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Abstract

Molecular oxygen abundance is a key parameter in understanding the chemical network of the interstellar medium. We estimate the molecular oxygen column density and abundance for a sample of Galactic massive star formation regions based on observations from the Submillimeter Wave Astronomy Satellite (SWAS) survey. We obtained an averaged O₂ spectrum based on this sample using the (SWAS) survey data (O₂, 487.249 GHz, N = 3-1, J = 3-2). No emission or absorption feature is seen around the supposed central velocity with a total integration time of $t_{\text{total}} = 8.67 \times 10^3$ hr and an rms noise per channel of 1.45 mK. Assuming a kinetic temperature $T_{\text{kin}} = 30$ K, we derive the 3σ upper limit of the O₂ column density to be 3.3×10^{15} cm⁻², close to the lowest values reported in Galactic massive star formation regions in previous studies. The corresponding O₂ abundance upper limit is 6.7×10^{-8} , lower than all previous results based on SWAS observations and is close to the lowest reported value in massive star formation regions. On a galactic scale, our statistical results confirm a generally low O₂ abundance for Galactic massive star formation regions. This abundance is also lower than results reported in extragalactic sources.

Full Text

Preamble

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Molecular Oxygen Abundance in Galactic Massive Star Formation Regions Based on SWAS Observations

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Abstract

Molecular oxygen abundance is a key parameter for understanding the chemical network of the interstellar medium. We estimate the molecular oxygen column density and abundance for a sample of Galactic massive star formation regions based on observations from the Submillimeter Wave Astronomy Satellite (SWAS) survey. We obtained an averaged O₂ spectrum for this sample using the SWAS data (O₂, 487.249 GHz, N₃₋₁, J₃₋₂). No emission or absorption feature is seen around the expected central velocity, with a total integration time of $t_{\text{total}} = 8.67 \times 10^3$ hr and an rms noise per channel of 1.45 mK. Assuming a kinetic temperature $T_{\text{kin}} = 30$ K, we derive the 3σ upper limit of the O₂ column density to be 3.3×10^{15} cm⁻², close to the lowest values reported for Galactic massive star formation regions in previous studies. The corresponding O₂ abundance upper limit is 6.7×10^{-8} , lower than all previous results based on SWAS observations and close to the lowest reported value in massive star formation regions. On a Galactic scale, our statistical results confirm a generally low O₂ abundance for Galactic massive star formation regions. This abundance is also lower than results reported for extragalactic sources.

Key words: ISM: molecules -galaxies: abundances -ISM: lines and bands - Galaxy: abundances

1. Introduction

In the interstellar medium (ISM), the most abundant species—such as H, H₂, O, C⁺, and N in diffuse clouds, and H₂, CO, and N₂ in molecular clouds (Tielens 2013, with He not included)—are composed of the most abundant elements and play important roles in both the chemical and physical evolution of the ISM. In turn, the resulting chemical composition affects energy transfer processes in the ISM. The formation and evolution of these species are highly dependent on the (kinetic) temperature, volume density, and radiation field in the ISM. Star formation is an important process in ISM evolution, with feedback from forming and newly-formed stars influencing these parameters and the most abundant molecular species in molecular clouds other than H₂/H and He.

Oxygen is the third most abundant element in the universe (Heiles 1971; Dalgarno & McCray 1972). O-bearing species are thus among the most abundant in both diffuse clouds and the molecular clouds where stars form. Therefore, it is necessary to study the forms of oxygen in the ISM and their abundances.

In diffuse gas subject to a strong interstellar far-ultraviolet (FUV) radiation field, oxygen and carbon atoms are predominantly ionized (Yamamoto 2017). With an ionization potential greater than that of hydrogen, in dense molecular gas where the FUV field is attenuated by dust absorption, elemental oxygen can exist within simple molecular species whose abundance and distribution are determined by gas-phase densities and temperatures, or by freezeout and surface chemistry on interstellar dust grains (Hollenbach et al. 2009; van Dishoeck et al. 2013; Wang et al. 2015; Zhang et al. 2020). Early theoretical calculations suggested that within well-shielded clouds, molecular oxygen (O₂), along with gas-phase H₂O, could be abundant reservoirs of elemental oxygen (Herbst & Klemperer 1973; Langer 1976) as well as major gas coolants (Goldsmith & Langer 1978). Because transitions between low-lying O₂ energy levels can be easily excited collisionally by H₂ at typical dense molecular cloud temperatures, molecular oxygen was once predicted to be comparable to CO and H₂O as a dominant molecular cloud gas coolant (Goldsmith & Langer 1978; Neufeld et al. 1995). Though no longer thought to be a major gas coolant, the abundance of molecular oxygen remains a largely unanswered question, with relevance to our understanding of interstellar chemistry.

Attempts to observe Galactic sources of O₂ from ground-based or airborne telescopes are prevented by the significant presence of O₂ in Earth's atmosphere. To avoid this obstacle, efforts have been made to observe highly redshifted O₂ from extragalactic sources (Goldsmith & Young 1989; Combes et al. 1991, 1997; Wang et al. 2020) as well as the isotopologue ¹⁶O¹⁸O toward Galactic sources (Goldsmith et al. 1985; Taquet et al. 2018). However, the best prospects for detecting O₂ remain space-based telescopes, well above the blocking effects of Earth's atmosphere. Observations with the Submillimeter Wave Astronomy Satellite (SWAS, Melnick et al. 2000), the Odin satellite (Frisk et al. 2003; Nordh et al. 2003), and the Herschel Space Observatory (Pilbratt et al. 2010)

