

The rotational spectrum of H₂ in AGB stars: Detection and analysis of the S(1) line in IRC+10216

José Pablo Fonfría

jpablo.fonfria@csic.es

Instituto de Física Fundamental (IFF)
Centro de Astrobiología (CAB)
Consejo Superior de Investigaciones Científicas (CSIC)

with the collaboration of

C. N. DeWitt, E. J. Montiel, J. Cernicharo & M. J. Richter

SOFIA Tele-Talk

July 6, 2022



Outline

- 1 Introduction
 - The spectrum of H₂
 - Detections in space
 - The mass-loss rate of evolved stars
- 2 H₂ observations toward IRC+10216 with SOFIA/EXES
- 3 Results
 - Where are the high excitation H₂ rotational lines?
 - Best fit – Mass-loss rate and CO abundance
 - Best fit – Physical conditions
 - Line identification at 17 μm
- 4 On-going work – Very preliminary results
- 5 Conclusions and Final remarks

Introduction: The spectrum of H₂

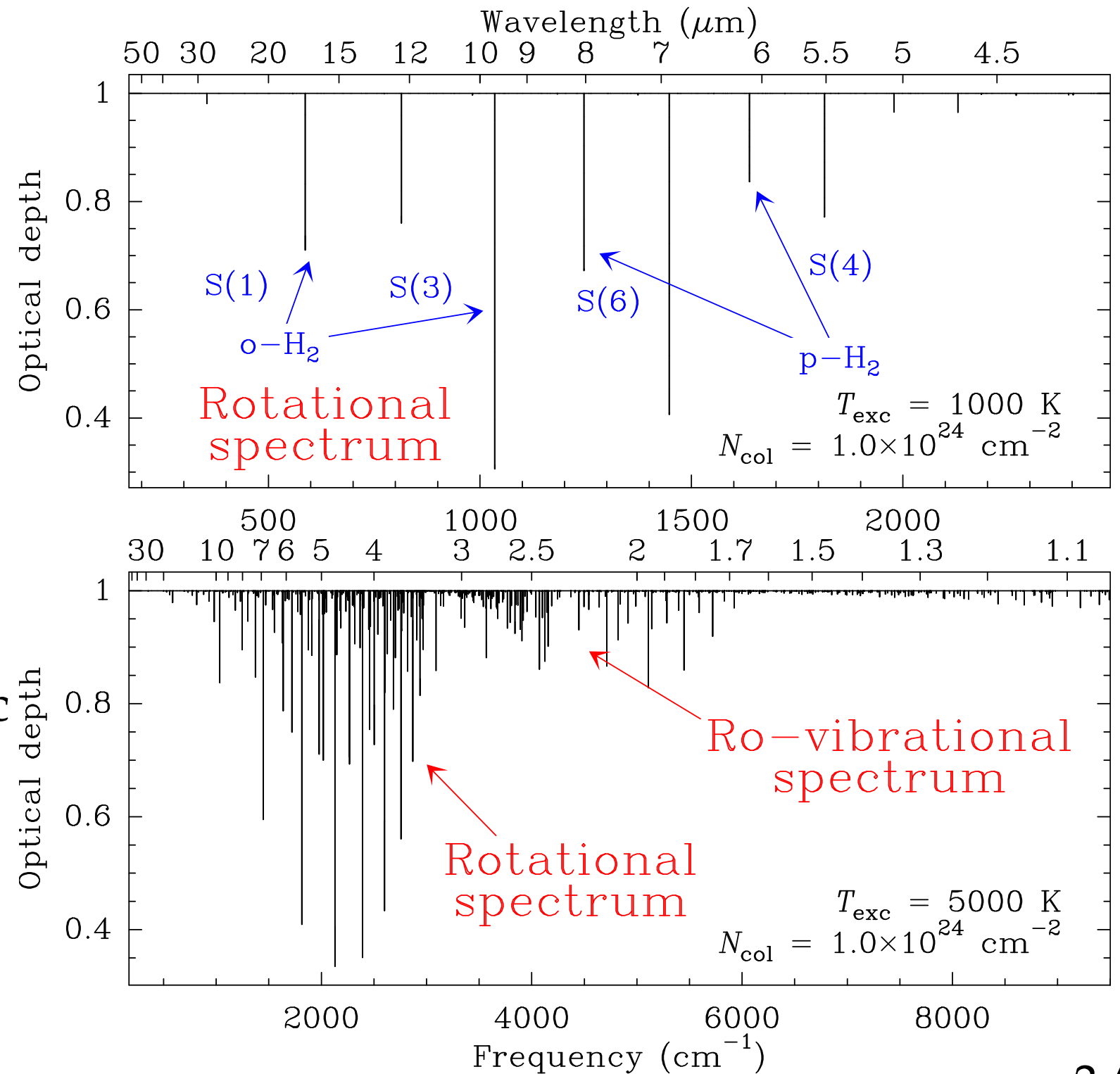
H₂ is a **diatomic, homonuclear** molecule



- Ortho-para ratio = 3
- Electric dipole transitions forbidden in the electronic ground state
- Electric dipole transitions allowed between electronic states
- Electric quadrupole and magnetic dipole transitions allowed in the same electronic state

