Multi-line detection of $O_2$ toward $\rho$ Oph A

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ABSTRACT

Context. Models of pure gas-phase chemistry in well-shielded regions of molecular clouds predict relatively high levels of molecular oxygen, $O_2$, and water, $H_2O$. These high abundances would imply large cooling rates, leading to relatively short time scales for the evolution of gravitationally unstable dense cores, forming stars and planets. Contrary to expectation, the dedicated space missions SWAS and Odin found typically only very small amounts of water vapour and essentially no $O_2$ in the dense star-forming interstellar medium.

Aims. Only toward $\rho$ Oph A did Odin detect a very weak line of $O_2$ at 119 GHz in a beam size of 10 arcmin. Line emission of related molecules changes on angular scales of the order of some tens of arcseconds, requiring a larger telescope aperture such as that of the Herschel Space Observatory to resolve the $O_2$ emission and to pinpoint its origin.

Methods. We use the Heterodyne Instrument for the Far Infrared (HIFI) aboard Herschel to obtain high resolution $O_2$ spectra toward selected positions in the $\rho$ Oph A core. These data are analysed using standard techniques for $O_2$ excitation and compared to recent PDR-like chemical cloud models.

Results. The $N_2$ = 3$\rightarrow$ 1 line at 487.2 GHz was clearly detected toward all three observed positions in the $\rho$ Oph A core. In addition, an oversampled map of the $N_2$ = 3$\rightarrow$ 1 transition at 773.8 GHz revealed the detection of the line in only half of the observed area. Based on their ratios, the temperature of the $O_2$ emitting gas appears to vary quite substantially, with warm gas ($\gtrsim$ 50 K) adjacent to a much colder region, where temperatures are below 30 K.

Conclusions. The exploited models predict $O_2$ column densities to be sensitive to the prevailing dust temperatures, but rather insensitive to the temperatures of the gas. In agreement with these model, the observationally determined $O_2$ column densities seem not to depend strongly on the derived gas temperatures, but fall into the range $N(O_2) = 3 \times 6 \times 10^{17}$ cm$^{-2}$. Beam averaged $O_2$ abundances are about $5 \times 10^{-8}$ relative to $H_2$. Combining the HIFI data with earlier Odin observations yields a source size at 119 GHz of about 4 to 5 arcmin, encompassing the entire $\rho$ Oph A core. We speculate that the general very low detection rate of $O_2$ sources might be explained by the transient nature of interstellar $O_2$ molecules.

Key words. ISM: abundances – ISM: molecules – ISM: lines and bands – ISM: clouds – ISM: individual objects: $\rho$ Oph A SM 1 – Stars: formation

1. Introduction

Despite the universal importance of oxygen, its molecular form, $O_2$, is an elusive species of the interstellar medium (ISM). This molecule was thought to be one of the main regulators of the energy balance in the ISM, as summarised by Goldsmith & Langer (1978). Consequently, large efforts, both from ground ($O^{18}O$) and space, had been devoted to obtain quantitative estimates of its abundance. The historical account of this essentially fruitless “$O_2$-struggle” was recently reviewed by Goldsmith et al. (2011).

Prior to Herschel, both SWAS (Melnick et al.2000; Goldsmith et al.2000) and Odin (Nordh et. al.2003; Pagani et al.2003) had already shown that abundances for both $O_2$ and $H_2O$ assumed by Goldsmith & Langer (1978) were much larger than actual values in the ISM and, with the exception of the $\rho$ Oph cloud, none of the $O_2$ lines were detected anywhere in the ISM. Goldsmith et al. (2002) announced the tentative detection by SWAS of the $O_2$ 487 GHz line in $\rho$ Oph A. The claimed signal appeared at an unusual velocity and was atypically broad. Pagani et al. (2003) showed that, on the basis of more sensitive $O_2$: 119 GHz observations with Odin, this was an erroneous result. This line was finally detected by Odin, at the correct LSZ-velocity and with a plausible, narrow line width (Larsson et al.2007). Here we report the detection of two more $O_2$ transitions in $\rho$ Oph A, viz. at 487 GHz and at 774 GHz, respectively.

