Warm $H_2O$ and OH in the disk around the Herbig star HD 163296*

D. Fedele1, S. Bruderer1, E. F. van Dishoeck1,2, G. J. Herczeg3, N. J. Evans II4, J. Bouwman5, Th. Henning3, and J. Green6

1 Max Planck Institut für Extraterrestrische Physik, Giessenbachstrasse 1, 85748 Garching, Germany  
2 Leiden Observatory, PO Box 9513, 2300 RA Leiden, The Netherlands  
3 Kavli Institute for Astronomy and Astrophysics, Yi He Yuan Lu 5, 100871 Beijing, PR China  
4 University of Texas at Austin, Department of Astronomy, 2515 Speedway, Stop C1400, Austin TX 78712-1205, USA  
5 Max Planck Institute for Astronomy, Königstuhl 17, 69117 Heidelberg, Germany

Received 16 May 2012 / Accepted 17 July 2012

ABSTRACT

We present observations of far-infrared ($50–200\,\mu m$) OH and $H_2O$ emission of the disk around the Herbig Ae star HD 163296 obtained with Herschel/PACS in the context of the DIGIT key program. In addition to strong $[O\,I]$ emission, a number of OH doublets and a few weak highly excited lines of $H_2O$ are detected. The presence of warm $H_2O$ in this Herbig disk is confirmed by a line stacking analysis, enabled by the full PACS spectral scan, and by lines seen in Spitzer data. The line fluxes are analyzed using a local-thermal-equilibrium slab model including line opacity. The $H_2O$ column density is $10^{15}–10^{16}\,cm^{-2}$, and the excitation temperature is $200–300\,K$, implying warm gas with a density $n > 10^4\,cm^{-3}$. For OH, we find $N_{\text{OH}}$ of $10^{14}–10^{15}\,cm^{-2}$ and $T_{\text{ex}}$ $\sim$ 300–500 K. For both species, we find an emitting region of $r \sim 15–20\,AU$ from the star. We argue that the molecular emission arises from the protoplanetary disk rather than the outflow. This far-infrared detection of both $H_2O$ and OH contrasts with near- and mid-infrared observations, which have generally found a lack of water in the inner disk around Herbig AeBe stars owing to the strong photodissociation of $H_2O$. Given the similar column density and emitting region, OH and $H_2O$ emission seems to arise from an upper layer of the disk atmosphere of HD 163296, which probes a new reservoir of water. The slightly lower temperature of $H_2O$ compared to OH suggests a vertical stratification of the molecular gas with OH located higher and $H_2O$ deeper in the disk, consistent with thermo-chemical models.

Key words. protoplanetary disks – stars: variables: T Tauri, Herbig Ae/Be – astrochemistry

1. Introduction

Water is a key molecule for the chemical and physical evolution of protoplanetary disks. Together with O and OH, it forms the main reservoir of oxygen. The formation of water ice layers on dust grains may improve their sticking behavior and thereby help the coagulation process toward larger particles that ultimately leads to the formation of planetesimals and planets. The growth of icy grains is also likely involved in the delivery of the main reservoir of oxygen. The formation of water ice layers in the main reservoir of oxygen. Together with O and OH, it forms the main reservoir of oxygen. The formation of water ice layers on dust grains may improve their sticking behavior and thereby help the coagulation process toward larger particles that ultimately leads to the formation of planetesimals and planets. The growth of icy grains is also likely involved in the delivery of the main reservoir of oxygen. Together with O and OH, it forms the main reservoir of oxygen. The formation of water ice layers on dust grains may improve their sticking behavior and thereby help the coagulation process toward larger particles that ultimately leads to the formation of planetesimals and planets. The growth of icy grains is also likely involved in the delivery of ore.