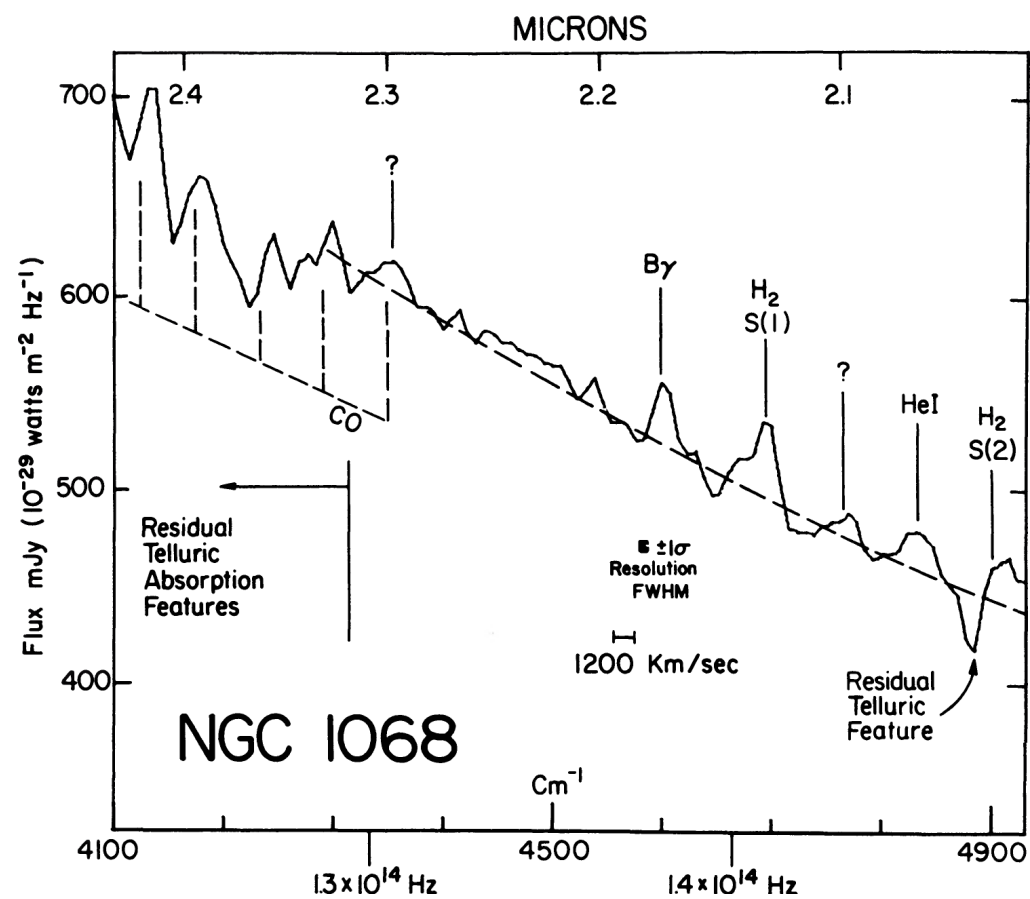


Very weak rotational and ro-vibrational spectra

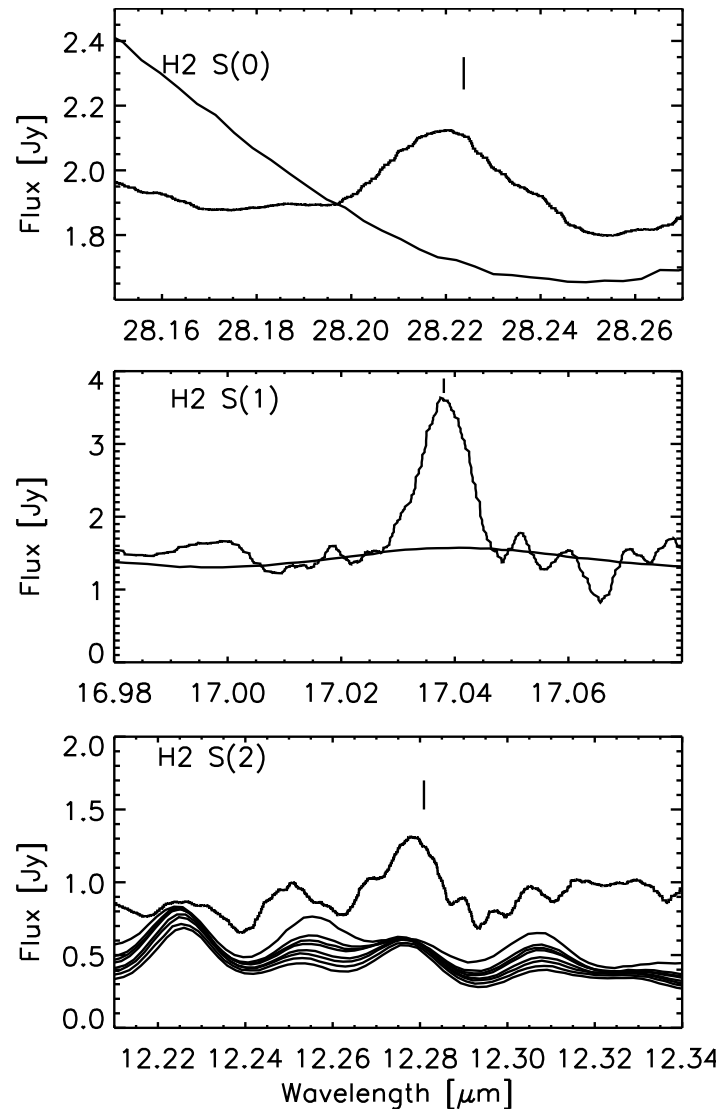


Introduction: Detections in space

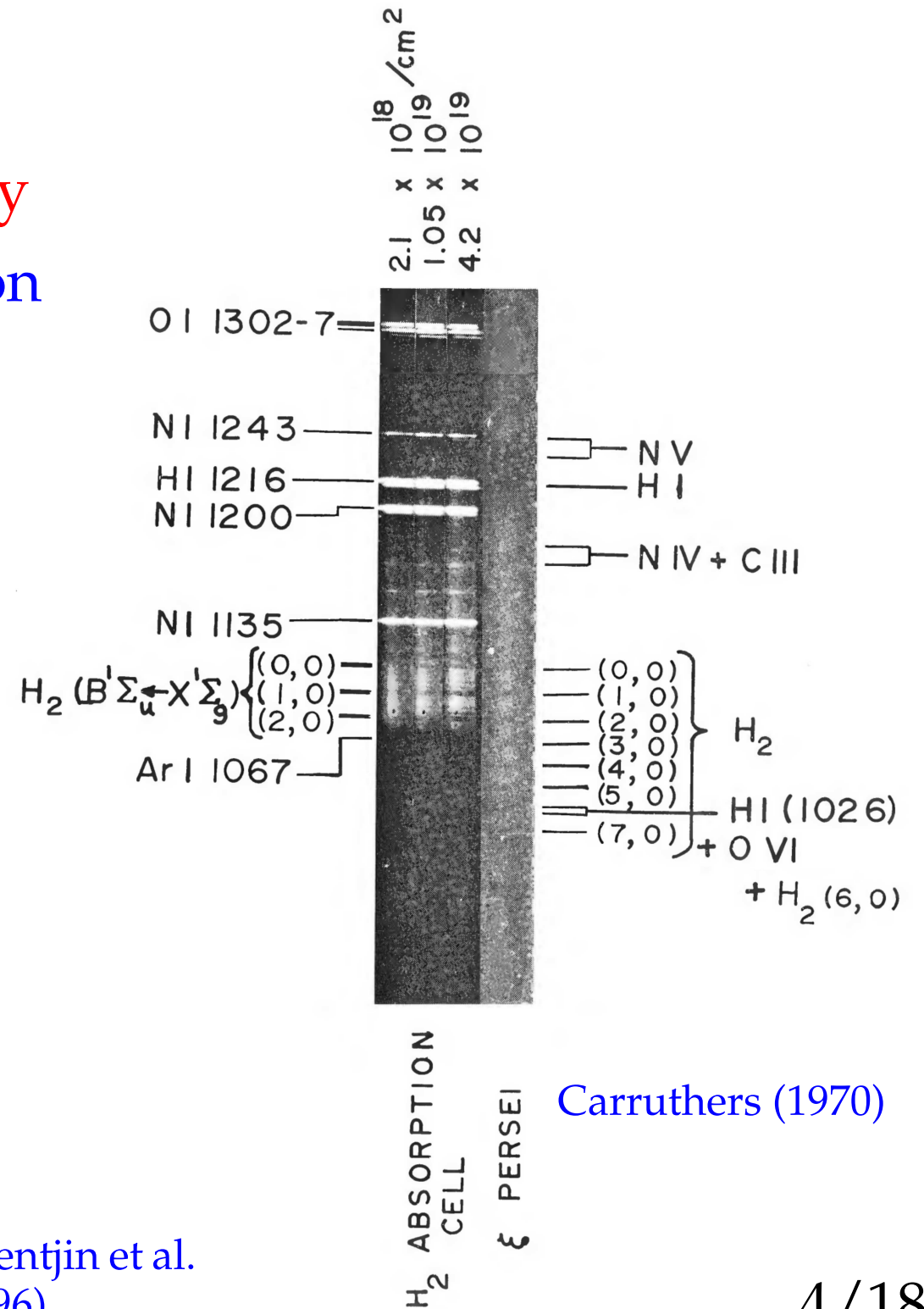
- First detection in space toward the O7 star ξ Persei (Carruthers, 1970). Vibronic bands of the Lyman system ($B^1\Sigma_u-X^1\Sigma_g$) at $0.11 \mu\text{m}$ in absorption \implies ISM of Milky Way
- First extragalactic detection (rotation-vibrational: Thompson et al., 1978; pure rotation: Valentjin et al., 1996 and Sturm et al., 1996)



Thompson et al. (1978)