Besides being relatively nearby (120–130 pc, Lombardi et al.2008; Snow et al.2008; Mamajek 2008; Loinard et al.2008) the $\rho$ Oph cloud distinguishes itself from other low-mass star forming regions in that it exhibits evidence (e.g., in $C^{18}O$ line emission) of gas at relatively high temperatures ($T \gtrsim 20$ K) over extended regions with high column densities ($N(H_2) \gg 10^{22}$ cm$^{-2}$, Liseau et al.2010). In addition, $\rho$ Oph A displays an interesting chemistry: For example, doubly deuterated formaldehyde ($D_2$CO) and hydrogen peroxide ($H_2O_2$) molecules, rarely seen elsewhere in the ISM have been found here (Bergman et al. 2011a, b). The overall impression is that the observable abundance of many species is the result of surface reactions on dust grains, a process which may also pertain to the production of oxygen molecules.
The motivation for the Herschel observations was, firstly, to pin down the precise location of the O$_2$ source inside the large, ten-arcminute beam of Odin. Secondly, to add observations of the O$_2$ 487.25 GHz (3-1) and 773.84 GHz (5-4) lines, which have upper level energies $E_{up}/k = 26\ K$ and $61\ K$, respectively, to the Odin data of the 118.75 GHz (1-0) transition ($E_{up}/k = 6\ K$). These observations should enable us to learn about the nature of the O$_2$ source in the p Oph cloud. This would then be compared to the physical and chemical conditions of other locations in the general ISM and potentially identify the characteristics and time scales of regions containing O$_2$ molecules.

The paper is organised as follows: in Sect. 2, our Herschel-HIFI observations and their reduction are discussed in considerable detail and our results are presented in Sect. 3. These results are discussed in Sect. 4, where the spectral line formation is analysed under different assumptions. Finally, in Sect. 5, our main conclusions are briefly summarised.

### 2. Observations and data reduction

**Herschel** is a space platform for far infrared and sub-millimetre observations (Pilbratt et al. 2010). It is orbiting the Sun about 1.5 million kilometres beyond the Earth (at L2) and its 3.5 m...
primary dish is radiatively cooled to its operational equilibrium temperature of about 85 K. The scientific instruments are placed in a liquid helium filled cryostat, limiting its cold lifetime to roughly 3.5 years. One of the three onboard instruments is the Heterodyne Instrument for the Far Infrared (HIFI, De Graauw et al. 2010) with continuous frequency coverage from 480 to 1250 GHz ($\lambda\lambda$ 624 – 234 $\mu$m) in 5 bands. In addition, the frequency range 1410 to 1910 GHz ($\lambda\lambda$ 213 – 157 $\mu$m) is covered by bands 6 and 7. The spectral resolving capability is the highest in a frequency range 1410 to 1910 GHz (486 km s$^{-1}$), which is detected in all three positions. Inspection of the individual on-off pairs suggests that the apparent absorption features next to the lines are not real but simply due to the noise. c: Similar to b but for the corresponding HRS data.

Table 2. Source designations and coordinates for $\rho$ Oph A, with positions observed in O3 in bold face.

| RA (h m s) | Dec (°′″) | 2000.0 | Source Designation | Reference |
|-----------|----------|--------|--------------------|----------|
| 16 25 24.32 | -24 27 56.57 | HD 147889 | SIMBAD: http://simbad.u-strasbg.fr/simbad/ |
| 16 26 17.5 | -24 23 13 | H 4, HH 313B | Dent et al. (1995), Garatti et al. (2006) |
| 16 26 19.0 | -24 23 08 | H 5, HH 313A | Dent et al. (1995), Garatti et al. (2006) |
| 16 26 21.36 | -24 23 06.4 | GSS 30, El 21 | Grasdalen et al. (1975), Elias (1978) |
| 16 26 25.7 | -24 23 24 | O1 | this paper |
| 16 26 25.7 | -24 23 57 | O2 | this paper |
| 16 26 26 | -24 23 14 | N2 H$^+$ N1 b (FWHM=0.29 km s$^{-1}$) | di Francesco et al. (2004) |
| 16 26 26.38 | -24 24 31.0 | VLA 1623 | Andre et al. (1999) |
| 16 26 27.1 | -24 23 30 | N5, 850 $\mu$m | di Francesco et al. (2004), Johnstone et al. (2000) |
| 16 26 27.2 | -24 24 04 | Deuterium peak | Bergman et al. (2011a) |
| 16 26 27.3 | -24 23 28 | SM 1N, 1.3 mm | Mottet et al. (1998) |
| 16 26 27.9 | -24 23 26 | O3, P2, C$^1$3O (3 - 2) | this paper, Liseau et al. (2010) |
| 16 26 27.9 | -24 23 57 | O4, P3, C$^1$3O (3 - 2); SM 1, 1.3 mm | this paper, Liseau et al. (2010), Mottet et al. (1998) |
| 16 26 34.19 | -24 23 28.2 | S 1, GSS 35, El 25 | Grasdalen et al. (1975), Elias (1978) |

