**OH emission from warm and dense gas in the Orion Bar PDR**

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ABSTRACT

As part of a far-infrared (FIR) spectral scan with *Herschel*/PACS, we present the first detection of the hydroxyl radical (OH) towards the Orion Bar photodissociation region (PDR). Five OH \((\mathrm{X}^2\Pi; \nu = 0)\) rotational \(\Lambda\)-doublets involving energy levels out to \(E_J/k = 511\) K have been detected (at \(\sim 65, \sim 79, \sim 84, \sim 119, \) and \(\sim 163\) \(\mu\)K). The total intensity of the OH lines is \(\Sigma I(\text{OH}) \approx 5 \times 10^{-4} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}\). The observed emission of rotationally excited OH lines is extended and correlates well with the high-\(J\) CO and CH\(^{+}\) \(J = 3\)–2 line emission (but apparently not with water vapour), pointing towards a common origin. Nonlocal, non-LTE radiative transfer models including excitation by the ambient FIR radiation field suggest that OH arises in a small filling factor component of warm \((T_k \gtrsim 10^4 \text{ K})\) and dense \((n_H \approx 10^6 \cm^{-3})\) gas with source-averaged OH column densities of \(\gtrsim 10^{17} \cm^{-2}\). High density and temperature photochemical models predict such enhanced OH columns at low depths \((A_V \lesssim 1)\) and small spatial scales \((\lesssim 10^5 \cm)\), where OH formation is driven by gas-phase endothermic reactions of atomic oxygen with molecular hydrogen. We interpret the extended OH emission as coming from unresolved structures exposed to far-ultraviolet (FUV) radiation near the Bar edge (photoevaporating clumps or filaments) and not from the lower density “interclump” medium. Photodissociation leads to OH/H\(_2\) abundance ratios (\(>1\)) much higher than those expected in equally warm regions without enhanced FUV radiation fields.

Key words. astrochemistry – infrared: ISM – ISM: abundances – ISM: molecules

1. Introduction

In quiescent regions irradiated by cosmic- or X-rays, the oxygen chemistry is initiated by the charge transfer from H\(^+\) and H\(_2^+\) to atomic oxygen, forming O\(^+\) and OH\(^+\). In warm environments it can also start with the reaction of atomic oxygen with H\(_2\)\((\nu = 0)\) to form OH. This endothermic reaction (by \(\sim 0.08\) eV) possesses an activation barrier of a few thousand K and high gas temperatures \((\gtrsim 400 \text{ K})\) are needed to produce significant OH abundances (e.g., in shocked gas). In molecular clouds exposed to strong far-ultraviolet (FUV) radiation fields, the so-called PDRs, the gas is heated to relatively high temperatures and there are also high abundances of FUV-pumped vibrationally excited molecular hydrogen H\(_2^\nu\)(\(\nu = 1, 2, \ldots\)) (Hollenbach & Tielens 1997). The internal energy available in H\(_2^\nu\) can be used to overcome the \(\mathrm{O}(^3\Pi) + \mathrm{H}_2(\nu = 0)\) reaction barrier (see Agúndez et al. 2010, and references therein). Although not well constrained observationally, enhanced OH abundances are expected in warm PDRs.

OH is a key intermediary molecule in the FUV-illuminated gas because further reaction of OH with H\(_2\), C\(^+\), O, N or S\(^+\) leads to the formation of H\(_2\)O, CO\(^+\), O\(_2\), NO or SO\(^+\) respectively. Besides, OH is the product of H\(_2\)O photodissociation, the main destruction route of water vapour in the gas unshielded against FUV radiation. Observations of OH in specific environments thus constrain different chemical routes of the oxygen chemistry.

Previous observations with KAO and ISO have demonstrated that OH is a powerful tracer of the warm neutral gas in shocked gas; from protostellar outflows and supernova remnants to extragalactic nuclei (e.g., Storey et al. 1981; Melnick et al. 1987; Gonzalez-Alfonso et al. 2004). Unfortunately, the poor angular resolution (\(>1\)) and sensitivity of the above telescopes prevented us from resolving the OH emission from interstellar PDRs.

