The Herschel Oxygen Project
Herschel Space Observatory
Open Time Key Project

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Herschel Oxygen Project

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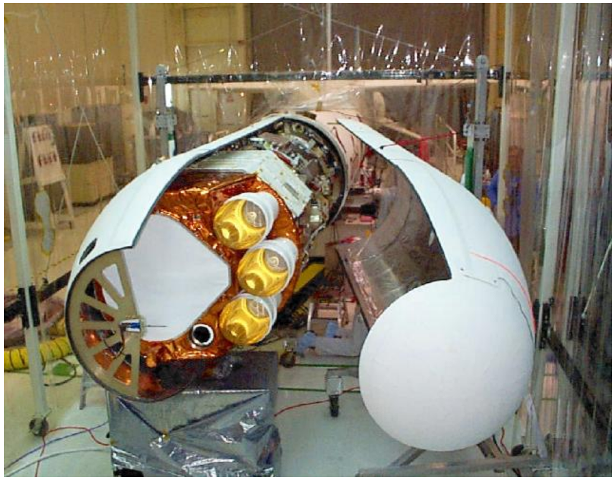
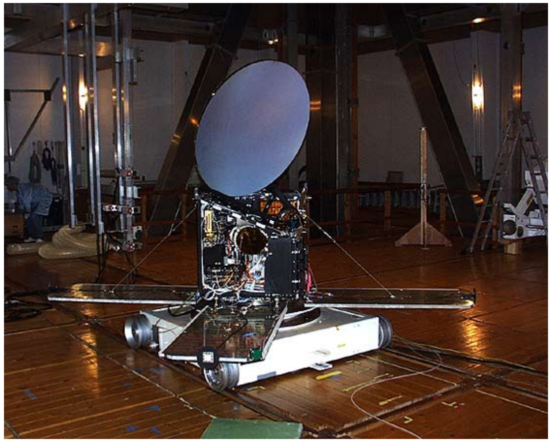
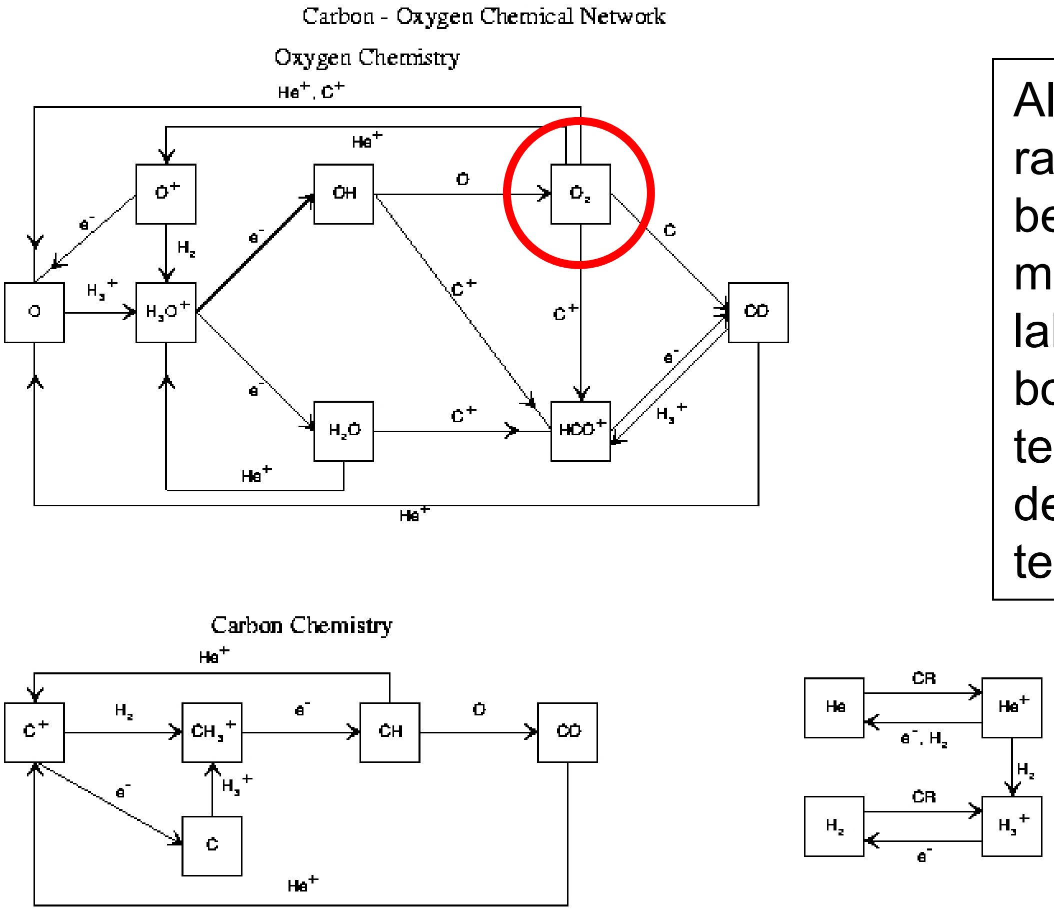
Why O_2 and Why at Submillimeter Wavelengths?





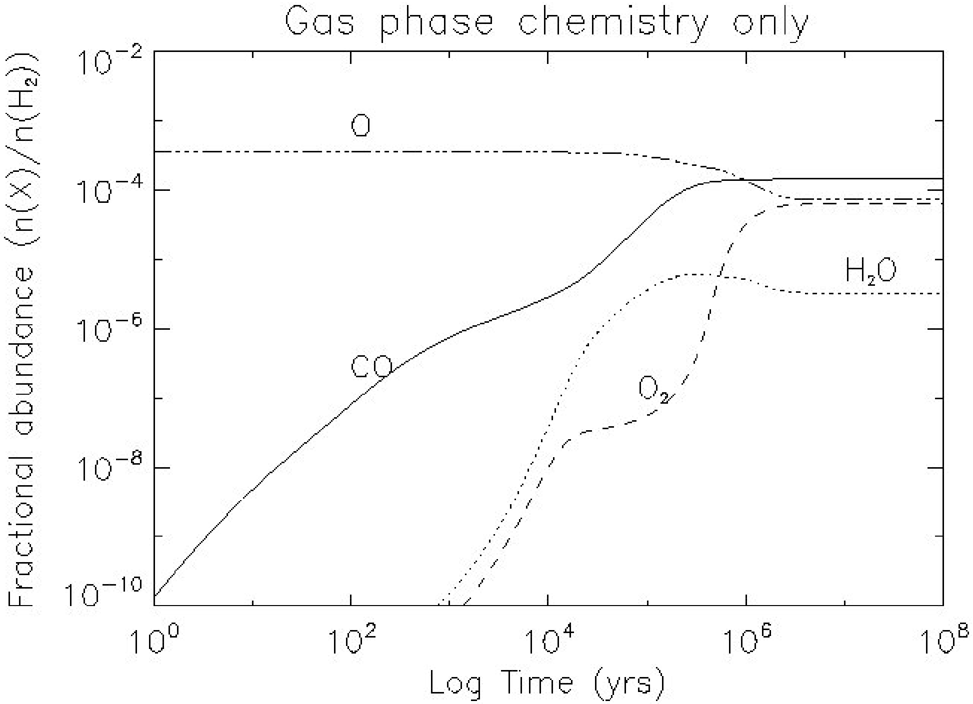
- **Astrophysical Importance** –O_2 is a simple molecule whose gas-phase chemistry is thought to be well understood
- **Large predicted abundance** - in relevant situations should be as large as $X(O_2) = n(O_2)/n(H2) = 3\text{x}10^{-5}$ making O_2 a major oxygen reservoir
- **Critical transitions** fall in THz range
- **O_2 was major objective** of SWAS and Odin satellites, which gave very surprising results
- **Connection with life**
- **Target of Herschel projects (GTKP & OTKP)**