2.1. 487 GHz observations

The 487 GHz observations with HIFI were performed on operating day OD 673 (2011 March 18). The three positions O1, O3 and O4 at the centre of the $\rho$ Oph A core (Table 2) were observed in double beam-switch mode (DBS), with beam throws of 3' in roughly the west and east directions (with a position angle of 101° E of N) and identified in Fig 1 by the numbers 6031 and 6032, respectively. For each position, the relative observing time spent on the east- and westward on-off pairs was 7.3 hr, and the total programme execution time was 21.9 hr. The DBS mode generally produces the highest quality data with HIFI and since the O2 signal is known to be weak, this was the observing mode chosen. Switching by only three arcminutes inside a molecular cloud is generally considered not a sensible option, as this potentially results in cancellation of the source signal. However,

Fig. 2. Averaged Double Side Band (DSB) spectra of H- and V-polarizations for the three positions O1, O3 and O4 in the $\rho$ Oph A cloud core, shown for the range 484.65 GHz to 489.85 GHz. The spectral lines are found exclusively in the Lower Side Band (LSB) and the LSR velocity, $v_{\text{LSR}}$, along the abscissa is in km s$^{-1}$ and the antenna temperature $T_A$ along the ordinate in mK. a: 5 GHz wide band of the WBS around the 487 O2 line (~1600, +1600 km s$^{-1}$). b: The WBS spectrum at expanded scale, showing the O2 line at 487 GHz, which is detected in all three positions. Inspection of the individual on-off pairs suggests that the apparent absorption features next to the lines are not real but simply due to the noise. c: Similar to b but for the corresponding HRS data.

Spectral line data and relevant characteristics of the instruments discussed in this paper have been compiled in Table 1.
a relatively large velocity gradient ($\gtrsim 0.3 \text{ km s}^{-1} / \text{arcmin}$) and/or two distinctly different velocity systems ($\Delta \nu \sim 1 \text{ km s}^{-1}$) are known to exist in $\rho$ Oph A (e.g., [Bergman et al. 2011a]). In addition, the $O_2$ line is known to be narrow (FWHM $\sim 1$ km s$^{-1}$), which taken together largely diminish the risk of signal cancellation. In fact, splitting the entire data set into two and reducing these two halves with only one off-spectrum used resulted in essentially the same spectral data. These off-beams were pointing at very different regions in $\rho$ Oph A (Fig. 1), but no traceable off-beam contamination was introduced by the DBS observations.

The receivers are double sideband and to counteract confusion in frequency space, we had selected for each observation 8 different LO-tunings inside HIFI-band 1a, spaced by 170 MHz to 260 MHz. During data reduction, this allowed sideband deconvolution and the identification of any “false” signal due to a strong feature in the other sideband, which might otherwise be folded over onto the weak $O_2$ feature.

Both the Wide Band Spectrometer (WBS) and the High Resolution Spectrometer (HRS) with respective resolutions 1.10 MHz and 250 kHz (0.68 and 0.15 km s$^{-1}$) were used. The positions of spikes and spectrometer artifacts are known and flagged and none of these interfered with the $O_2$ observations. Initial data reduction and calibrations were performed with the standard Herschel pipeline HIPE version 7.1 and the subsequent data analysis was made with a variety of other software packages. The quality of the HIFI data is excellent and it was sufficient to subtract a low order baseline for each LO setting prior to averaging. The intensity calibration accuracy is estimated to be 10%.

The frequency dependent beam widths (HPBW) and main beam efficiencies ($\epsilon_{mb}$) were adopted from [Roelfsema et al. 2012]. Before averaging the data for a given position, the $H$- and $V$-polarization spectra were all inspected individually in order to avoid the suppression of weak spectral lines or the generation of artificial features.

### 2.2. 774 GHz observations

The 774 GHz observations with HIFI Band 2 were made on OD 583 (2011 September 15). A 6 × 6 map, aligned with the equatorial celestial coordinates (Fig. 3), was obtained with 10″ regular spacing, oversampling the 28″ beam by nearly a factor of three and allowing for potentially increased spatial information of the emission regions. Both the WBS ($0.43 \text{ km s}^{-1}$) and the HRS ($0.097 \text{ km s}^{-1}$) were used. The 774 GHz data were also obtained in DBS mode, with the offset positions displaced by 3′ and in nearly the same chopping direction as before (along $pa = 98^\circ$). With 500 s on-source integrations at each position, the total observing time was 12 hr.

### 3. Results

In the figures showing HIFI data, brightness is given as antenna temperature, $T_A$. When more than one telescope had been used, the data are presented on the main beam brightness temperature scale, $T_{mb}$, where the main beam efficiency is $\epsilon_{mb} = 0.75$ for...
both HIFI transitions (Roelfsema et al. 2012) and 0.9 for the Odin transition (Frisk et al. 2005) and where we use the relation $T_A/\eta_{mb} = T_{mb}$. For completeness, we also provide in Table 3, together with the HIFI data, the results of the Odin observations.

