné et al. (2009) on the basis of the purely rotational lines of H$_2$ that trace the PDR. This supports the scenario of an expanding PDR in which the highest velocities are associated to the molecular gas closer to the UC H$\alpha$ regions, i.e., the warm HI/H$_2$ layer traced by the PAHs and the H$_2$ rotational lines. However, the possible contribution of an outflow component cannot be discarded, especially to the southwest, where the outflow detected by Xu et al. (2006) has its maximum emission.

### 4.2. H$_2$O emission

Because the H$_2$O lines are heavily self-absorbed at central velocities, we concentrated our LVG analysis on the emission in the red wings, in the velocity interval $\Delta_{\nu_c}$. Emission from $^{12}$CO (9-8) and o-H$_2$O (1$_{1,0}$→0$_{0,1}$) is expected to arise in similar physical conditions, because both lines need relatively high temperatures and densities to be excited. We modeled the intensity of the o-H$_2$O emission and the ratio $R_{H_2O}$ in the 9-8) to derive the water abundance in the line wings.

Assuming a beam filling factor $\eta_B=1$, which would imply an angular extension of the region emitting in the red wings of $\sim38''$, we only found solutions for o-H$_2$O abundances between $10^{-8}$ and $10^{-7}$ relative to H$_2$. The highest water abundance corresponds to a molecular hydrogen density of $\sim 5 \times 10^5$ cm$^{-3}$ and gas kinetic temperature of about 70 K. For an abundance $\sim 10^{-8}$, densities of several $10^5$ cm$^{-3}$ and temperatures $\sim 50$ K are needed to reproduce the measured line intensities. Since both set of values are within the range of physical conditions that we can accept for this region, we cannot easily distinguish between them.

To assume a beam filling factor of 1, however, is a limiting case, since the high-velocity wings are concentrated in the PDR around the UC H$\alpha$ region. A beam filling factor $\eta_B=0.1$ would correspond to the case of an emission region extending only in the plane of the sky with a thickness of $\sim2''$ and a diameter of $20''$, which is consistent with the size of the PDR traced by PAH emission around this region (Berné et al. 2009). Assuming these lower values of $\eta_B$, we found a water abundance $X$(o-H$_2$O) in the range $[10^{-6} - 10^{-7}]$ for reasonable physical conditions in this region ($\eta_B$, of several $10^3 - 10^4$ cm$^{-3}$ and $T_\text{K}$ between 50 and 100 K). These values of molecular hydrogen density are consistent with the physical conditions derived by Berné et al. (2009) on the basis of the purely rotational lines of H$_2$ that trace the PDR. This supports the scenario of an expanding PDR in which the highest velocities are associated to the molecular gas closer to the UC H$\alpha$ regions, i.e., the warm HI/H$_2$ layer traced by the PAHs and the H$_2$ rotational lines. However, the possible contribution of an outflow component cannot be discarded, especially to the southwest, where the outflow detected by Xu et al. (2006) has its maximum emission.

### 4.3. NH$_3$

We used the same approach to estimate the o-NH$_3$ abundance in $\Delta_{\nu_c}$. The profiles of the o-NH$_3$ lines are not self-absorbed, and can be used to obtain a direct estimate of the column density of this species for all velocity intervals. In contrast to water, the $R_{NH_3}$ ratio decreases at higher velocities, corroborating our interpretation that the NH$_3$ emission does not come from the innermost part of the PDR, but from the bulk of the molecular cloud.

We have fitted the intensity of the o-NH$_3$ line and its ratio to the C$^{18}$O (5→4) line using the collisional rate coefficients from Danby et al. (1988). The results for $\Delta_{\nu_c}$ are reported in Fig. 4. Assuming a beam filling factor of $\sim1$, consistent with the large extension observed with HIFI, our data are reasonably well re-

| Species | Units | $\Delta v_p$ [4.5-8.5] km s$^{-1}$ | $\Delta v_e$ [8.5-12.5] km s$^{-1}$ | $\Delta v_v$ [12.5-20.5] km s$^{-1}$ |
|---------|-------|-----------------|----------------|----------------|
| $^{13}$CO (2→1) | [K] | 0.58 | 2.93 | 0.093 |
| $^{13}$CO (5→4) | [K] | 0.29 | 2.93 | 0.08 |
| $^{12}$CO (9→8) | [K] | 5.11 | 24.86 | 2.83 |
| o-NH$_3$ (1$_{1,0}$→0$_{0,1}$) | [K] | $\ll0.01$ | 0.052 | $\ll0.01$ |
| $R_{NH_3}/^{12}$CO | - | 0.018 | - | - |
| X(o-NH$_3$)kR | - | [10$^{-8} - 10^{-7}$] | - | - |

