

Molecular Oxygen in the ISM: An Astrochemical Dilemma

Herschel Oxygen Project “HOP”

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for the HOP Team

***with special thanks to Jo-Hsin Chen, Ron Snell, Darek Lis, Umut Yildiz, and
Michael Kaufman***

***The Universe as seen by Herschel
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Herschel Oxygen Project

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Why O₂ and Why Observe this Molecule at Submillimeter Wavelengths?

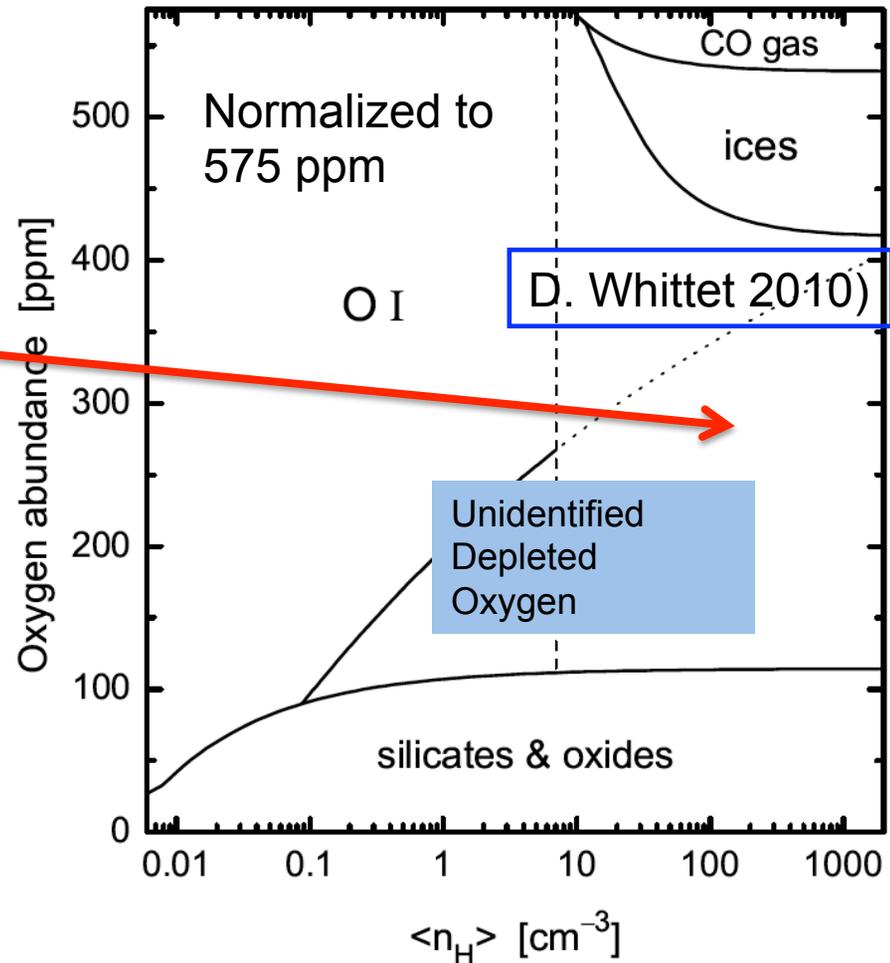
- **Astrophysical Importance** – O₂ is a simple molecule whose gas-phase chemistry is thought to be well understood
- **Large predicted abundance** - in relevant situations $X(\text{O}_2) = n(\text{O}_2)/n(\text{H}_2)$ should be as large as 3×10^{-5} making O₂ a major oxygen reservoir
- **Critical O₂ transitions** fall in the THz range
- **O₂ was a major objective** of SWAS and Odin satellites, which gave very surprising results. This has kept interest alive, with result that **O₂ is a target of Herschel projects (OTKP, OT1, OT2)**

Part of a Bigger Question: Oxygen is 3rd Most Abundant Element. Where is it in the Dense ISM?

- Oxygen's form in the Dense ISM is very unclear – O I ??
- Should O₂ be in this figure??

Caux et al. 1999;
Vastel et al. 2000:
Using ISO absorption measurements:
O I/CO = 10 – 50

What kind of region
are they observing?

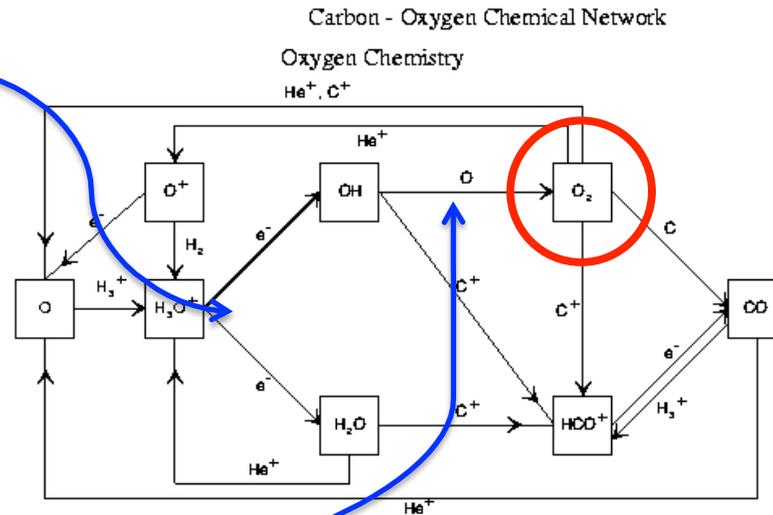


Gas Phase Chemistry for O, H₂O, O₂ and CO is Relatively Simple

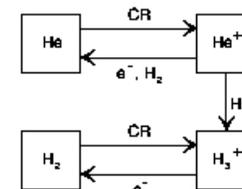
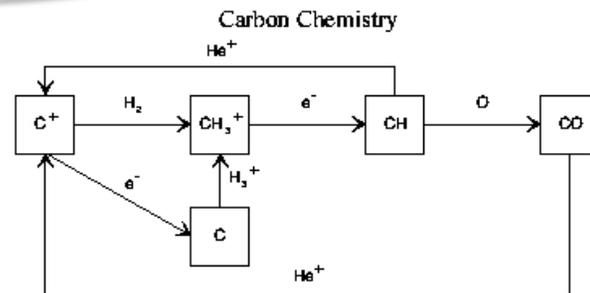
Branching ratio measured by ASTRID and CRYRING experiments (Jensen et al. 2000; Neau et al. 2000) $f(\text{H}_2\text{O}):f(\text{OH}) = 0.25:0.75$

$\text{OH} + \text{O} \rightarrow \text{O}_2$ is an exothermic neutral-neutral reaction

