Multi-line detection of O$_2$ toward $\rho$ Ophiuchi A


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ABSTRACT

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$_2$O. These high abundances imply high cooling rates, leading to relatively short timescales for the evolution of gravitationally unstable dense cores, forming stars and planets. Contrary to expectations, the dedicated space missions SWAS and Odin typically found only very small amounts of water vapour and essentially no O$_2$ in the dense star-forming interstellar medium. Despite the universal importance of oxygen, its molecular abundances in the 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, from both the ground (O$_2$(O)) and space, were made to obtain quantitative estimates of its abundance. The historical account of this essentially fruitless “O$_2$-struggle” was reviewed by Goldsmith et al. (2011). Prior to Herschel, both SWAS (Melnick et al. 2000; Goldsmith et al. 2000) and Odin (North et al. 2003; Pagani et al. 2003) had already shown that the abundances of both O$_2$ and H$_2$O assumed by Goldsmith & Langer (1978) were much higher 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, based on more sensitive O$_2$ 119 GHz observations with Odin, this was an erroneous result. This line was finally detected by Odin, at the correct local standard of rest (LSR) 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 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 ($T \geq 20$ 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: doubly deuterated formaldehyde (D$_2$CO) and hydrogen peroxide (H$_2$O$_2$) molecules, rarely seen elsewhere in the ISM,
Table 1. Instrumental reference.

<table>
<thead>
<tr>
<th>Transition$^a$</th>
<th>Frequency$^b$</th>
<th>Wavelength</th>
<th>Energy $E_{up}/k$ (K)</th>
<th>Observatory/Instrument</th>
<th>Beam width HPBW (')</th>
<th>Efficiency $\eta_{ob}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1_1-1_0$</td>
<td>118750.34</td>
<td>2526</td>
<td>5.7</td>
<td>Odin</td>
<td>9.96</td>
<td>0.91</td>
<td>Frisk et al. (2003)</td>
</tr>
<tr>
<td>$3_3-3_2$</td>
<td>487249.26</td>
<td>616</td>
<td>26.4</td>
<td>SWAS</td>
<td>3.5 x 5.0</td>
<td>0.90</td>
<td>Melnick et al. (2000)</td>
</tr>
<tr>
<td>$5_3-3_4$</td>
<td>773839.512</td>
<td>388</td>
<td>60.7</td>
<td>HIFI</td>
<td>0.73</td>
<td>0.757</td>
<td>Roelfsema et al. (2012)</td>
</tr>
</tbody>
</table>

Notes. (a) An energy level diagram is provided by, e.g., Goldsmith et al. (2011). (b) Frequencies are from the JPL-catalogue http://spec.jpl.nasa.gov/cgi-bin/catform

Table 2. Source designations and coordinates for ρ Oph A, with positions observed in O$_2$ in bold face.