Gas Phase Chemistry of H_2O, O_2, and CO is Relatively Simple



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

Standard Gas-Phase Chemistry Models Predict Lots of O_2

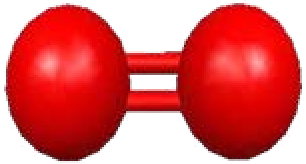


The time dependent evolution of a gas phase chemistry model. The physical conditions are n(H_2) = 10^4 cm^{-3}, T = 10 K, and A_v = 10 mag. The oxygen is initially atomic (K. Willacy).

Molecular Oxygen Structure

- O_2 is a homonuclear molecule with zero permanent electric dipole moment
- Last 2 electron spins are parallel, yielding S = 1
- Symmetry demands that rotational quantum number N must be odd
- Spin magnetic moment interacts with molecular rotation, splitting each rotational level into three levels having J = N-1, N, N+1
- Magnetic dipole transitions connect different levels but transitions are 10^4 times weaker than those of H_2O
- Level populations easily thermalized by collisions (LTE)
- Photon trapping is unimportant but O_2 is difficult to detect because emission per molecule is so weak

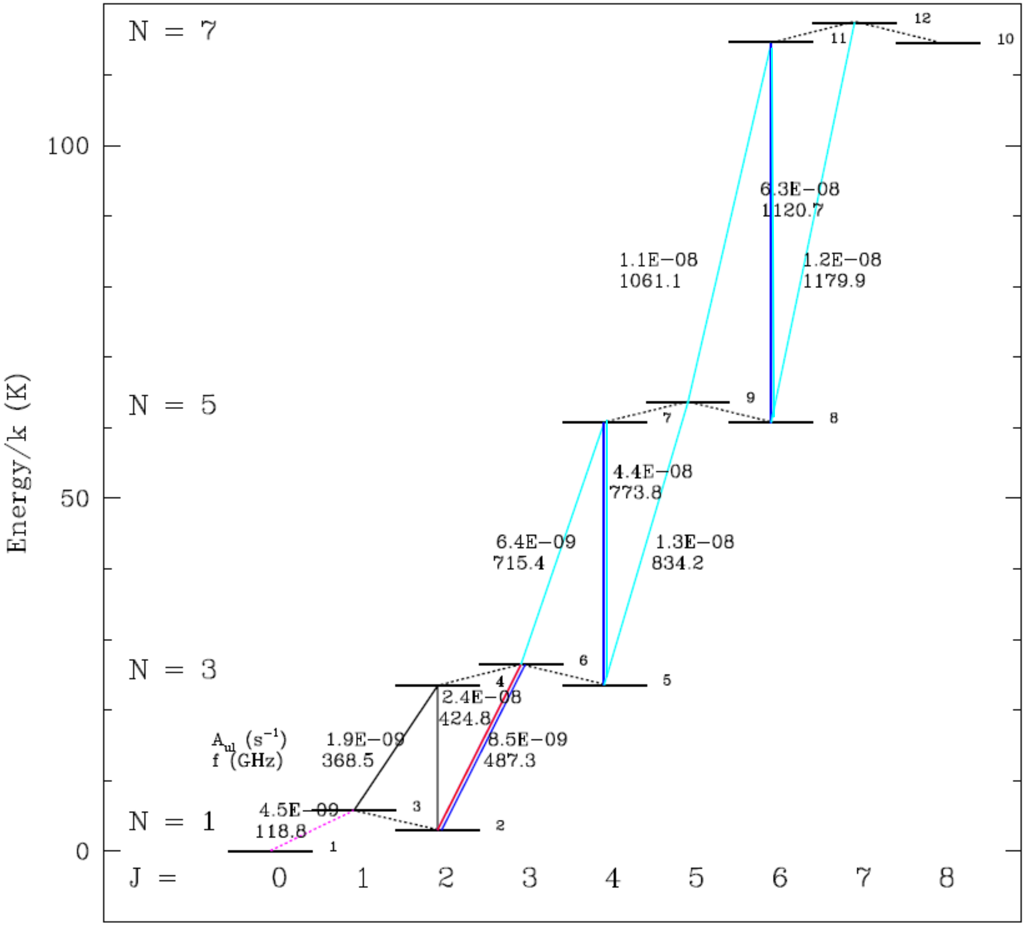
Lower Rotational Levels and Transitions of O_2



