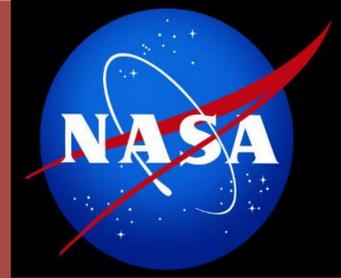


Depletion Cores – the O₂ hideout?



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The interstellar O₂ problem

Molecular oxygen has proven to be the most elusive molecule in the interstellar medium. Gas-phase chemical models predict that dense molecular clouds should contain large fractional abundances of O₂ (see Figure 1) due to the lack of atomic carbon (C), which efficiently destroys O₂. However, despite extensive searches in various astronomical environments by SWAS, ODIN, and Herschel (with respective beam sizes of 9', 4' and <1'), O₂ has only been detected in two, potentially three sources. In addition, upper limits in many other sources are at levels of 100-1000 times less abundant than predicted.

Currently, the most generally accepted explanation is that, once CO formation is complete, the simple process of oxygen atom (OI) accretion and ice formation on cold dust grains is responsible for the lack of O₂ (e.g. Roberts & Herbst 2002). These models show that once atomic carbon has been fully converted into CO (cloud ages in excess of ~10⁵ years), significant OI depletion is necessary to prevent the O₂ abundance from violating the observed limits. Most O₂ ice in these models come from direct accretion.

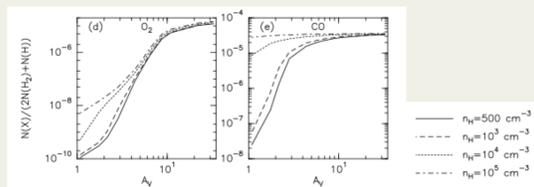


Figure 1. Pure gas-phase model abundances of O₂ and CO as a function of the total visual extinction throughout clouds of different hydrogen density (from Marechal et al. 1997)

Observations

In order to test whether O₂ abundances can be significantly enhanced in high density depletion cores, a small scale survey of the O₂ N_J=3₃-1₂ transition at 487.249 GHz was conducted with Herschel HIFI. Based on the starless core surveys by Crapsi et al. (2005) and Caselli et al. (2008), the four sources with highest CO depletion factors, f_D(CO), were selected (see Table 1). Maps of Oph D in Figure 4 show that the depletion cores, traced by N₂D⁺, can be significantly offset from continuum core positions. We were therefore careful to target the N₂D⁺ peaks in this study.

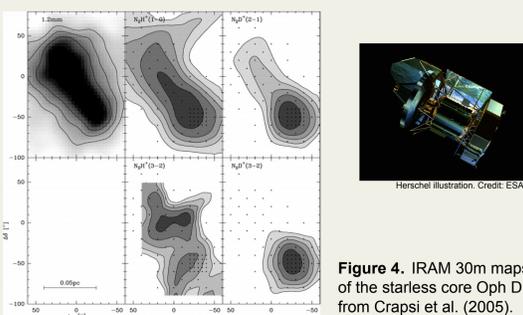


Figure 4. IRAM 30m maps of the starless core Oph D from Crapsi et al. (2005).

Source	f _D (CO)	n(H ₂) (cm ⁻³)	O ₂ / H ₂
L1544	19	2×10 ⁶	<6.3×10 ⁻⁸
L694-2	16	9×10 ⁵	<1.6×10 ⁻⁷
L429	20	6×10 ⁵	<9.2×10 ⁻⁸
Oph D	19	5×10 ⁵	<1.1×10 ⁻⁷

Table 1. Depletion factor and H₂ density (Caselli et al., 2008), as well as O₂ abundance upper limits in core sample (Wirström et al. 2013b).

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OI and O₂ chemistry

Several studies provide observational evidence for high OI/CO ratios and a large fractional abundance of OI (≈10⁻⁴) in L1544 and other depletion cores (Caselli et al. 2002; Cordiner et al. 2011).

Does OI not in fact freeze out efficiently in dense cores? If not – can the O₂ formed from it remain in the gas-phase at observable abundances?

Figure 2 illustrates how oxygen atoms are generally assumed to become incorporated in water ice mantles upon collision. However, the efficiency of atom accretion has been questioned. The reason might be that OI instead attach to grain ices by *chemical fixing* – i.e. reacts with HI upon collision and the resulting OH molecule attach to the surface water ice by hydrogen-bonding. The probability for OI to desorb upon collision is then finite. The gas-phase OI/HI ratio determines how efficiently OI is removed from the gas-phase: At high densities HI is converted into H₂ more efficiently and OI/HI increase, leading to OI build-up in the gas.

Model: Introduce an OI desorption rate taken as a fraction of HI desorption.

Gas-phase CO freeze out onto cold dust grains leading to severe CO depletion in cold dense cores. CO, N₂ and O₂ have similar physisorption binding energies leading to similar thermal desorption rates. However, CO seems to have a lower freeze-out density limit than N₂ which could potentially be connected to N₂ being non-polar. If this is the case we might expect that O₂ will behave like N₂ and persist after CO has become depleted.

Model: Set O₂ sticking efficiency to zero.

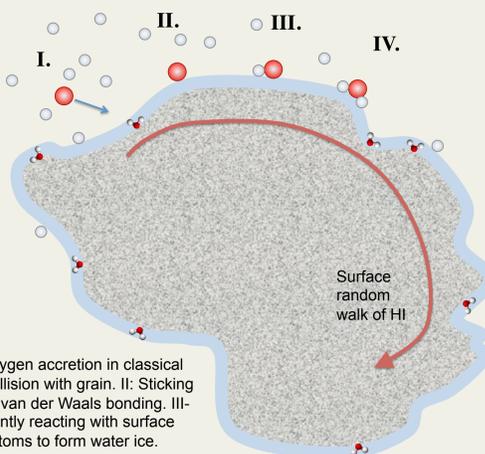


Figure 2. Oxygen accretion in classical model – I: Collision with grain. II: Sticking to surface by van der Waals bonding. III-IV: Subsequently reacting with surface scanning H atoms to form water ice.