* Self-absorbed profile.
produced with a density of \( \sim 10^4 \) – \( 10^5 \) cm\(^{-3}\), a gas kinetic temperature of \( \sim 50\)K and an ammonia abundance \( \sim 10^{-8} \) – \( 10^{-9}\). The opacity of the o-NH\(_3\) line are of the order of \( \tau \sim 10\), so the lines are very optically thick. Lower values of the NH\(_3\) abundances are associated to higher densities that have no evidence in MonR2.

5. A simple spherical model of MonR2

In this section, we test a simple geometrical model of the region to reproduce the observed line profiles. The model assumes an expanding spherical structure composed of concentric layers with given physical conditions (gas temperature and local density), kinematical information (turbulent and expansion velocities), and molecular abundances. We note in advance that with such a simple, spherically symmetric model is impossible to account for all asymmetries in the velocity structure of the observations, which may reflect large-scale structures such as the outflow, small-scale inhomogeneities (clumpiness) and other kinematical effects such as rotation. Yet, we propose it as a useful step toward a better understanding of this region.

In a first step, we fit the CO observations to fine-tune the physical structure of the molecular cloud and its associated PDR. This structure is then used to fit the H\(_2\)O observations by varying their abundance profiles across the cloud. To keep the model as simple as possible, we assume a double step-function abundance profile. For NH\(_3\), our observations consist of a single, optically thick line that does not provide a reliable probe of the detailed spatial distribution of the o-NH\(_3\) abundance, and we therefore exclude this molecule from this toy model.

### 5.1. The physical structure

The physical structure (in terms of the length of each layer, their density and temperature) is derived based on previous observational data and modeling (Berné et al. 2009; Fuente et al. 2010). A first estimate of the gas temperature was obtained using an up-
dated version (1.4.3) of the Meudon PDR code\(^4\) (Le Petit et al. 2006; Goicoechea & Le Bourlot 2007; Gonzalez García et al. 2008; Le Bourlot et al. 2012, cf. also Sect. 6.2 and Table 3).

The density structure in Mon R2 can be assumed to be similar to other PDRs associated to star-forming regions, such as NGC 7023 and the Orion Bar (Joblin et al. 2012, in prep.). The first layer \((\sim 1-2 \, \lambda_V)\) of the PDR is where most of the [C\(\text{ii}\)] and PAH emission originates from (Habart et al. 2003; Joblin et al. 2010; Pilleri et al. 2012). This is generally followed by a high-density layer (or “filament”) with \(n_H \geq 10^4 \text{cm}^{-3}\), which can be several magnitudes thick and is responsible for the emission in the high-J rotational lines of CO. Finally, the bulk of the molecular cloud is usually at a lower density, and accounts for the emission of molecular tracers that are easily photo-dissociated.

In our model, the outermost layer (3 mag thick) is heated from the outside, in agreement with the large large-scale PAH emission detected at \(8 \mu\text{m}\), which testifies to the presence of an external source of heating, especially to the north of the H\(\alpha\) region (Ginard et al. 2012).

In our spherical model, the central core of the ‘onion’ is represented by an H\(\alpha\) region with a very low density that is free of molecular gas. The H\(\alpha\) region is surrounded by a warm and relatively low-density expanding layer \((L_{\text{PDR}})\). For this layer we adopted the density derived by Berné et al. (2009) from the \(H_2\) rotational lines. The next layer is the high-density layer, \(L_{\text{HD}}\), which is extended for a few 0.001 pc (\(\sim 10\) mag) and is required to explain the emission of high wavelength molecular tracers such as CS, C-C\(\text{H}_2\) and HCO\(^+\) (Ginard et al. 2012).