Owing to its proximity and nearly edge-on orientation, the interface region between the Orion Molecular Cloud 1 (OMC1) and the H\(_2\) region illuminated by the Trapezium cluster, the Orion Bar, is the prototypical warm PDR (with a FUV radiation field at the ionization front of \(x \approx 2.5 \times 10^4\) times the mean interstellar field in Draine units; Marconi et al. 1998). The most commonly accepted scenario is that an extended gas component, with mean gas densities \(n_H \approx 10^{2} \cm^{-3}\), causes the chemical stratification seen in the PDR (Hogerheijde et al. 1995). Most of
the low-J molecular line emission arises in this extended “interclump” medium (Tielens & Hollenbach 1985; Simon et al. 1997; van der Wiel et al. 2009; Habart et al. 2010). In addition, another component of higher density clumps was introduced to fit the observed H2, high-J CO, CO+ and other high density and temperature tracers (Burton et al. 1990; Parmar et al. 1991; Störzer et al. 1995; van der Werf et al. 1996; Young Owl et al. 2000). Owing their small filling factor this clumpy structure would allow FUV radiation to permeate the region. The presence of dense clumps is still controversial.

In this letter we present initial results from a spectral scan of the Orion Bar taken with the PACS instrument (Poglitsch et al. 2010) on board Herschel (Pilbratt et al. 2010) as part of the “HEXOS” key programme (Bergin et al. 2010). PACS observations of OH lines towards young stellar objects have recently been reported by Wampfler et al. (2010). Here we present the first detection of OH towards this prototypical PDR.

2. Observations and data reduction

PACS observations were carried out on 7 and 8 September 2010 and consist of two spectral scans in Nyquist sampling wavelength range spectroscopy mode. The PACS spectrometer uses photocarrier detectors and provides 25 spectra over a 47′′ × 47′′ field-of-view resolved in 5 × 5 spatial pixels (“spaxels”), each with a size of ∼9.4′′ × 9.4′′ on the sky. The measured width of the spectrometer point-spread function (PSF) is relatively constant at λ ≤ 125 μm but it increases above the spaxel size for longer wavelengths. The resolving power varies between λ/Δλ ∼ 1000 (R1 grating order) and ∼5000 (B3A). The central spaxel was centred at δ2000: 5h35m20.61s, ε2000: −5°25′14.0″ target position. Observations were carried out in the “chop-nodded” mode with the largest chopped throw of 6 arcmin. Nominal capacities (0.14μF) were used. The integration time was 3.2h for the 1342204117 observation (B2B and R1) and 2.7h for the 1342204118 observation (B3A and R1). The data were processed with HIPPE using a pipeline upgraded with a spectral flatfield algorithm that reduces the spectral fringing seen in the Nyquist-sampled wavelength spectra of bright sources. Figure 1 shows the resulting OH lines towards the OH emission peak and Fig. 3 shows the intensities measured in each of the 25 spaxels for several lines of OH, CO, CH+, H2O and [N II]. In order to better sample the PSF and obtain accurate line intensities to be reproduced with our models, we fit the OH emission averaged over several adjacent spaxels in Sect. 4 (see also Appendix A).

3. Results

Of all the observed OH lines only the ground-state lines at ~119 μm show widespread bright emission at all positions. The ~119 μm lines mainly arise from the background OMC1 complex (the same applies to most ground-state lines of other species). Figure 2 shows the spatial distribution of the rotationally excited OH J = 7/2 → 5/2 lines at ~84 μm (Eu/k = 291 K) superimposed over the CO J = 6−5 peak brightness temperature (colour image from Lis et al. 1998) and over the brightest H2 v = 1−0 S(1) line emission regions (white contours from Walmsley et al. 2000). The emission from the other OH A-doublets at ~79 and ~163 μm (see Fig. B.2 in Appendix B) displays a similar spatial distribution that follows the “bar” morphology peaking near the H2 v = 1−0 S(1) bright emission region and then decreases with distance from the ionization front (note that H2 shows lower level extended emission with small-scale structure in the entire observed field; van der Werf et al. 1996). The excited OH spatial distribution, however, does not follow the CO J = 6−5 emission maxima, which approximately trace the gas temperature in the extended “interclump” component.