1 Appendices are available in electronic form at http://www.aanda.org

2. Observations and data reduction

HD 163296 was observed on April 03 2011 with the PACS instrument (Poglitsch et al. 2010) onboard the Herschel Space Observatory (Pilbratt et al. 2010) as part of the DIGIT key program (KPOT_nevans_1, PI: N. Evans). The target was observed in range spectroscopy mode covering the wavelength range $50–220\,\mu m$ with $R \sim 1000–3000$ (obsid: 1342217819, 1342217829). The observations were carried out in chopping/nodding mode with a chopping throw of $6\,\arcsec$. The total
on-source integration time is 6176 s for the B2A (51–73 \μm) and short R1 (70–105 \μm) modules and 8360 s for the B2B (70–105 \μm) and long R1 (140–220\μm) modules. The data were reduced with HIPE 8.0.2489 using standard calibration files from level 0 to level 2. The data for the two nod positions were reduced separately (oversampling factor = 3, up-sampling factor = 1 to ensure that the noise in each spectral point is independent) and averaged after a flat-field correction.

The spectrum was extracted from the central spaxel (9.4” square) to optimize the signal-to-noise ratio. Owing to the large point spread function of the telescope, some flux leaks into the other spaxels of the PACS array. To recover the absolute flux level, we applied a correction factor using the spectrum extracted from the other spaxels of the PACS array. To recover the absolute flux level, we applied a correction factor using the spectrum extracted from the central 9 spaxels (3×3 extraction); this was performed by fitting a third-order polynomial to each of the two extracted spectra (central spaxel and 3×3) and multiplying by a correction defined to be the ratio of these two fits. Finally, the spectrum was scaled so that the spectrum matched the PACS photometry (from Meeus et al., in prep.) at 70 \μm and 160 \μm.

The line flux ($F_{\text{line}}$) was measured by fitting a Gaussian function and the uncertainty ($\sigma$) was given by the product $STD_e \sqrt{\text{FWHM}} \delta$, where $STD_e$ (W m$^{-2}$ \μm$^{-1}$) is the standard deviation of the (local) spectrum, $\delta$ is the wavelength spacing of the bins (\μm), and $FWHM$ is the full width at half maximum of the line (\μm).

### 3. Results

We clearly detect the strong [O I] 63.2 \μm line as well as five OH far-infrared features above 3\σ (i.e. having $F_{\text{line}}/\sigma > 3$, Table 1). Spectra of selected lines are shown in Fig. 1. The OH lines are readily recognized because of their doublet pattern; only intra-ladder transitions, which have the largest Einstein coefficients, are found. In the case of the $^3\Pi_{1/2} 7/2-5/2$ doublet at 71 \μm, only one of the two lines is detected, although the non-detection of the second line is hardly significant within the noise. Asymmetric line intensities of A-doublets are predicted at high temperature (Offer & van Dishoeck 1992), but because of the noise this doublet is not considered in our analysis below.

Three lines of H$_2$O are detected slightly above 3\σ (Table 2). The H$_2$O $R_{18-7}_{07}$ line at 63.32 \μm is seen not only in our data but also in the GASPS spectrum shown by Tilling et al. (2012), although they do not claim a detection. The H$_2$O $4_{33-312}$ line at 78.74 \μm is seen here with a flux of 1.8 (±0.4) × 10$^{-17}$ W m$^{-2}$, while Tilling et al. (2012) report only a 3\σ upper limit of 1.5 × 10$^{-17}$ W m$^{-2}$. Meeus et al. (2012) claim a detection of far-infrared H$_2$O emission toward this source based on new

\[ \text{This formula comes directly from the error propagation of the sum } \Sigma(F_i), \text{ where } F_i \text{ is the flux of the } i\text{th spectral bin.} \]

---

![Fig. 1. PACS spectrum (continuum-subtracted) of selected lines. The (blue) dashed line indicates the root mean square of the baseline multiplied by three. The presented spectrum has been smoothed (smooth width = two bins) for clarity. The red line is a Gaussian fit to the detected lines.](image)