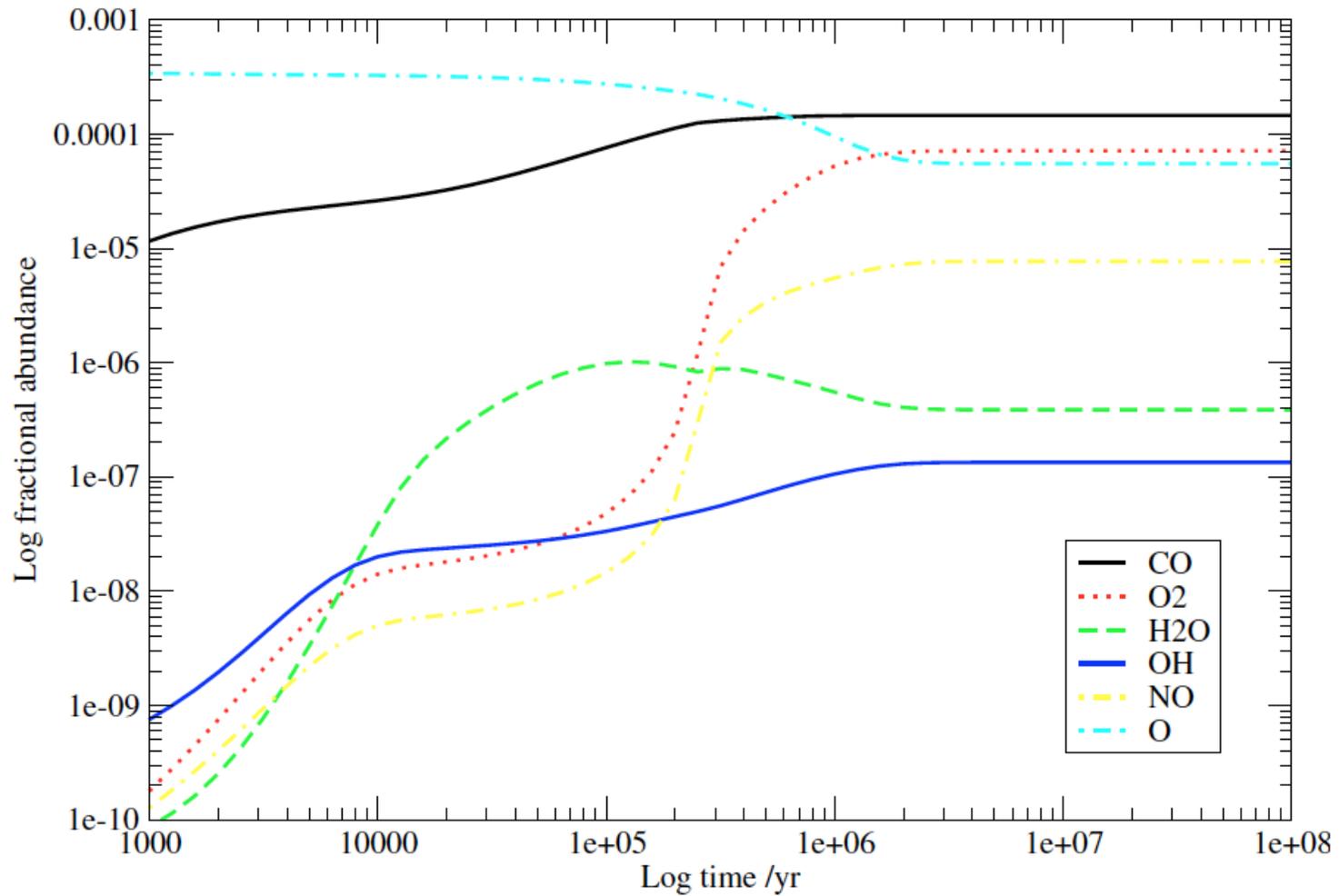
Measurements (Carty et al. (2006) and full quantum calculations (Lique 2010) indicate \sim temp-indep. rate from 300 K to very low temperatures $\approx 4 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$



All key reaction rates have been measured in laboratory, both at room temperature & at temperatures of dense interstellar clouds



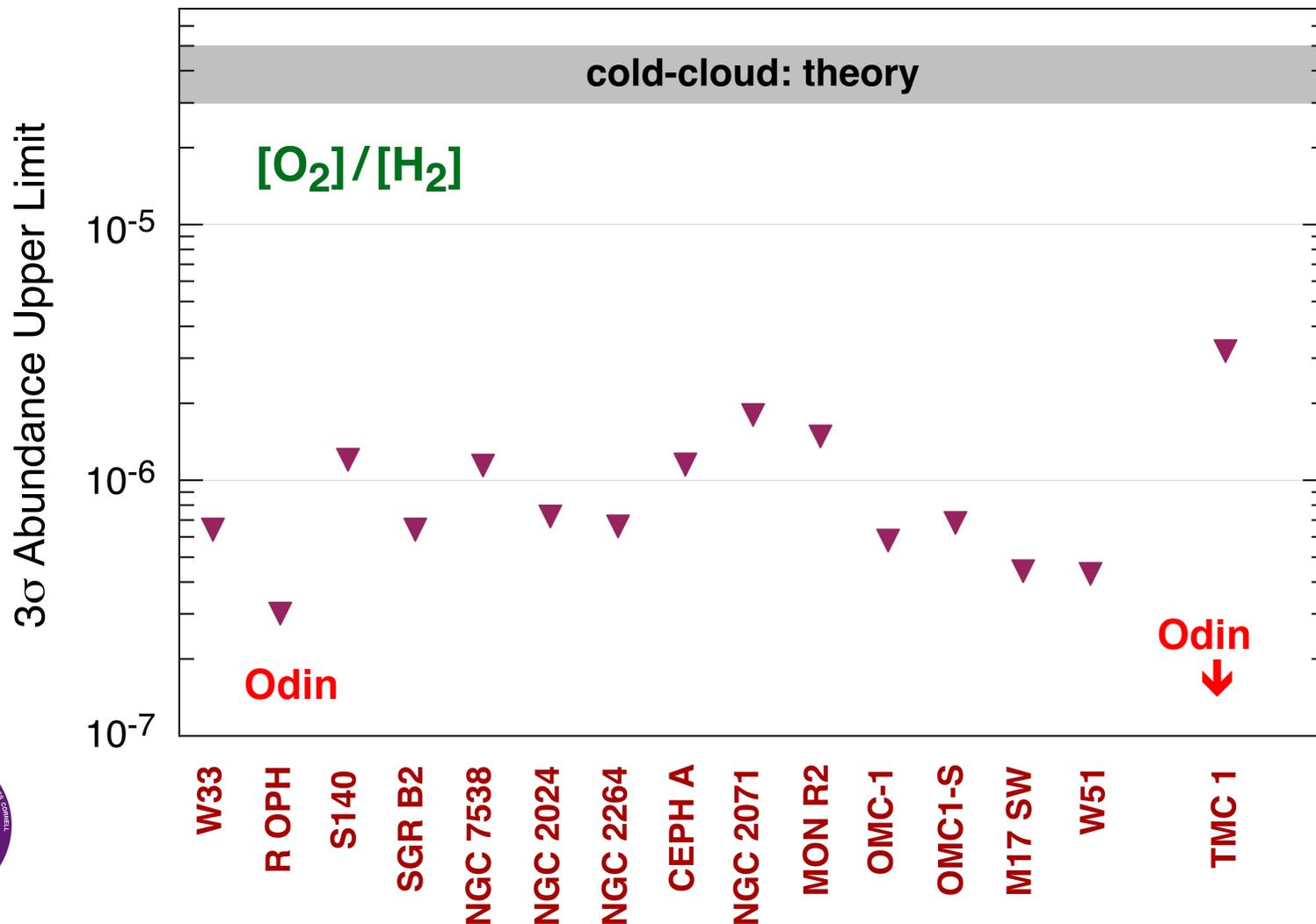
Standard Gas-Phase Chemistry Models Predict Large Abundance of O₂