Figure 1 shows the detected OH A-doublets (at ~65, ~79, ~84, ~119 and ~163 μm) towards the position where the higher excitation OH lines peak. The total intensity of the observed FIR lines is I(Δν) = 5 × 10−4 erg cm−2 s−1 Hz−1. All OH doublets appear in emission, with intensity asymmetry ratios up to 40% (one line of the A-doublet is brighter than the other).

Note that the upper energy level of the 2Π1/2 J = 9/2 → 7/2 transition at ~65 μm lies at Eu/k ~ 511 K. The critical densities (ncr) of the observed OH transitions are high, ncr ≥ 105 cm−3. For much lower gas densities, and in the presence of strong FIR radiation fields, most lines would have been observed in absorption, especially those in the 2Π1/2 ladder (Goicoechea & Cernicharo 2002). Hence, the observed OH lines must arise in a widespread component of warm and dense gas.

Although our PACS observations do not provide a fully sampled map, the line emission observed in the 25 spaxels can be used to carry out a first-order analysis on the spatial correlation of different lines (neglecting perfect PSF sampling, line opacity and excitation effects). Except for the OH ground-state lines at ~119 μm (that come from the background OMC1 cloud), we find that the rotationally excited OH lines correlate well with the high-J CO and CH+ emission but, as expected, they do not correlate with the ionized gas emission. Figure 3 (lower panel) compares the observed OH ~84.597 μm line intensities with those of CO J = 21−20 (Eu/k ~ 1276 K), CH+ J = 3−2

Fig. 1. OH (X 2Π; ν = 0) rotational lines detected with Herschel/PACS towards the δ2000: 5°35’19.9″, ε2000: −5°25′06.7″ position where the higher excitation OH line peak is observed (see Fig. 2). The red dotted lines show the expected wavelength for each A-doublet (see Fig. B.1 in Appendix B for a complete OH rotational energy diagram). Small intensity asymmetries are observed in most OH A-doublets. Transition upper level energies and Aij spontaneous transition probabilities are indicated.

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Asymmetries are significantly reduced when collisions with ortho to the gas temperature, e.g., \( \sim \) H\textsubscript{13}CN field (van der Werf et al. 1996). Violet stars shows the position of the \(*\) the brightest regions of H\textsuperscript{\(\alpha\)} well correlated, while the OH and H\textsubscript{2}O emission is not (within the PSF sampling caveats). Note the decrease of OH line intensity with distance from the ionization front.

\[ (E_{\text{u}}/k \sim 240 \text{ K}) \text{ and } [\text{N}\textsubscript{II}] 121.891 \mu\text{m} \] (all observed with a similarly PSF) and also with the CO \( J = 15-14 \) (\( E_{\text{u}}/k \sim 663 \text{ K} \)), H\textsubscript{2}O 3\( 0\)-\( 2 \) (\( E_{\text{u}}/k \sim 163 \text{ K} \)) and OH \( \sim 163.397 \mu\text{m} \) lines (upper panel). This simple analysis suggests that the excited OH, high-J CO and CH\textsuperscript{+} \( J = 3-2 \) lines arise from the same gas component. It also shows that the emission from different excited OH lines is well correlated, while the OH and H\textsubscript{2}O emission is not (within the PSF sampling caveats).

4. OH column density determination

Determining the OH level populations is no trivial excitation problem. In addition to relatively strong asymmetries in the collisional rate coefficients\(^1\) between each \( \Lambda \)-doubling component (Offer & Van Dishoek 1992), radiative and opacity effects (pumping by the ambient IR radiation field and line trapping) can play a significant role if the gas density is much lower than \( n_{\text{ex}} \). Here we use a nonlocal and non-LTE code that treats the OH line and continuum radiative transfer (see appendix in Goicoechea et al. 2006). The continuum measured by PACS and SPIRE in the region (Arab et al., in prep.) can be approximately reproduced by a modified blackbody with a colour temperature of \( \sim 55 \text{ K} \) and a opacity dependence of \( \sim 0.05(100/\lambda)^{1.75} \).

\(^1\) We used collision rate coefficients of OH with para- and ortho-H\textsubscript{2} from Offer & Van Dishoek (1992) and Offer et al. (1994). Strong differences in the intensity of each OH \( \Lambda \)-doublet component due to asymmetries in the collisional rates between OH and para-H\textsubscript{2} were predicted (e.g., \( I(84.597)/I(84.420) > I(119.441)/I(119.234) > 1 \)). Asymmetries are significantly reduced when collisions with ortho-H\textsubscript{2} are included (i.e., in the warm gas) and when FIR radiative pumping plays a role. We assume that the H\textsubscript{2} ortho-to-para ratio is thermalized to the gas temperature, e.g., \( \sim 1.6 \) at 100 K and \( \sim 2.9 \) at 200 K.