Finally, everything is surrounded by a lower-density envelope, \(L_{\text{env}}\) (Fuente et al. 2010). The inner radius of the PDR, \(r_{\text{PDR}}\), is 0.08 pc (\(\sim 20\)″), is determined by the angular size of the H\(\alpha\) region, and the outer radius of the envelope, \(r_{\text{out}}=0.34\) pc, is fixed on basis of the extension of the 12\(\text{CO}\) 2\(\rightarrow\)1 and \(\text{C}^{18}\text{O}\) 2\(\rightarrow\)1 line emissions (Fig. 1). The values of \(r_{\text{PDR}}\) and \(r_{\text{HD}}\) are tuned to fit the CO (and isotopologues) lines. Summarizing:

\[
\begin{align*}
n_H(r) &= \begin{cases} 
2 \times 10^5 \text{cm}^{-3} & \text{if } r_{\text{PDR}} < r < r_{\text{HD}} \rightarrow L_{\text{PDR}} \\
3 \times 10^6 \text{cm}^{-3} & \text{if } r_{\text{PDR}} < r < r_{\text{HD}} \rightarrow L_{\text{HD}} \\
5 \times 10^4 \text{cm}^{-3} & \text{if } r_{\text{HD}} < r < r_{\text{out}} \rightarrow L_{\text{env}} 
\end{cases}
\end{align*}
\]

For the kinematics, we adopted the expansion velocity law

\[V_{\exp}(r) = V_{\text{out}} \times (r_{\text{out}}/r),\]

where \(r\) is the radial distance from the center of the sphere and \(V_{\text{out}}\) is the expansion velocity at \(r_{\text{out}}\). This law mimics the expansion velocity profiles commonly used to model H\(\alpha\) regions, with the surrounding envelope expanding at a lower velocity compared to the PDR and the H\(\alpha\) region (Lebrón et al. 2001).

Finally, we included a continuum source in our model to reproduce the fluxes measured with Herschel. The continuum fluxes toward the IF are well reproduced by a modified black body at the temperature of 500 K and with an opacity of 0.1 at 50 \(\mu\text{m}\), an exponent for the opacity law of 1 and a radius of 0.03 pc. This enables one to adequately fit the continuum levels toward the IF, but underestimates it at larger offsets. The presence of other continuum sources in the background might help to reproduce the continuum levels at large distance from the IF, but these are not included in our model for simplicity.

5.2. CO lines

We used our non-local radiative transfer code (Cernicharo et al. 2006b) to fit the line profiles at various offsets along the HIFI stripes. We adopted a standard 12\(\text{CO}\) abundance relative to \(H_2\) of \(10^{-4}\) and the isotopic abundance ratios of \(^{12}\text{C}/^{13}\text{C}=50\) and \(^{18}\text{O}/^{16}\text{O}=500\).

Assuming the density structure described above and the gas kinetic temperature derived with the Meudon PDR code, we fine-tuned the values of \(r_{\text{PDR}}\) and \(r_{\text{HD}}\) and the kinematical parameters to best reproduce the CO observations. The integrated intensities are well-fitted with \(r_{\text{PDR}}\) and \(r_{\text{HD}}\) being 0.082 pc and 0.083 pc, respectively. To improve the fit of the CO lines, the mean kinetic temperature of the outermost 3 mag of the cloud is set to 50 K, which corresponds to an external radiation field of \(G_0^{\text{ext}} \gtrsim 1\). This value is consistent with an extended PDR at a distance of \(\sim 100\)″, which is illuminated by the UV field produced by IRS1.

The best fit to the line profiles was obtained using the velocity law of Eq. 1 with \(V_{\text{out}} = 0.125 \text{km s}^{-1}\). We have also varied the turbulent velocities to improve the fit of the wings of the 12\(\text{CO}\) lines. The best solution is found with a turbulent velocity of 1 km s\(^{-1}\) in \(L_{\text{HD}}\) and 1.5 km s\(^{-1}\) in \(L_{\text{env}}\). To reproduce the high-velocity wings, we fixed the expansion and turbulent velocity in \(L_{\text{PDR}}\) to 2 km s\(^{-1}\) and 5 km s\(^{-1}\), respectively. We stress that because the model has so many parameters, other solutions may be found that reproduce the CO emission well, especially in the wings. Higher resolution observations will be very useful to improve our knowledge of the structure of this region. Figure 5 shows a summary of the physical structure and the velocity profile across the PDR.