Woodall et al. (2007)

Reality Intrudes:

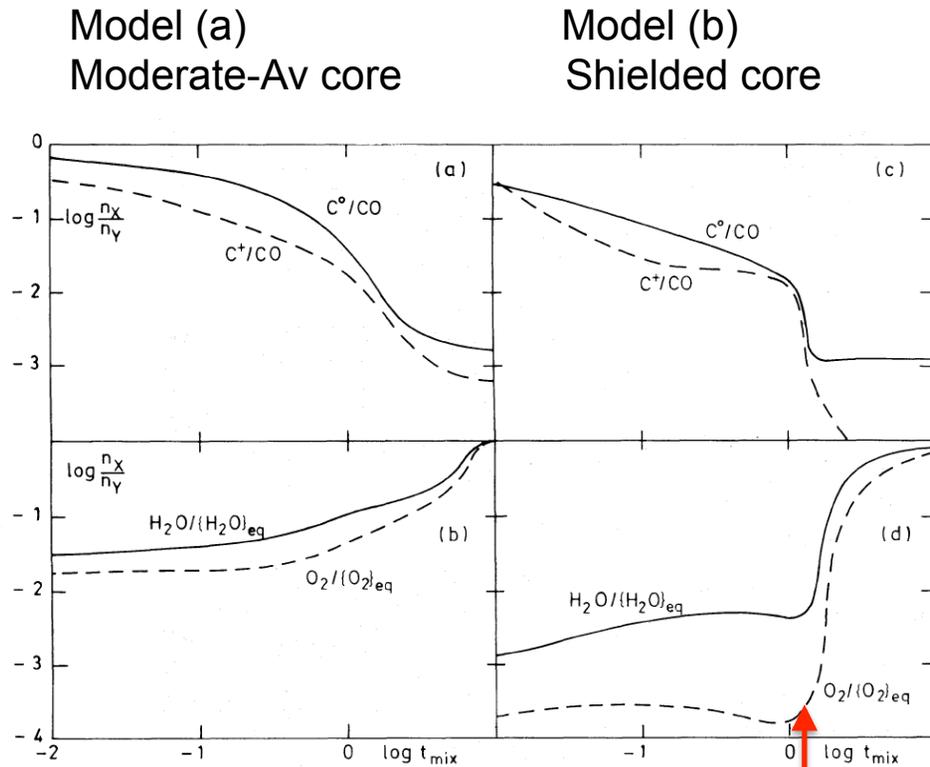
X(O₂) in IS Clouds from Odin & SWAS is More Than 100X Below that Predicted by Gas-Phase Chemistry



Why is the O₂ Abundance so Low? - I

Dynamical Mixing (circulation)

Chièze & Pineau des Forêts 1989

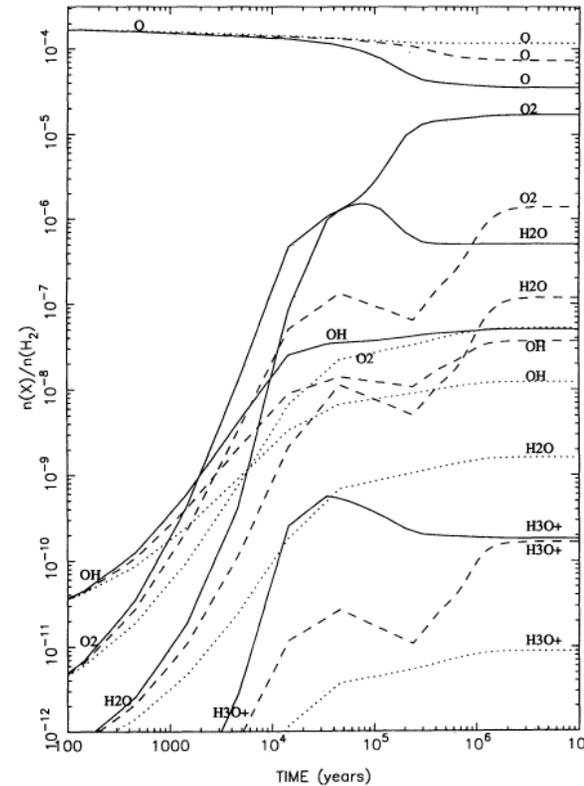


t_{mix} in units of 10^6 yr

Significant impact when dynamical timescale < chemical timescale $\sim 10^6$ yr

Turbulent Diffusion

Xie, Allen, & Langer (1995)



$K=0$

$K=10^{23}$

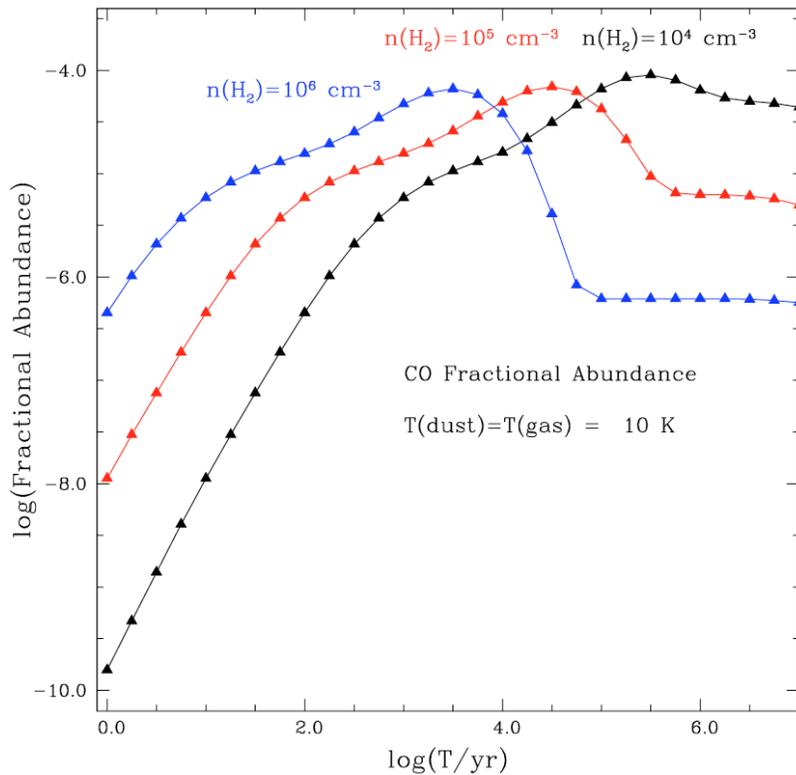
$K=10^{24}$

Transport due to concentration gradient
 $K = \text{turbulent diffusion coefficient} = \langle v_L L \rangle$
 Turbulent velocity $\sim 1 \text{ km s}^{-1}$
 Mixing length due to turbulence very uncertain.
 $K = 1 \times 10^{23} \text{ cm}^2 \text{ s}^{-1}$ (?)