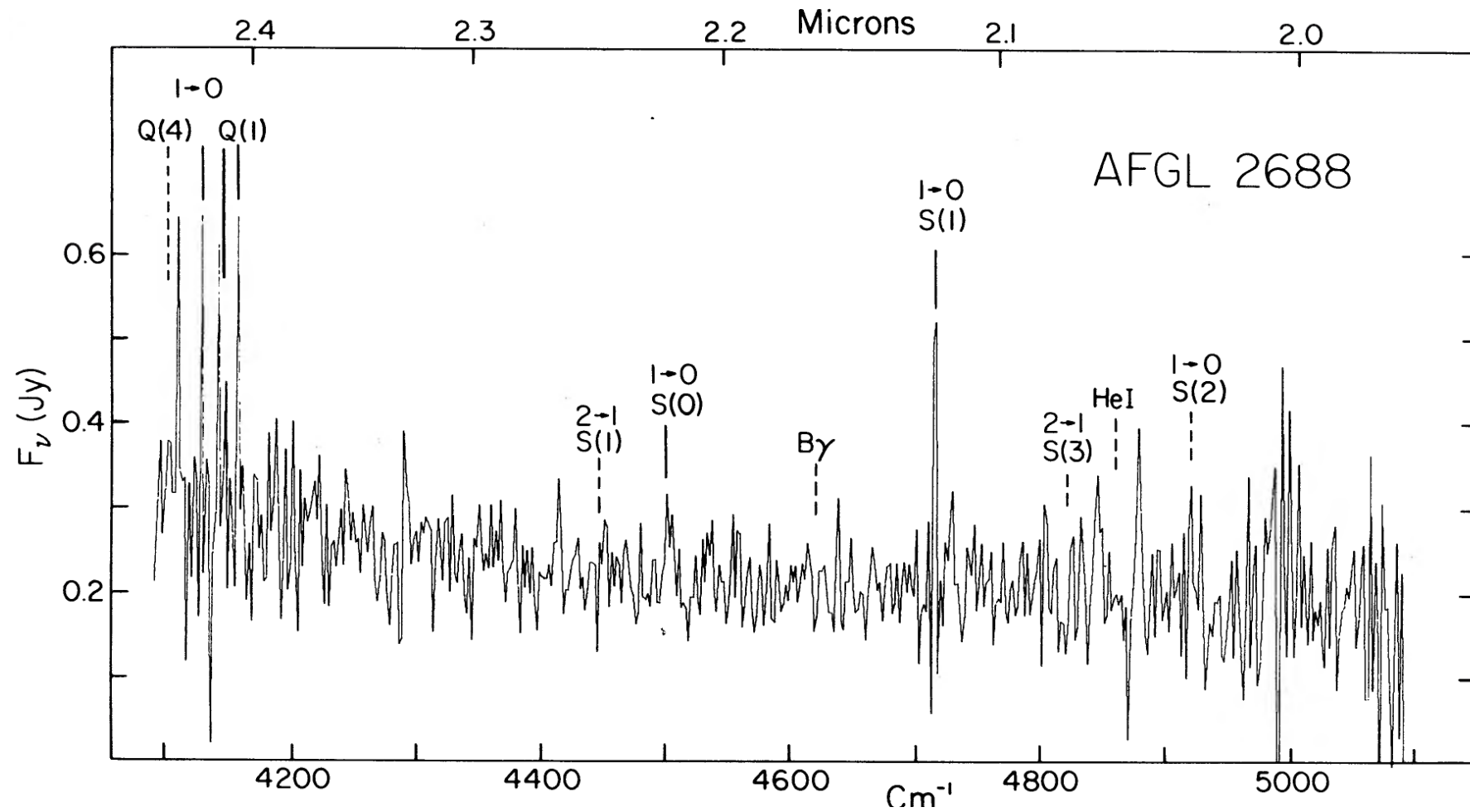
Valentjin et al. (1996)



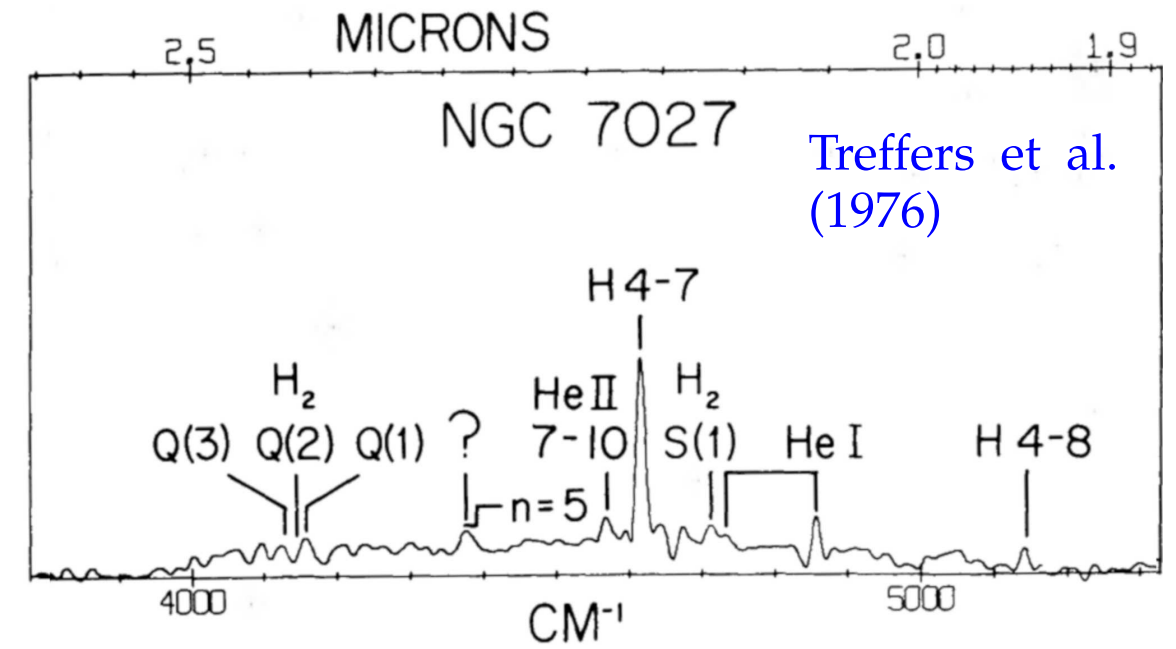
Carruthers (1970)

Introduction: Detections in space (post-AGB stars)

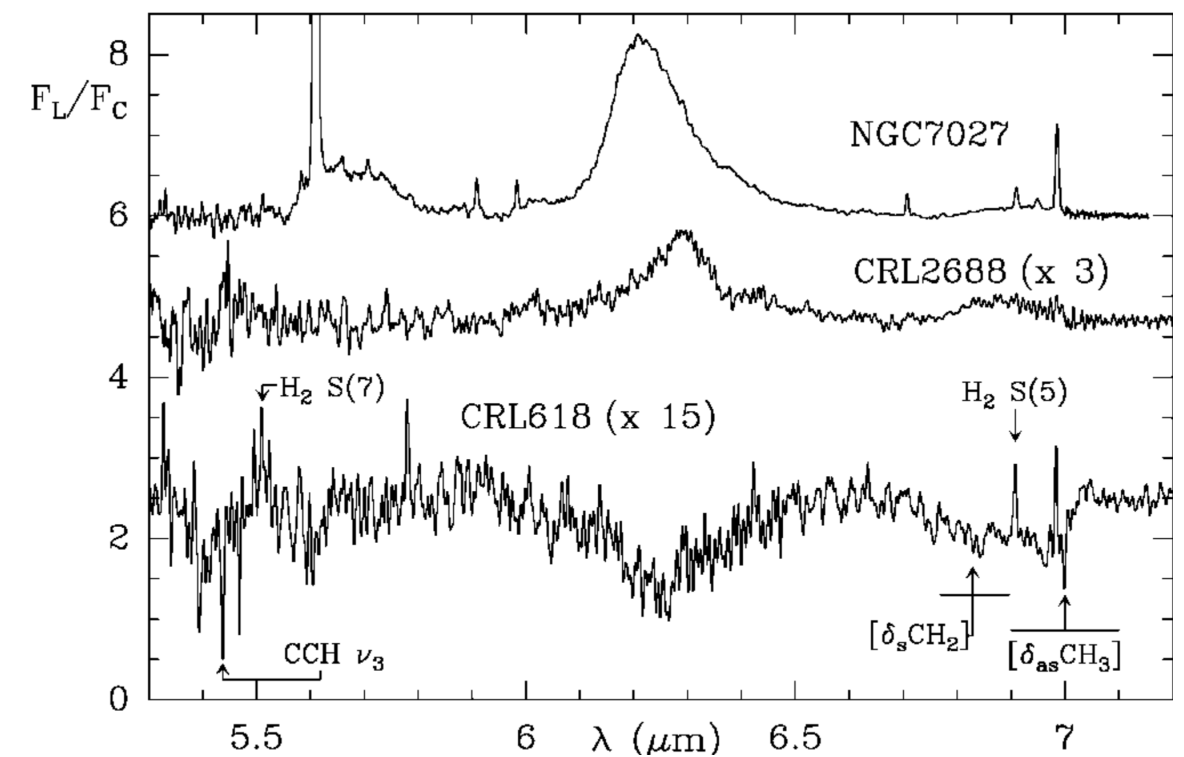
- Detection in PNe (Treffers et al., 1976)
- Detection in PPNe (rotation-vibration: Thronson, 1982; pure rotation: Cernicharo et al., 2001)



Thronson (1982)