have confirmed a much lower O_2 abundance (upper limit) in Galactic dense gas (generally from 5×10^{-8} to 10^{-6}), more than two orders of magnitude below the earlier predictions of cold-cloud gas-phase chemical models (Goldsmith et al. 2000, 2011; Pagani et al. 2003; Bergin & Melnick 2005; Larsson et al. 2007; Sandqvist et al. 2008, 2015; Liseau et al. 2012; Yildiz et al. 2013; Chen et al. 2014; Wirström et al. 2016). The only two Galactic O_2 detections—in Orion (Goldsmith et al. 2011; Chen et al. 2014) and Rho Ophiuchi A (Rho Oph A, with a tentative detection included) (Goldsmith et al. 2002; Larsson et al. 2007; Liseau et al. 2012)—are both local warm spots likely heated by shocks, resulting in enhanced O_2 emission due to the release of O_2 from grain surfaces (Goldsmith et al. 2011; Liseau et al. 2012; Chen et al. 2014) or, alternatively, from gas-phase chemistry within post-shock regions behind FUV-illuminated shocks (Melnick & Kaufman 2015). Generally, the corresponding O_2 abundance values are less than 10^{-7} relative to H_2 . The limited post-shock distances over which the O_2 abundance is enhanced, combined with geometric effects—i.e., the angle the shock presents to the observer—may be reasons why confirmed O_2 detections are rare (Melnick & Kaufman 2015). Similar shock enhancement mechanisms may also apply to extragalactic sources, such as the ultra-luminous infrared galaxy Mrk 231, which led to a detection with an inferred O_2 abundance greater than 1×10^{-4} (Wang et al. 2020). Within the central region of Mrk 231 and other observed extragalactic sources (the Small Magellanic Cloud (SMC), NGC 6240 and B0218+357), the O_2 abundance remains very low, comparable to the Galactic sources (Wang et al. 2020; Wilson et al. 2005; Combes et al. 1991, 1997). The O_2 abundance is commonly very low in dense molecular gas, and the significant surplus of oxygen in solar abundance (the interstellar “O crisis,” Whittet 2010a) remains. Obtaining improved constraints on the upper limit to the O_2 abundance from non-detections toward Galactic massive star formation regions provides critical data for time-dependent gas-grain interstellar chemistry models (Zhang et al. 2020) and can help us gain a better understanding of the oxygen life-cycle in the Galaxy (Vastel et al. 2002; Whittet et al. 2010; Whittet 2010b).

In this paper, we estimate the average molecular oxygen upper limit based on a large sample of Galactic massive star formation regions using the SWAS survey data. The paper is organized as follows: in Section 2 we briefly describe the SWAS survey observations and data; in Section 3 we describe our data reduction steps; the results are presented in Section 4. We compare our results with previous studies in Section 5. Finally, in Section 6 we present our conclusions.

2. SWAS Observation

The SWAS mission lasted for 5.5 years and the survey covers hundreds of Galactic molecular clouds (Bergin & Melnick 2005). The sources were observed at single or multiple positions via intermittent sampling. For every observed position, four molecular lines were observed simultaneously by two double sideband receivers (DSBs): Receiver 1 (C I, $^3\text{P}_1$ - $^3\text{P}_0$, 492.161 GHz; O_2 , 3,3-1,2, 487.249

GHz) and Receiver 2 (H_2O , $1_{10}-1_{01}$, 556.936 GHz; ^{13}CO $J = 5-4$, 550.926 GHz), respectively (Melnick et al. 2000). SWAS' s beam size is $3.5' \times 5.0'$ for Receiver 1 and $3.3' \times 4.5'$ for Receiver 2, and the main beam efficiency is 0.90 (Melnick et al. 2000). We obtained data for all 386 sources from the SWAS spectrum service at the NASA/IPAC Infrared Science Archive.

3. Data Reduction

We assumed that for every observed position in the SWAS survey, the C I line ($^3\text{P}_1-^3\text{P}_0$, 492.161 GHz) and O_2 line (3,3-1,2, 487.249 GHz) sampled simultaneously by Receiver 1 have the same central velocities. This assumption is consistent with C I and O_2 line observations in the only two previous Galactic O_2 detection cases in Rho Oph A (Larsson et al. 2007; Liseau et al. 2012) and Orion (Goldsmith et al. 2011) molecular clouds (see Appendix A for more details).

We analyzed the C I and O_2 spectra of the observed massive star formation regions in the SWAS survey, but excluded sources in the Orion molecular cloud and near/toward the Galactic center. We selected positions whose C I spectra have only one clear single emission peak for our statistical analysis sample. To reduce the influence of weighting differences among spectra due to different integration times, we only selected positions with sufficiently long total integration time (not less than 10,000 s, on+off, see Appendix D) and used the corresponding O_2 and C I spectra to compose the overall averaged O_2 and C I spectra. Subsequently, based on the overall averaged spectra, we estimated a statistical O_2 abundance upper limit.

For every observed position, all sampled C I and O_2 spectra were combined to generate the corresponding C I and O_2 average spectra, respectively. The C I average spectrum was fitted with a Gaussian and the centroid velocity was adopted as the central velocity of the corresponding O_2 average spectrum. This central velocity was aligned to 0 km s^{-1} in our spectral plots. The antenna temperatures were then corrected for SWAS' s main beam efficiency of 0.90. A linear baseline was fitted based on spectra outside the -20 to 20 km s^{-1} velocity interval and subtracted from the spectra. The average spectra of different positions were then combined to generate an overall O_2 average spectrum and corresponding C I average spectrum for the sample of massive star formation regions. These operations were performed using the GILDAS CLASS software. Considering the varying integration times among different observed positions, the mode of “weighting by time” was adopted.