Figure 6 displays the model results and the comparison with the observations. Although the overall quality of the low-J lines is very good, there are some discrepancies. The model falls short of the high-J \((J_{\text{up}} > 9)\) CO lines at offsets [-20″, -20″] to [+20″, +20″]. This is not unusual in PDR, because current PDR models fail to reproduce the intensity of the high-J lines of CO. There are various effects that can be invoked to explain this missing intensity, i.e. clumpiness and an erroneous description of the microphysics of PDRs, which may influence the heating and the chemistry of PDRs (Joblin et al. 2012, in prep). The presence of a high-velocity outflow, or the inclusion of rotation may all be possible ways to improve the fit. However, this accurate level of modeling is beyond the scope of this paper.

5.3. H\(_2\)\(^{18}\)O and H\(_2\)O

We used the physical and kinematical structure derived above to constrain the abundance of water in each layer of the cloud. We assumed an abundance profile defined as a double step-function and the standard ortho-to-para ratio of 3. We varied the abundances in the three regions to reproduce the line profiles of all H\(_2\)O lines.

The emission of H\(_2\)\(^{18}\)O is optically thin and does not present significant emission in the wings, and therefore its intensity is influenced mainly by the low-velocity layers \(L_{\text{HD}}\) and \(L_{\text{env}}\). We were able to reproduce the intensity and profile of this transition at all offsets by assuming an abundance \(X(\text{H}_2\text{O}) \approx 3 \times 10^{-6}\) in \(L_{\text{HD}}\) and 1 \times 10^{-8} in \(L_{\text{env}}\). These values are consistent with the results of the local LVG modeling assuming a beam filling factor \(\lesssim 0.1\) and with the previous estimate reported in Fuente et al. (2010). With the assumed physical structure, small variations of the water abundances (more than a factor of 2) from these values do not allow one to fit the observed intensities and spatial distribution. However, the main source of uncertainty is the assumed values for \(n_H\) and \(T_{\text{kin}}\). Considering the range of physical conditions that is observed in Mon R2, we can estimate our final error bars in the water abundances to be of one order of magnitude.

\(^4\) http://pdr.obspm.fr/PDRcode.html
Fig. 6. Comparison of the continuum-subtracted HIFI spectra (black) and the results of the non-local radiative transfer modeling (red) assuming a spherical symmetry for Mon R2.

With the same velocity profile, we tried to reproduce both the ortho- and para-H$_2$O lines at all offsets (See Fig. 6). However, both lines are very optically thick and variations in the morphology and kinematics of the cloud can strongly modify the line profiles. Therefore, we concentrated our efforts on the modeling of the red wings only, which are optically thin and therefore less sensible to small variations of the detailed velocity structure. To reproduce the line wings, we varied the abundance of H$_2$O in the layer $L_{PDR}$. Our best fit is obtained with an abundance of $X$(o-H$_2$O) $\approx 1 \times 10^{-7}$ in this layer, consistent with the results of the LVG modeling assuming a density of a few $10^4$ and high kinetic temperature (between 50 and 150 K). Similarly to H$_{18}$O, the main source of uncertainty for H$_2$O are the model parameters. However, the physical conditions in this layer are relatively well constrained (Berné et al. 2009) and the corresponding water abundances are in the range $[10^{-7} - 10^{-6}]$ relative to H$_2$. As mentioned above, the complete velocity profile of the main isotopologues is very dependent on the assumed kinematics and abundance. Therefore, it is difficult to obtain a very good fit of all spectra with a very simple model like ours. There are a few discrepancies between the observed H$_2$O profiles and the model. The observations are not symmetric between positive and negative offsets, and there is often an excess emission in the blue wings. These differences are most likely due to the unrealistic assumption that our cloud is perfectly spherical and symmetric under any point of view. The PV diagram of [C II] clearly shows that the kinematical pattern is not symmetric. The wings are wider at red velocities, probably because of the cometary shape of the nebula. In our model, we have used the red wings as the basis for our expansion pattern which is very likely incorrect for the blue part.

Summarizing, we derived a relatively constant ($1 - 3 \times 10^{-8}$) abundance of water in the high-density region and in the envelope, and a larger abundance ($1 \times 10^{-7}$) in the high-velocity gas. With these abundances, we obtained very good fits to all three water lines at the same time. With the assumed physical structure, the abundances are relatively well constrained (within a factor of 2), since small variations of the water abundance have a strong impact on all the lines. Larger variations from these values do not enable one to reproduce all the lines at the same time. However, since the density and velocity structure are not very well constrained and because of the degeneracy between density and abundance, we speculate that a reasonable uncertainty on the water abundance is one order of magnitude.
forming regions, Lefloch et al. (2010) studied the water emission in the bipolar outflow of L1157, determining a water abundance varying between few $10^{-7}$ in the warm and dense ($n > 10^7 \text{ cm}^{-3}$, $T_k \sim 100 \text{ K}$) extended part of the outflow and few $10^{-5}$ in the high-velocity hot component ($T_k > 100 \text{ K}$) that arises from the bow shock. Kristensen et al. (2010, 2011) derived similar abundances in the early stages of low-mass star-forming regions.