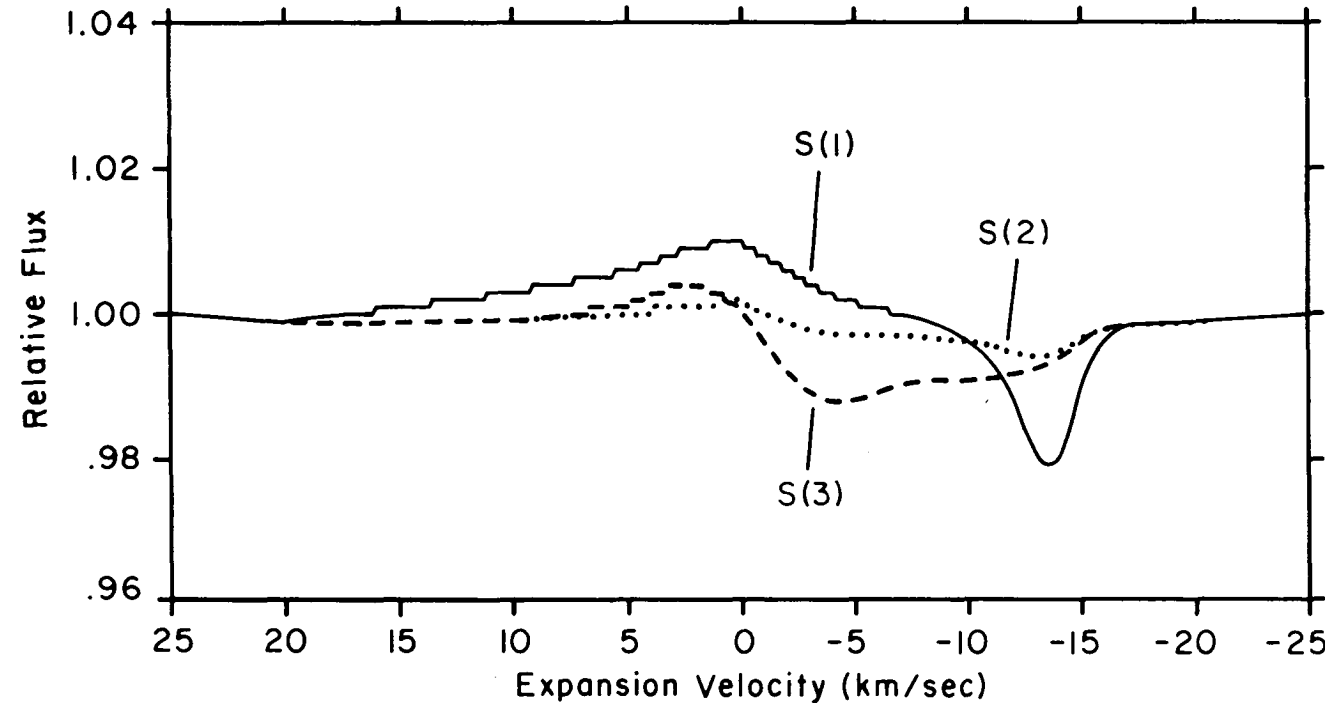
Treffers et al. (1976)



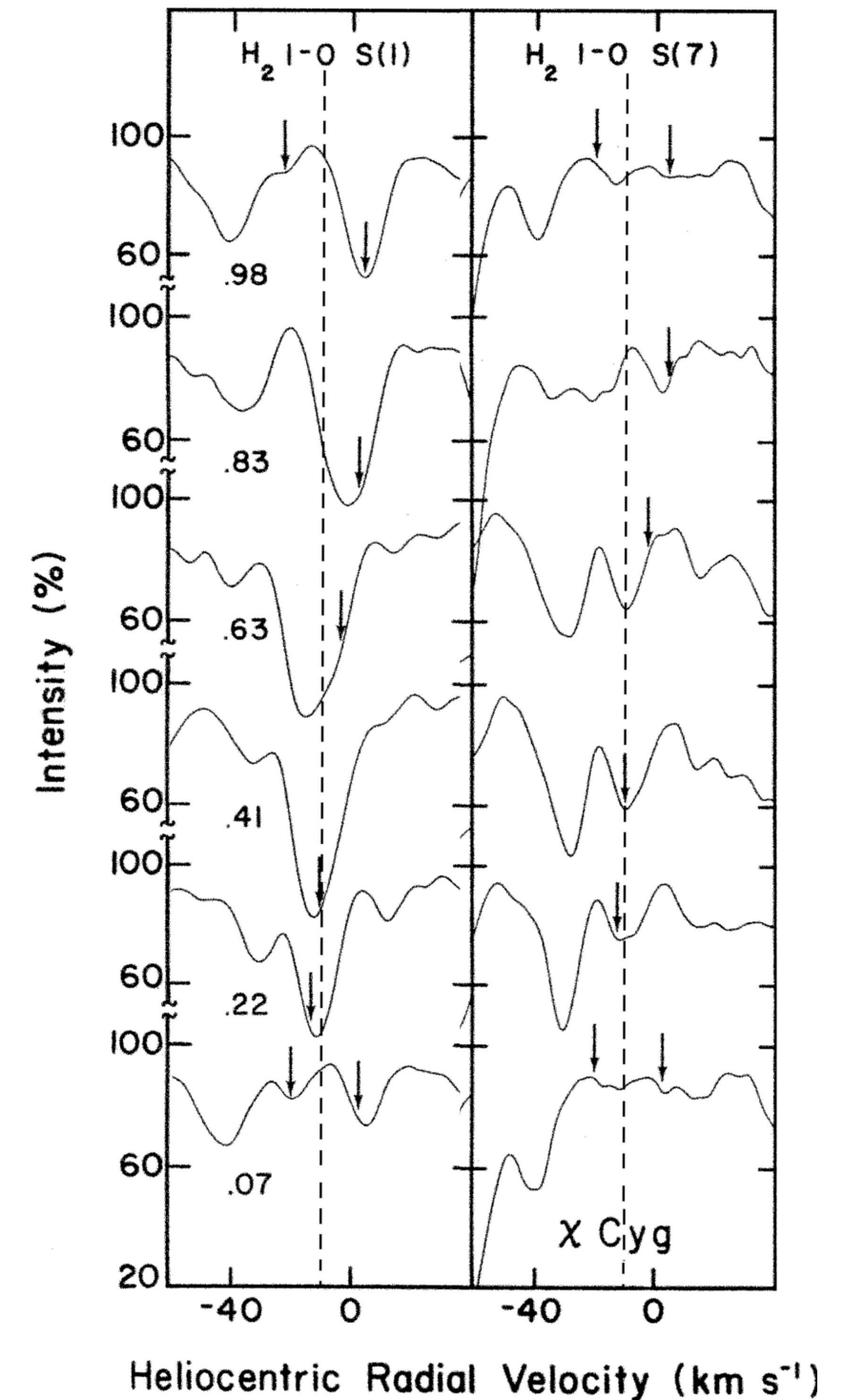
Cernicharo et al. (2001)

Introduction: Detections in space (AGB stars)

- Detection of rotation-vibration bands in many AGBs (Hinkle et al., 2000)
- However, **no rotational line of H₂ has been detected so far in AGB stars**
- Keady & Ridgway (1993) predicted the rotational lines of H₂ in IRC+10216



Keady & Ridgway (1993)



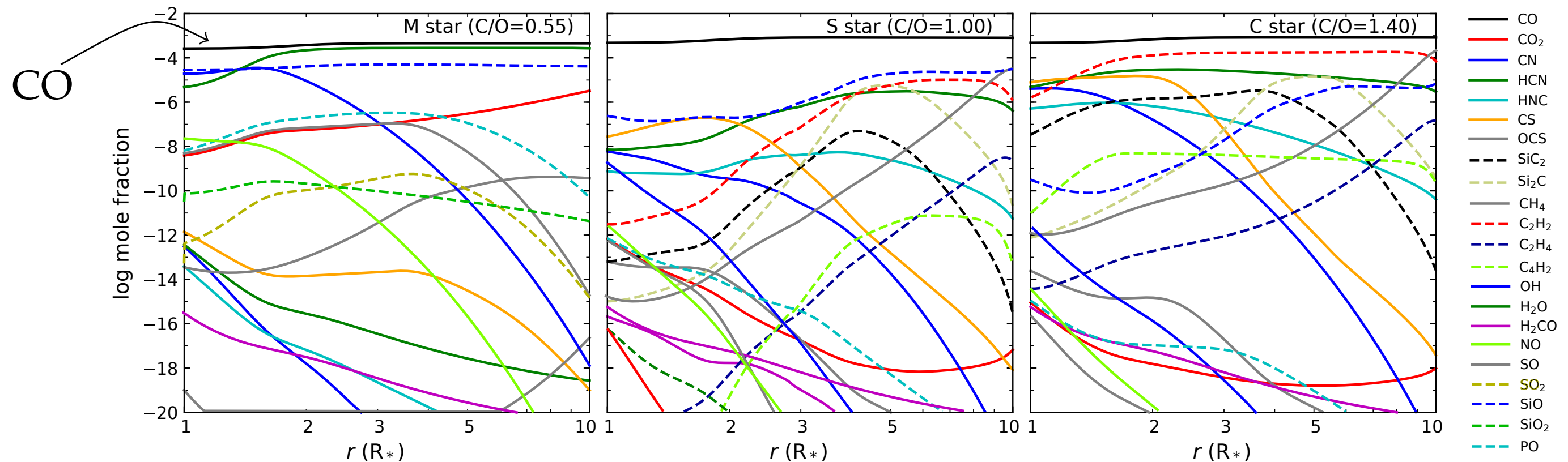
Hinkle et al. (2000)