<table>
<thead>
<tr>
<th>RA (h:m:s) J2000.0</th>
<th>Dec ('&quot;:&quot;) J2000.0</th>
<th>Source designation</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 25 24.32</td>
<td>−24 27 56.57</td>
<td>HD 147889</td>
<td>SIMBAD: <a href="http://simbad.u-strasbg.fr/simbad/">http://simbad.u-strasbg.fr/simbad/</a></td>
</tr>
<tr>
<td>16 26 17.5</td>
<td>−24 23 13</td>
<td>H 4, HH 313B</td>
<td>Dent et al. (1995), Caratti o Garatti et al. (2006)</td>
</tr>
<tr>
<td>16 26 19.0</td>
<td>−24 23 08</td>
<td>H 5, HH 313A</td>
<td>Dent et al. (1995), Caratti o Garatti et al. (2006)</td>
</tr>
<tr>
<td>16 26 21.36</td>
<td>−24 23 06.4</td>
<td>GSS 30, El 21</td>
<td>Grasdalen et al. (1973), Elias (1978)</td>
</tr>
<tr>
<td>16 26 25.7</td>
<td>−24 23 24</td>
<td>O1</td>
<td>this paper</td>
</tr>
<tr>
<td>16 26 25.7</td>
<td>−24 23 57</td>
<td>O2</td>
<td>this paper</td>
</tr>
<tr>
<td>16 26 26.1</td>
<td>−24 23 14</td>
<td>N$_2$H$^+$ N1 b ($FWMH = 0.29$ km s$^{-1}$)</td>
<td>di Francesco et al. (2004)</td>
</tr>
<tr>
<td>16 26 26.38</td>
<td>−24 24 31.0</td>
<td>VLA 1623</td>
<td>André et al. (1990)</td>
</tr>
<tr>
<td>16 26 27.1</td>
<td>−24 23 30</td>
<td>N5, 850$\mu$m</td>
<td>di Francesco et al. (2004), Johnstone et al. (2000)</td>
</tr>
<tr>
<td>16 26 27.2</td>
<td>−24 24 04</td>
<td>Deuterium peak</td>
<td>Bergman et al. (2011a)</td>
</tr>
<tr>
<td>16 26 27.3</td>
<td>−24 23 28</td>
<td>SM 1, 1.3 mm</td>
<td>Motte et al. (1998)</td>
</tr>
<tr>
<td>16 26 27.9</td>
<td>−24 23 26</td>
<td>O3, P2, C$^{18}$O (3 - 2)</td>
<td>this paper, Liseau et al. (2010)</td>
</tr>
<tr>
<td>16 26 27.9</td>
<td>−24 23 57</td>
<td>O4, P3, C$^{18}$O (3 - 2); SM 1, 1.3 mm</td>
<td>this paper, Liseau et al. (2010), Motte et al. (1998)</td>
</tr>
<tr>
<td>16 26 34.19</td>
<td>−24 23 28.22</td>
<td>S 1, GSS 35, El 25</td>
<td>Grasdalen et al. (1973), Elias (1978)</td>
</tr>
</tbody>
</table>

have for example 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 that may also pertain to the production of oxygen molecules.

The first motivation behind our Herschel observations was to pin down the precise location of the O$_2$ source inside the large, ten-arcminute beam of Odin. Secondly, we wished to add observations of the O$_2$ 487.25 GHz (3$_3$−1$_2$) and 773.84 GHz (5$_3$−3$_4$) 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$_1$−1$_0$) transition ($E_{up}/k = 6$ K). These observations should enable us to learn something about the nature of the O$_2$ source in the ρ Oph cloud. This could then be compared to the physical and chemical conditions of other locations in the general ISM and potentially identify the characteristics and timescales 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 orbits the Sun about 1.5 million kilometres beyond the Earth (at L 2) 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 GHz to 1250 GHz (4.624 – 234 lm) in 5 bands. In addition, the frequency range 1410 GHz to 1910 GHz (4.6213 – 157 lm) is covered by bands 6 and 7. The spectral resolving capability is the highest available on Herschel, i.e. up to 10$^7$ corresponding to 30 m s$^{-1}$, and is required to resolve the profiles of very narrow lines of cold sources, which have temperatures of the order of 10 K or less.

Spectral line data and the relevant characteristics of the instruments discussed in this paper have been compiled in Table 1.

2.1. The 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 ρ 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 h, and the total programme execution time was 21.9 h. The DBS mode generally produces the highest quality data with HIFI and since the O$_2$ signal is known to be weak, this was the observed mode chosen. Switching by only three arcminutes inside a molecular cloud is generally considered not to be a sensible option, as this potentially results in the cancellation of the source signal. However, a relatively large velocity gradient (>0.3 km s$^{-1}$/arcmin) and/or two distinctly different velocity systems ($\Delta$υ ~ 1 km s$^{-1}$) are known to exist in ρ Oph A (e.g., Bergman et al. 2011a). In addition, the O$_2$ line is known to be narrow ($FWMH \sim 1$ km s$^{-1}$). Hence, all of these factors taken together suggest that the risk of signal cancellation is low. Splitting the entire data set into two and reducing these two halves with only one of the off-spectra used resulted in essentially the
Fig. 1. Herschel beams of O$_2$ 487 GHz (44″) superposed onto a grey scale C$^{18}$O (3−2) map of ρ Ophi A (Liseau et al. 2010). The + and × symbols designate the positions of the H- and V-polarization beam centres of HIFI, respectively, with a separation of 6″. The heavy circles show the positions of the sources O1, O3, and O4 (see Table 2), with the corresponding off-source reference positions shown by the displaced symbols to the east and west and identified by their observation numbers, 6032 and 6031 respectively, above the double arrows. The origin is at $16^h26^m24^s.6$, $-24^\circ23'54''$ J(2000.0) and offsets in RA and Dec are in arcsec. At the distance of 120 pc, 40″ corresponds to about 0.02 pc. The star symbols identify the positions of the star S1, the young stellar object GSS 30 and the Class 0 source VLA 1623, where the contours depict red- and blueshifted CO (3−2) emission of its bipolar outflow. The filled squares identify the known Herbig-Haro objects H1 through 5 and the direction to the dominating B-star HD 147889, about 15′ away, is indicated by the heavy arrow.