Stochastic chemistry model

A correct treatment of the gas-grain interaction of oxygen requires a fully stochastic treatment of the kinetics involving solution of the chemical master equation (Gillespie, 1976). We have used a revised version of a unified gas-grain stochastic simulation code (Wirström et al. 2013), which was based on earlier simulation codes (Charnley 1998, 2001). The code only needs specification of the rates of the different surface processes (collision and physisorption, tunnelling, hopping, reaction and desorption) to compute the evolution of the gas-phase and ice mantle populations.

Figure 3 shows a stochastic gas-grain simulation in a cloud core at a temperature of 7 K and a hydrogen density of 2×10⁶ cm⁻³, with the kinetics highlighted in red to the left implemented. This version has 73 species and 742 reactions. At these high densities we found that at times when CO is significantly depleted (as is C), there is a possibility for elevated O₂ abundances, as high as a few times 10⁻⁶. At later times the O₂ is destroyed by H⁺ and He⁺; the OI and O⁺ so-formed are channeled into water which then freezes out. Note that a large OI/HI ratio also reduces the probability of O₂ hydrogenation on dust.

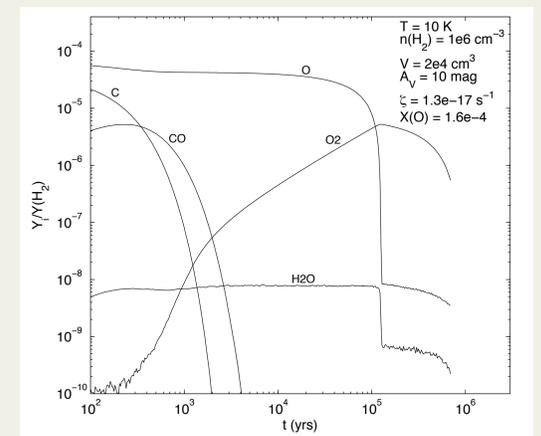


Figure 3. Time evolution of chemical abundances relative to H₂ for a stochastic gas-grain simulation in a reaction volume V, where O₂ does not stick to the grains and the desorption rate for O atoms, ξ(O), is 10⁻³×ξ(H), and elemental C/O=0.6. The assumed physical conditions are shown to the upper right.

Results

Figure 5 shows the observed Herschel HIFI Wide Band Spectrometer (WBS) polarization-averaged spectra towards the four sources in this study. Linear baselines have been subtracted and frequency axes shifted to the respective source velocity. Resulting noise rms varies between 3-7 mK.

Molecular oxygen was not detected towards any of the cores. We use the RADEX non-LTE radiative transfer code to model the level populations of O₂ molecules and 3σ line intensity upper limits. The molecular data file is based on spectroscopic data from Drouin et al. (2010) and collision rates scaled from He + O₂ collision rates of Lique (2010). Physical conditions of the cores are adapted from Caselli et al. (2008). The rightmost column of Table 1 shows the beam averaged upper limits on O₂ abundances based on these calculations.

Discussion

We did not detect molecular oxygen at abundances as high as 10⁻⁶ in the depletion cores of the survey. The derived upper limits of ~10⁻⁷ or less are similar to those obtained elsewhere and lower than recently reported in the NGC 1333 molecular cloud (Yildiz et al., 2013).

Our model probably overestimates the O₂ abundance by assuming that O₂ molecules have zero sticking probability. Rather, upon collision they will remain on the grain for some finite time before desorption. These O₂ molecules can be hydrogenated to H₂O and retained in the ice mantle (Oba et al., 2009), which would lead to a slow decline for the gas-phase O₂ abundance in Figure 3.

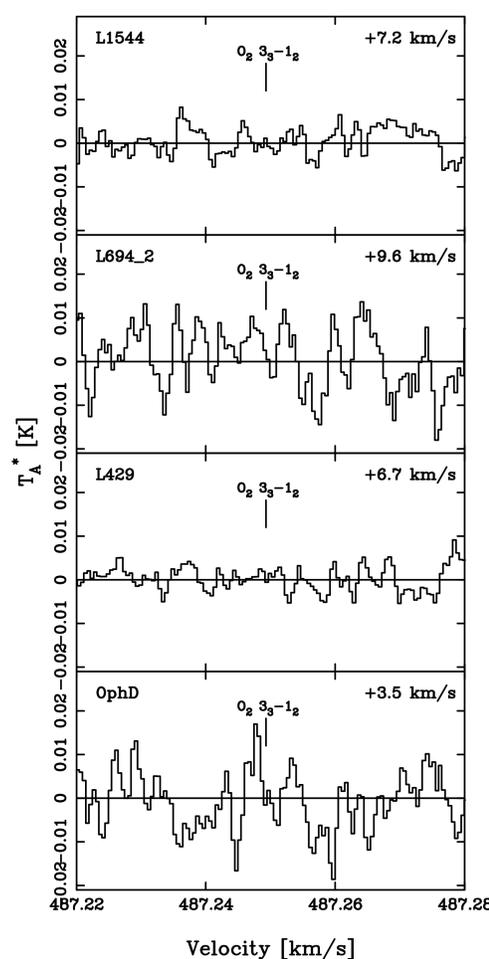


Figure 5. Spectra taken with HIFI WBS towards the four sources in this study. Frequency axes are shifted to the respective v_{LSR}, given in the upper right corner of each spectrum, and the position of the O₂ line is marked.

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