4. Results

4.1. Overall Averaged O_2 and C I Spectra

The observed positions in the massive star formation regions analyzed in this paper are listed in Table D1 in Appendix D. The total integration time (on+off)

is 3.12×10^7 s (8.67×10^3 hr). The long-term integration capability of SWAS receivers has been investigated and confirmed in Wang et al. (2024), and a noise floor has not been reached even after such a long total integration time.

Figure 1 [Figure 1: see original paper] shows the overall averaged O₂ and C I spectra of these observed positions, with the assumed central velocities aligned to 0 km s⁻¹. In the averaged O₂ spectrum, there is no obvious emission or absorption feature around the central velocity. The rms noise per channel is 1.33×10^{-3} K, which is very close to the theoretical value of 1.24×10^{-3} K. The corresponding overall averaged C I spectrum has a clear single emission peak. The central velocity is 0.010 ± 0.016 km s⁻¹ and the line width (full width at half maximum, FWHM) is 6.3 ± 0.043 km s⁻¹ according to the Gaussian fitting results.

4.2. Molecular Oxygen Column Density and Abundance Upper Limit

4.2.1. O₂ Radiative Transitions, Collisional Excitation and Thermalization As a homonuclear molecule, O₂ has no permanent electric dipole moment and thus has no pure rotational transitions (Kaiser et al. 1999) (i.e., electric-dipole rotational transitions, Liszt & Vanden Bout 1985). However, the coupling of the electron spin angular momentum of the unpaired electrons (designated as S, whose associated moment is a purely magnetic dipole moment, Gordy & Cook 1984) and the non-spin angular momentum (designated as N, see Gordy & Cook 1984) causes the splitting of N and thus generates the resultant total angular momentum J (excluding nuclear spin, according to Gordy & Cook 1984). The allowed transitions between J and/or N levels are magnetic dipole transitions, with selection rules $\Delta N = 0, \pm 2$ and $\Delta J = 0, \pm 1$ (Maréchal et al. 1997; Brown & Carrington 2003).

The allowed radiative transitions between the lowest 48 energy levels all have small spontaneous emission coefficients (10^{-10} - 10^{-7} s⁻¹, Drouin et al. 2010). For lower O₂ energy levels, these slow rates result in relatively low critical densities and thus the levels are easily thermalized. The low transition strength and low molecular oxygen abundance make the 487 GHz O₂ (3,3-1,2) transition almost certainly optically thin.

SWAS generally observed dense molecular clouds with molecular hydrogen volume density $n_{\text{H}_2} > 10^3$ cm⁻³ and kinetic temperature $T_{\text{kin}} > 10^3$ K (Melnick 1995). When $T_{\text{kin}} \sim 30$ K, the O₂ (3,3) level is essentially thermalized (Goldsmith et al. 2000). Further calculations suggested that $n_{\text{H}_2} > 10^3$ cm⁻³ is enough to keep the (3,3) energy level, with the upper energy level being close to local thermal equilibrium (LTE) at a temperature of 100 K (Goldsmith et al. 2011).

For the massive star formation regions we analyzed in the SWAS survey, we can expect even higher H₂ volume density on average, but not likely higher kinetic temperature. To estimate the average O₂ column density and abundance upper limits, we adopted the median values of H₂ volume density and T_{kin} of

seven giant cloud cores from Table 1 in Goldsmith et al. (2002) as the assumed average values for our sample of massive star formation regions. The seven giant cloud cores are Mon R2, M17SW, W49, W51, S140, Cep A, and NGC 7538. All of them were studied individually based on SWAS O₂ (3,3-1,2) and Five College Radio Astronomical Observatory (FCRAO) C¹⁸O J = 1-0 observations in Goldsmith et al. (2000) and were also included in our sample. With the H₂ volume density and T_{kin} values adopted as described above, we assumed an average n_{H₂} = 10^{5.6} cm⁻³ and average T_{kin} = 30 K for the sample of massive star formation regions in our estimations.

4.2.2. Average O₂ Column Density Upper Limit for Galactic Massive Star Formation Regions When the O₂ (3,3) level is thermalized, for the O₂ (3,3-1,2) transition, its excitation temperature T_{ex} = T_{kin}. Assuming the observed molecular clouds fill the SWAS beam and ignoring the background continuum radiation at 2.73 K, the O₂ column density in the (3,3) upper level of the 487 GHz transition is given by the quasi-Planck expression (see Appendix B). The O₂ total column density is then obtained using the correction factor CF.

Here, A_{ul} is the Einstein A coefficient, and CF is the correction factor, the inverse of the fractional population of a given level. For the thermalized O₂ (3,3) level in our calculation, CF = 1/0.128 = 7.81 (see Section 4.2.1).

The 3σ integrated line intensity upper limit for the overall averaged O₂ spectrum in Figure 1 is calculated as 3σ_{rms}√(Δvδv), where σ_{rms} = 1.33 × 10⁻³ K is the rms noise per channel of the overall averaged O₂ spectrum, δv = 0.64 km s⁻¹ is the velocity resolution, and Δv is the assumed line width (see more in Appendix C.2), which we take as the line width of the corresponding overall averaged C I spectrum (6.3 km s⁻¹). With A_{ul} of O₂ (3,3-1,2) as 8.66 × 10⁻⁹ s⁻¹ (Drouin et al. 2010), the 3σ average O₂ column density upper limit is 3.3 × 10¹⁵ cm⁻². With corrections for the O₂ rms noise per channel and the assumed O₂ line width, this column density upper limit at 30 K is 3.3 × 10¹⁵ cm⁻² (see Appendices C.1 and C.2). For a thermalized O₂ (3,3) level at T_{kin} = 20-40 K, the O₂ column density upper limit is 1.0-1.05 times the value at the assumed T_{kin} = 30 K (see Appendix C.3).