### 3.1. 487 GHz

The reduced WBS spectra for the three positions O1, O3 and O4 are shown in the frequency range 484.65 GHz to 489.85 GHz in Fig. 2a. The Upper Side Band (USB) is completely line-free, i.e. all line detections refer to the LSB only. The presented data are DSB in order to suppress the noise. Centered on the O2 line, radial velocities span −1600 to +1600 km s$^{-1}$. In addition to the detected O$_2$ 487.25 GHz lines near an LSR velocity of 3 km s$^{-1}$ in all three positions, the spectra show a number of other emission features which correspond to identified molecular lines, due to, e.g., CS, CH$_3$OH, NH$_2$D and SO, to mention only the strongest ones. Also these spectra reveal variations in intensity and line width on angular scales of only some tens of arcsec. This remarkable behaviour of different molecular species toward the ρ Oph A core has been known for some time, and has recently been documented by Bergman et al. (2011a). The multi-line HIFI data will not be discussed further here but be presented elsewhere (Larsson et al., Pagani et al., in preparation).

Figure 2b shows the WBS spectra zoomed in on the O$_2$ 487 GHz transition. This line too displays varying intensity levels in the three positions. In particular, the line toward the O1 position appears, by comparison, rather strong and broader than those toward O3 and O4. The HRS data shown in Fig. 2 suggest the line at O1 to be a composite of two different, narrow components, blending into a single broad feature at the lower resolution of the WBS. Henceforth we will refer to this spectral component at $\nu_{\text{LSR}} \approx +3.6$ km s$^{-1}$ as O1,2, whereas the one closer to 2.8 km s$^{-1}$ is referred to as O1,1.

We summarise the spectral characteristics of the O$_2$ 487 GHz line in Table 3. Within the errors, the WBS line centroids and widths are in agreement with the Gaussian fittings of the HRS data. Also, the average intensities for positions O1,2, O3 and O4 with the WBS (8.3 ± 1.8 mK km s$^{-1}$) and the HRS (9.1 ± 1.9 mK km s$^{-1}$), respectively, are consistent with each other.

In addition, the O$_2$ line centroid and width also conform with values of other optically thin species, e.g. $^{13}$C$^{18}$O (3–2) (Liseau et al. 2010), N$_2$H$^+$ (1–0) (di Francesco et al. 2004), deuterated molecules (Bergman et al. 2011a) and the recently discovered H$_2$O$_2$ (HOOH, Bergman et al. 2011b). Regarding the 2.8 km s$^{-1}$ feature, we can at present entirely exclude the possibility that it is due to an unidentified species. If so, the line transition frequency should be $\nu_0 = (487250.548 ± 0.098)$ MHz (1σ).

### 3.2. 774 GHz

The convolved and averaged 774 GHz spectra are compared to 487 GHz spectra in Fig. 4 and the $6 \times 6$ map of the 774 GHz observations, convolved to the beam at 487 GHz, is displayed in Fig. 5. The line was not detected toward the east side of the cloud, i.e. toward O3 and O4, with 1σ-upper limits of 3 mK km s$^{-1}$, but clearly detected toward the west side of the cloud, i.e. toward O1 and O2, at $S/N = 4 - 6$. The derived line parameters for the 774 GHz spectra, convolved to the 487 GHz beam, are reported in Table 3. We note that only the 3.6 km s$^{-1}$ component is seen at the O1 position.

The O$_2$ 774 GHz line falls in the lower side band (LSB: 770.75–775.65 GHz). The entire observed spectral region is however totally dominated by the $^{13}$CO(7–6) transition at 771.2 GHz. This line exhibits significant variations on small angular scales which is clearly evident in individual pointings of the 774 GHz beam of 28″ (FWHM). In the spectrum farthest to the northeast, the line reaches a peak $T_{mb}$ of 25 K, whereas in the opposite corner in the southwest the intensity has decreased to less than 5 K.

In addition, in the upper side band (USB: 783.15–786.815 GHz), the strongest and clearly detected line is due to the C$\equiv$O (7–6) transition at 786.3 GHz (Larsson et al., in preparation). In contrast to $^{13}$CO, the line of C$\equiv$O has its maximum of almost 3 K at the O1 position.

### 4. Discussion

#### 4.1. Observed quantities: Temperature, line width, column density and size of the O$_2$ emission region

The O$_2$ 487 GHz and 774 GHz lines are clearly detected toward multiple positions. From the observation of more than one transition, some basic physical parameters of the source can be derived, where we assume that all transitions trace the same gas along the line of sight. In the case of the observed O$_2$ emission, this should be straightforward, as detailed computations of statistical equilibrium and radiative transfer for a multi-level system demonstrate this emission to be optically thin and to originate in conditions of local thermodynamic equilibrium (LTE).