Introduction: The mass-loss rate of evolved stars

- Mass-loss rates can be estimated from pure rotational lines of ubiquitous molecules such as CO, H₂, SiO, HCN, C₂H₂,...
- Chemistry is a serious problem and molecular abundances are typically extremely variable
- CO(2 – 1) is widely used

$$\dot{M}_{\text{H}_2} = 5.1 \times 10^{-15} T_A \frac{v_e^2 B^2 D^2}{f_x} \frac{Z(T_x) v^2}{g_u A_{ul}} \exp\left(\frac{E_l}{T_x}\right) \times \left\{ \int_{r_i}^{r_e} \exp\left[-4(\ln 2) \left(\frac{r}{BD}\right)^2\right] dr \right\}^{-1}$$

Adapted from Olofsson et al. (1993)



Adapted from Agúndez et al. (2020)

H₂ observations toward IRC+10216 with SOFIA/EXES



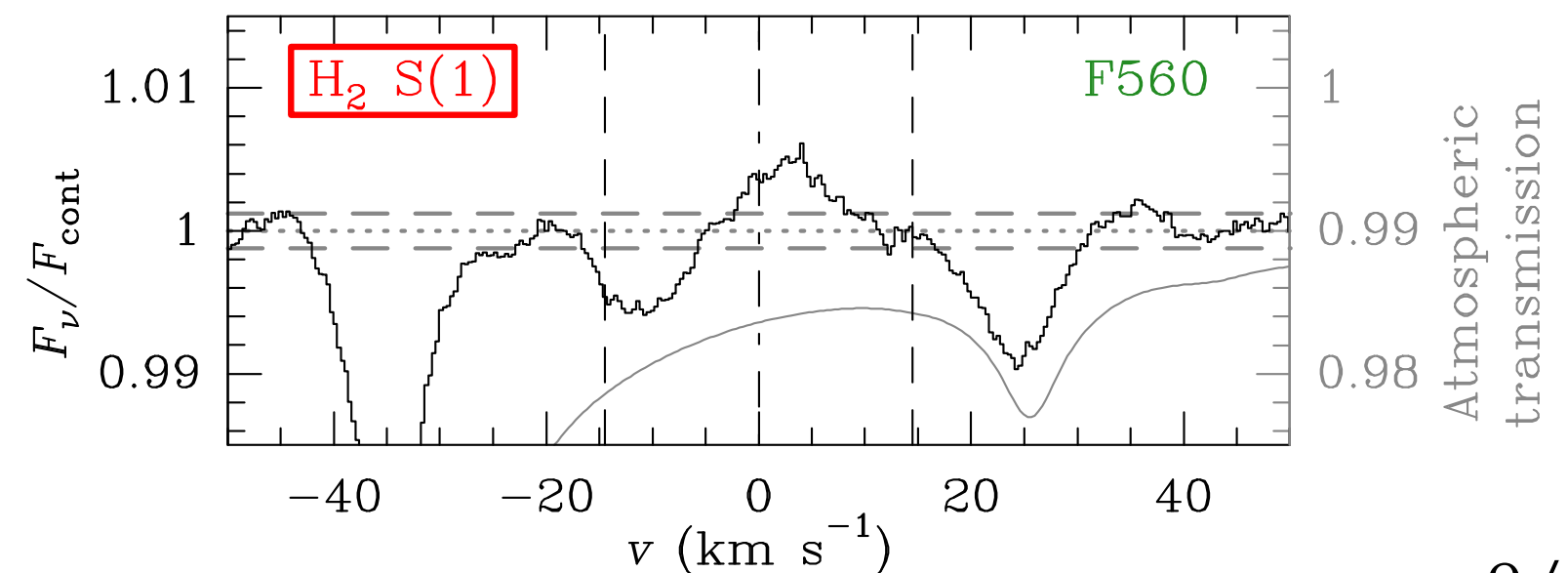
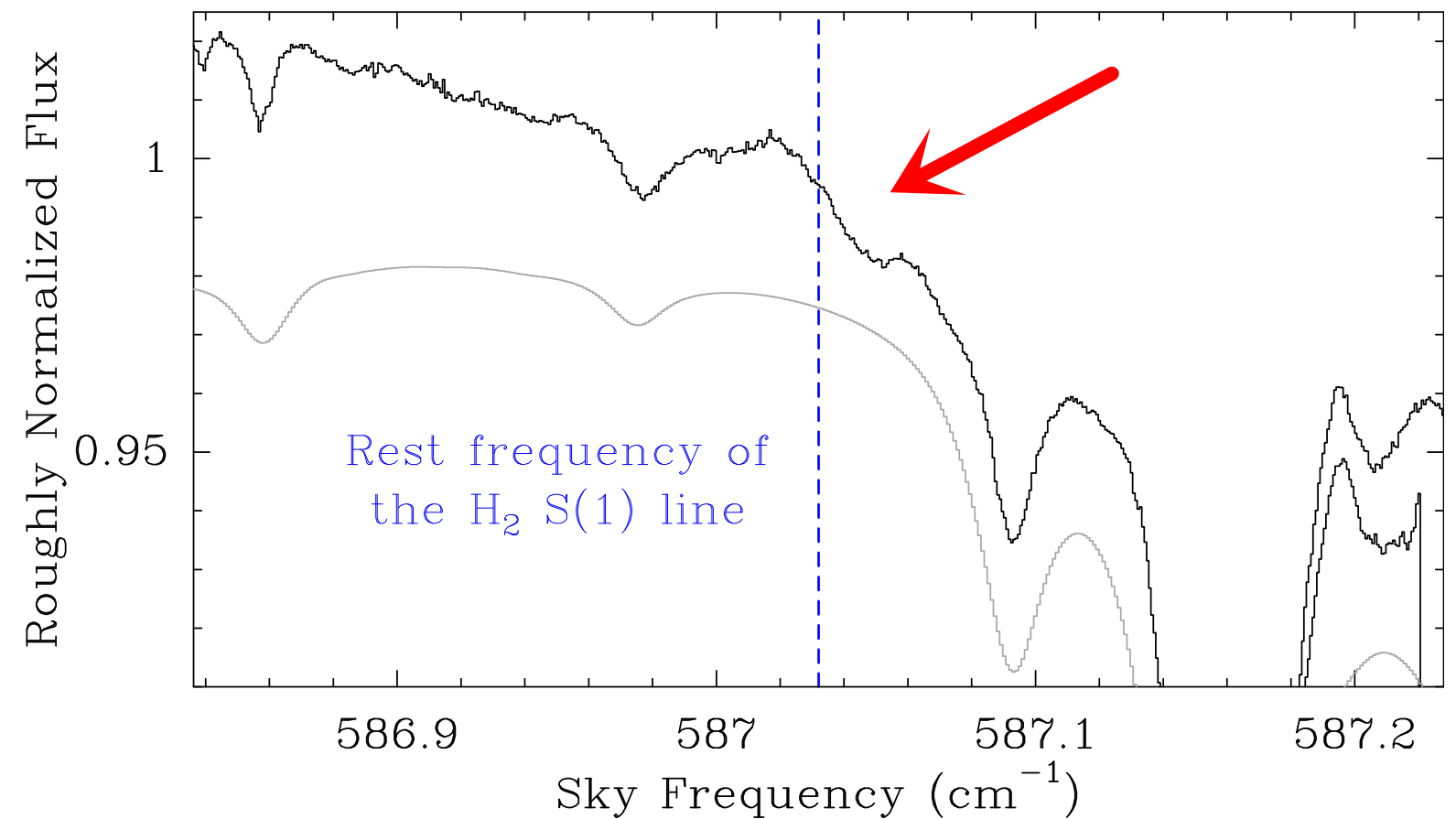
The observations were taken during flights F519, F520, and F560 that took place in 2018 and 2019 (P.I.: J. P. Fonfría; programs: 06_0172 and 07_0084):