5. OH chemistry and line emission origin

We used the Meudon PDR code (Le Petit et al. 2006; Goicoechea & Le Bourlot 2007) to estimate the OH column density in a slab of gas at different densities \( n_{\text{H}} \) from \( 5 \times 10^{4} \) to \( 10^{17} \text{ cm}^{-3} \). The adopted FUV radiation field, \( \chi = 10^{4} \), roughly corresponds to the attenuation of the FUV field at the ionization front by a column density of \( N_{\text{H}} \approx 10^{21} \text{ cm}^{-2} \) in a \( n_{\text{H}} \approx 10^{3} \text{ cm}^{-3} \) medium. This attenuation is equivalent to a spatial length of...
Gas temperatures around $\sim 10^3$ cm, consistent with the observed decrease of excited OH emission with projected distance from the ionization front (see Fig. 2). Given the high gas temperature, FUV field and moderate grain temperature ($T_{gr} \sim 70–100$ K) in the regions traced by FIR OH, CO and CH$^+$ lines, we neglected molecule freeze-out and ice desorption (which are important deeper inside at $A_V \gtrsim 3$; Hollenbach et al. 2009). In our models OH is a surface tracer that reaches its peak abundance at $A_V \lesssim 1$ (Fig. 4) where OH formation is driven by the endothermic reaction O$^+(3P) + H_2 \rightarrow OH + H$, slightly enhanced by the O$^+(3P) + H_2$ reaction (included in our models; see Agúndez et al. 2010).

Gas temperatures around $1000–5000$ K are predicted near the slab surface at $A_V = 0.01$ and around $100$ K at $A_V \gtrsim 1$. In these H$_2$ gas transition layers where the OH abundance peaks, the electron density is still high ($\lesssim$[e$^-$/H]$_{n_{OH}}$) and hydrogen is not fully molecular, with $f$(H$_2$) = 2n(H$_2$)/[n(H) + 2n(H$_2$)] $\gtrsim$ 0.5. In general, the higher the gas temperature where enough H$_2$ has formed, the higher the predicted OH abundance.

In the $A_V \lesssim 1$ layers, OH destruction is dominated by photodissociation (OH + $h\nu$ → O + H) and to a lesser extent, by reactions of OH with H$_2$ to form H$_2$O (only when the gas temperature and density are very high). Water vapour photodissociation (H$_2$O + $h\nu$ → OH + H) in the surface layers limits the H$_2$O formation and leads to OH/H$_2$O abundance ratios ($>1$), much higher than those expected in equally warm regions without enhanced FUV radiation fields (e.g. in C-shocks). The lack of apparent correlation between the excited OH and H$_2$O 3$_{0}$−2$_{1}$ lines (see Fig. 3) and the absence of high excitation H$_2$O lines in the PACS spectra (only weak H$_2$O 2$_{1}$−2$_{1}$, 2$_{1}$−1$_{0}$ and 3$_{0}$−2$_{1}$ lines are clearly detected) suggests that the bulk of OH and H$_2$O column densities arise from different depths.

As the temperature decreases inwards, the gas-phase production of OH also decreases. The spatial correlation between excited OH, CH$^+$ J = 3–2 and high-J CO lines is a good signature of their common origin in the warm gas at low $A_V$ depths.