### Table 1. [O I] and OH line fluxes.

| Transition | $F_{\text{line}}$ | $E_{\text{u}}$ | $\log A_{\text{d}}$ |
|------------|------------------|---------------|------------------|
| [O I]      |                  |               |                  |
| $^2\Pi_{1/2} 9/2^-7/2^-$ | 55.8 ± 1.1 | 6.7 | 0.34 |
| $^2\Pi_{1/2} 9/2^-7/2^+$ | 55.9 ± 1.1 | 6.7 | 0.34 |
| $^2\Pi_{1/2} 9/2^-7/2^-$ | 65.1 ± 1.4 | 5.9 | 0.11 |
| $^2\Pi_{1/2} 9/2^-7/2^+$ | 65.2 ± 1.0 | 5.9 | 0.10 |
| $^2\Pi_{1/2} 7/2^-5/2^-$ | 84.6 ± 2.4 | 2.8 | 0.28 |
| $^2\Pi_{1/2} 7/2^-5/2^+$ | 84.4 ± 2.4 | 2.8 | 0.28 |
| $^2\Pi_{1/2} 5/2^-3/2^-$ | 119.2 ± 1.2 | 0.9 | 0.86 |
| $^2\Pi_{1/2} 5/2^-3/2^+$ | 119.4 ± 0.9 | 0.9 | 0.86 |

Notes. Column $F_{\text{line}}$ reports the line flux predicted by the best-fit model.

$^a$ Blended with o-H$_2$O 6$_{25}$–5$_{14}$

### Table 2. H$_2$O line fluxes.

| Transition | $F_{\text{line}}$ | $E_{\text{u}}$ | $\log A_{\text{d}}$ |
|------------|------------------|---------------|------------------|
| p-H$_2$O   |                  |               |                  |
| $4_{31}-3_{22}$ | 56.31 | 2.7 ± 1.6 | 2.5 | 0.16 |
| o-H$_2$O   |                  |               |                  |
| $9_{09}-8_{10}$ | 56.82 | 0.9 ± 1.6 | 1.5 | 0.39 |
| $8_{18}-7_{07}$ | 63.32 | 2.0 ± 0.6 | 2.0 | 0.24 |
| $7_{07}-6_{16}$ | 71.95 | 2.2 ± 0.5 | 1.9 | 0.43 |
| o-H$_2$O   |                  |               |                  |
| $4_{23}-3_{12}$ | 78.74 | 1.8 ± 0.4 | 1.7 | 0.32 |
| o-H$_2$O   |                  |               |                  |
| $5_{17}-5_{16}$ | 82.03 | 0.8 ± 0.8 | 1.5 | 0.06 |
| p-H$_2$O   |                  |               |                  |
| $3_{32}-2_{21}$ | 89.89 | 0.9 ± 0.9 | 0.8 | 0.45 |
| o-H$_2$O   |                  |               |                  |
| $2_{14}-1_{10}$ | 108.07 | 0.7 ± 0.5 | 0.7 | 0.59 |
| o-H$_2$O   |                  |               |                  |
| $4_{16}-3_{10}$ | 113.54 | 0.7 ± 0.4 | 0.6 | 0.61 |

Notes. (a) Flux integrated over 5 bins centered at the expected line position.

---

GASPS data. Pontoppidan et al. (2010) also provide tentative detections of H$_2$O lines in the mid-infrared Spitzer wavelength range. Table 2 summarizes our fluxes and includes the fluxes measured at the position of some (undetected) key H$_2$O lines that are used later in the analysis.

The detected lines have upper level energies over a wide range of values of $E_u/k \sim 120–900$ K (OH) and $E_u/k \sim 400–1300$ K (H$_2$O). Most of the lines are detected in the blue part of the spectrum.

### 3.1. Confirmation of H$_2$O by line stacking

Since only three H$_2$O lines are marginally detected above 3\σ, we used the availability of the full DIGIT PACS spectrum to confirm the presence of warm water in this disk through a stacking
analysis. Line stacking is commonly used in extragalactic surveys to detect the faint emission lines from the outer regions of galaxies (e.g., Schruba et al. 2011). Warm water has many lines spread throughout the far-infrared wavelength region that can be used for this purpose. In this work, we stacked spectra centered at the location of different H$_2$O lines based on the far-infrared lines detected with PACS toward the protostar NGC 1333 IRAS 4B (Herczeg et al. 2012). The 95–100 μm range is excluded because of spectral leakage (produced by overlap of grating orders). Blended lines are excluded from this analysis and OH and [O I] lines are masked. The remaining number of H$_2$O lines available for the analysis is 54. The stacked spectrum is the weighted average of 54 spectra, each of which is 100 bins wide centered at the position of a water line $F_j = \frac{\sum_{i=1}^{54} w_i F_i}{\sum_{i=1}^{54} w_i}$, where $F_j$ is the (continuum-subtracted) spectrum centered at the $j$th water line and $w_j$ is the weight of the line. The weight corresponds to $STD_j^{-1}$, where $STD_j$ is the standard deviation in the continuum-subtracted spectrum $F_j$. The lines are stacked in bins because the spectral resolution in velocity space varies but is approximately constant in bins.