O_2 Rotational Levels are Connected by Weak Magnetic Dipole Transitions

Level Populations in LTE

Emission will be Optically Thin



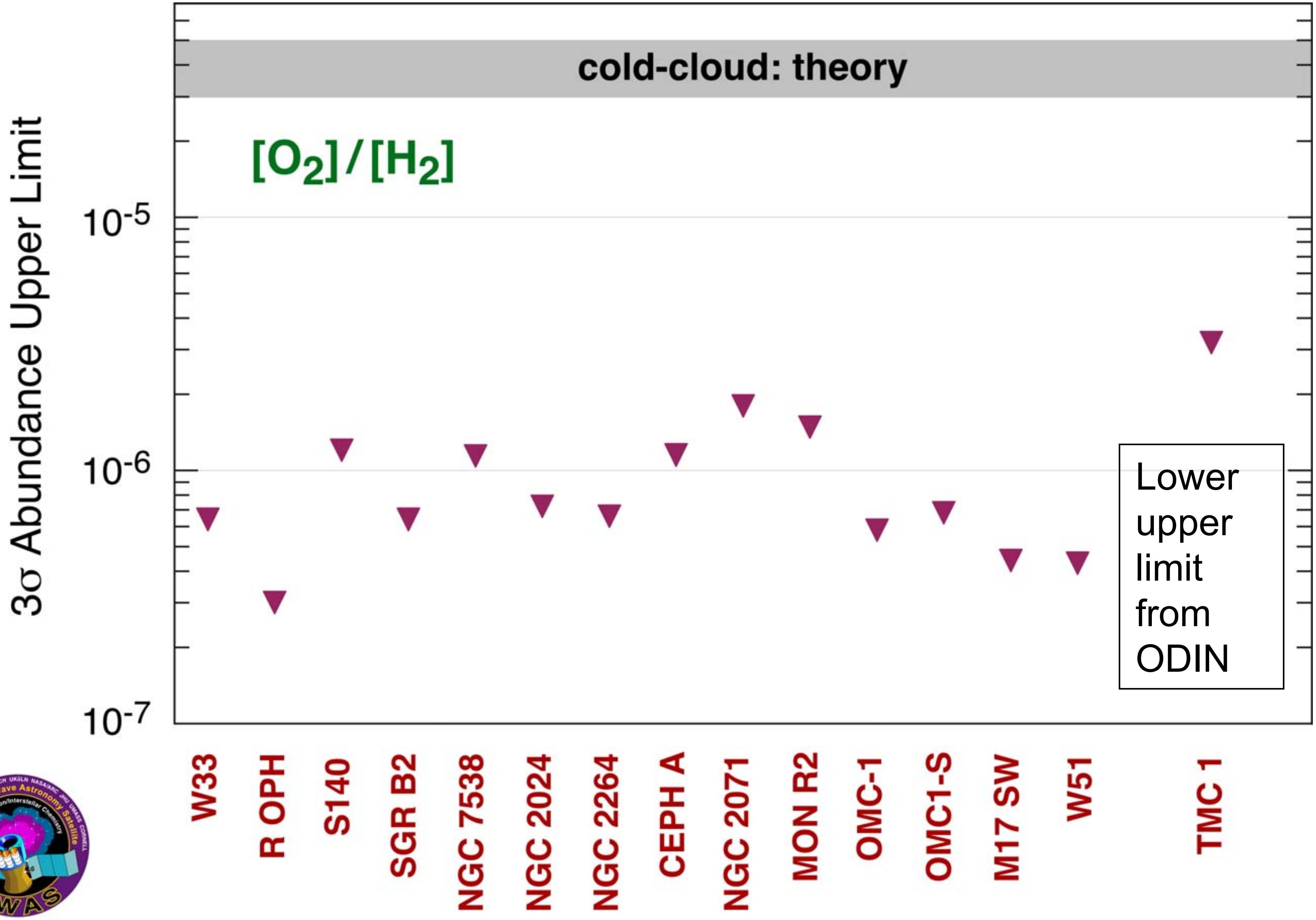
Observed by SWAS

Observed by Odin

Observable with Herschel

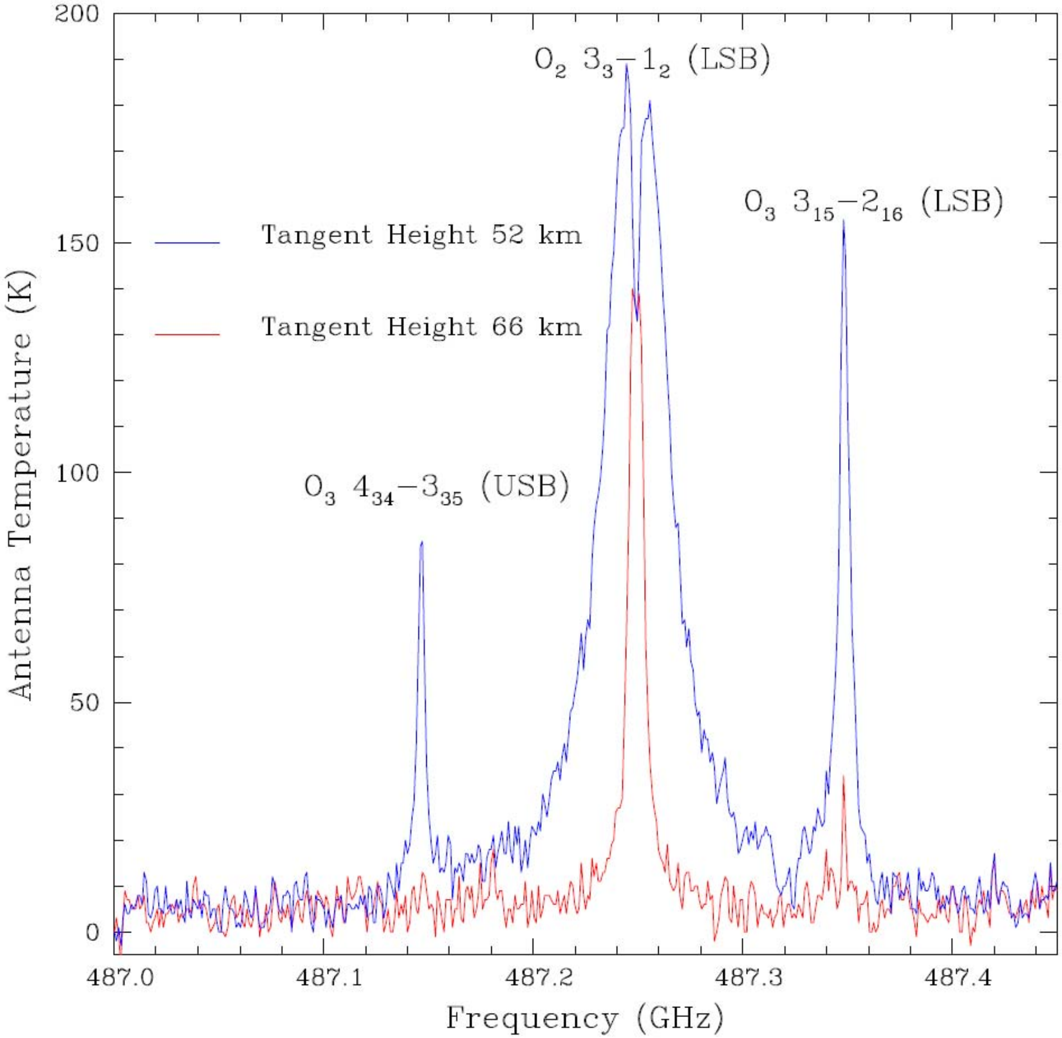
Most favorable transitions for Herschel

O_2 Interstellar Cloud Abundance from SWAS



Lower upper limit from ODIN

SWAS Spectra of Terrestrial O_2



Atmospheric Limb Sounding

For path including only very high altitude, we see pure emission with narrow line width and relatively weak lines