##### 4.1.1. Temperature

At O1, the observed source extent of the 487 GHz and 774 GHz lines seems similar so that the ratio of the beam fillings $f_{487}/f_{774}$ is probably not far from unity. In addition, the main
From FIR continuum measurements with a 40\(^\circ\) resolution, of both the dust and the gas temperature toward O1. The actual temperatures would be even higher. Our value can be in agreement with the beam filling at 774 GHz were smaller than that at 487 GHz, yielding \(v_{\text{non-th}} = 0.72 \pm 0.80 \text{ km s}^{-1}\) for the cold region including O3 and O4 (Table 4). Hence, we find that the line broadening is totally dominated by the non-thermal random motions, being more than twice as high as the thermal ones. On the other hand, in the warm region O1 and O2, the thermal motions dominate over the non-thermal ones (0.57 km s\(^{-1}\) versus \(< 0.44 \text{ km s}^{-1}\) for \(T = 78 \text{ K}\)) or being comparable at the lower limit temperature of 47 K. This could suggest that, if the non-thermal motions are identified with turbulence at O1 and O2, much of this turbulence has been dissipated and converted into heat.

The O2 source is seen in projection close to the outflow from VLA 1623 and judging from its position (Figs. 1 and 2), it is possible that the gas at O2 is enriched by shock processed material. At the border of the outflow, a broader line might be expected due to enhanced turbulent motions. In fact, the 774 GHz line width appears (marginally) broader than that toward O1 (Table 3), but the uncertainties are large and the significance is low.

### 4.1.3. Source size

Having determined the temperature, we can use the theoretical line ratio for another transition and equate it to the ratio of the respective beam fillings, e.g. \(R = (I_{119}/I_{487})_{\text{beam}}(T)/(I_{119}/I_{487})_{\text{obs}} = f_{119}/f_{487}\). The relevant 119 GHz data have been adopted from Larson et al. (2007) and are compiled in Table 5 and all lines are displayed on the \(T_{\text{mb}}\) scale in Fig 6. For a Gaussian beam at 119 GHz, the beam filling factor is given by \(f_{119} = \theta_{119}^2/(\theta_{119}^2 + \theta_{\text{O2}}^2)\), where \(\theta_{119}\) is the size of the source and \(\theta_{\text{O2}}\) is that of the beam at 119 GHz. Re-arranging, this reads \(\theta_{119} = \theta_{\text{O2}}\sqrt{1/f_{119} - 1}\) or \(\theta_{119}/\theta_{\text{O2}} = \sqrt{f_{119}/f_{487}} - 1\), where \(\theta_{\text{O2}} = 10\)\(^\prime\).

The 487 GHz source seems to be extended on the scale of at least the beam width, i.e. \(f_{487} \geq 0.5\), and for the average values of \(<O1, O3, O4>\) results in a value of about 20 to 25 K, which is entirely consistent with earlier determinations, based on a variety of techniques. Temperatures between 9 K and 49 K have been derived, but with most values clustering around 20–30 K (e.g., Harvey et al. 1979; Loren et al. 1980; Ward-Thompson et al. 1989; Motte et al. 1998; Stamatellos et al. 2007; Bergman et al. 2011a; Ade et al. 2011).

As is evident from Fig. 5, a temperature gradient or two distinctly different temperature regimes, i.e. with larger than about 50 K and distinctly lower than 30 K, exist within the boundaries of our limited map of roughly one square arcminute (see also Figs. 1 and 2).

### 4.1.4. Column density

For the warm region O1, an O2 column density of \(5 \times 10^{13} \text{ cm}^{-2}\) is derived, whereas for the cold O4, \(N(O_2) > 6 \times 10^{16} \text{ cm}^{-2}\) (Table 4). These estimations are based on the assumption of optically thin emission in LTE at the kinetic gas temperature.
Fig. 5. Left: The regridded 6 × 6 map of the WBS 774 GHz spectra, weighted by the Gaussian profile of the 487 GHz beam of 44″. The darker area shows roughly the region inside that Half Power Beam Width (HPBW). The $v_{LSR}$ and $T_A$ scales are indicated in the upper right corner. Right: Same as to the left but shown as an image of the spatial distribution of the integrated intensity, $\int T_A d\nu$, with observed positions shown as plusses. The circles show the 487 GHz and 774 GHz beams, respectively.