4.2.3. Average O₂ Column Abundance Upper Limit for Galactic Massive Star Formation Regions We used the weighted integrated intensity ratio method from Goldsmith et al. (2000) to estimate a 3σ upper limit for the average O₂ abundance in Galactic massive star formation regions. This method derives the fractional abundance of O₂ from the C¹⁸O fractional abundance through the ratio of their column densities N(O₂)/N(C¹⁸O).

The C¹⁸O total column density can be calculated from the corresponding C¹⁸O J = 1-0 (109.782 GHz) spectrum (Goldsmith et al. 2000), also using Equation (B8) from Appendix B. The weighted ratio W is defined as the ratio of O₂ integrated line intensity to C¹⁸O integrated line intensity, weighted by the C¹⁸O main beam

brightness temperature in each channel when both O₂ and C¹⁸O spectra share the same velocity resolution. $A_{ul}(C^{18}O, J = 1)$ and $A_{ul}(O_2, 3,3-1,2)$ are the Einstein A coefficients for the C¹⁸O J = 1 and O₂ (3,3-1,2) transitions, respectively.

For the overall averaged O₂ spectrum without any feature around the expected central velocity, we derive a 3σ upper limit for the average O₂ abundance from the uncertainty of the weighted ratio.

The C¹⁸O abundance corresponds to the entire C¹⁸O J = 1-0 line, which also corresponds to the weighted integrated intensity. The O₂ rms noise per channel is the rms uncertainty in one channel, and the corresponding weighted rms uncertainty of O₂ line intensity in a single channel is $\sigma_{weighted} = \sigma_{rms} \times (T_{C^{18}O}/T_{C^{18}O,peak})$, where $\sigma_{rms} = 1.33 \times 10^{-3} K$ is the rms noise per channel of the overall averaged O₂ spectrum and the velocity resolution is 0.64 km s^{-1} . For random noise in independent O₂ channels, the weighted rms uncertainty of the O₂ integrated line intensity is $\sigma_{int} = \sigma_{weighted} \times \sqrt{n}$, where n is the total number of channels included in the O₂ integrated line intensity. The weighted rms uncertainty of the ratio of O₂ and C¹⁸O integrated line intensities is then $\sigma_{ratio} = \sigma_{int}/W$.

The overall averaged C I spectrum has a near-Gaussian profile. Assuming a Gaussian line profile for the corresponding J = 1-0 C¹⁸O spectrum, we obtain T_0 , $C^{18}O_{1,0}$ and Δv_{FWHM} , $C^{18}O_{1,0}$ as the peak temperature and line width (FWHM) of the overall averaged C¹⁸O (1-0) spectrum, respectively. The channel width dv_{O_2} is the same as the velocity resolution (0.64 km s^{-1}). The analytical expression for the weighted ratio uncertainty is given by Equation (10), which corresponds to Equation (4) in Goldsmith et al. (2000).

We adopted the median value of 1.1 K (range 0.8-1.3 K) for the seven Galactic giant molecular cloud cores described in Section 4.2.1 as the assumed peak temperature of the corresponding overall averaged C¹⁸O (1-0) spectrum under the same spatial resolution as SWAS. The Δv_{FWHM} values for the giant molecular cloud cores were not listed in Goldsmith et al. (2000). We adopted the line width of the overall averaged C I spectrum, 6.3 km s^{-1} , as the assumed C¹⁸O J = 1-0 line width.

We performed RADEX non-LTE analysis (van der Tak et al. 2007) for C¹⁸O total column densities of 10^{14} - 10^{18} cm^{-2} at $T_{kin} = 30 \text{ K}$, with $n_{H_2} = 10^{5.6} \text{ cm}^{-3}$ as assumed in Section 4.2.1. The C¹⁸O population of the J = 1 energy level ranges from 0.221 to 0.216, all very close to the LTE value of 0.215. We adopted $CF(C^{18}O, J = 1) = 4.54$ (from the results for $N(C^{18}O) = 10^{16} \text{ cm}^{-2}$ in the RADEX analysis) in our calculation.

Substituting three times Equation (10) into Equation (5) together with $A_{ul} = 6.266 \times 10^{-8} \text{ s}^{-1}$ for C¹⁸O (1-0) (from the Leiden Atomic and Molecular Database) and $X_{C^{18}O} = 1.7 \times 10^{-7}$ (Frerking et al. 1982), we derived a 3σ average O₂ abundance upper limit of 5.6×10^{-8} for Galactic massive star formation regions. With corrections for the O₂ rms noise per channel and the assumed

C^{18}O $J = 1-0$ line width, this abundance upper limit at 30 K is corrected to 6.7×10^{-8} (see Appendices C.1 and C.2). When both the C^{18}O ($J = 1$) and O_2 (3,3) levels are thermalized, at $T_{\text{kin}} = 20-40$ K, the O_2 abundance upper limit is 0.8-2.1 times the value at the assumed $T_{\text{kin}} = 30$ K (see Appendix C.3).

5. Discussion

With a total integration time (on+off) of 3.12×10^7 s and rms noise per channel of 1.45×10^{-3} K, we derived a 3σ average O_2 column density upper limit of 3.3×10^{15} cm^{-2} and O_2 abundance upper limit of 6.7×10^{-8} for Galactic massive star formation regions based on SWAS survey data. These values are lower than previous values based on SWAS observations toward individual sources or regions in Goldsmith et al. (2000) and Goldsmith et al. (2002).