The stacked spectrum is shown in Fig. 2. The warm H$_2$O signal is clearly detected and centered on the central bin. The integrated H$_2$O signal is seven times its uncertainty. The false alarm probability (FAP), i.e. the probability of detecting a 7σ signal by stacking random portions of the PACS spectrum, is <0.03% based on 10,000 randomized tests (see Appendix B).

This analysis confirms the presence of warm H$_2$O in the PACS spectrum of HD 163296. Stacking H$_2$O lines separately in spectra from the two nod positions also yields >3σ detections. The H$_2$O signal is only detected in the central spaxel and not in off-source spaxels. These last two tests exclude the contamination from an extended and/or off-source emission and confirm that the H$_2$O lines detected in the PACS spectrum are associated with HD 163296.

4. Analysis

We analyze the OH and H$_2$O excitation using a uniform slab of gas in local thermal equilibrium (LTE) and including the effect of line opacity (see Appendix A for details). The limited number of lines and their large uncertainties do not warrant a more sophisticated non-LTE treatment. The analysis is based on the data in Tables 1 and 2, including the mid-infrared lines detected with Spitzer/IRS (Pontoppidan et al. 2010). The free parameters of the model are the excitation temperature $T_{ex}$ (K) and the molecular column density $N_{mol}$ (cm$^{-2}$). The size of the emitting region, given by its radius $r$, is not a free parameter since it can be determined uniquely for every given combination of $T_{ex}$ and $N_{mol}$. Comparison between models and data is done based on the reduced $\chi^2$ values.

The range of models that yields acceptable agreement is shown in Fig. 3. Overplotted are contours for the radius $r$. For H$_2$O, the data are best-fitted (1σ, $p = 68.3\%$) by models with $T_{ex} \sim 200–350$ K, and $N_{mol} \sim 10^{14}–10^{16}$ cm$^{-2}$, and $r \sim 15–20$ AU. For OH, the data are best-fitted by models with $N_{mol} \sim 10^{14}–10^{15}$ cm$^{-2}$, $T_{ex} \sim 300–500$ K, and $r \sim 20$ AU. The Spitzer/IRS spectrum of selected lines is shown in Fig. 4, along with the best-fit model.

Further constraints on the H$_2$O column density and temperature come from individual line-flux ratios. In particular, the ratio of far- to mid-infrared lines (e.g. $\nu_07–\nu_6/\nu_03$–$\nu_5$) constrains the column density to be $>10^{14}$ cm$^{-2}$. On the other hand, the
The primary result of this Letter is a detected signal of H₂O, in addition to OH, toward a Herbig star. The H₂O emitting region is found to be 15–20 AU in size, demonstrating that H₂O can survive the UV radiation further away from the star, while likely being photodissociated in the inner part of the disk.

Given that a bipolar microjet is known to be associated with HD 163296 (Wassell et al. 2006), the question arises of whether the far-infrared molecular line emission presented here indeed arises from the disk or whether it comes from such a jet. There are several arguments in favor of the disk. First, we note that HD 163296 is isolated and not associated with a molecular cloud. No evidence of a molecular outflow has been reported to date (e.g. Bae et al. 2011). Second, the spectrally resolved CO J = 3–2 line in the sub-millimeter shows the characteristic double-peaked profile of gas in Keplerian rotation (Thi et al. 2001; Dent et al. 2005). At much shorter wavelengths (4.7 μm), the CO ro-vibrational emission lines are also characterized by a double-peaked profile (Salyk et al. 2011). Thus, there is no hint of any significant small- or large-scale molecular outflow in these data that could dominate the PACS emission. Third, the PACS data show no evidence of extended/off-source emission beyond the central spaxel, not even for the strong [O I] 63 μm line, which places the warm H₂O within 500 AU of the central star.