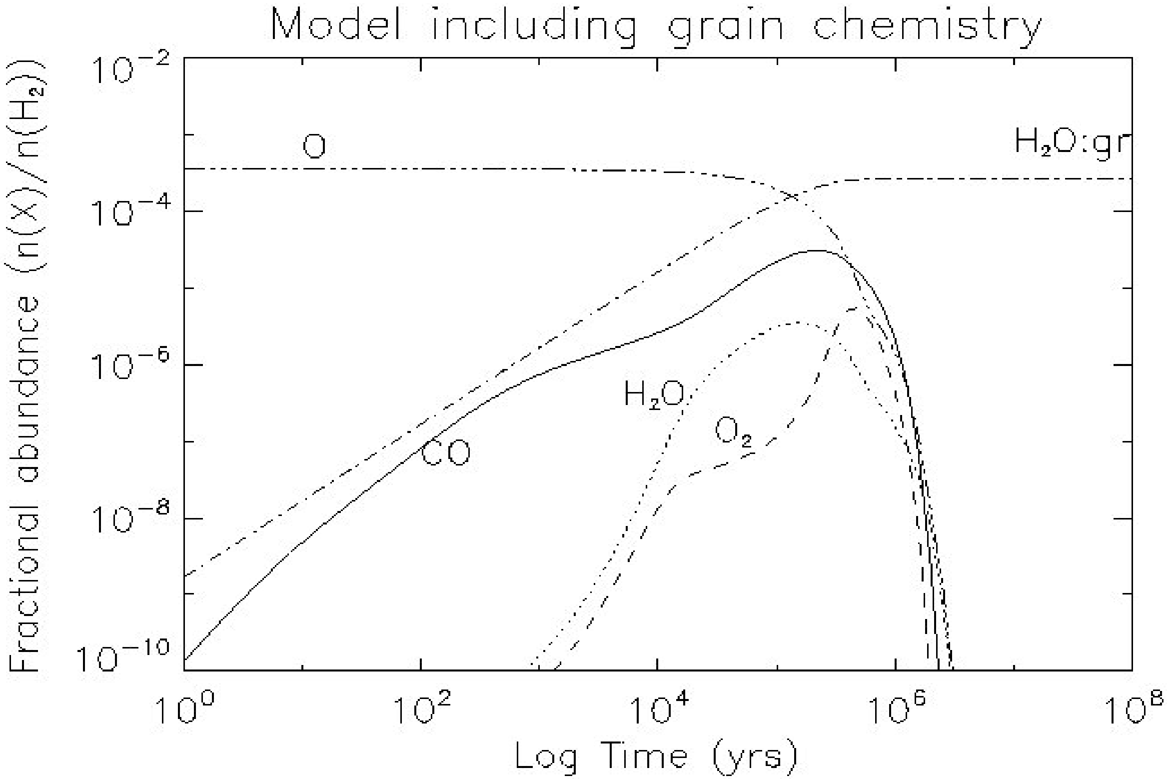
For path including lower altitudes, we see stronger emission with greater line width for O_2 and O_3

O_2 shows self-absorption produced by colder gas at higher altitude

Note: Sideband gain ratio implied by O_3 lines is ~ unity

(This option is not available for Herschel)

To Reduce X(O_2) in Dense ISM Gas Phase – Bring in the Grains



Addition of (cold) grains results in freezout of O_2 in few x 10^6 yr at $n(H_2) = 10^4$ cm^{-3}. No desorption included. One problem is that observed upper limits to O_2 on grains make this unlikely. Another problem is that entire gas phase other than H_2 disappears as well!

Reducing Gas Phase O_2 (2)

- **Atomic oxygen** may stick to grains. Binding energy is NOT well known, but assumed to be 800 K (Tielens & Allamandola 1987); this value now considered dubious.
- **Atomic oxygen** may also react with species on grain surfaces, e.g. to form H_2O which may remain bound on surface or may be returned to gas phase.
- If abundance of O in gas phase is reduced to be less than that of C, all O will be locked up in CO, dramatically reducing $X(O_2)$ and $X(H_2O)$.

Reducing Gas Phase O_2 (3)

Several molecular cloud models were developed *prior* to SWAS and Odin results which do predict lower $X(O_2)$ and $X(H_2O)$ as consequence of

- Circulation of material between well-shielded regions and outer (UV-exposed) regions. The UV-exposed material has increased CI & CII and lower O_2 & H_2O abundances (Chièze & Pineau des Forêts 1989).
- Turbulent diffusion, which effectively increases the communication between inner and outer regions of cloud, having a similar effect (Xie, Allen, & Langer 1995).

These models have not been pursued because of issues of physics as well as tendency to reduce most molecular abundances along with those of O_2 and H_2O.

What Herschel Offers HOP

- **Small Beam Size** (20” to 46”) - [compared to 4.2’ for SWAS and 10’ for Odin] allows probing compact, warm regions in which gas-phase chemistry should be dominant
- **Increased Sensitivity** - greatly improved due to L-He cooled submillimeter SIS and HEB receivers [20 X lower noise than SWAS]
- **Broad Frequency Coverage** - increases chance of unambiguous assignment of weak lines in sources having rich submm spectra [3 lines selected to cover range of source conditions]

Key Regions for Probing O_2 in the Dense ISM

- **High column density regions** with embedded heating sources ♦ Grains too warm for significant atomic or molecular depletion $\Rightarrow$ decisive test of gas phase chemistry
- **Photon dominated regions** (*PDRs*)♦ Probe O_2 in transition zone between photodissociated outer layer and highly depleted inner region where oxygen has frozen on grains
- **X-Ray Dominated Regions** (*XDRs*) ♦ Explore effects of X-rays which are predicted to photodissociate CO making atomic O which $\rightarrow O_2$
- **Shock-Heated Regions** ♦ High temperatures enhance $O + H_2 \rightarrow OH + H$ which then $\rightarrow O_2$
- **Infrared Dark Clouds** (*IRDCs*) ♦ Turbulence and accompanying dissipation may affect grain surfaces and/or promote disequilibrium chemistry

Warm Dust Surrounding Embedded Sources $\Rightarrow$ Large $X(O_2)$

Consider region of a GMC surrounding an embedded massive star with $N(H_2) = 10^{23}$ to 10^{24} cm^{-2}.