Why is the O₂ Abundance so Low?

Depletion of molecules onto dust grain surfaces in cold clouds (e.g. Bergin+ 2006; Maret & Bergin 2007)

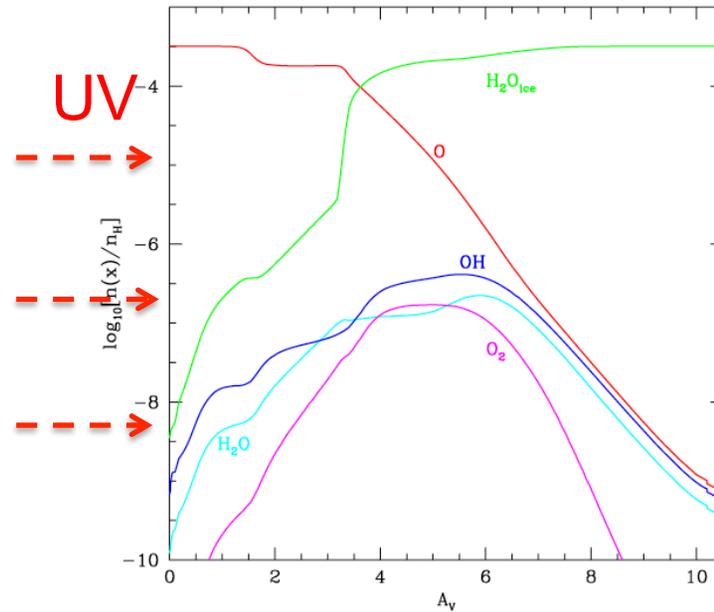
Same process will occur for O atoms, reducing gas-phase oxygen to form O₂



$$t_{\text{dep}} = 10^{10} \text{ yr}/n(\text{H}_2)$$

Photodestruction – Limits O₂ abundance at cloud edges

Hollenbach et al. (ApJ 2009) combine gas phase photochemistry with grain surface freezeout in cloud interior.



O₂ and H₂O are confined to a “layer” 3 ≤ A_v ≤ 7 in which X ≅ 10⁻⁷ so that N(O₂) ~ 1x10¹⁵ cm⁻². Think of O₂ COLUMN DENSITY rather than fractional abundance

The Herschel Oxygen Project (HOP) – A *Herschel* Open Time

Key Project to search for O₂ in variety of such environments to detect and measure molecular oxygen, and improve our understanding of astrochemistry

- Deep searches in three transitions of O₂
487 GHz, 774 GHz, and 1121 GHz
- Probe a variety of sources and environments
- Test chemical models
- Source list pruned after early observations showed that O₂ is a challenge even for HIFI

HOP Sources

Orion Bar	PDR
AFGL2591	XDR
Orion H ₂ Pk1	Postshock
Orion (S)	Embedded Source
NGC1333 IRS4A	“
NGC6334	Protostellar cluster
ρ Oph	Intermediate mass YSO
Sgr A	50 km s ⁻¹

OT1

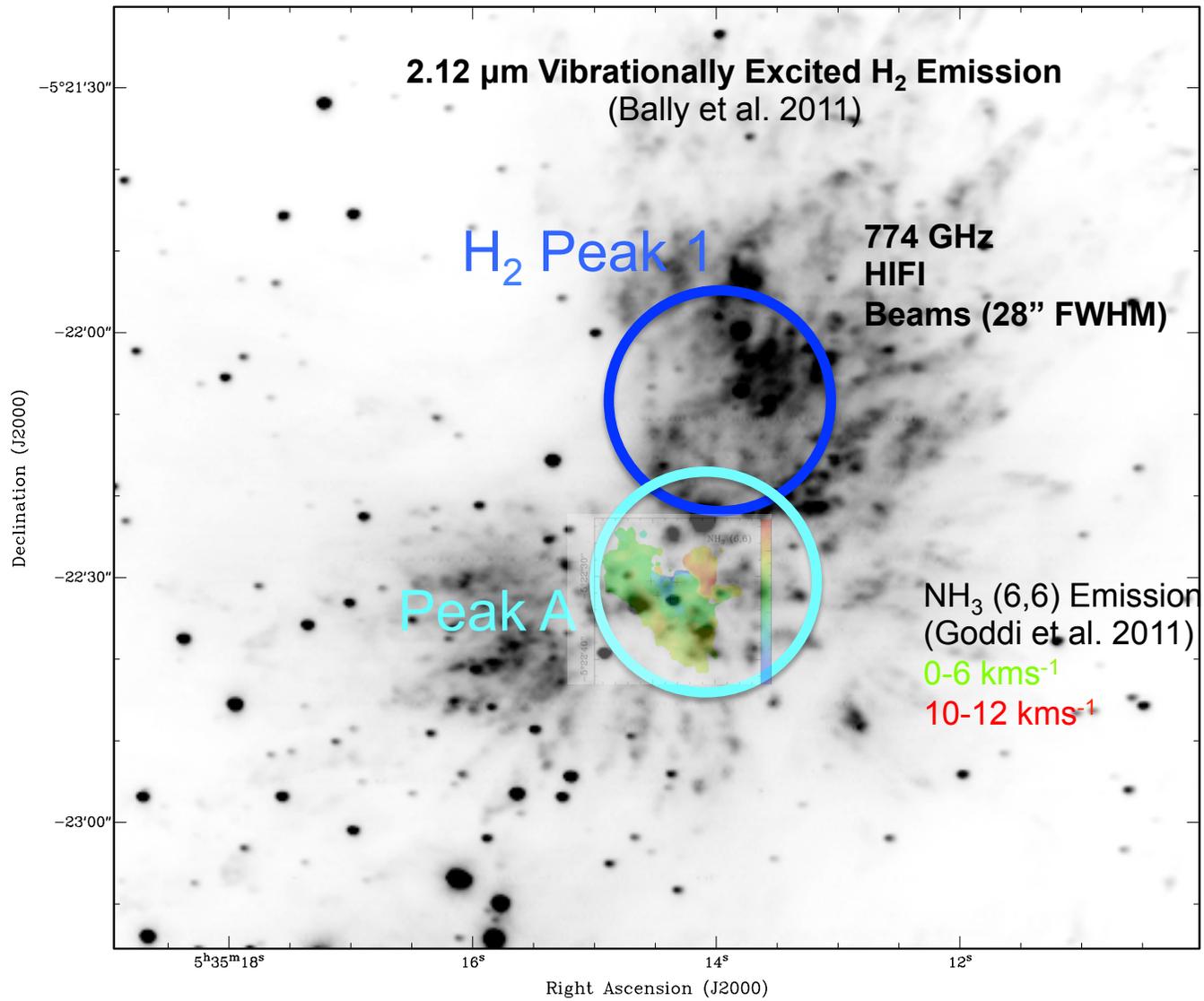
Orion Peak A (Hot Core)