same spectral data. These off-beams were pointed at very different regions in ρ Oph A (Fig. 1), but no traceable off-beam contamination was introduced by the DBS observations.

The receivers are double side-band and to counteract confusion in frequency space, we selected for each observation 8 different LO-tunings inside HIFI-band 1a, spaced by 170 MHz to 260 MHz. During data reduction, this allowed us to perform a sideband deconvolution and identify any “false” signal due to a strong feature in the other sideband, which might otherwise have been folded over onto the weak O$_2$ feature.

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 a 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 km s$^{-1}$) and the HRS (0.097 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″). With 500 s on-source integrations at each position, the total observing time was 12 h.

3. Results

In the figures showing HIFI data, brightness is given as the 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 $\eta_{mb}$ = 0.75 for both HIFI transitions (Roelfsema et al. 2012) and 0.9 for the Odin transition (Frisk et al. 2003; Hjalmarson et al. 2003) 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.
Table 3. O2 line observations of Ρ Oph A.

<table>
<thead>
<tr>
<th>Position/ Average</th>
<th>$T_{\text{int}, o}$ (mK)</th>
<th>$v_{\text{LSR}}$ (km s$^{-1}$)</th>
<th>FWHM (km s$^{-1}$)</th>
<th>$10^7 \frac{\tilde{T}<em>{\text{int}}}{T</em>{\text{int}}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1 HRS</td>
<td>14.4 ± 1.8</td>
<td>3.05 ± 0.10</td>
<td>1.63 ± 0.23</td>
<td>19.8 ± 2.4</td>
</tr>
<tr>
<td>O1_1$^b$</td>
<td>24.2 ± 3.3</td>
<td>2.79 ± 0.05</td>
<td>0.46 ± 0.08</td>
<td>15.5 ± 1.7</td>
</tr>
<tr>
<td>O1_2</td>
<td>19.6 ± 3.5</td>
<td>3.58 ± 0.04</td>
<td>0.41 ± 0.09</td>
<td>8.7 ± 1.7</td>
</tr>
<tr>
<td>O3 HRS</td>
<td>7.6 ± 2.2</td>
<td>3.59 ± 0.12</td>
<td>0.80 ± 0.27</td>
<td>5.7 ± 1.3</td>
</tr>
<tr>
<td>O4 HRS</td>
<td>11.5 ± 2.5</td>
<td>3.75 ± 0.07</td>
<td>0.84 ± 0.16</td>
<td>13.0 ± 1.6</td>
</tr>
<tr>
<td>O1 WBS</td>
<td>9.4 ± 2.0</td>
<td>2.89 ± 0.20</td>
<td>1.91 ± 0.46</td>
<td>18.4 ± 1.6</td>
</tr>
<tr>
<td>O1_1</td>
<td>9.6 ± 1.4</td>
<td>2.70 fix</td>
<td>0.90 fix</td>
<td>9.2 ± 1.4</td>
</tr>
<tr>
<td>O1_2</td>
<td>6.9 ± 1.4</td>
<td>3.60 fix</td>
<td>0.90 fix</td>
<td>6.6 ± 1.4</td>
</tr>
<tr>
<td>O3 WBS</td>
<td>5.7 ± 3.4</td>
<td>3.66 ± 0.26</td>
<td>0.87 ± 0.60</td>
<td>5.3 ± 1.5</td>
</tr>
<tr>
<td>O4 WBS</td>
<td>10.3 ± 2.6</td>
<td>3.78 ± 0.12</td>
<td>0.99 ± 0.28</td>
<td>10.3 ± 1.5</td>
</tr>
<tr>
<td>(O3, O4) WBS</td>
<td>7.8 ± 3.0</td>
<td>3.69 ± 0.20</td>
<td>0.90 ± 0.47</td>
<td>7.8 ± 1.5</td>
</tr>
</tbody>
</table>