In agreement with previous estimates of the water abundance toward Orion KL based on the IRAM-30m telescope (Cernicharo et al. 1994) and ISO data (Cernicharo et al. 2006a), most recent observations with Herschel (Melnick et al. 2010) have derived a water abundance of $\sim 10^{-5}$ in the outflow, much higher than that derived in this work. Using spatially resolved PACS observations, Habart et al. (2010) derived an upper limit to the water abundance in the Orion Bar of a few $10^{-7}$. This value is very consistent with our results. Still unpublished data from the WADI consortium show that water is detected also in PDRs not associated with outflows, such as NGC 7023, Ced 201 and the Horsehead nebula (Teyssier et al., in prep.). The water abundance derived in the Horsehead nebula seems to be much lower than that in MonR2, most likely because the dust temperature is very low ($\sim 30 \text{ K}$), and sticking on grains is more efficient. Interestingly, in the PDR associated to the protoplanetary disk TW Hydra, Hogerheijde et al. (2011) derived an upper limit to the abundance of water of $0.5-2\times10^{-7}$, which is consistent with the values detected in the PDR of Mon R2.

Summarizing, the abundances measured in Mon R2 are lower than those obtained in shocked regions, similar to those observed in the outer layers of pre-stellar cores and the envelopes of young stellar objects, and consistent with the upper limit derived toward the Orion Bar.

### 6. Discussion

#### 6.1. H$_{2}$O abundances in MonR2 and the ISM

The results of the previous sections on the water abundance can be summarized as follows. In the gas at low velocities, the abundance of water is $<10^{-8}$ relative to H$_2$. The spatial distribution and the radiative transfer analysis of the H$_2$O line suggests that the low-velocity water emission arises in a region of enhanced density and relatively small volume centered toward the IF. This corresponds to the physical conditions of the high-density PDR proposed by Rizzo et al. (2003).

In the high-velocity gas, the abundance seems to be about an order of magnitude higher and the origin of the wing emission is more doubtful. In our simplistic ‘onion’ model of Mon R2, both the red emission and blue absorption are due to the expanding gas associated with the PDR surrounding the H$_n$ region (Rizzo et al. 2005; Fuente et al. 2010). In this scenario, the emission in the red wing of the $\alpha$-H$_2$O line would be related to the PDR around the UC H$_n$ region. This is consistent with the high-velocity wings observed in typical PDR tracers such as c-C$_3$H$_2$ and the small linewidth of shock tracers such as SiO (Rizzo et al. 2003). However, our simple model cannot reproduce the detailed spectral profiles of the H$_2$O lines. In particular, our model overestimates the blue-shifted emission at every position in the strip and it cannot reproduce the red wings at the offsets (-40",-40") and (-60",-60") (see Fig. 6). An asymmetric expanding PDR, and the contribution of the molecular outflow to the water line profiles are very likely the cause of this discrepancy.

The values derived in this work for the water abundances are similar to those commonly found in massive star-forming regions, and somewhat lower than those usually found in outflows and hot cores. In early-stage massive star-forming regions such as W3 IRS5, the abundance of water has been shown to vary between $10^{-9}$ in the outer and cold envelope and $10^{-4}$ in the inner hot cores (Chavarría et al. 2010). Concerning lower mass star-forming regions, Lefloch et al. (2010) studied the water emission in the bipolar outflow of L1157, determining a water abundance varying between few $10^{-7}$ in the warm and dense ($n > 10^7 \text{ cm}^{-3}$, $T_k \sim 100 \text{ K}$) extended part of the outflow and few $10^{-5}$ in the high-velocity hot component ($T_k > 100 \text{ K}$) that arises from the bow shock. Kristensen et al. (2010, 2011) derived similar abundances in the early stages of low-mass star-forming regions.