\[ T_{\text{kin}}, \text{i.e. for unit beam filling the O}_2 \text{ column is given by} \]
\[ N(O_2) = \int T_{mb} d\nu \times \Phi(T_{\text{kin}}) \text{ cm}^{-2} \]
when the integral is expressed in K cm s\(^{-1}\) and where
\[ \Phi(T_{\text{kin}}) = \left( \frac{2\pi c}{\hbar} \right)^3 \frac{T_{\text{kin}}^2}{h_0 A_d} \frac{F_{\nu}(T_{\text{kin}})}{F_{\nu}(T_{\text{mb}})} Q(T_{\text{kin}}) \exp(T_{\text{up}}/T_{\text{kin}}), \]
in K\(^{-1}\) cm\(^{-3}\) s (cgs units throughout). Here, the transition temperature is $T_{\text{mb}} \equiv h\nu/k$, the quasi-Planck function is $F_\nu(T) \equiv T_\nu/(e^{h\nu/T} - 1)$, the partition function is $Q(T)$, the upper level energy is $T_{\text{up}} = E_{\text{up}}/k$ and the other symbols have their usual meaning. The background temperature is that of the cosmic microwave background, i.e. $T_{bg} = T_{\text{CMB}}$.\(^1\) The frequencies were adopted from Drouin et al. (2010) and the Einstein A-values from Marečal et al. (1997) (see also Black & Smith (1984).

If on the other hand <O1, O3, O4> can be taken as a representative for $\rho$ Oph A as a whole, column densities lower than 5 × 10\(^{15}\) cm\(^{-2}\) would be indicated. Although there is a considerable range in gas kinetic temperature, the O3 column densities seem not to vary much. However, with the observed inhomogeneity of the emission in mind, the significance of such an average could be questioned.

4.2. O\(_2\) abundance

Once the O\(_2\) column density is known, the line of sight average O\(_3\) fractional abundance, with respect to H\(_2\) or H-nuclei, can be measured if the column density of H\(_2\) molecules is available. The hydrogen column density along the appropriate lateral and depth scales is not well known from observation. However, we can get an approximate idea from the C\(^{18}\)O observations by Liseau et al. (2010), where it was suggested on the basis of the line profiles that the $J=3–2$ line was a reasonably good proxy for the O\(_2\) 119 GHz line observed with Odin (Larsson et al. 2007). If the O\(_2\) molecules are indeed cospatial with those of CO and its isotopic variants, their optically thin lines could be used to infer the H\(_2\) column densities relevant also for O\(_2\). We derive “local” C\(^{18}\)O column densities taking C\(^{18}\)O intensity and O\(_2\) temperature variations into account. The gas and dust peaks coincide spatially (see also Table 2), i.e. there is no indication of significant CO freeze out (at levels higher than a factor of 2 to 3, see Fig. 10 of Bergman et al. 2011a). The C\(^{18}\)O column density varies by less than 20% for 20 K ≤ $T_{\text{kin}}$ ≤ 50 K. Assuming that C\(^{18}\)O/H\(_2\) = 1.5 × 10\(^{-7}\) (likely within about 30%, e.g. Wannier et al. 1976) (Goldsmith et al. 2000), H\(_2\) columns are found to be 1 × 10\(^{25}\) cm\(^{-2}\).

Hence, for the O\(_2\) column densities in Table 2, we find that $X(O_2) = 5 \times 10^{-8}$ relative to H\(_2\) in the warm gas toward the west, at O1 (and likely also toward O2), and higher than that toward the east, at the colder O4. The C\(^{18}\)O lines are slightly optically thick, implying that these H\(_2\) column densities are lower limits and need to be adjusted upwards by a factor of the order of $1/(1-e^{-\tau}) \geq 2$, for $\tau \sim 2$. Hence, these O\(_3\) abundances are upper limits, i.e. the fractional abundance of O\(_2\) in the gas phase is less than indicated above.

A way to obtain a more detailed picture of the source is to use detailed theoretical models to predict the O\(_2\) abundance or column and to compare these models with the observations. This will be the topic of the next section.

\(^1\) In our numerical radiative transfer calculations (Sect. 4.1), also the dust continuum is included. These calculations make use of the collision data of Lique (2010).
Fig. 6. Averaged data for the HIFI O₂ observations (774 and 487 GHz) and the Odin 119 GHz spectrum toward ρ Oph A. For proper comparison, these spectra are given in the $T_{\text{mb}}$ scale and for reference, a vertical dotted line is shown at $v_{\text{LSR}} = +3.5 \text{ km s}^{-1}$.