Figure 2 [Figure 2: see original paper] shows O_2 column density and abundance (or their 3σ upper limits) from previous studies, together with the values derived in this paper. The results include Galactic sources and the SMC (Wilson et al. 2005). The observed targets circled in black dashed lines are in massive star formation regions. Symbols in red, green, and blue represent results based on observations via SWAS, Odin, and Herschel, respectively. The symbols linked with solid black lines are O_2 detections or tentative detections, showing the ranges. Symbols linked by dotted black lines represent results for different positions of the same object in the same study. The black arrows suggest possible lower limits.

The beam-averaged O_2 column density upper limit (3.3×10^{15} cm^{-2}) we derived is lower than those values except one (Orion A, 1.9×10^{15} cm^{-2} , Pagani et al. 2003) in massive star formation regions. The abundance upper limit (6.7×10^{-8}) we derived is very close to the lowest value (G34.3+0.2, 5.2×10^{-8}) based on Odin observations for the 119 GHz O_2 line in Pagani et al. (2003) in a massive star formation region.

Compared with our results based on the O_2 487 GHz line, in cold and warm (50K in Pagani et al. 2003) molecular gas, the larger population in the upper level (Goldsmith et al. 2011) and lower frequency 119 GHz transition together lead to lower column density and/or abundance upper limits in non-detection cases, even when the rms noises are much higher. The lowest O_2 abundance (upper limit) values ($1.3-2.1 \times 10^{-8}$ and 5.7×10^{-9}) are based on Herschel observations toward molecular clouds and envelopes around NGC 1333 IRAS 4A (a low-mass Class 0 protostar) at 487 GHz, with observed and assumed line widths of 1.3 and 1 km s^{-1} respectively, and the lowest rms noise in all studies of 1.3×10^{-3} K (Yildiz et al. 2013, assuming $T_{\text{kin}} = 30$ K).

The O_2 column density upper limits we derived are lower than previous upper limit results (see Table E1 in Appendix E) in massive star formation regions like the Orion Bar (Melnick et al. 2012) and Rho Oph A (Class 0 protostar IRAS 16293-2422, based on $^{16}\text{O}^{18}\text{O}$ line, Taquet et al. 2018).

The statistical average O_2 column density and abundance upper limit based on this sample of massive star formation regions under SWAS' s beam size can be treated as a kind of average result on the Galactic scale. When converted to the corresponding 1σ value, our O_2 abundance upper limit is lower than those for other extragalactic sources (NGC 6240, Combes et al. 1991; in front of B0218+357, Combes et al. 1997; the center of Mrk 231, Wang et al. 2020).

6. Conclusions

1. We obtained an overall averaged O_2 spectrum for a large sample of Galactic massive star formation regions based on SWAS survey data. The rms noise per channel of the overall averaged O_2 spectrum is 1.45×10^{-3} K for the total integration time $t_{\text{total}} = 8.67 \times 10^3$ hr. There is no O_2 emission or absorption around the expected central velocity of the overall averaged O_2 spectrum.
2. At an assumed $T_{\text{kin}} = 30$ K, the 3σ average O_2 column density and abundance upper limits for Galactic massive star formation regions based on the thermalized O_2 487 GHz line are 3.3×10^{15} cm^{-2} and 6.7×10^{-8} , respectively. The column density upper limit we derived is close to the lowest values in Galactic massive star formation regions from previous studies. The corresponding abundance upper limit is lower than previous results based on SWAS observations and close to the lowest reported value in massive star formation regions.
3. On a Galactic scale, our results confirm that O_2 abundance is very low in Galactic massive star formation regions. The O_2 abundance upper limit we derived is lower than previous results for extragalactic sources.

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Appendix A: C I and O₂ Central Velocity in Galactic O₂ Detection Cases

Observations of C I and O₂ emission toward the same position can be seen in the only two Galactic O₂ detection cases so far: Rho Oph A and the Orion molecular cloud, as mentioned in the Introduction. The results support our assumption that C I and O₂ lines along the same line of sight have the same central velocity.

In the Rho Oph A O₂ detection case, O₂'s 119 GHz transition (1₁-1₀) observed by Odin (Larsson et al. 2007), as well as its 487 GHz (3₃-1₂) and 774 GHz (5₄-3₄) transitions observed by Herschel (Liseau et al. 2012), all show emission features with central velocities around 3.5 km s⁻¹. SWAS' s C I spectra in the corresponding area ((0, 0) and (0, 1.6) relative to R.A. = 16:26:23.4, decl. = -24:23:02 (J2000)) show roughly consistent central velocities (3.60 km s⁻¹ and 3.44 km s⁻¹, respectively) with the O₂ observations, though with different velocity and spatial resolution (beam size).

A similar situation applies to the O₂ detection case in the Orion molecular cloud. In multi-line O₂ observations via Herschel HIFI toward the northwest maximum of H₂ rovibrational emission in Orion, the 487 GHz O₂ spectrum presents a velocity component whose peak is between 11 and 12 km s⁻¹ (10.96 km s⁻¹, FWHM = 3.05 km s⁻¹). This velocity is consistent with those of transitions between higher energy levels, such as 740 GHz (10.96 km s⁻¹, FWHM = 2.91 km s⁻¹) and 1121 GHz (11.87 km s⁻¹, FWHM = 2.87 km s⁻¹) (Goldsmith et al. 2011). In SWAS' s beam covering the same position, the C I 492.161 GHz spectra show a central velocity at 9.69 km s⁻¹. The difference between the O₂ 487 GHz line and C I 492 GHz line central velocities is acceptable for our assumption.