- Observed H₂ rotational lines: S(1), S(5), and S(7)
- S(3) is strongly overlapped with an ozone band and S(*J*), with *J* even (p-H₂), are significantly weaker. None of them were observed
- Settings roughly centered at 17.04, 6.91, and 5.51 μm to observe S(1), S(5), and S(7), respectively
- EXES was configured in its High_Medium mode with the S19 slit. We nodded along the slit, which had a length of 19''
- Effective resolving power $R \simeq 88,000 - 95,000 \implies$ Spectral resolution of 3.1 – 3.4 km s⁻¹
- The sky frequencies of the S(5) and S(7) lines were not seriously overlapped with telluric features during every flight. The **Doppler shift was favorable** to observe the S(1) separated from strong telluric lines only during flight F560
- RMS noise of 0.04 %, 0.12 %, and 0.09 % of the continuum at 17.04, 6.91, and 5.51 μm

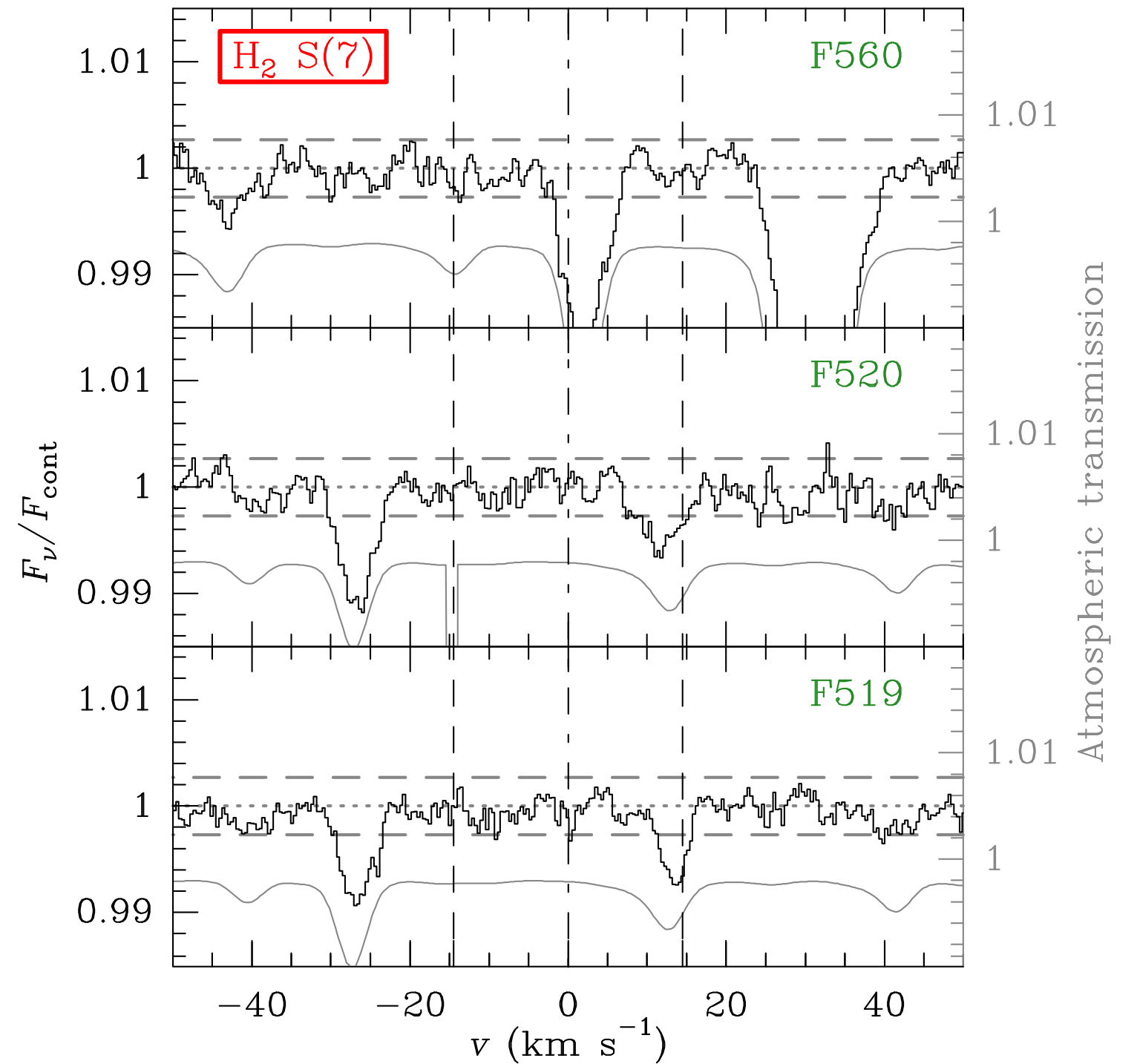
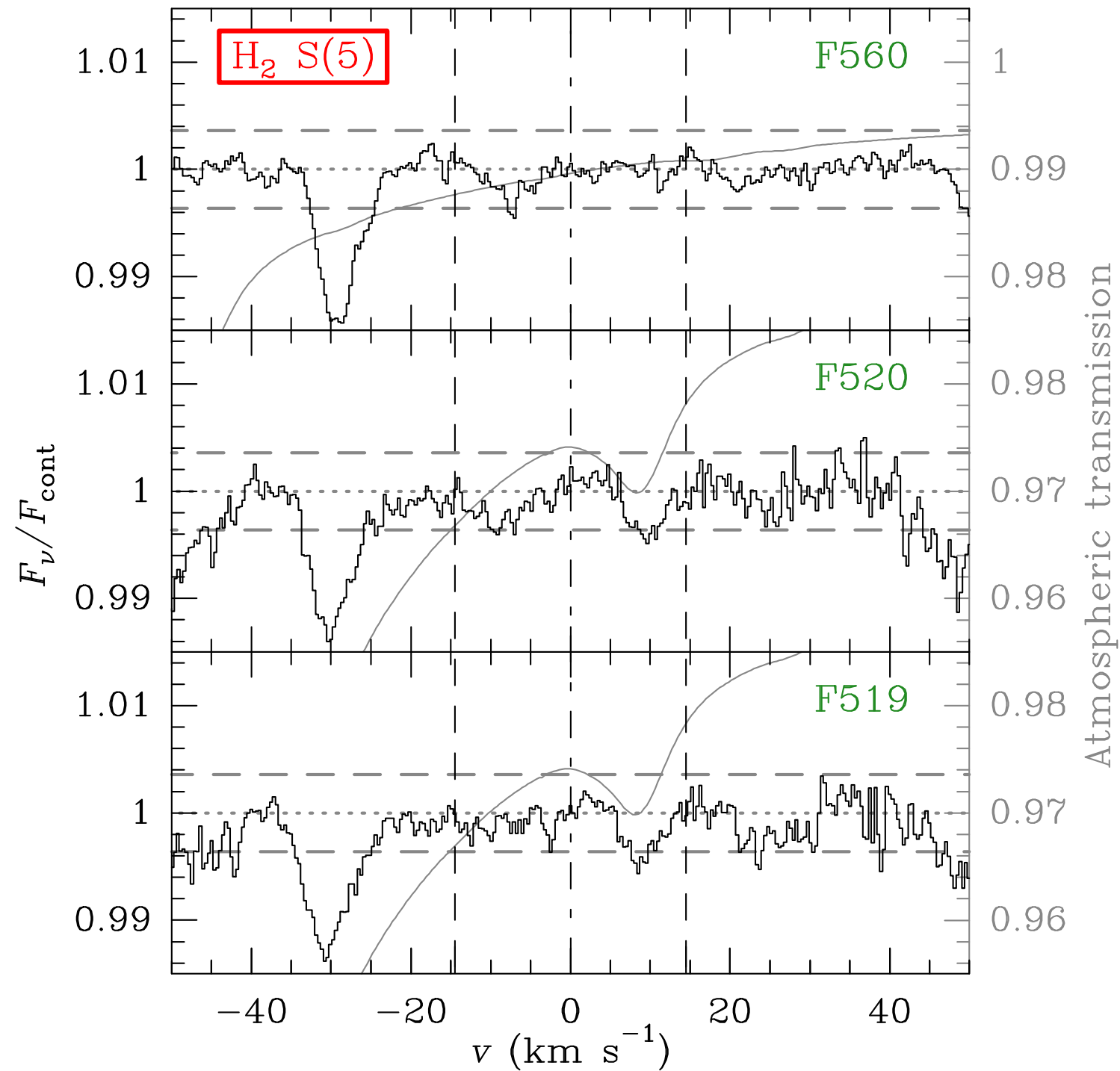
H₂ observations toward IRC+10216 with SOFIA/EXES