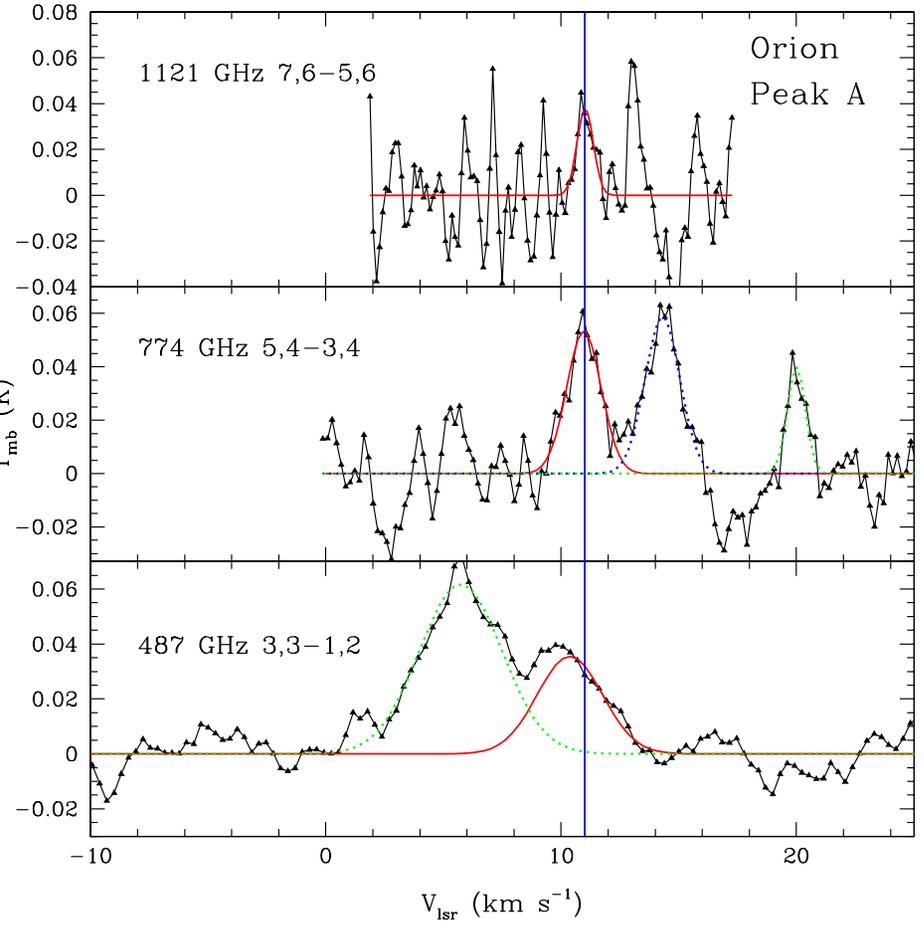
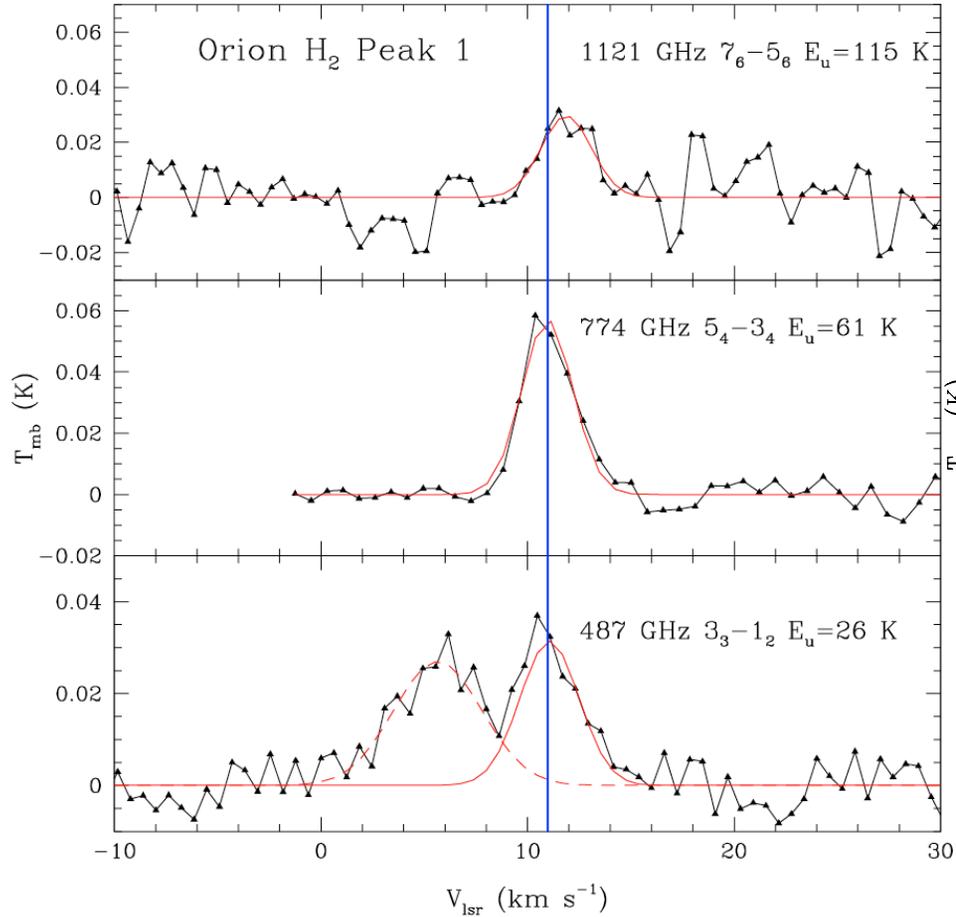
OT2

Rho Oph mapping –

Larsson et al. poster

3 O₂ Transitions Observed at 2 Positions in Ori A





Beam Sizes: 487 GHz 44" 774 GHz 30" 1121 GHz 20"
 Integration times up to 8 hr
 3 transitions observed with $v_{\text{lsr}} = 11 \text{ km s}^{-1}$ $\delta v = 2.9 \text{ km s}^{-1}$