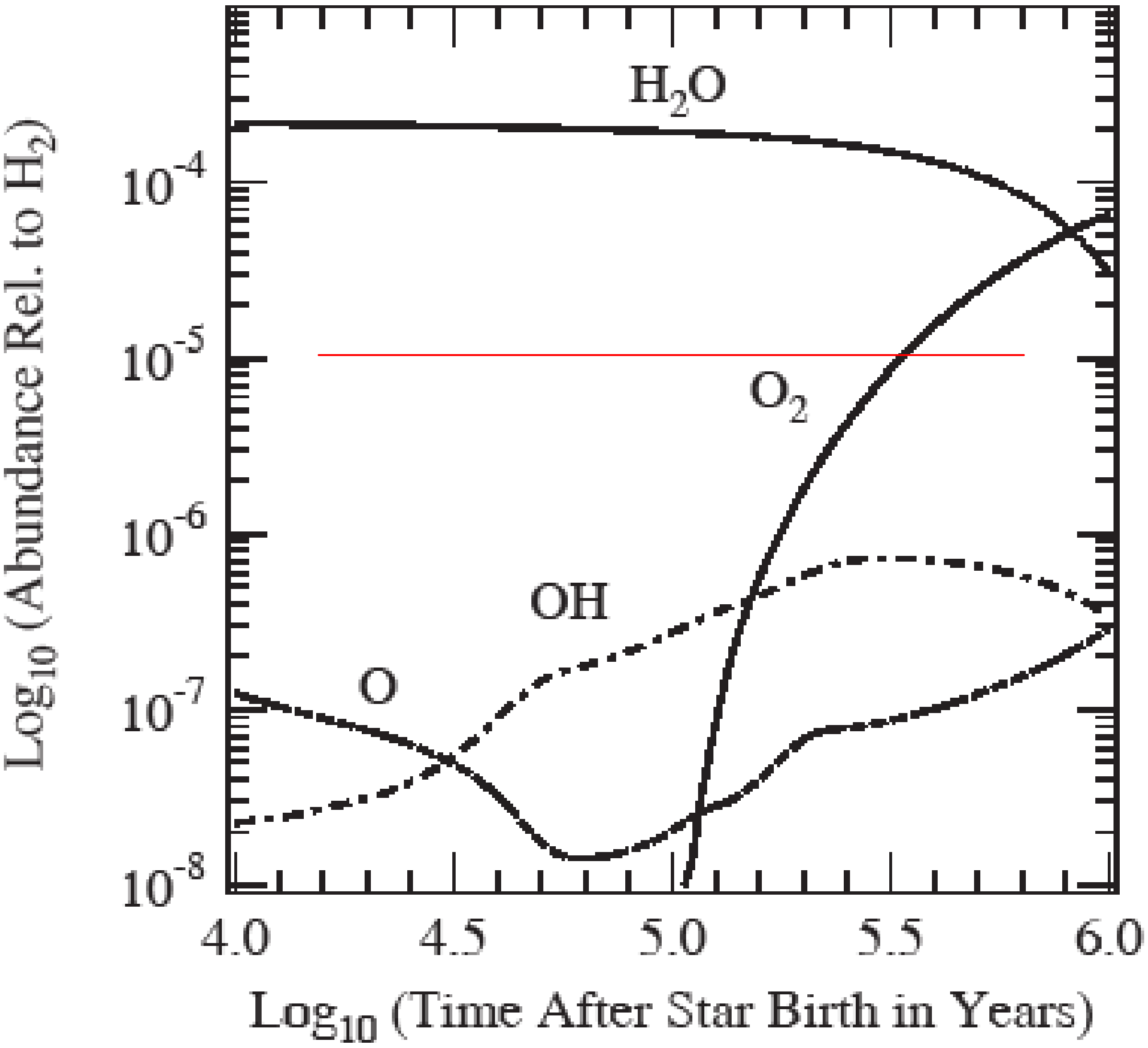
- Dust rapidly degrades dissociating UV and visible photons and is heated by IR radiation.
- O_2 binding very weak compared to that of H_2O so there will be ~ no O_2 on grains (Acharyya et al. 2007).
- Atomic O will start desorbing when T_g exceeds 25 K (Hasegawa & Herbst 1993).
- When T_g exceeds 110 – 130 K, H_2O will start desorbing
- With gas phase H_2O present, “normal” gas-phase chemistry will reassert itself in ~ 10^5 – 10^6 yr, depending on density. Expect $X(O_2)$ at least 10^{-5} in “warm dust” regions.

Time-dependence of O_2 subsequent to massive star formation

Initial conditions: T_{gas} = T_{dust} = 20 K; Most oxygen is on grain surfaces as water ice

T = 0: star turns on; dust grains in this single-zone model are heated to 150 K

Evolution: Gas phase O_2 abundance starts to rise and reaches ~ 10^{-5} in 3×10^5 yr



Observing “Warm Dust” Sources

Orion KL - L = 10^5 L_{sun}. $T_{dust} > 150$ K for $r < 5\times10^{16}$ cm ↔ 15” @ 450 pc

Within this region $n(H_2) = 10^6$ cm^{-3} so $N(H_2) = 10^{23}$ cm^{-2}. For $X(O_2) = 10^{-5}$, $N(O_2) = 10^{18}$ cm^{-2}

Herschel beam dilution factor ~ 2 ⇒ Ta = 0.14 K (easy detection)

Distant source such as Sgr B2 (D = 8.5 kpc) has larger column density of warm dust (2×10^{24} cm^{-2}), but greater beam dilution factor (40). Still easily detectable.

Note: Beam dilution factor for SWAS ≈ 3000.

The three “best” Herschel O_2 transitions are all good candidates for observation with Herschel HIFI instrument

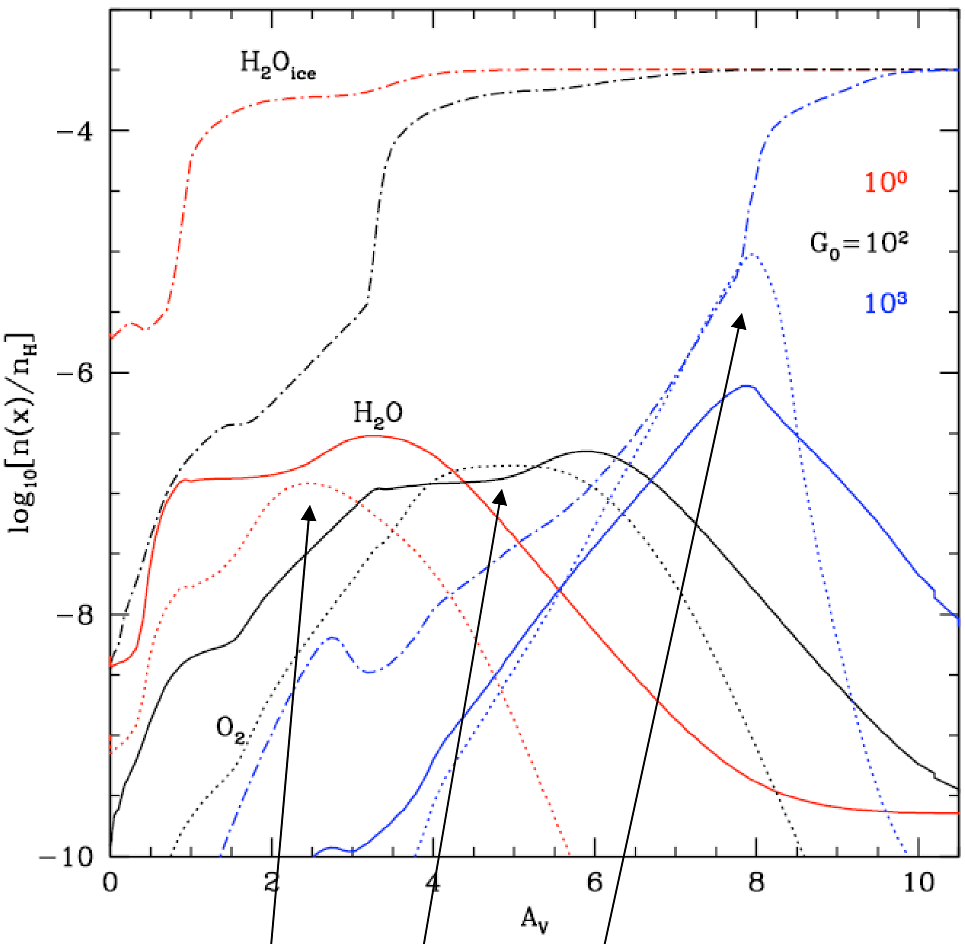
Water & Molecular Oxygen in PDRs

External radiation field

- Destroys molecules by photodissociation (low Av)
- Heats grains

Molecules deplete on grain surfaces in well-shielded regions where grains are cold