$774$ GHz, $N_{\text{J}} = 3_1 - 2_0$

(01, O2) HRS

22.3 ± 9.9          3.59 ± 0.03          0.57 ± 0.10        13.2 ± 4.0

O1 WBS

17.9 ± 4.2          3.67 ± 0.07          0.61 ± 0.16        11.4 ± 2.9

O2 WBS

14.5 ± 3.8          3.59 ± 0.09          0.72 ± 0.22        10.9 ± 2.8

(01, O2) WBS

15.9 ± 2.8          3.62 ± 0.06          0.67 ± 0.17        11.2 ± 2.0

O3 WBS

...               ...                        ...                ...                ...

O4 WBS

...               ...                        ...                ...                ...

(O3, O4) WBS

...               ...                        ...                ...                ...

$119$ GHz, $N_{\text{J}} = 2_1 - 1_0$

Odin$^a$

19.3 ± 0.6          3.5 ± 0.5           1.5 ± 0.5          26.7 ± 4.4

Notes. $^{a)}$ Gaussian fits: peak intensity, central velocity and full width half maximum of line. $^{b)}$ O1_1 and O1_2 refer to two velocity components (see Sect. 3.1). $^{c)}$ 10' beam centred on ρ Oph A (Larsson et al. 2007).

3.1. 487 GHz

The reduced WBS spectra for the three positions O1, O3, and O4 are shown for 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. Centred on the O2 line, radial velocities span $-1600$ to $+1600$ km s$^{-1}$. In addition to the detected O2 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 that correspond to identified molecular lines, e.g., CS, CH$_3$OH, NH$_2$D, and SO, to mention only the strongest ones. In addition these spectra reveal variations in intensity and line width on angular scales of only some tens of arcsec. The remarkable behaviour of these different molecular species toward the ρ Oph A core has been known for some time, and was recently documented by Bergman et al. (2011a). Our multi-line HIFI data will not be discussed further here but will be presented elsewhere (Larsson et al.; Pagani et al., in prep.).

Figure 2b shows the WBS spectra zoomed in on the O$_2$ 487 GHz transition. The intensity of this line also varies at 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. 2c suggest that the line at O1 is a composite of two different, narrow components, blended into a single broad feature at the lower resolution of the WBS. Henceforth, we refer to this spectral component at $v_{\text{LSR}} \sim +3.6$ 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 agree with the Gaussian fittings of the HRS data. In addition, the average intensities at the 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)
Fig. 3. Outline of the oversampled 6 × 6 regular map with 10″ spacings of the O2 774 GHz observations. At this frequency, the beam of the 3.5 m Herschel telescope has a size of 28″ (small blue circles). The beam centres for the H- and V-polarisations are separated by 4″5. Larger (black) circles correspond to the 487 GHz beam positions (44″; cf. Fig. 1) and as before, north is up and east is to the left. Background image is courtesy of Spitzer IRAC-MIPS (blue: 3.6 μm, green: 8 μm, red: 24 μm).

Fig. 4. The WBS spectra toward the positions O1 to O4 are shown for both the 774 GHz (upper) and 487 GHz (lower) lines in each frame. The average 774 GHz data are convolved to the 487 GHz beam of 44″. Offsets relative to the origin O4 are shown along the upper and right-hand scales.