First MULTITRANSITION DETECTION OF MOLECULAR OXYGEN IN THE ISM

Far more line confusion @ Peak A than H₂ Peak 1. Green = CH₃OCHO; Blue – U-line
 487 GHz and 774 GHz lines detected @ 11 km s⁻¹
 5 km s⁻¹ feature is primarily CH₃OCHO
 11 km s⁻¹ feature is ~ same intensity as at H₂ Peak 1

SOURCE IS NOT PEAK A OR HOT CORE

Possible Explanations for O₂ Seen in Orion

If at Peak A/Hot Core: Dust heated by nearby massive stars:

Desorb water ice mantles; initially, there is spike in gas-phase X(H₂O), but eventually we regain “standard” gas-phase chemistry with large X(O₂)

Almost all species having emission in 10 - 12 km s⁻¹ range have local maximum at Peak A/Western Clump/MF4/Cnt D location

BUT THE INTENSITY OF 774 GHz LINE SHOULD HAVE BEEN > 10X GREATER AT PEAK A THAN AT H₂ PEAK 1

MEASUREMENTS SHOW ABOUT THE SAME INTENSITY! - Peak A/Hot Core is NOT the source!

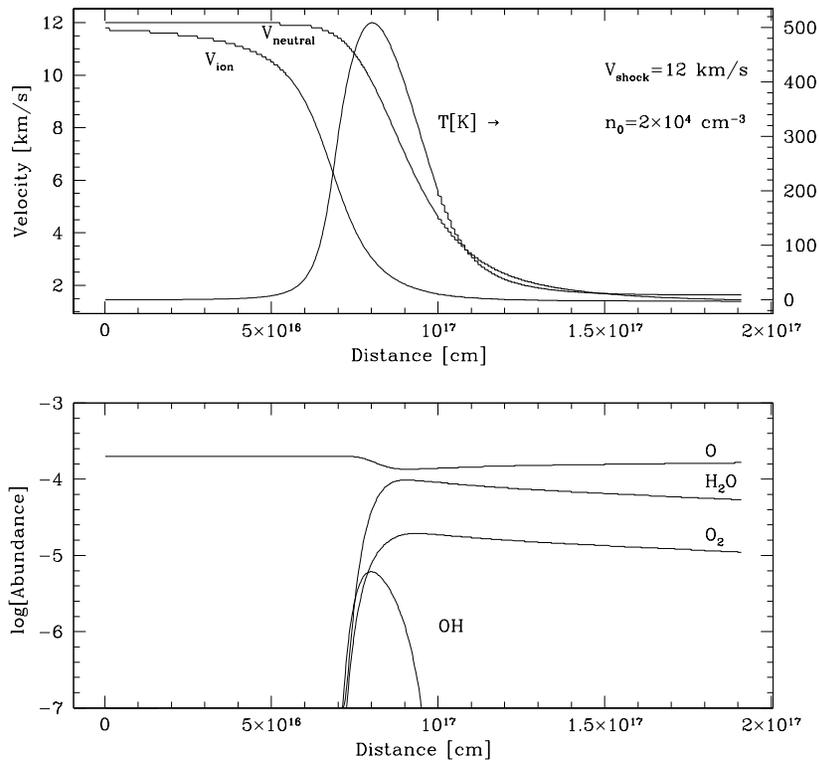
Where is the source?

Combined analysis of two sets of spectra gives best fit (for a single source) of size ~ 8” located about 7” from H₂ Peak 1

Relatively LOW Excitation Temperature, 30 K – 50 K. Since in LTE, this is from RELATIVELY COOL GAS

Location and Low Gas Temperature suggest postshock gas behind moderate velocity shock driven by disruptive event in center of Orion ~ 500 yr ago

Low-velocity Shocks are Effective at Producing O_2



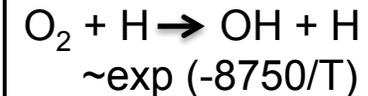
$V > 10$ km/s gives sufficient heating to allow rapid



Followed by



$V > 15$ km/s produces high enough T to allow back reaction



$N(O_2)$ can be as high as 10^{17} cm $^{-2}$

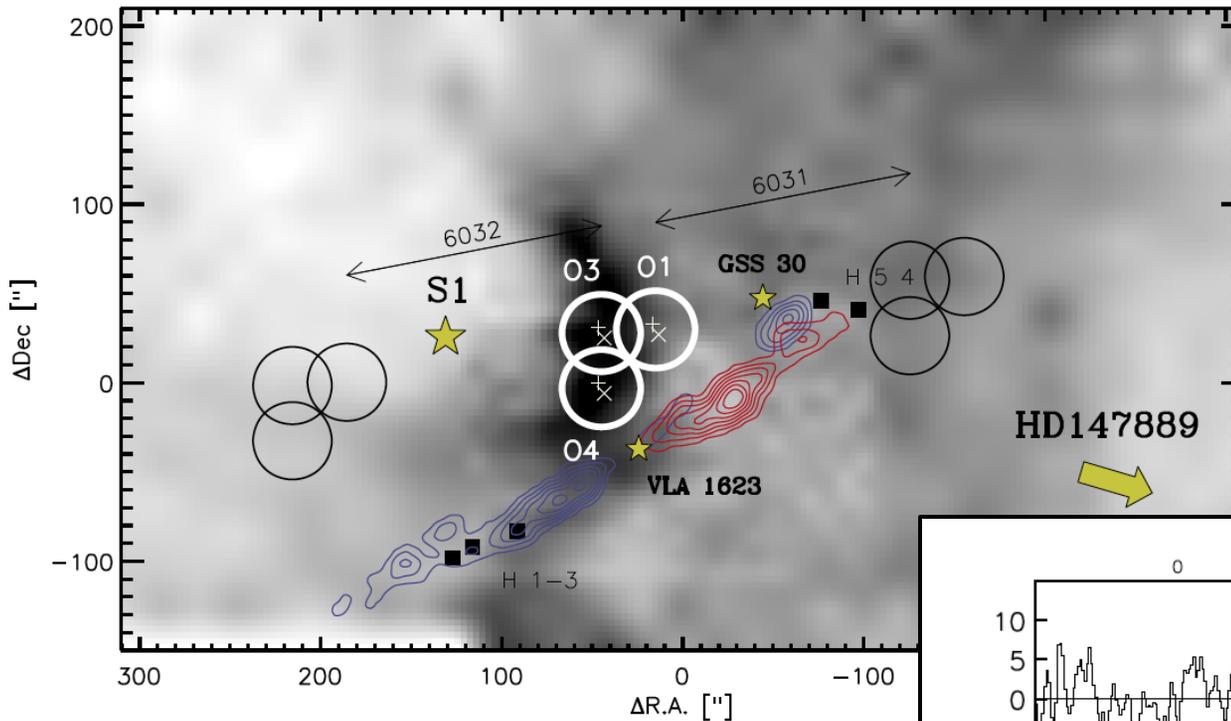
(from M. Kaufman)