⇒Result is a “layer” of enhanced abundance of H_2O and O_2



Region of enhanced $X(O_2)$ moves inwards as G0 increases and $N(O_2)$ increases

Hollenbach, Kaufman, Bergin, & Melnick (ApJ 2008)

Embedded X-Ray Sources Increase X(O_2)

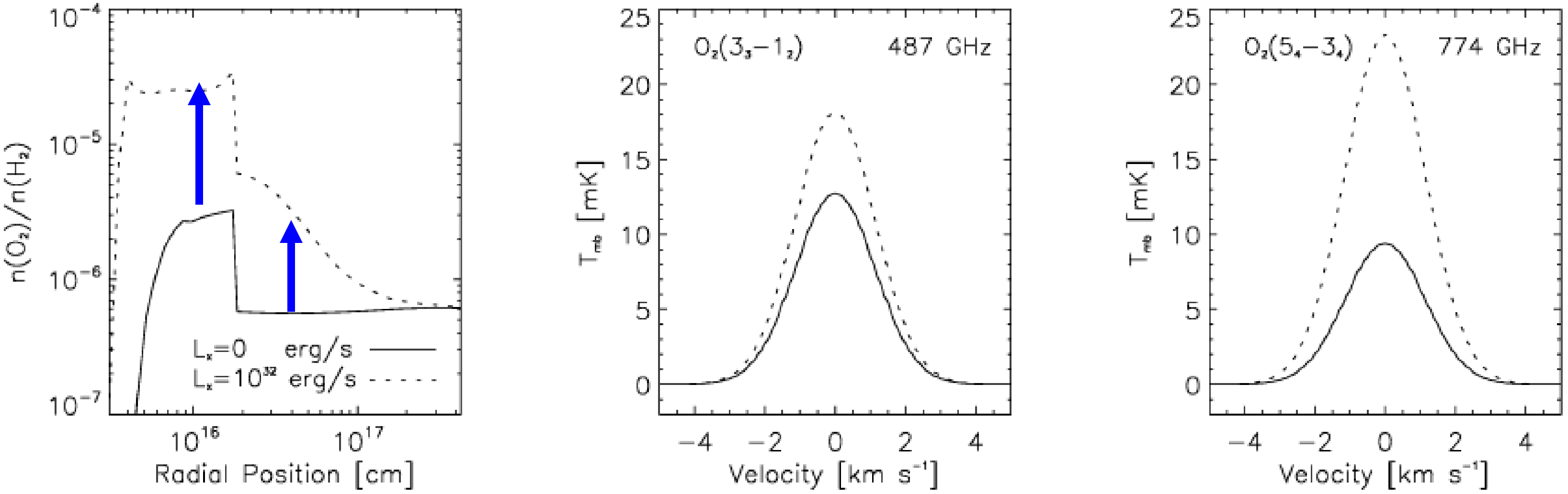
1 – 100 keV radiation penetrates deeply into surroundings of YSOs

Dissociate CO_2 yielding increased abundance of atomic oxygen

X-ray enhanced species HCO^+ and H_3O^+ react with H_2O yielding H3O$^+$ which dissociatively recombines to form OH

Enhanced formation rate of O_2 via OH + O → O_2 + H

Studied by Stauber et al. (2005)



Model of YSO AFGL 2591 at chemical age of 104 yr (Doty et al. 2006)

Non-Dissociative Shocks Impact Specific Molecular Abundances

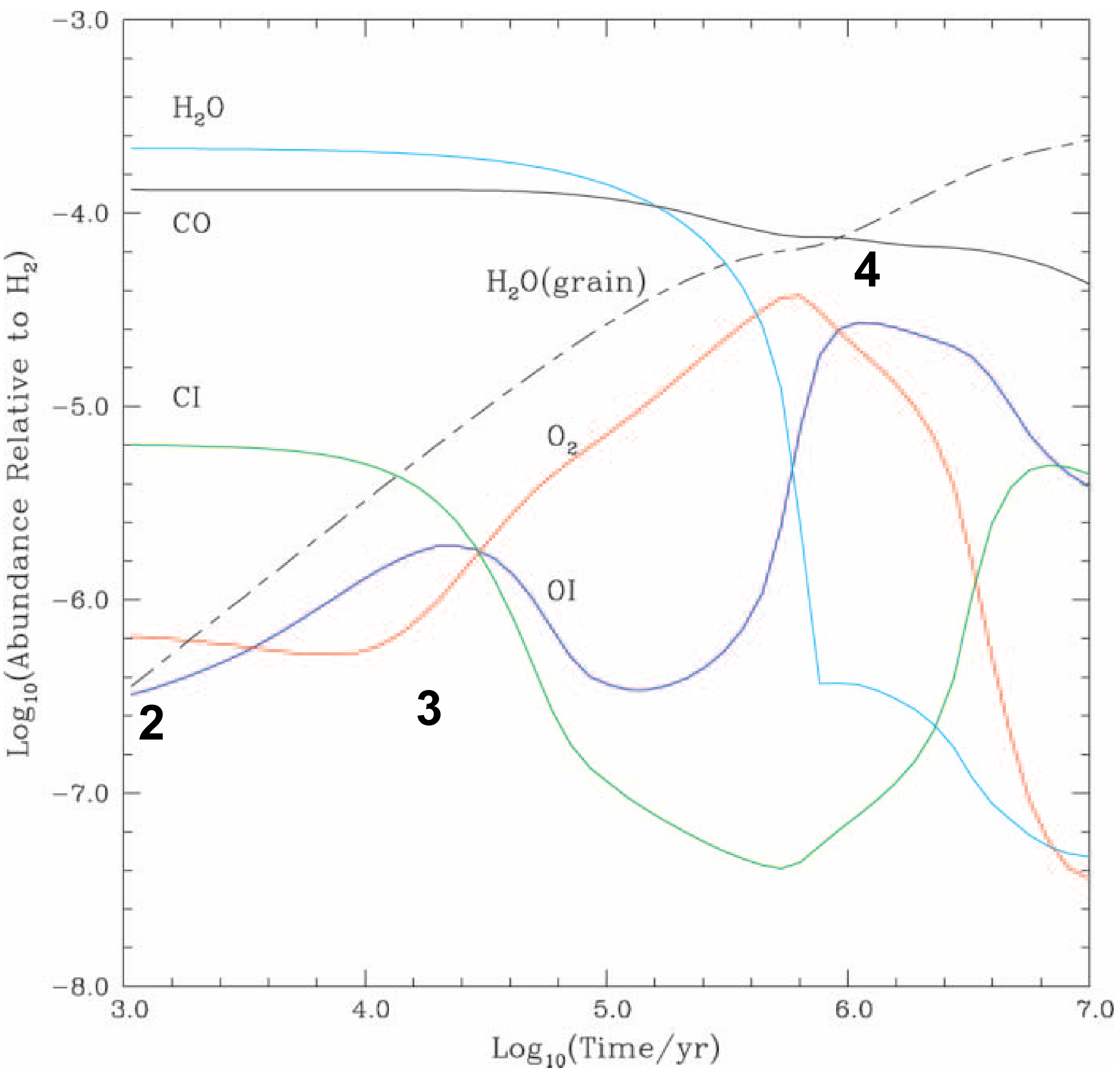
- Shocks heat gas to ≥ 100’s of K
- Pre-existing O reacts rapidly with H_2 via the endothermic reaction $O + H_2 \rightarrow OH + H$ for $T > 300$ K (Draine, Roberge, & Dalgarno 1983)
- OH reacts with O to give O_2
- Fractional abundance $X(O_2)$ can reach 10^{-6} in postshock gas, while $X(H_2O)$ can get as high as 10^{-4}
- If H_2O is on grain surfaces in preshock gas, the shock will likely return it to gas phase, and shock-produced UV will result in enhanced gas phase oxygen abundance leading to increased O_2 as above
- Example:

H_2 Peak 1 in Orion found to have $N(H_2O) = 8 \times 10^{17}$ cm^{-2} (Snell et al. 2007).

$\Rightarrow N(O_2) \sim 10^{16}$ cm^{-2} which should be detectable with Herschel HIFI

Multistage Cloud Model

1. Cloud with gas (n = 5000 cm^{-3}; T = 10 K) and grains evolves for 10^6 yr.
2. Cloud shocked – heated to 1000 K then cools to 20 K and density 10^4 cm^{-3} in 100 yr.
3. After 10^4 yr, gas-phase chemistry reasserts itself in the postshock gas. X(O_2) reaches $3x10^{-5}$ after $6x10^5$ yr.
4. Grain depletion becomes dominant, reducing available oxygen. X(O_2) drops.



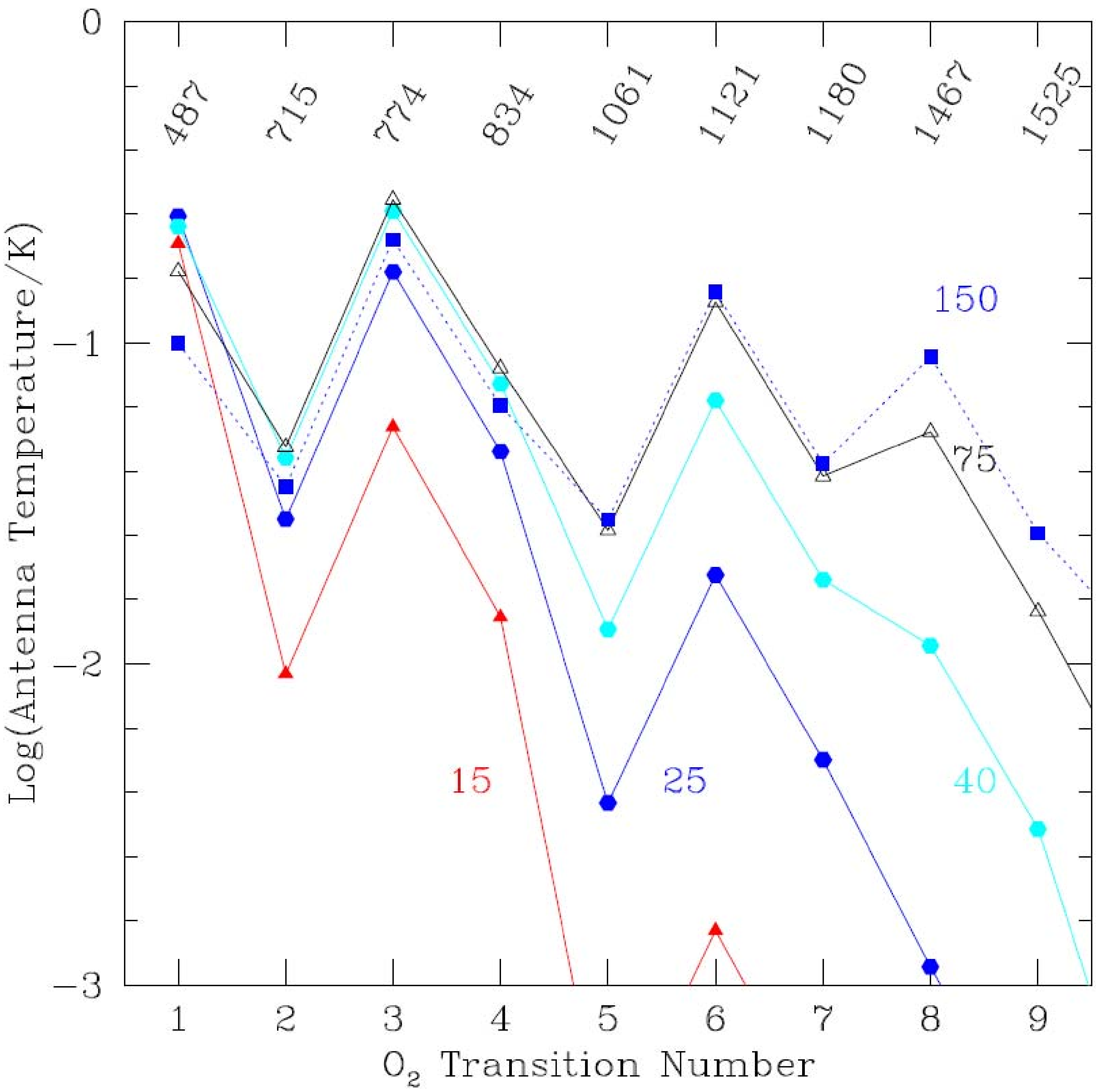
Goldsmith et al. (2002)

HOP Sources and Strategy

- Observe 487 GHz, 774 GHz, and 1121 GHz transitions in a selection of sources
- Typical observing times are 3 hours per transition per source (plus additional “deep integration” time
- RMS antenna temperature sensitivity in 3 hr integration is 3 mK (487 GHz) to 15 mK (1121 GHz) with 1σ column density sensitivity for T_k = 100 K ~ 5×10^{15} cm^{-2}.
- The H_2 column density in Herschel beam can significantly exceed 10^{23} cm^{-2}, so that we should be sensitive to O_2 fractional abundances as low as ~ 10^{-8}.