3.2. 774 GHz

In Fig. 4 the convolved and averaged 774 GHz spectra are compared to the 487 GHz spectra, and the 6 × 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 a signal-to-noise ratio of 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 O2 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 13CO (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 width 28″ (FWHM). In the spectrum farthest to the northeast, the line reaches a peak Tmb 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 C17O (7−6) transition at 786.3 GHz (Larsson et al., in prep.). In contrast to 13CO, the line of C17O reaches 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 O2 emission region

The O2 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 O2 emission, this should be straightforward, as detailed computations of statistical equilibrium and radiative transfer for a multi-level system demonstrate that this emission is optically thin and originates 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 appears to be similar, hence the ratio of the beam fillings f487/f774 is probably not far from unity. In addition, the main beam efficiencies at these frequencies are also about equal (Table 1). Therefore, the observed ratio of integrated intensities I(487)/I(774)obs is directly comparable to the theoretical one, I(487)/I(774)theo, obtained from LTE calculations for optically thin O2 radiation, which depends only on the gas temperature (Fig. 7).

From Table 4, we see that the measured intensity ratio of the 487 GHz to 774 GHz lines toward O1 implies a temperature of nearly 80 K, with the large error allowing a large range, from about 50 K to very much higher than 100 K (see also Fig. 7). If the beam filling at 774 GHz were smaller than that at 487 GHz, the actual temperatures would be even higher. Our value can
be compared to earlier estimates, obtained at comparable spatial resolution, of both the dust and the gas temperature toward O1. From FIR continuum measurements with a 40′′ beam, Harvey et al. (1979) obtained the dust temperature $T_d = 41$ K. Zeng et al. (1984) derived from NH$_3$ observations, also with a 40′′ beam, the temperature of the gas, $T_g = 45$ K.

For the dense spot O4 (P3, SM1), the 3σ upper limit to the 774 GHz line yields a temperature that is strictly lower than 31 K, which would agree with the value of $T_g = 22 \pm 3$ K obtained by Bergman et al. (2011b). For the dense core ρ Oph A, the average for (O1, O3, O4) results in a value of about from 20 K 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. higher than about 50 K and strictly lower than 30 K, exist within the boundaries of our limited map of roughly one square arcminute (see also Figs. 1 and 3).

### 4.1.2. Line width

Comparing the observed line widths, FWHM, of Table 3 with the resolutions offered by the HRS and WBS, we see that the HRS data for the 487 GHz line are all well-resolved ($\Delta \nu = 0.15$ km s$^{-1}$), whereas the 774 GHz line toward O1 and O2 is just barely resolved with the WBS ($\Delta \nu = 0.43$ km s$^{-1}$). However, the average 774 GHz spectrum (O1, O2) is well-resolved with the HRS and the line has a comparable width to that observed with the WBS. It is remarkable that the lines in the cold regions O3 and O4 are observed to be broader than those in the warmer O1 and O2.

The non-thermal contribution to the observed width, $\Delta \nu = FWHM$, of an unblended line is $\Delta \nu_{\text{th}} = (\Delta \nu^2 - \Delta \nu_{\text{nh}}^2)^{1/2}$, where all radial velocities are expressed in terms of their FWHM. For $T$ in the range 18 K to 30 K, $\Delta \nu_{\text{th}} = 0.27$ to 0.35 km s$^{-1}$, yielding $\Delta \nu_{\text{th}} = 0.72$ to 0.80 km s$^{-1}$ for the cold region including O3 and O4 (Table 4). Hence, we find that there the line broadening is totally dominated by the non-thermal random motions, which are 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 $\leq 0.44$ km s$^{-1}$ for $T = 78$ K) or are 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.