- Doppler shift (F560):
 $v_{\text{rad}} \simeq +8.40 \text{ km s}^{-1}$
- The rest frequency of the S(1) line is in the wing of a strong telluric feature and between two weak features
- There is a line compatible with the rest frequency and with a P-Cygni profile
- The wing of the telluric line was corrected with a cubic spline fit avoiding the creation of high frequency ripples
- The **shape and intensity** of the normalized line are **as expected** for the H₂ S(1) line and it is **at the right frequency**



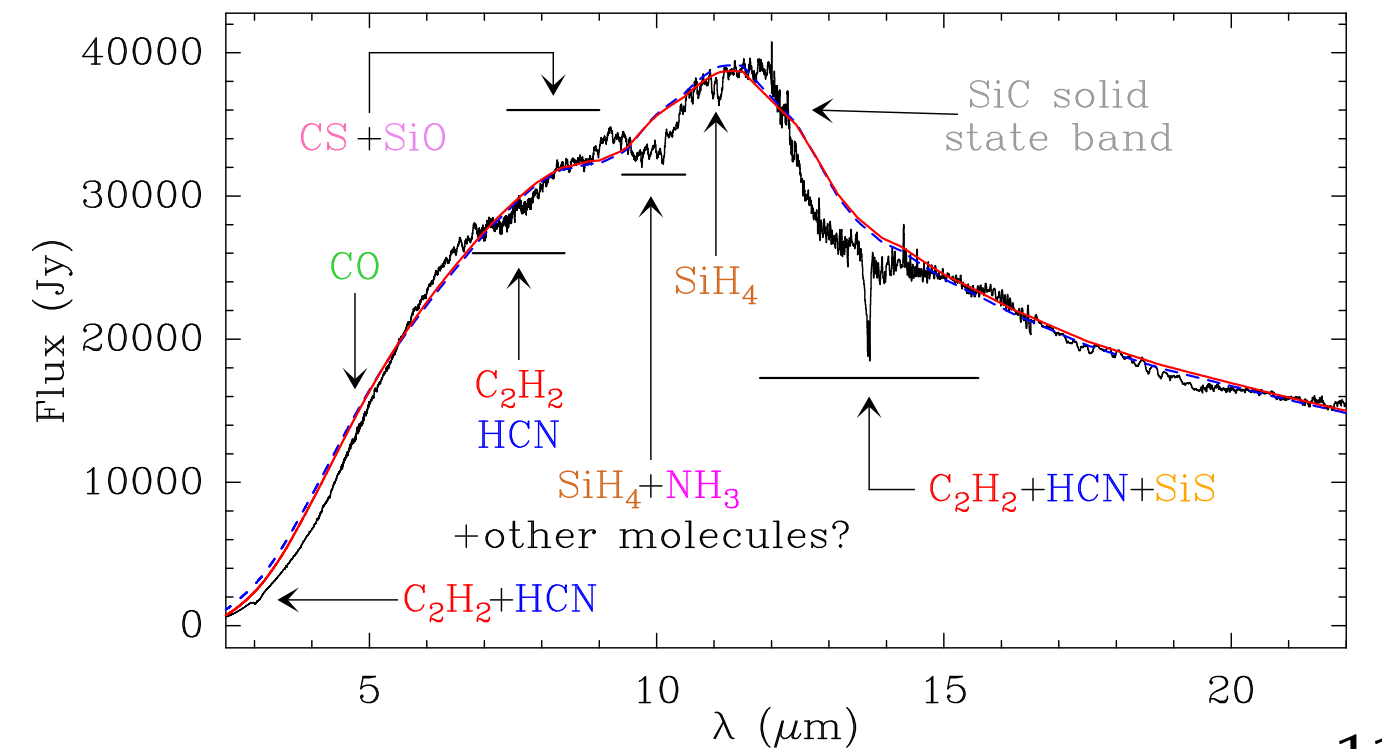
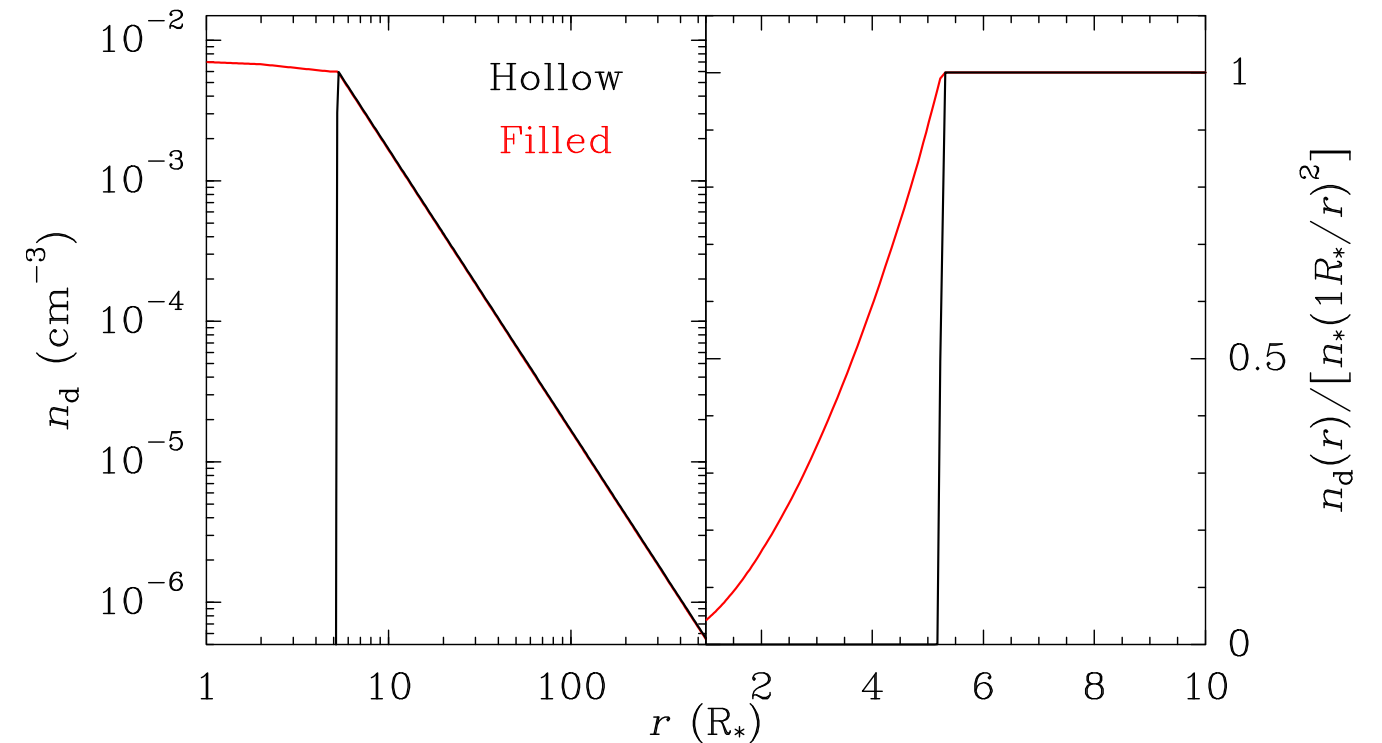
H₂ observations toward IRC+10216 with SOFIA/EXES