4.3. Chemical models

Specifically for O₂ (and H₂O), [Hollenbach et al. (2009)] constructed theoretical models of Photon-Dominated Regions (PDRs, Hollenbach & Tielens 1997), invoking also grain surface chemistry, including freeze-out and desorption of the species. These new models are models of the whole cloud, to arbitrary values of the extinction, and showing that most of the gas phase O₂, OH and H₂O is found at values of $A_V \sim 3$–10 mag, where the details depend, as in a conventional PDR, on the ratio $G_0/n_H$. In many aspects, these models are similar to the traditional dense PDR models including chemistry and gas heating which have been developed to explain the abundances and column densities of other molecules (including radicals and ions) at intermediate depths into the clouds (e.g., Fuente et al. 1993; Sternberg & Dalgarno 1995; Jansen et al. 1995; Simon et al. 1997; Pety et al. 2005). The current models are extended even deeper into the cloud where external UV photons play no role anymore in the chemistry, only cosmic-ray induced photons.

In the direction of ρ Oph A, a number of spectroscopic indicators suggest the presence of a PDR [Liseau et al. (1999) inferred that the PDR is situated on the rear side of ρ Oph A, as seen from the Sun, and excited by the two stellar sources HD 147889 and S 1 (see Fig. 1 and Table 2) by their combined UV fields, corresponding to $G_0 \sim 10^2$. For the densest parts of the cloud, atomic recombination lines of carbon, $^{12}$C, and sulfur, $^{33}$S, (Cesarsky et al.1976; Pankonin & Walmsley 1978), fine structure lines: [C I] 492.2 GHz, (Kamegai et al. 2003), [C I] 809.3 GHz (Kamegai et al. 2003; Kulesa et al. 2005), [C II] 157 μm (Yui et al. 1993; Liseau et al. 1999), [O I] 63 μm (Ceccarelli et al. 1997; Liseau et al. 1999), [O I] 145 μm (Liseau et al. 1999; Liseau & Justtanont 2009) and mid-infrared PAH emission: (Liseau & Justtanont 2009).

Fig. 7. Upper: LTE computations of the O₂ column density $N(O_2)$ as function of the temperature $T$ for an extended homogeneous source, to yield a line intensity of 1.0 K km s$^{-1}$. For optically thin emission, intensity and column density are linearly related. 119 GHz: blue dots; 487 GHz: black solid line; 774 GHz: red short dashes. Lower: The ratio of the 487 GHz integrated line intensity to that at 774 GHz is shown by the curve for a range of temperatures. For O1 ($=O_1$ and $O_1$), the error shown by the dashed line formally extends to the unphysical result of nearly 10$^3$ K. For O4, the limit symbols are for the lower limit on the intensity ratio and the upper limit on the temperature, respectively.
the [C II] emitting $\rho$ Oph A-PDR these authors derived empirically $n_{\text{H}} = 5 \times 10^4$ cm$^{-3}$ and over more extended regions, 1 to $3 \times 10^3$ cm$^{-3}$.

The model of [Hollenbach et al. 2009] predicts columns of O$_2$ between about 10$^{4.5}$ and a few times 10$^{6}$ cm$^{-2}$ depending on the grain temperature in the O$_2$-emitting region, with higher columns in regions with warmer dust. Warmer ($T_d > 20$ K) dust produces more O$_2$ column because O atoms evaporate from grains before they can react with atomic hydrogen sticking to the grains. This increases the elemental gas phase O available to make O$_2$, whose abundance in the $\rho$ Oph model can reach locally above 10$^{-3}$ for $T_d = 25$ K. The results are quite insensitive to the gas temperature in the O$_2$-emitting region for the range 10 K $< T_d < 100$ K.

However, the [Hollenbach et al. 2009] models predict gas temperatures of only ~20 K, as would all thermochemical models with only cosmic ray heating and heating by the penetrating FUV. Gas temperatures as high as 80 K, as derived here, suggest other heating mechanisms, such as slow shocks or turbulent dissipation (e.g., Goldsmith et al. 2010). Our observations show a slight increase in O$_2$ column in cooler gas. If the dust is also cooler in the cooler gas region, as would be expected for the derived densities above 10$^7$ and, centrally, higher than 10$^7$ cm$^{-3}$, this contradicts the predictions of this particular model.

On the other hand, geometry also plays a role in determining the column of O$_2$ observed along the line of sight. The [Hollenbach et al. 2009] models assume an illuminated slab face-on. However, clumpiness and more edge-on geometry could increase the observed column in some beams, and could explain the slightly increased column of O$_2$ in the region with somewhat cooler gas. We conclude that these models are modestly consistent with the observations, but likely require some additional gas heating in the O$_2$-emitting region. We defer detailed thermochemical modeling of these $\rho$ Oph observations to a future paper.