### Table 4. Observed O$_2$ line intensity ratios.

<table>
<thead>
<tr>
<th>Spectrum/Position</th>
<th>$I_{487}$/c</th>
<th>$T_{\text{kin}}$ (K)</th>
<th>$N$(O$_2$) (cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1_1 (2.8 km s$^{-1}$)</td>
<td>&gt;0.9 (3σ)</td>
<td>&lt;40</td>
<td>$&gt;2 \times 10^{15}$</td>
</tr>
<tr>
<td>O1_2 (3.6 km s$^{-1}$)</td>
<td>0.58±0.19</td>
<td>78</td>
<td>5.4 $\times 10^{15}$</td>
</tr>
<tr>
<td>O2</td>
<td>0.39 (1σ)</td>
<td>47</td>
<td>5.0 $\times 10^{15}$</td>
</tr>
<tr>
<td>O3</td>
<td>&gt;0.61 (3σ)</td>
<td>&gt;70</td>
<td>$&gt;3 \times 10^{15}$</td>
</tr>
<tr>
<td>O4</td>
<td>&gt;1.14 (3σ)</td>
<td>&gt;31</td>
<td>$&gt;6 \times 10^{15}$</td>
</tr>
<tr>
<td>O1, O3, O4</td>
<td>1.43±0.94</td>
<td>25</td>
<td>3.4 $\times 10^{15}$</td>
</tr>
</tbody>
</table>

Notes. (a) Errors are $\pm (I_2/I_1)\sqrt{(\delta I_1/I_1)^2 + (\delta I_2/I_2)^2}$. (b) For HIFI, $\eta_{\text{HI}}(487) = \eta_{\text{HI}}(737) = 0.75$. (c) Similar to O3 for 1σ limit on 774 GHz intensity (1.47 ± 1.26).

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**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 within the half power beam width (HPBW). The $\nu_{\text{LSR}}$ and $T_A$ scales are indicated in the upper right corner. Right: same as left panel but as an image of the spatial distribution of the integrated intensity, $\int T_s d\nu$, with observed positions shown as pluses. The circles show the 487 GHz and 774 GHz beams, respectively.
The O2 source is seen in projection close to the outflow from VLA 1623 and judging from its position (Figs. 1 and 3), 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. 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. $R = \frac{(I_{119}/I_{487})_{\text{theo}}(T)}{(I_{119}/I_{487})_{\text{obs}}}$ (Larsson et al. 2007). The relevant 119 GHz data were adopted from Larsson et al. (2007); they are compiled in Table 3 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 $f_{119} = \frac{\theta_{119}^2}{\sqrt{f/\theta_{119}^2 + f/\theta_{119}^2}}$, where $\theta_{119}$ is the size of the source and $\theta_{\text{odin}}$ that of the beam at 119 GHz. Rearranging, this reads $\theta_{119} \approx \frac{\theta_{\text{odin}}}{\sqrt{f/\theta_{119}^2}} = \theta_{\text{odin}}/\sqrt{f}$, where $\theta_{\text{odin}} \approx 10^\circ$.

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) in Table 4, we find a size of the Odin source of $\geq 4$ arcmin, for gas at from 18 to 25 K, i.e. for $(I_{119}/I_{487})_{\text{theo}}(T) = 11$ to 8, respectively. The solution for much warmer gas (127 K for $-1\sigma$ in Table 4) ought to be excluded, as the calculated source size would exceed 9', whereas the 774 GHz line that traces high temperature gas is expected only within a limited region ($\approx 1'$).

The O2 source is seen in projection close to the outflow from Odin 119 GHz spectrum toward Oph A. Proper comparison, these spectra are given on the $T_{\text{mb}}$ scale and for reference, a vertical dotted line is shown at $T_{\text{mb}} = +3.5$ km s$^{-1}$.

![Graph](image-url)

**Fig. 6.** Average data for the HIFI O$_2$ observations (774 and 487 GHz) and the Odin 119 GHz spectrum toward Oph A. For proper comparison, these spectra are given on the $T_{\text{mb}}$ scale and for reference, a vertical dotted line is shown at $T_{\text{mb}} = +3.5$ km s$^{-1}$.