Our PDR models predict OH column densities in the range $\sim$10$^{12}$ cm$^{-2}$ to $\sim$10$^{15}$ cm$^{-2}$ at $A_V \lesssim 1$ for gas densities between $n_{HI} = 5 \times 10^3$ and 10$^7$ cm$^{-3}$ respectively. Hence, even if we take into account possible inclination effects, high density and temperature models produce OH columns closer to the values derived in Sect. 4 just from excitation considerations (note that a precise determination of the gas density would require knowing the collisional rate coefficients of OH with H atoms and electrons). The OH abundance in these dense surface layers is of the order of $\sim$10$^{-6}$ with respect to H nuclei. However, optical depths of $A_V \lesssim 1$ correspond to spatial scales of $\sim$10$^{15}$ cm (i.e., much smaller than the H$^{13}$CN clumps detected by Lis & Schilke 2003, deeper inside the cloud), but we detect extended OH emission over $\sim$10$^{17}$ cm scales. Therefore, we have to conclude that the observed OH emission arises from a small filling factor ensemble of unresolved structures that are exposed to FUV radiation (overdense clumps or filaments). Note that owing to the lower grain temperature compared to the gas, the expected FIR continuum emission from these clumps will still be below the continuum levels observed by Herschel/PACS.

The minimum size of the dense clumps is $\sim$10$^{15}$ cm (from OH photochemical models) with a maximum size of $\sim$10$^{16}$ cm (from the inferred beam dilution factor). Both correspond to $\lesssim 0.2'' - 2''$ at the distance of Orion. As an example, H$_2$ photo-evaporating clumps of $\sim$10$^{16}$ cm size have been unambiguously resolved towards S106 PDR Noel et al. (2005). However, higher angular resolution observations (e.g., with 8–10 m telescopes) are needed to resolve smaller H$_2$ clumps from the H$_2$ interclump emission in the Orion Bar.

If the observed FIR OH line emission does not arise from such a high density gas component, a different non-thermal excitation mechanism able to populate the OH $^1$H$^1$/2 $J = 9/2$ and 7/2 levels would be needed. Two alternative scenarios can be explored, at least qualitatively. First, OH molecules produced by H$_2$O photodissociation are expected to form mostly in the ground electronic and vibrational state but in unusually high energy $J > 70/2$ levels (a few thousands K; van Harrevelt & van Hemert 2000). Nevertheless, they will cascade down radiatively to lower energy rotational ladders extremely rapidly. Although very excited suprathermal OH $J \approx 70/2$–15/2 lines have been reported towards the HH 211 outflow and were interpreted as H$_2$O photodissociation (Tappe et al. 2008), we did not find any of them in the SWS or in the IRS spectra of the Orion Bar (taken and processed by us from the ISO and Spitzer basic calibrated data archives). Besides, even if photodissociation is the main H$_2$O destruction mechanism in the $A_V \lesssim 1$ warm layers, this is not the main production pathway of OH (the O$^+(3P)$ + H$_2$ reaction dominates).

Second, experiments and quantum calculations suggest that reaction of O$^+(3P)$ atoms with H$_2$(ν = 1) can produce significant OH in the ν = 1 vibrationally excited state, with OH(ν = 1)/OH(ν = 0) population ratios $\gtrsim$1 for moderate kinetic energies (0.05–0.1 eV; e.g., Balakrishnan 2004). Complementarily, absorption of near- and mid-IR photons (from the continuum or from bright overlapping H$_2$ and ionic lines) can also pump OH to the ν = 1 state. In both cases, subsequent de-excitation through the ν = 1–0 rotation–vibration band at $\sim$2.80 $\mu$m would populate the OH(ν = 0) rotationally excited levels that we observe with PACS. However, the OH ν = 0–1 band at $\sim$2.80 $\mu$m is not present in the ISO/SWS spectra. Even assuming that the O$^+(3P)$+H$_2$(ν = 1) reaction only forms OH(ν = 1), significant gas column densities at very hot temperatures ($T_k \sim 2000$ K) will be needed to match the observations if $n_{HI} = 10^{5–6}$ cm$^{-3}$. Studying the OH vibrationally-pumping mechanism quantitatively is beyond the scope of this work but these chemical and pumping effects could contribute to the excitation of FIR OH lines in lower density gas.

Different scenarios for the origin and nature of photoevaporating clumps have been proposed (Gorti & Hollenbach 2002), but without a more precise determination of their sizes and densities it is hard to conclude on any of them. Subarcsec resolution
Owing to the broader PSF width in co-adding the measured fluxes over four adjacent spaxels (the [3,4], [3,3], [2,4] and [2,3]). Owing to the broader PSF width at long wavelengths, the entire array was used to extract the OH ~ 163 μm line intensities. 