ISSUES:

Need to have atomic oxygen in preshock gas; would lead to O_2 on longer timescale w/o shock
Narrow line width and lack of significant velocity shift

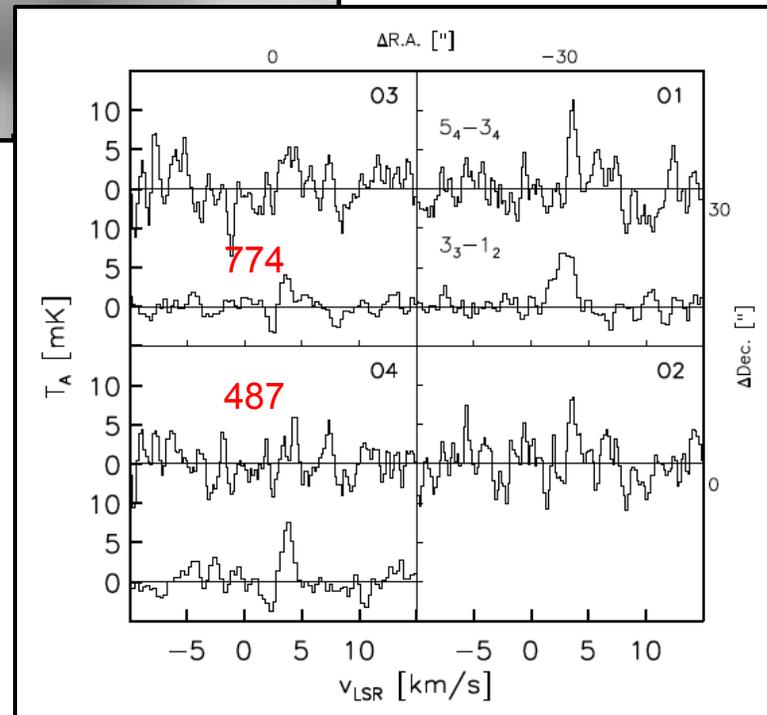
O₂ in Rho Oph

Liseau et al. A&A 2012
 Larsson et al. poster this conference: more extensive mapping results



Pos.	N(O ₂) /cm ⁻²
O1	5x10 ¹⁵
O4	> 6x10 ¹⁵
ALL	< 5x10 ¹⁵

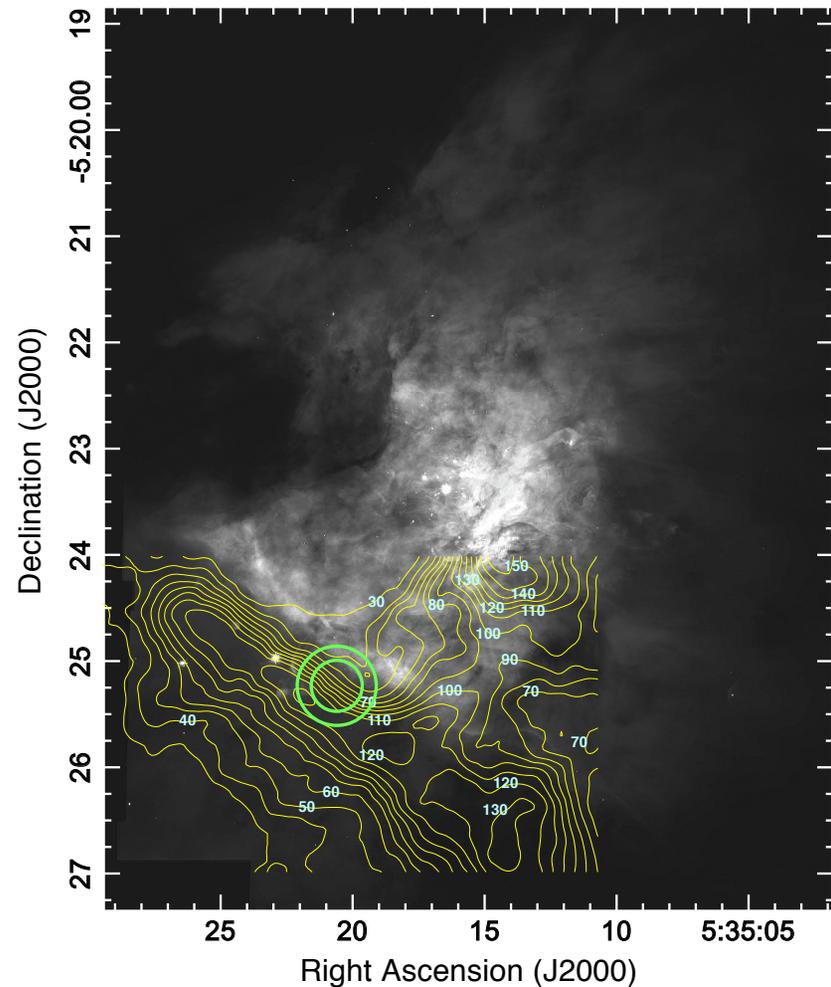
X(O₂) ~ 5x10⁻⁸ (relative to total N)



Narrow lines at quiescent cloud velocity. Fair agreement with PDR model (G₀ = 200). Geometry and source are not clear. **OT2 data: Larsson poster**

Non-detection: Orion Bar (Melnick et al. 2012)

- Up to 12 hrs integration towards the surface layers of the FUV-illuminated Orion Bar
 - the thermal evaporation of O from the grain surfaces is enhanced
- Non-detection at both 487 and 774 GHz
- Upper limit $N(\text{O}_2) \sim 4 \times 10^{15} \text{ cm}^{-2}$ (face-on)



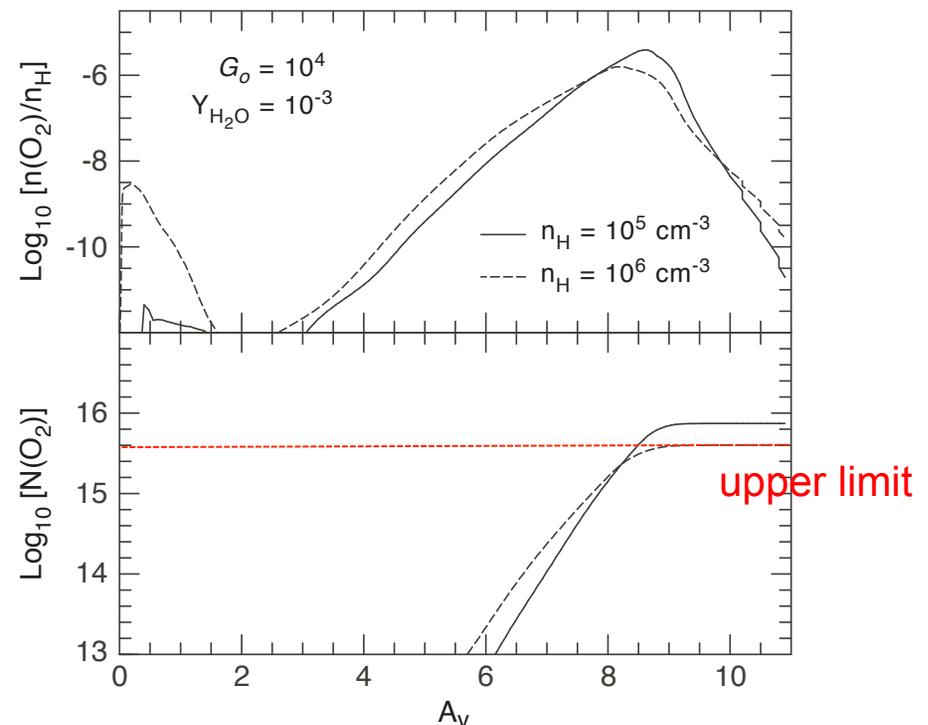
HST image (O'Dell & Wong 1996)
with ^{13}CO 3-2 contours (Lis &
Schilke 2003)