### 6.2. Comparison with gas-phase PDR chemical models

It is interesting to compare our observational results with the predictions of the Meudon PDR chemical model to understand where gas-phase chemistry is sufficient to explain the observed water abundances, and where gas-grain chemistry needs to be taken into account. The input parameters to the code are reported in Table 3. We have tested the impact of using different extinction curves (a standard galactic and the Orion Bar’s) as well as varying the cosmic ray ionization rate. We did not find significant differences in the predicted water abundances in the gas phase.

| Parameter          | Value       |
|--------------------|-------------|
| $G_0$              | $5 \times 10^5$ |
| $G_{\text{ext}}$   | 100         |
| $A_V$              | 50 mag      |
| $R_V$              | 3.1         |
| $\zeta$            | $5 \times 10^{-17} \text{ s}^{-1}$ |
| $\alpha_{\text{min}}$ | $3 \times 10^{-7} \text{ cm}$ |
| $\alpha_{\text{max}}$ | $3 \times 10^{-5} \text{ cm}$ |
| $\sigma$           | 3.5         |
| He/H               | 0.1         |
| O/H                | $3.2 \times 10^{-4}$ |
| C/H                | $1.3 \times 10^{-4}$ |
| N/H                | $7.5 \times 10^{-5}$ |
| S/H                | $1.8 \times 10^{-5}$ |

Table 3. Input parameters for the Meudon PDR code
The water abundance predicted by the Meudon PDR code (middle panel in Fig. 7) shows significant variations with $A_V$. Following a very low abundance in the most exposed layers ($A_V \leq 1$), the code predicts a water abundance of $X(\text{H}_2\text{O}) \sim 10^{-7} - 10^{-5}$ in a compact layer of about 1 mag. Subsequently, the water abundance strongly dips to $10^{-11}$ in the high-density layer at about $-5$ mag, and increases again and reaches its maximum value of $\sim 10^{-9}$ for $A_V \gtrsim 10$.

Our results show that the o-\text{H}_2\text{O} abundance is $\sim 10^{-7}$ in the first layers of the PDR ($L_{PDR}$). This is consistent with the value predicted by the Meudon code under the assumption that the outflow has only a minor contribution to the wing emission at central positions. In this layer, water is formed in gas phase via

$$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}.$$  

This reaction has a high activation barrier ($\sim 4000$ K) and is significant only at $T_K \gtrsim 250$ K. The internal energy available in vibrationally excited $\text{H}_2$ can help to overcome this barrier (Agúndez et al. 2010). Photodissociation is the main destruction mechanism.

In the rest of the cloud, the gas-phase predictions and the observational results do not agree. In the high-density region, the predicted water abundance is lower than $10^{-10}$, whereas the $\text{H}_2\text{O}$ measurements point to a relatively high abundance of $\sim 10^{-8}$. An additional water supply mechanism, such as desorption (photo-desorption, mechanical sputtering, thermal desorption) from the grain mantles, is required. In contrast, the measured $\text{H}_2\text{O}$ abundance in the envelope is at least two orders of magnitude lower than the abundances derived by the chemical model. The freeze-out of water onto grain mantles is very likely an efficient gas-phase water destruction mechanism in this colder region. Although it is difficult to compare these results without a precise profile for the water abundance, these results clearly show that gas-phase chemistry is not sufficient to account for the water emission in this PDR.

We have also compared our results with the predictions from the PDR model of Hollenbach et al. (2009), which includes freeze-out and photo-desorption processes but does not consider turbulence. Our observational value of the water abundance in the envelope ($1 \times 10^{-8}$) is consistent with the model predictions assuming a typical photo-desorption yield $Y_{\text{H}_2\text{O}} = 1 \times 10^{-3}$ and a grain cross sectional area $\sigma_H = 2 \times 10^{-21}$ cm$^{-2}$. Indeed, the Hollenbach et al. (2009) model predicts that freeze-out and photo-desorption are the dominant processes to explain the water abundance starting at $A_V \gtrsim 5$ for the physical conditions of the Mon R2 envelope.

Summarizing, our observational results agree well with gas-phase chemical models only in the very first layers of the PDR, $A_V \leq 1$, where high-temperature chemistry dominates the formation and photo-dissociation is the main destruction mechanism. The water abundance in the high-velocity gas is consistent with pure gas-phase chemistry, characteristic for PDRs. In the more quiescent gas, desorption from grains must play a role. This could be provided by photo-desorption according to the PDR model of Hollenbach et al. (2009), by turbulence, or by grain destruction in shocks. Deeper into the cloud, freeze-out into grains needs also to be taken into account for taking out $\text{H}_2\text{O}$ molecules from the gas phase. A complete treatment of the gas-grain chemistry is required to explain the observational results.