Appendix B: Calculation of Column Density—Approximations and Assumptions

For a system in thermal equilibrium (TE), the radiative spectral distribution at temperature T and frequency ν is given by the Planck equation. In radio astronomy, in the Rayleigh-Jeans case ($h\nu \ll kT$), the effective source radiation temperature is described by the quasi-Planck function (Kutner & Ulich 1981):

$$J(\nu, T) = \frac{h\nu/k}{\exp(h\nu/kT) - 1}$$

where $J(\nu, T)$ is the radiation temperature of a radio source at temperature T .

For particles in a two-level system with spontaneous emission and collisional excitation/de-excitation, the Rayleigh-Jeans approximation can also apply to the line brightness temperature T_L . For an observed extended source that fills the main beam of the telescope, the main beam brightness temperature $T_{mb} \approx T_L$.

When the particles are in TE and follow a Boltzmann distribution, in the optically thin case ($\tau \ll 1$), the column density of the upper level is given by the quasi-Planck expression:

$$N_u = \frac{8\pi\nu^3}{c_{ul}^{3A}} \left[\frac{1}{\exp(h\nu/kT_{ex}) - 1} - \frac{1}{\exp(h\nu/kT_{bg}) - 1} \right]^{-1} \int T_{mb} dv \quad (\text{B3})$$

where T_{ex} is the excitation temperature, $T_{bg} = 2.73$ K is the cosmic background temperature, and A_{ul} is the Einstein A coefficient of the radiative transition from the upper to lower level. The total column density is:

$$N_{tot} = N_u \times CF \quad (\text{B4})$$

where CF is the correction factor.

When the upper level is thermalized, $T_{ex} \approx T_{kin}$. If we replace all T_{ex} terms in Equation (B3) with T_{kin} , we obtain the expression used for the upper level O_2 column density in calculations of O_2 total column density (Liseau et al. 2012).

In Equation (B3), when $T_{ex} \approx T_{kin}$, the ratio of the cosmic microwave background radiation temperature term (term A) to the O_2 radiation temperature term (term B) is:

$$\frac{T_{bg}}{T_{ex}} = \frac{h\nu/k}{\exp(h\nu/kT_{bg}) - 1} \bigg/ \frac{h\nu/k}{\exp(h\nu/kT_{ex}) - 1}$$

For a given frequency, this ratio decreases monotonically as T_{ex} increases. For the O_2 487 GHz line at an assumed $T_{kin} = 30$ K ($T_{ex} \approx T_{kin}$), term A is negligible compared to term B, so Equation (B3) reduces to:

$$N_u \approx \frac{8\pi\nu^3}{c_{ul}^{3A}} [\exp(h\nu/kT_{kin}) - 1] \int T_{mb} dv \quad (\text{B6})$$

This is analytically equivalent to the commonly used expression (Equation B7), which ignores term A and adopts the Rayleigh-Jeans approximation for both term B and term C in Equation (B3) when $T_{ex} \approx T_{kin}$:

$$N_u \approx \frac{8\pi\nu^{2k}}{hc_{ul}^{3A}} T_{kin} \int T_{mb} dv \quad (\text{B7})$$

The total column density is then:

$$N_{tot} \approx \frac{8\pi\nu^{2k}}{hc_{ul}^{3A}} T_{kin} \int T_{mb} dv \times CF \quad (B8)$$

Equation (B8) has been adopted in estimations of O₂ column density in earlier studies (Goldsmith et al. 2000, 2002, 2011). When $T_{ex} \approx T_{kin}$, the difference between Equation (B4) (the quasi-Planck expression) and Equation (B8) (the Rayleigh-Jeans expression) is caused by the cosmic microwave background radiation term (term A). Although in our calculations $h\nu = kT_{kin}$ does not strictly apply at 487 GHz for the O₂ (3,3-1,2) transition, we adopt Equation (B8) for total column density calculations for both O₂ and C¹⁸O, as the difference is negligible (<1% for O₂ at $T_{ex} > 8$ K and <5% for C¹⁸O J = 1-0 at $T_{ex} > 30$ K; see Mangum & Shirley 2015).

Appendix C: Corrections and Deviations for Parameters in Calculations of O₂ Column Density and Abundance Upper Limits

C.1. Correction for O₂ rms Noise Per Channel

The baseline noise performance of the overall averaged O₂ spectrum was checked following the method in Wang et al. (2024). The “clean” baseline velocity intervals without spikes or ripples in the average O₂ spectra of every observed position were aligned and added. The rms noise per channel of the “clean” interval of the overall added spectrum is 1.13×10^{-3} K, lower than the theoretical value of 1.24×10^{-3} K (calculated according to Goldsmith et al. 2002 and Tolls et al. 2004) by a factor of 1.09. A similar phenomenon has been reported in Goldsmith et al. (2000) and Goldsmith et al. (2002), possibly caused by larger-than-theoretical effective noise bandwidth (Wang et al. 2024). Thus, we corrected the rms noise per channel of the overall averaged O₂ spectrum from 1.33×10^{-3} K to 1.45×10^{-3} K by multiplying by this factor of 1.09.