4.1.4. Column density

For the warm region O1, an O$_2$ column density of $5 \times 10^{15}$ cm$^{-2}$ is derived, whereas for the cold O4, $N(O_2) > 6 \times 10^{15}$ cm$^{-2}$ (Table 4). These estimations are based on the assumption of optically thin emission at LTE at the kinetic gas temperature $T_{\text{kin}}$, i.e. for unit beam filling the O$_2$ column is given by

$$N(O_2) = \int T_{\text{mb}} \, d\nu \times \Phi(T_{\text{kin}}) \, \text{cm}^{-2}$$

when the integral is expressed in K cm s$^{-1}$ and where

$$\Phi(T_{\text{kin}}) = \frac{2\pi^{1/2}}{\hbar c} \frac{T_{\text{kin}}^2}{\theta_{\text{odin}}^2} \times \frac{F_\nu(T_{\text{kin}})}{F_\nu(T_{\text{bg}})} Q(T_{\text{kin}}) \exp(T_{\text{up}}/T_{\text{kin}}),$$

in K$^{-1}$ cm$^{-3}$ s (cgs units throughout). Here, the transition temperature is $T_\nu = \nu/k$, the quasi-Planck function is $F_\nu(T) = T_\nu/(e^{T_\nu/\nu} - 1)$, the partition function is $Q(T)$, the upper level energy is $E_{\text{up}} = E_{\text{bg}}/k$ and the other symbols have their usual meaning.

The hydrogen column density along the appropriate lateral and depth scales is not well-known from observations. However, we can get an approximate idea from the C$^{18}$O observations by Liseau et al. (2010), where it was suggested, based on the line profiles, that the $J = 3\to 2$ line was a reasonably good proxy for the O2 119 GHz line observed with Odin (Larsson et al. 2007). If the O$_2$ molecules were indeed cosmicall with those of CO and its isotopic variants, their optically thin lines could be used to infer the H$_2$ column densities relevant also to O$_2$. We derive “local” C$^{18}$O column densities by 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

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1. In our numerical radiative transfer calculations (Sect. 4.1), the dust continuum is also included. These calculations use the collision data of Lique (2010).
For O$_4$, the limit symbols are for the lower limit on the intensity by the dashed line formally extends to the unplausible result of nearly of the 487 GHz integrated line intensity to that at 774 GHz is shown by 487 Ghz: black solid line; 774 GHz: red short dashes.

Upper: LTE computations of the O$_2$ column density $N$(O$_2$) as a 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; $-\alpha$ as a function of the temperature $T$.

$10^2 K$. For O$_4$, the limit symbols are for the lower limit on the intensity ratio and the upper limit on the temperature, respectively.

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 $\leq T_{\text{kin}} \leq 50$ K. Assuming that C$^{18}$O/H$_2$ = $1.5 \times 10^{-7}$ (likely within about 30%, e.g. Wannier et al. 1976; Goldsmith et al. 2000), H$_2$ columns are found to be $1 \times 10^{21}$ cm$^{-2}$.

Hence, for the O$_2$ column densities in Table 4, we find that $X$(O$_2$) = $5 \times 10^{-8}$ relative to H$_2$ in the warm gas toward the west, at O$_1$ (and likely also toward O$_2$), and higher than that toward the east, at the colder O$_4$. 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 $\tau/(1 - e^{-\tau}) \geq 2$, for $\tau \sim 2$. Hence, these O$_2$ 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 is the topic of the next subsection.

4.3. Chemical models

Specifically for O$_2$ (and H$_2$O), 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 show that most of the gas phase O$_2$, OH, and H$_2$O is found at values of $A_V \sim 3$–10 mag, where the details depend, as in a conventional PDR, on the ratio $G_0/m_H$. In many aspects, these models are similar to the traditional dense PDR models that include chemistry and gas heating and that 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 no longer play a role in the chemistry, only cosmic-ray induced photons.

In the direction of $\rho$ Oph A, a number of spectroscopic indicators suggest the presence of a PDR$^2$. Liseau et al. (1999) inferred that the PDR is situated on the rear side of $\rho$ 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 [C II] emitting $\rho$ Oph A-PDR, these authors empirically derived $n_H = 5 \times 10^2$ cm$^{-3}$ and over more extended regions, from 1 to $3 \times 10^3$ cm$^{-3}$.

The model of Hollenbach et al. (2009) predicts columns of O$_2$ between about $10^{15}$ and a few times $10^{16}$ 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 locally reach above $10^{-5}$ 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 $\sim 20$ 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 that there are 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 colder gas.