Fig. 7. Results of the modeling of MonR2 with the Meudon PDR code. The angular and physical distances refer to the projected distances from the IF in the plane of the sky. The two curves for the dust temperature are for grains of radius $3.6 \times 10^{-7}$ and $3.6 \times 10^{-5}$ cm.

6.3. Ammonia abundances

Figure 7 shows the predicted abundance for $\text{NH}_3$ as a function of the distance from the cloud center: qualitatively, ammonia is expected to be highly abundant only in the more shielded part of the envelope. This is consistent with our observational results, which show that emission of o-$\text{NH}_3$ is very extended, peaks outside the H$\alpha$ region and does not present high-velocity wings. This is also consistent with the results of the LVG modeling presented in Sect. 3, which were obtained with a beam filling factor of 1, densities between $5 \times 10^4$ cm$^{-3}$ and $1 \times 10^5$ cm$^{-3}$ and temperatures of $\sim 50$ K. Lower densities would result in higher $\text{NH}_3$ abundances. Comparing the abundances in the envelope obtained with the LVG modeling (few $10^{-9}$ for $n_\text{H}_2 = 5 \times 10^4$ cm$^{-3}$) and with the Meudon PDR code ($10^{-8}$), it seems that gas-phase chemistry slightly over-predicts the observed values, although for less than an order of magnitude.

7. Summary and conclusions

In this work, we have presented spatially and spectrally resolved observations of [C$\text{ii}$], CO, o-\text{H}_2\text{O}, p-\text{H}_2\text{O} and $\text{NH}_3$ along a strip crossing the PDR that surrounds the UCH$\alpha$ region MonR2. Using a local and non-local radiative transfer model and assuming a spherical approximation for the whole cloud, we have fitted the line profiles and intensities of the CO, $\text{H}_2\text{O}$ and $\text{NH}_3$ lines observed with Herschel.
The o-H$_2$O line has a narrow profile that peaks at ~ 11 km s$^{-1}$, the rest velocity of the cloud. The emission of this line is not very extended, and reaches it maximum toward the H ii region, suggesting that there is a significant fraction of the water emission arising from relatively quiescent gas associated to the innermost parts of the cloud. This is consistent with our modeling, which yielded an abundance of water of ~ 1 - 3 x 10$^{-8}$ relative to H$_2$ in a thick layer of 10 mag surrounding the PDR and in the envelope.

The o-H$_2$O abundance is higher, ~ 10$^{-7}$ relative to H$_2$, in red high-velocity gas. The origin of the red wings that appear in the H$_2$O and in the high-J $^{12}$CO lines is more doubtful. The red wings of all species toward the H ii region can be well reproduced by assuming an expanding PDR with relatively high expansion and turbulent velocities of 2 km s$^{-1}$ and 5 km s$^{-1}$, respectively. Yet, the red wings could also have an outflow origin, particularly to the southwest half of the strip. In any case, the density of this gas is not very well constrained and therefore the precise values of the abundance need to be taken with caution, at an order-of-magnitude significance.

Moreover work still remains to be done on the abundance of water in PDRs. The comparison of the derived abundances with gas-phase chemical modeling shows that gas-phase PDR chemistry can reproduce the observed abundances in the very first hot layer of the PDR up to an $A_V$ of 1. In this innermost layer, high-temperature chemistry is the main source of production of gas-phase water in the innermost layers of the PDR. However, the outflow can contribute to the H$_2$O emission at these high velocities. In the more shielded layers of the molecular cloud, the observational abundances differ by several orders of magnitude from the predictions of the gas-phase chemical model, suggesting that the freeze-out and photo-desorption mechanisms are the dominant processes at these cloud depths. Similarly, gas-phase chemical models overpredict the abundance of ammonia in the envelope by about one order of magnitude, suggesting that freeze-out into the grain surface needs to be taken into account for this species.

Acknowledgements. We acknowledge F. van der Tak for useful suggestions in improving this manuscript. We also acknowledge S. Treviño-Morales and A. Sanchez-Monge for their help with complementary data. We also thank the anonymous referee for his constructive report.

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