O_2 Transitions Observable with Herschel

- Small A-coeffs ⇒ LTE will hold for any reasonable density
- Emission optically thin
- Curves are for various kinetic temperatures
- Once you have heating sources, strongest lines are 487, 774, and 1121 GHz



$N(O_2)/\delta v = 10^{17} cm^{-2}/kms^{-1}$

HOP Sources and Strategy (2)

- Total observing time = 140 hr
  - 6 Low mass embedded sources (incl. ρ Oph)
  - 6 High mass embedded sources
  - 2 PDRs
  - 1 XDRs
  - 1 Shock-heated sources
  - 2 IRDCs
- Observe 2 or 3 lines, with 487 GHz and 774 GHz having largest time allocation; 1121 to be observed only in regions expected to have T > 50 K.
- Use mini-spectral scan mode: 5 different LO settings employed with double beam switching.
  - Assumes relatively small source size
  - Allows resolving sideband ambiguity to be resolved
  - Should ensure good baseline quality necessary to exploit long integrations
- Various other transitions of interesting species will be (surely or plausibly or possibly) detected as result of very high sensitivity (e.g. SO, H_2O, $H_2{}^{18}O$, CS, HDCO, D_2CO, ^{13}CO)

Herschel – 2nd Generation Submm Space Mission

3.5m diameter SiC Cass telescope

3 L-He cooled instruments

670 μm → 60 μm range

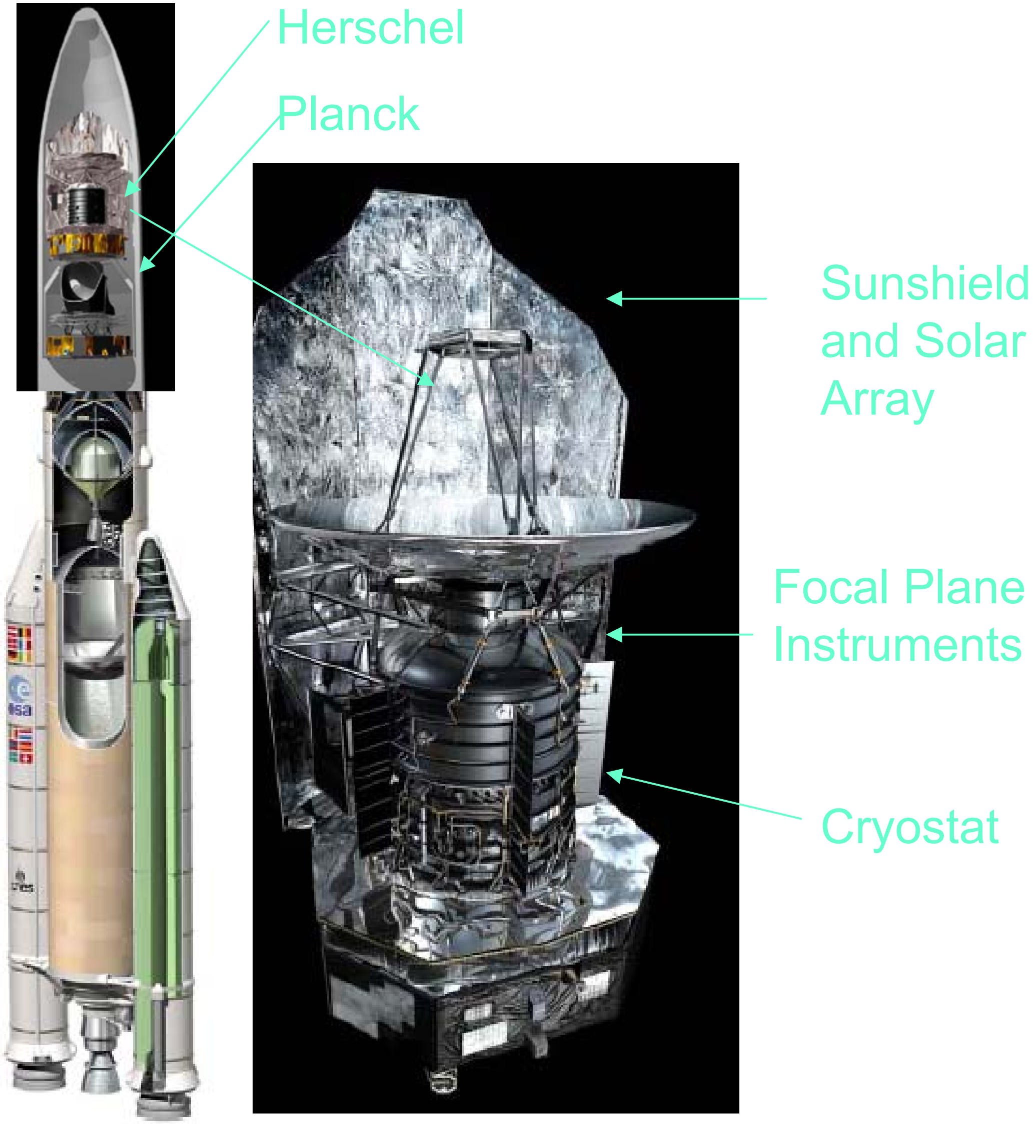
Wavefront error < 6μm rms

$\Delta\theta = 50'' \rightarrow 9''$

L2 orbit

Minimum 3.5 yr mission lifetime

Ariane 5 Dual launch with Planck CMB satellite



The Three Herschel Instruments

Two are imaging photometers and spectrometers

- Photodetector Array Camera and Spectrometer (PACS)
  60 μm – 210 μm PI = Albrech Poglitsch, MPE, Garching [Germany]
  2 bolometer arrays w/ 32x16 and 64x32 pixels
  R up to 4000 at shortest wavelength with grating w/ 25 spatial x 16 spectral pixels

- Spectral and Photometric Imaging Receiver (SPIRE)

  200 μm – 670 μm PI = Matt Griffin, Cardiff Univ. [UK]
  R up to 1200 using FTS with 19/37 detectors; 43/88/139 pixel photometer arrays (long → short wavelengths)

The third is a high resolution heterodyne spectrometer

- Heterodyne Instrument for the Far Infrared (HIFI)
  157 μm – 212 μm & 240 μm – 625 μm PI = Thijs de Graauw (now Frank Helmich SRON [Netherlands]; US PI = Tom Phillips, CIT
  R up to 10^6; 1 pixel x 2 polarizations at each frequency

Herschel will be launched into an L2 orbit

Current launch date: April 12, 2009