4.4. Source(s) of O$_2$ or the dearth of O$_2$

The discussed models could be expected to apply quite generally to all externally illuminated molecular clouds developing PDR-like parts. It is surprising therefore that O$_2$ has been detected only toward the dense cloud core $\rho$ Oph A (Larsson et al. 2007 and this work) and a spot in OMC-1 (Goldsmith et al. 2011), in spite of numerous searches toward other regions. For instance, surveying twenty sources, Goldsmith et al. (2000) obtained limiting O$_2$ abundances $N$(O$_2$)/$N$(H$_2$) of a few times 10$^{-7}$, whereas Pagani et al. (2003) derived limiting O$_2$ columns of 10$^{15}$ to a few times 10$^{16}$ cm$^{-2}$ for nearly a dozen objects. These surveys included dark clouds, regions of low mass star formation in the solar neighbourhood and of high mass star formation at different galactocentric distances, i.e. these surveys sampled a wide range of cloud properties and energetics, from quiescent cold clouds to turbulent shock heated gas due to mass infall and molecular outflows. Yet, most escaped detection, although their limiting O$_2$ column densities fall within the range predicted by the theoretical models.

One possibility could be that this apparent mismatch is due to observational bias, such as source distance and beam dilution. For instance, the limit on the O$_2$ column in Ori A determined by Pagani et al. (2003) is entirely consistent with the HIFI beam-averaged detection obtained by Goldsmith et al. (2011), if proper correction for dilution in the Odin-beam is applied. We recall that the detected spot is not toward the Orion-PDR (Melnick et al. 2012), as one might have expected, but close to the outflow in the vicinity of IRc2.

However, the difference in distance aside, with differing $G_0/n_{\text{H}}$, $\rho$ Oph A and Ori A represent very different environments, viz. cold core deuterium versus hot core grain chemistry (Bergman et al. 2011a; Bisschop et al. 2007; Ceccarelli et al. 2007; Ratijczak et al. 2011). Star forming regions like IRAS 16293 in Ophiuchus, NGC 7333 in Perseus or the Serpens core near S 68 are more akin to the conditions in $\rho$ Oph A, yet no O$_2$ detections have been reported. These complexes are at the same or within at most twice the distance to $\rho$ Oph A, so that beam dilution issues should be much reduced. It is conceivable that the viewing geometry of $\rho$ Oph A could be particularly favourable for the observability of O$_2$ and that this aspect is not shared by other regions.

However, a clear difference is suggested by the fact that hydrogen peroxide (H$_2$O$_2$) has so far only been detected in $\rho$ Oph A (Bergman et al. 2011b). H$_2$O$_2$ is thought to be a clear indicator of grain surface chemistry and relatively abundant at about 30 K (e.g., Cazaux et al. 2010). The simultaneously detectable abundance of O$_2$ and H$_2$O$_2$ may perhaps be used to infer the evolutionary chemical state of the cloud, hence its “age”, if interstellar gas phase O$_2$ is relatively transient (Du et al. 2012). In that case, it could explain the paucity of known O$_2$ line emitters.

5. Conclusions

• We have successfully detected the $3_1-1_2$ transition of O$_2$ at 487 GHz with HIFI onboard Herschel toward three positions in the $\rho$ Oph A core. In addition, we have also obtained a $6 \times 6$ oversampled map with 10$''$ spacings in the $5_2-3_2$ transition at 774 GHz.

• The telescope pointings were toward two cold, high density cores, i.e. O4 [C$^{18}$O P3 = SM 1] and O3 [C$^{18}$O P2, near SM 1N], and two positions 30$''$ west of these, labelled O2 and O1, respectively. All three observed positions (O1, O3 and O4) were detected in the 487 GHz line, with significant variations of the line intensity on scales as small as 30$''$. At 774 GHz, emission was detected from only the western part of the map, including O1 and O2.

• Combining the 487 GHz and 774 GHz data leads to the column density of $N$(O$_2$) $> 6 \times 10^{15}$ cm$^{-2}$, at the 3$\sigma$ level and at T $< 30$ K, in the high density region O3 and O4, whereas in the warmer region of O1 and O2, $N$(O$_2$) $= 5.5 \times 10^{15}$ cm$^{-2}$ (T $> 50$ K). There, standard analysis yields an abundance of $N$(O$_2$)/$N$(H$_2$) $< 5 \times 10^{-8}$ in the warm gas and somewhat higher in the cold region.

• This result is in agreement with $\chi$(O$_2$) based on the observation of the 119 GHz line with Odin (Larsson et al. 2007), assuming that the O$_2$ source size has an angular extent of about 5$''$.

• Comparing our results with the predictions from theoretical chemical models, we find good agreement between observed and predicted O$_2$ column densities. Less convincing agreement regards theoretical and observed temperatures, the reasons for which are not clear.

• The question why O$_2$ is such an elusive molecule in the ISM is still unanswered. In the special case of $\rho$ Oph A, there is some evidence suggesting that detectable amounts of gas phase O$_2$ might be a relatively transient phenomenon, which could explain why interstellar O$_2$ is generally not detected.

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