C.2. Line Width of O₂, C¹⁸O, and C I

Models for photodissociation regions suggest that CO and its isotopic variants are generally co-spatial and co-temporal with O₂ in star-forming gas (Hollenbach et al. 2009; Draine 2011). The line width of C¹⁸O J = 1-0 was adopted as a proxy for the O₂ line width to estimate its column density upper limit in a previous study (Pagani et al. 2003). C¹⁸O has also been used to estimate O₂ abundance via X-C¹⁸O in previous studies (based on J = 3-2 or multi-transitions in Pagani et al. 2003; Larsson et al. 2007; Liseau et al. 2012; Yildiz et al. 2013; based on J = 1-0 in Goldsmith et al. 2000, 2002; Pagani et al. 2003; Sandqvist et al. 2015).

In the detected case of O₂ 119 GHz emission in Rho Oph A (Larsson et al. 2007), the C¹⁸O J = 3-2 spectrum shows consistent central velocity and line width

with those of the 119 GHz O_2 spectrum despite very different beam sizes (15 versus 9). The $C^{18}O$ $J = 1-0$ line width can therefore serve as a proxy for the corresponding O_2 spectrum line width. In this paper, we adopted the line width of the overall averaged C I spectrum as the assumed value for the corresponding $C^{18}O$ $J = 1-0$ and O_2 (3,3-1,2) spectra.

A larger line width than that of $C^{18}O$ can be expected. C I is distributed more extensively than CO isotopic variants due to different optical depths (Yamamoto 2017). Therefore, in observations with different spatial resolutions, the C I spectrum shows a larger line width than $C^{18}O$ low-J transitions. In SWAS observations toward Rho Oph A, the C I ($^3P_1-^3P_0$) line width is 2.7 km s^{-1} while the $C^{18}O$ (1-0) line toward the same position has a line width of 1.5 km s^{-1} (Goldsmith et al. 2002). At this same position, the 119 GHz O_2 (1_1-1_0) spectrum has a line width of 1.5 km s^{-1} (Larsson et al. 2007).

In observations toward the molecular cloud core HH24-26 with the James Clerk Maxwell Telescope (JCMT) (Gibb & Little 1998), C I ($^3P_1-^3P_0$) spectra have larger line widths than corresponding $C^{18}O$ (2-1) spectra (with angular resolution 23 versus 10) over six positions within the clump. The line width ratios vary from 1.0 to 2.3. These cases suggest that the C I 492 GHz line likely has a larger line width than the $C^{18}O$ (1-0) spectrum.

For the seven giant molecular cloud cores in massive star formation regions (see Section 4.2.1) whose parameters we adopted, we derived their $C^{18}O$ (1-0) line widths from Table 1 in Goldsmith et al. (2000) using Equation (10) from this paper. The median and average $C^{18}O$ (1-0) line widths are 5.6 and $6.5 \pm 4.4 \text{ km s}^{-1}$, respectively. At the same SWAS spatial resolution, the average C I spectra toward individual positions all have larger line widths. The median and average C I line widths are 6.2 and $7.8 \pm 3.9 \text{ km s}^{-1}$, respectively. The average C I to $C^{18}O$ (1-0) line width ratio for each of the seven sources is 1.21 ± 0.25 . Based on this average value, we corrected the assumed $C^{18}O$ (1-0) line width from that of the overall averaged C I spectrum (6.3 km s^{-1}) to 5.2 km s^{-1} . We therefore corrected the assumed line width for the overall averaged O_2 spectrum to this value (5.2 km s^{-1}) as well, matching that for $C^{18}O$ (1-0), in our estimation of the O_2 column density upper limit.

C.3. O_2 Column Density and Abundance Upper Limit at Different T_{kin}

If the O_2 (3,3) level is thermalized, the O_2 column density upper limit is 1.26 times the value at 30 K for $T_{\text{kin}} = 15 \text{ K}$, and 1.0-1.06 times the value at 30 K for $T_{\text{kin}} = 20-40 \text{ K}$. When the $C^{18}O$ $J = 1$ level is also thermalized, at $T_{\text{kin}} = 30 \text{ K}$, $CF(O_2, 3,3)/CF(C^{18}O, J = 1) = 1.67$. For $T_{\text{kin}} = 15-40 \text{ K}$, $CF(O_2, 3,3)/CF(C^{18}O, J = 1) = 3.43-1.40$. Thus, the O_2 abundance upper limit can be 0.84-2.05 times the value at 30 K. The O_2 abundance upper limit can be as high as twice the value we derived for $T_{\text{kin}} = 30 \text{ K}$.

Appendix D: Massive Star Formation Regions Analyzed in This Paper

Table D1: Massive Star Formation Regions Analyzed in This Paper

Source	t_{total} (on+off, h)	RA Offset (deg)	Dec Offset (deg)
CEPHA	189.10	-0.15	-43.77
CEPHA	190.85	-2.47	-43.66
CEPHA	194.63	-0.35	-43.66
CEPHA	192.26	-0.20	-43.72
CEPHA+15	193.97	-2.28	-43.72
CEPHA+15-NO	192.78	-0.79	-43.72
CEPHA-30	192.11	-1.71	-43.77
CEPHA-30	191.22	-1.60	-43.77
CEPHA-30	192.74	-383.62	-43.77
CEPHA-30	193.89	-1.11	-43.82
CEPHB	192.71	-2.21	-43.82
CEPHB	193.87	-3.06	-43.82
CEPHB	194.03	-1.33	-43.82
CEPHB	190.85	-0.85	-43.82
CEPHB	192.05	-0.99	-47.48
CEPHB	191.67	-0.12	-47.43
G265.1+1.5	193.57	-189.67	-47.43
G265.1+1.5	193.10	-192.66	-47.43
G265.1+1.5	193.10	-193.10	-47.48
...

Note: The complete table is available in the electronic version of the article. Coordinates are offsets relative to the source reference position.