The inferred OH and H₂O excitation temperatures of several hundred Kelvin indicate warm emitting regions. The high critical densities of the H₂O lines, n_c ≥ 10⁷ cm⁻³, implies that the density of the gas should also be high (n ≥ 10⁸ cm⁻³; e.g. Herczeg et al. 2012). These conditions and the arguments above suggest that the OH and H₂O emission arises from the atmosphere of the disk associated with HD 163296 at radial distances >10 AU from the star.

If we assumed that the OH/H₂O far-infrared lines are emitted by the disk, which zone would this emission trace? Models of the water chemistry in Herbig disks suggest at least three chemically distinct zones (e.g., Woite et al. 2009; Glassgold et al. 2009; Walsh et al. 2010, 2012; Vasyunin et al. 2011; Najita et al. 2011): (i) an inner-disk water reservoir (few AU) with a chemistry close to LTE; (ii) a cold water belt at large distances (>250 AU) where gaseous H₂O results primarily from photodesorption of water ice; and (iii) hot water layers at both intermediate distances of 1–50 AU and medium heights with water formation driven by high-temperature neutral-neutral reactions. The derived parameters for our OH and H₂O lines are consistent with the existence of zone (iii) (see also Tilling et al. 2012); zone (i) is probed by the near-infrared data and zone (ii) can be targeted by HIIF observations of low-J lines. Thus, the PACS data reveal that there is an additional water reservoir in disks.

6. Conclusions
We have presented new Herschel/PACS observations of the disk around the Herbig Ae star HD 163296. We have detected far-infrared lines of warm OH and H₂O toward this Herbig star. The presence of warm H₂O is confirmed by a line stacking analysis (7μ detection) enabled by the full PACS spectral scan. Our LTE slab-model analysis including optical depth effects indicates emission from the intermediate radii of the disk. Combined with near-infrared and sub-millimeter data, the oxygen chemistry can now be probed over the entire disk range.

References
Bae, J.-H., Kim, K.-T., Youn, S.-Y., et al. 2011, ApJS, 196, 21
Banzatti, A., Meyer, M. R., Bruderer, S., et al. 2012, ApJ, 745, 90
Carr, J. S., & Najita, J. R. 2008, Science, 319, 1504
Dent, W. R. F., Greaves, J. S., & Coulson, I. M. 2005, MNJAS, 359, 663
Fedele, D., Pascucci, I., Brittain, S., et al. 2011, ApJ, 736, 102
Glassgold, A. E., Meijerink, R., & Najita, J. R. 2009, ApJ, 701, 142
Grady, C. A., Polomski, E. F., Henning, T., et al. 2001, AJ, 122, 3396
Herczeg, G. J., Karska, A., Bruderer, S., et al. 2012, A&A, 540, A84
Hogerheijde, M. R., Bergin, E. A., Brinch, C., et al. 2011, Science, 334, 338
Isella, A., Testi, L., Natta, A., et al. 2007, A&A, 469, 213
Mandell, A. M., Munnum, M. J., Blake, G. A., et al. 2008, ApJ, 681, L25
Mandell, A. M., Bast, J., van Dishoeck, E. F., et al. 2012, ApJ, 747, 92
Mannings, V., & Sargent, A. I. 1997, ApJ, 490, 792
Meens, G., Montesinos, B., Mendoza, J. I., et al. 2012, A&A, 544, A78
Najita, J. R., Adámkovics, M., & Glassgold, A. E. 2011, ApJ, 743, 147
Offer, A. R., & van Dishoeck, E. F. 1992, MNJAS, 257, 377
Pilbratt, G. L., Riedinger, J. R., Passvogel, T., et al. 2010, A&A, 518, L1
Poghosian, A., Wailekens, C., Geis, N., et al. 2010, A&A, 518, L2
Pontoppidan, K. M., Salyk, C., Blake, G. A., et al. 2010, ApJ, 720, 887
Riviere-Marichalar, P., Ménard, F., Thi, W. F., et al. 2012, A&A, 538, L3
Salyk, C., Pontoppidan, K. M., Blake, G. A., et al. 2008, ApJ, 676, L49
Salyk, C., Blake, G. A., Boogert, A. C. A., & Brown, J. M. 2011, ApJ, 743, 112
Schura, A., Leroy, A. K., Walter, F., et al. 2011, AJ, 142, 37
Thi, W. F., van Dishoeck, E. F., Blake, G. A., et al. 2001, ApJ, 561, 1074
Tilling, I., Woitek, P., Meeus, G., et al. 2012, A&A, 538, A20
van der Tak, F. S. J., Black, J. H., Schöier, F. L., Jensen, D. J., & van Dishoeck, E. F. 2007, A&A, 468, 627
van Leeuwen, F. 2007, A&A, 474, 653
Vasyunin, A. I., Wiebe, D. S., Birnstiel, T., et al. 2011, ApJ, 727, 76
Walsh, C., Millar, T. J., & Nomura, H. 2010, ApJ, 722, 1607
Walsh, C., Nomura, H., Millar, T. J., & Aikawa, Y. 2012, ApJ, 747, 114
Wassell, E. J., Grady, C. A., Woodgate, B., Kimble, R. A., & Bruderer, F. C. 2006, ApJ, 650, 985
Woitek, P., Kamp, I., & Thi, W. 2009, A&A, 501, 383
Appendix A: Slab model