$^2$ 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 $\mu$m (Yui et al. 1993; Liseau et al. 1999), [O I] 63 $\mu$m (Ceccarelli et al. 1997; Liseau et al. 1999), [O I] 145 $\mu$m (Liseau et al. 1999; Liseau & Justtanont 2009), and mid-infrared PAH emission (Liseau & Justtanont 2009).
If the dust is also cooler in the cooler gas region, as would be expected for the derived densities above 10^4 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 O2 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 higher column of O2 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 O2-emitting region. We defer detailed thermochemical modelling of these ρ Oph observations to a future paper.

4.4. Source(s) of O2 or the dearth of O2

The discussed models could be expected to apply quite generally to all externally illuminated molecular clouds developing PDR-like parts. It is therefore surprising that O2 has been detected only toward the dense cloud core ρ Oph A (Larsson et al. 2007, and this work) and a spot in OMC-1 (Goldsmith et al. 2011), despite numerous searches toward other regions. For instance, surveying twenty sources, Goldsmith et al. (2000) obtained limiting O2 abundances N(O2)/N(H2) of a few times 10^{-7}, whereas Pagani et al. (2003) derived upper limits to the O2 column density 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 caused by mass infall and molecular outflows. Nevertheless, most of these regions escaped detection, although their limiting O2 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 O2 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 corrections for dilution in the Odin-beam are 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 IRC 2.

However, the difference in distance aside, ρ Oph A and Ori A represent very different environments in terms of the parameter G_0/n_H2, viz. cold-core deuteration versus hot-core grain chemistry (Bergman et al. 2011a; Bisschop et al. 2007; Ceccarelli et al. 2007; Ratnajitkz et al. 2011). Star-forming regions such as IRAS 16293 in Ophiuchi, NGC 1333 in Perseus, or the Serpens core near S 68 are more akin to the conditions in IRAS 16293 in Ophiuchus, NGC 1333 in Perseus, or the Serpens cloud. If that is the case, this may also explain the paucity of known O2 line emitters.

In the specific model for ρ Oph conditions, Du et al. (2012) find that H2O2 is reasonably abundant only for some 10^7 yr (their Fig. 1). A similar, only slightly broader, profile is displayed by the abundance of O2, rendering this molecule essentially undetectable after about 2 × 10^7 yr. Compared to other molecular species, which have attained chemical equilibrium and/or are abundant on much longer timescales (>10^8 yr), the abundances of both H2O2 and O2 appear transient. Therefore, one may expect that the simultaneously detectable abundance of O2 and H2O2 could be used to infer the evolutionary chemical state of the cloud. If that is the case, this may also explain the paucity of known O2 line emitters.

5. Conclusions

We now summarise the main results of our present study:

- We have successfully detected the 3_{1}−1_{1} transition of O2 at 487 GHz with HIFI onboard Herschel toward three positions in the ρ Oph A core. In addition, we have also obtained a 6 × 6 oversampled map with 10″ spacings in the 5_{1}−3_{1} transition at 774 GHz.
- The telescope pointings targeted two cold, high density cores, i.e. O4 [C^{18}O,P3 = SM1] and O3 [C^{18}O,P2, near SM1N], 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 in 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(O2) > 6 × 10^{15} cm^{-2}, at the 3σ level and at T < 30 K, in the high density region O3 and O4, whereas in the warmer region of O1 and O2, N(O2) = 5.5 × 10^{15} cm^{-2} (T > 50 K). There, our standard analysis yields an abundance of N(O2)/N(H2) ∼ 5 × 10^{-8} in the warm gas and somewhat higher in the cold region.
- This result agrees with that for X(O2) based on the observation of the 119 GHz line with Odin (Larsson et al. 2007), assuming that the O2 source size has an angular extent of about 5″.
- The question of why O2 is such an elusive molecule in the ISM is still unanswered. In the special case of ρ Oph A, there is some evidence that detectable amounts of gas phase O2 might be a relatively transient phenomenon, which could explain why interstellar O2 is generally not detected.

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