Appendix E: Molecular Oxygen Column Density and Abundance Upper Limits from Literature

Table E1: O_2 Column Density and Abundance Upper Limits from Literature

Source	$N(O_2)$ Upper Limit (cm^{-2})	$X(O_2)$ Upper Limit	Temperature (K)	Telescope	References
NGC 2024	$<2.6 \times 10^{15}$	$<6.1 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
NGC 2071	$<7.3 \times 10^{15}$	$<1.5 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)

Source	N(O ₂) Upper Limit (cm ⁻²)	X(O ₂) Upper Limit	Temperature (K)	Telescope	References
NGC 2071	$<6.8 \times 10^{14}$	$<1.5 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
Mon R2	$<1.1 \times 10^{15}$	$<1.3 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
NGC 2264	$<5.0 \times 10^{15}$	$<5.6 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
Sgr B2	$<5.6 \times 10^{16}$	$<4.6 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
DR 21	$<1.6 \times 10^{15}$	$<5.4 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
DR 21(OH)	$<5.2 \times 10^{15}$	$<1.9 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
Cep A	$<1.1 \times 10^{15}$	$<3.6 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
NGC 7538	$<5.0 \times 10^{15}$	$<1.0 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
M17SW	$<1.1 \times 10^{15}$	$<1.5 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
TMC-1	$<1.4 \times 10^{15}$	$<9.4 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
TMC1-NH ₃	$<9.7 \times 10^{14}$	$<3.7 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
L134N	$<1.2 \times 10^{15}$	$<5.7 \times 10^{-7}$	20	SWAS	Goldsmith et al. (2000)
L134N-NH ₃	$<2.7 \times 10^{15}$	$<2.9 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
NGC 6334I	$<1.7 \times 10^{15}$	$<7.7 \times 10^{-8}$	20	SWAS	Goldsmith et al. (2000)

Source	N(O ₂) Upper Limit (cm ⁻²)	X(O ₂) Upper Limit	Temperature (K)	Telescope	References
G0.26-0.01	$<1.2 \times 10^{15}$	$<1.3 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2000)
S68FIRS	1.8×10^{15}	$<9.2 \times 10^{-8}$	20	SWAS	Goldsmith et al. (2000)
G34.3+0.2	1.4×10^{16}	$<1.1 \times 10^{-7}$	20	Odin	Pagani et al. (2003)
NGC 1333	$<1.0 \times 10^{16}$	$<6.3 \times 10^{-8}$	30	Herschel	Yildiz et al. (2013)
NGC 1333 IRAS 4 Pro-to-star	$<1.2 \times 10^{15}$	$<5.7 \times 10^{-9}$	30	Herschel	Yildiz et al. (2013)
NGC 1333 IRAS 4 cloud	$(2.8-4.3) \times 10^{15}$	$(1.3-2.1) \times 10^{-8}$	30	Herschel	Yildiz et al. (2013)
IRAS16293-2422	1.5×10^{16}	$<1.6 \times 10^{-7}$	100	Herschel	Taquet et al. (2018)
Rho Oph A	$<8.2 \times 10^{15}$	$<1.3 \times 10^{-6}$	20	SWAS	Goldsmith et al. (2002)
Rho Oph A	$<2 \times 10^{15}$	$<5 \times 10^{-8}$	50	Herschel	Larsson et al. (2007)
Rho Oph A	$(3-6) \times 10^{15}$	$(0.3-7.3) \times 10^{-6}$	65-120	Herschel	Liseau et al. (2012)
Orion H ₂ Peak 1	2.3×10^{16}	$<1.0-1.5 \times 10^{-5}$	125-200	Herschel	Goldsmith et al. (2011)
Orion bar	$<3.4 \times 10^{15}$	$<9.3 \times 10^{-8}$	Tex = 15 K or higher	Herschel	Melnick et al. (2012)

Source	N(O ₂) Upper Limit (cm ⁻²)	X(O ₂) Upper Limit	Temperature (K)	Telescope	References
Orion H ₂ Peak 1 (Hot Core)	$<1.1 \times 10^{18}$	$<1.2 \times 10^{-6}$	150-300	Herschel	Chen et al. (2014)
Oph D	$<1.1 \times 10^{16}$	$<1.3 \times 10^{-6}$	30	Herschel	Wirström et al. (2016)
L1544	$<1.4 \times 10^{16}$	$<1.3 \times 10^{-6}$	30	Herschel	Wirström et al. (2016)
L694-2	$<1.1 \times 10^{16}$	$<1.3 \times 10^{-6}$	30	Herschel	Wirström et al. (2016)
Sgr A +20-50 km s ⁻¹	$<1.1 \times 10^{16}$	$<1.3 \times 10^{-6}$	30	Herschel	Wirström et al. (2016)
Sgr A (Scutum Arm)	$<1.1 \times 10^{16}$	$<1.3 \times 10^{-6}$	30	Herschel	Wirström et al. (2016)
NGC 6240	$<6 \times 10^{16}$	$<1.2 \times 10^{-7}$	30	IRAM 30m	Combes et al. (1991)
B0218+357 (in front of)	357.5×10^{16}	$<1 \times 10^{-6}$	30	IRAM 30m	Combes et al. (1997)
Mrk 231 (2 kpc in center)	$<8.9 \times 10^{16}$	$<2 \times 10^{-3}$	30	IRAM 30m	Wang et al. (2020)

Source	N(O ₂) Upper Limit (cm ⁻²)	X(O ₂) Upper Limit	Temperature (K)	Telescope	References
Mrk 231 (out-flow)	$>1 \times 10^{15}$	$>1 \times 10^{-4}$	30	IRAM 30m	Wang et al. (2020)

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