Orion Bar O₂ Observations: Test of Current Models of Externally FUV-illuminated Gas

- X(O₂) is predicted to peak at intermediate depth of $A_V \sim 8$
 - Some gas phase O is provided by FUV photodesorption of water ice
 - Most O₂ formed in gas phase
- Observed upper limit is a factor of a few below model prediction
- The discrepancy between models and observations can be resolved in a number of ways. One promising one is if

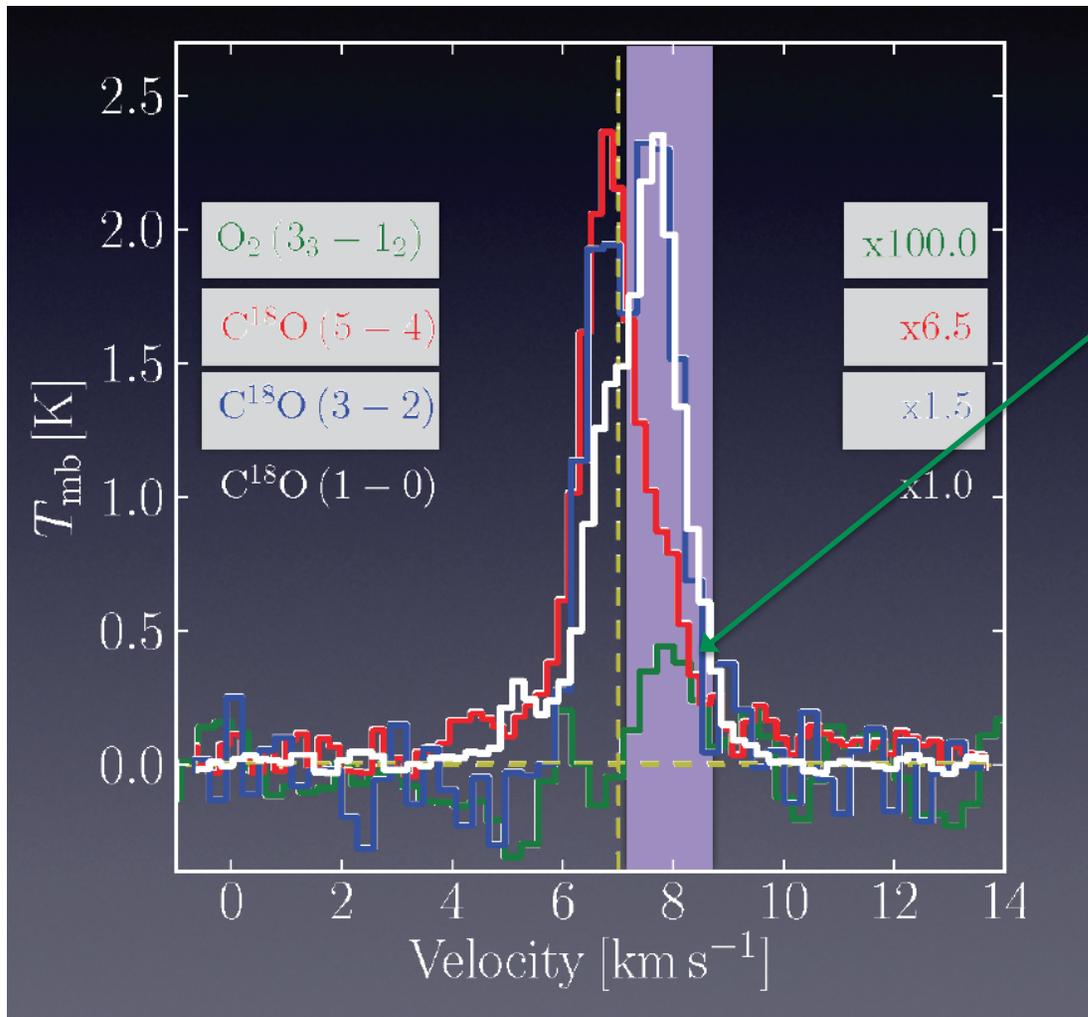
The adsorption energy of O on dust grains is greater than 800 K

- Keeps O on grains and thus ready for hydrogenation and in consequence keeps gas-phase abundance of O very low
- Results are **lower abundances of O₂ and H₂O** in the gas phase



O₂ in NGC1333 IRS4A

(Yildiz et al. 2013)



O₂ emission velocity agrees with C¹⁸O 1-0 from cold 8 kms^{-1} cloud

$$X(\text{O}_2) \approx 10^{-8}$$

Binary Class 0 protostar has $v = 7.0 \text{ km s}^{-1}$

$$X(\text{O}_2) < 6 \times 10^{-9}$$

C¹⁸O 3-2 has 8 kms^{-1} and 6.5 kms^{-1} components

Cloud collision ?

Conclusions

With limited data available, mostly in lowest frequency transition, most sources show **no** detectable O₂ emission with Herschel HIFI

The broad-brush interpretation is that in regions of modest temperature, the **O₂ abundance is extremely low**, with limits between few x10⁻⁹ and few x10⁻⁸ if compared to total N(H₂) along line of sight

These results confirm and extend SWAS and Odin results: O₂ is **not** a significant coolant and is **not** a major contributor to overall oxygen budget.

O₂ in ρ Oph has been confirmed with 2 Herschel lines (+ Odin 118 GHz line)

Detection in NGC1333 cloud (not protostar envelope) with X(O₂) ~ 10⁻⁸

Significant detections of three O₂ transitions in Orion: narrow lines with velocity 11 – 12 km/s; most likely due to shock chemistry

Complete HOP data set

- confirms that pure gas-phase chemistry is not applicable to dense regions of molecular clouds
- suggests that PDR chemistry, while promising, may need adjustment
- indicates that shock chemistry could be important in some regions



**Thanks to all who worked for so long to make
Herschel a great success!**