For an optically thin line from a point-like source, the flux can be written by

\[ F_{ul} = \Omega_s \frac{\hbar \nu_{ul} A_{ul} N_{mol} g_u e^{-E_u / kT}}{Q(T)} \]  

(A.1)

for the solid angle of the source \( \Omega_s \), the line frequency \( \nu_{ul} \), the Einstein-A coefficient \( A_{ul} \), the molecular column density \( N_{mol} \), the statistical weight of the upper level \( g_u \), the energy of the upper level \( E_u \), and the partition function \( Q(T) \). The solid angle of the emitting region can be written as \( \Omega_s = \pi r^2 / d^2 \), for the radius of the emitting region \( r \) and a distance of \( d = 118 \) pc to HD 163296. For an optically thick line, the integrated intensity is obtained from

\[ I_{ul} = \Delta v \nu_{ul} B_{ul}(T_{ex})(1 - e^{-\tau_{ul}}) \]  

(A.2)

where the opacity at the line center is

\[ \tau_{ul} = \frac{A_{ul} c^3}{8 \pi \nu_{ul}^3 \Delta \nu} \left( \frac{N_l g_l}{N_u g_u} - 1 \right) \]  

(A.3)

The (thermal) width of the lines is assumed to be \( \Delta v \sim 1 \) km s\(^{-1}\), which is appropriate for gas at several hundred K and we assume a simple square-like line profile as e.g. used in the RADEX code (van der Tak et al. 2007).

Appendix B: False alarm probability of water detection in the stacked spectrum

We performed a simulation to measure the probability of detecting a signal with an integrated value, \( S > 7 \sigma \). This provides the false alarm probability (FAP) of a detection based on the stacked spectrum. We performed 10,000 random stackings of 54 (equal to the number of water lines) parts of the PACS spectrum of HD 163296. After 10,000 iterations, we measured the distribution of the ratio of the integrated signal to its uncertainty (measured as in Sect. 3.1). We masked the bins containing H\(_2\)O, OH, and [O\(_i\)] emission. Figure B.1 shows the distribution of \( S / \sigma \). The distribution is well-fitted by a Gaussian function (red line, \( \tilde{\chi}^2 = 0.03 \)), centered (as expected) at \( S / \sigma = 0 \) (i.e. an equal number of positive and negative peaks). The number of occurrences with \( S / \sigma > 7 \) is less than thee, which corresponds to FAP <0.03% according to Bayesian statistics.