The best-fit OH radiative transfer model was obtained by finding the minimum \( \chi^2 \)-value defined as

\[
\chi^2 = \frac{1}{n - p} \sum_{i=1}^{n} \left( \frac{I^\text{obs}_i - I^\text{mod}_i}{\sigma^\text{obs}_i} \right)^2 ,
\]

where \( n \) is the number of observed OH lines, \( p \) is the number of free parameters in the fit, \( I^\text{obs} \) and \( I^\text{mod} \) are the observed and modelled line integrated intensities, and \( \sigma^\text{obs} \) is the 1σ uncertainty of \( I^\text{obs} \). Therefore, we fit absolute intensity values and not line intensity ratios. Figure A.1 shows the best grid of radiative transfer models with a density of \( n_{\text{grid}} = 10^3 \) cm\(^{-2} \) and a beam filling factor \( \eta = 1 \), defined as \( \eta = \frac{a}{\Omega} \), where \( \Omega \) and \( \Omega^\text{PSF} \) are the sky solid angles subtended by the source and by the PACS PSF respectively. Figure A.1 shows the best source-averaged OH column densities, where \( N(\text{OH})^\text{beam} \approx \eta \times N(\text{OH})^\text{source} \).

The list of OH line intensities around the position where the higher excitation OH lines peak is shown in Table A.1. In order to better sample the spectrometer PSF in these extended emission observations, the OH line intensities were computed by co-adding the measured fluxes over four adjacent spaxels (the [3,4], [3,3], [2,4] and [2,3]).

## Table A.1. PACS OH line intensities towards the Orion Bar PDR. 

| \( \lambda \) (μm) | OH transition | \( \bar{I}_{\text{obs}} \) (\( \sigma_{\text{obs}} \)) |
|-----------------|---------------|------------------------------------------|
| 119.441 | \( ^2 \Pi_{1/2} J = 5/2 - 3/2 \) | 10.09 (0.21) |
| 119.234 | \( ^2 \Pi_{1/2} J = 5/2 - 3/2 \) | 9.44 (0.21) |
| 84.597 | \( ^2 \Pi_{1/2} J = 7/2 - 5/2 \) | 4.07 (0.79) |
| 84.420 | \( ^2 \Pi_{1/2} J = 7/2 - 5/2 \) | 2.38 (0.91) |
| 163.396 | \( ^2 \Pi_{1/2} J = 3/2 - 1/2 \) | 1.34 (0.17) |
| 163.015 | \( ^2 \Pi_{1/2} J = 3/2 - 1/2 \) | 0.53 (0.26) |
| 79.179 | \( ^2 \Pi_{1/2} J = 1/2 - 1/2 \) | 1.97 (1.30) |
| 79.115 | \( ^2 \Pi_{1/2} J = 1/2 - 1/2 \) | 0.96 (1.54) |
| 65.279 | \( ^2 \Pi_{1/2} J = 9/2 - 7/2 \) | 1.02 (0.49) |
| 65.131 | \( ^2 \Pi_{1/2} J = 9/2 - 7/2 \) | 1.32 (0.54) |

**Notes.** (a) Near the OH emission peak: \( \delta_{2000} \approx 8^h 35^m 21.9^s \), \( \alpha_{2000} \approx 5^h 25^m 06.7^s \).
Appendix B: Figures

**Fig. B.1.** Rotational energy diagram of $^{16}\text{OH}$ showing the lines detected by *Herschel/PACS* (in microns). Detected transitions are shown in black while other pumping transitions discussed in the text are shown in red. OH $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ rotational ladders are produced by the spin-orbit interaction, while the $\Lambda$-doubling splitting of each rotational level is produced by the nuclei rotation and the unpaired electron motion. The $\Lambda$-doubling splitting has been enhanced for clarity. Hyperfine structure is not shown.

**Fig. B.2.** Same as Fig. 2 for the OH $^2\Pi_{1/2}$ $^2\Pi_{3/2}$ $J = 1/2 \rightarrow 3/2$ cross-ladder lines at $\sim 79\mu m$, the OH $^2\Pi_{1/2}$ $J = 5/2 \rightarrow 3/2$ ground-state lines at $\sim 119\mu m$, and the OH $^2\Pi_{1/2}$ $J = 3/2 \rightarrow 1/2$ excited lines at $\sim 163\mu m$. Note the decrease of OH line intensity with distance from the ionization front.