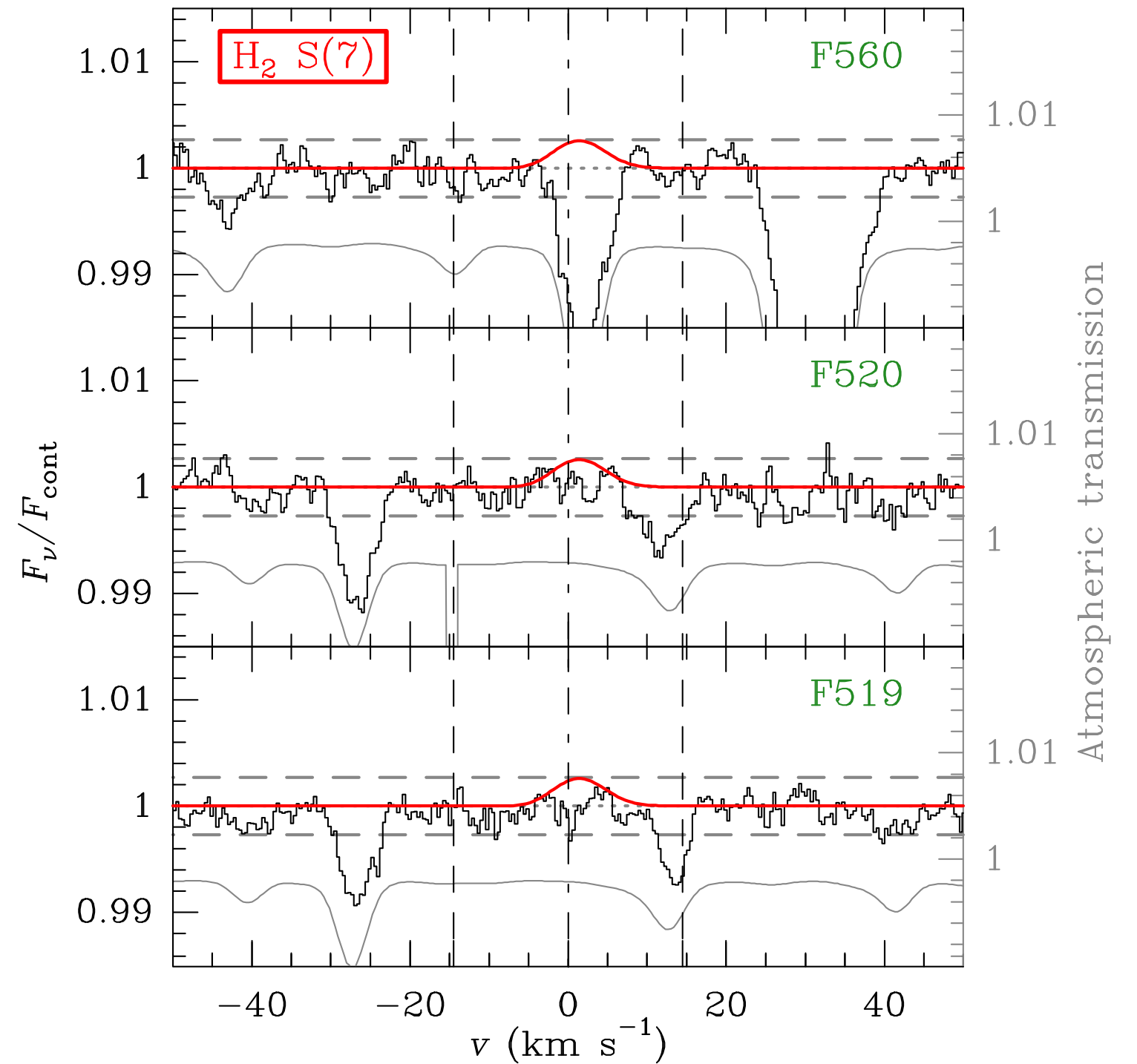
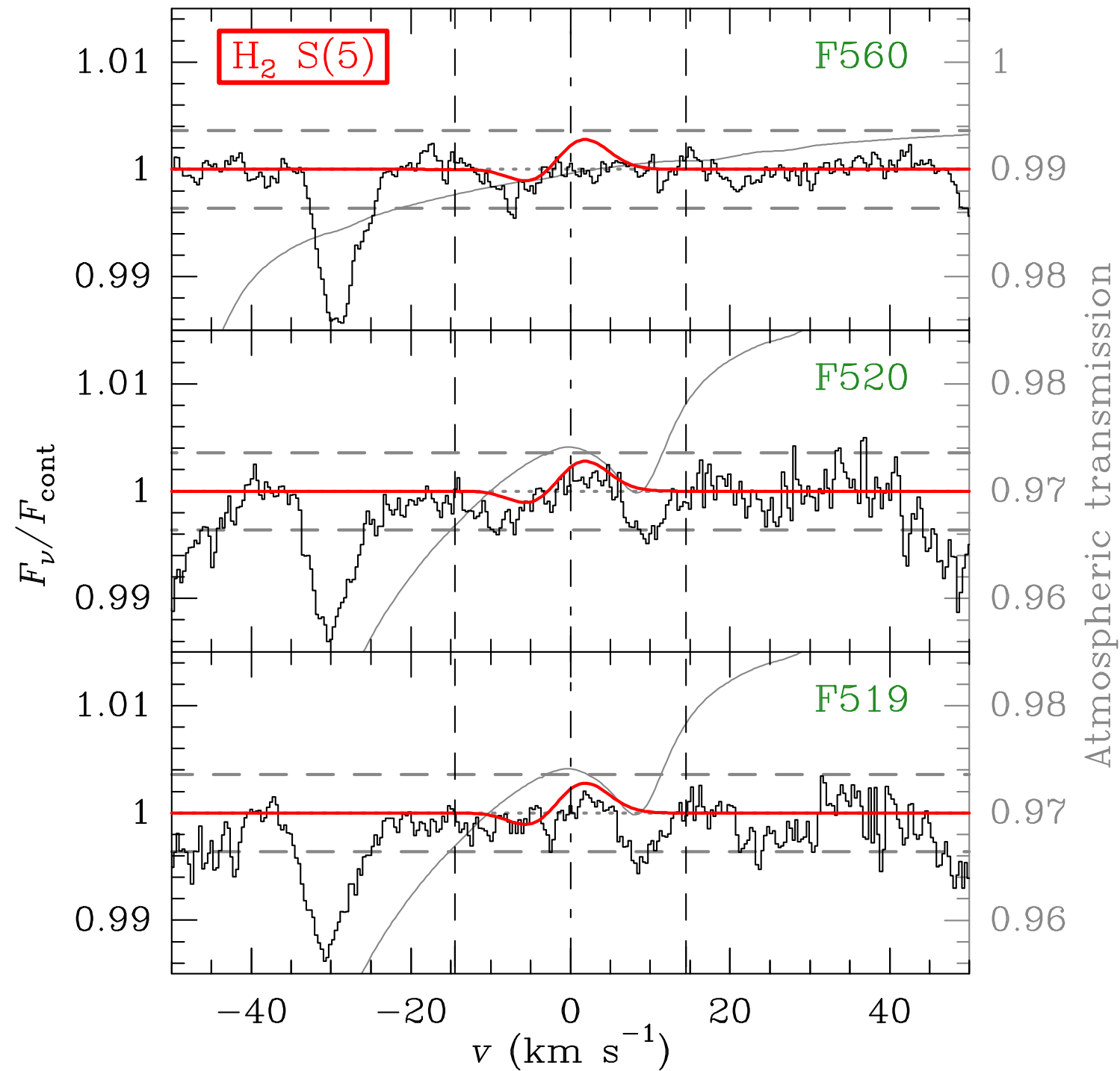
Results: Where are the high excitation H₂ rotational lines?

- Dust grain seeds are supposed to form at the photosphere but the bulk of dust forms at a few R_\star beyond
- It is possible to reproduce the ISO continuum emission (SED) of IRC+10216 with dust formed at $5R_\star$
- The S(1) line forms over the region of the CSE up to $\simeq 150R_\star$ from the star but the S(5) and S(7) lines form in the region $r = 1 - 5R_\star$
- Is it possible to add dust between the photosphere and $5R_\star$ to make S(5) and S(7) disappear without modifying the SED?

YES!

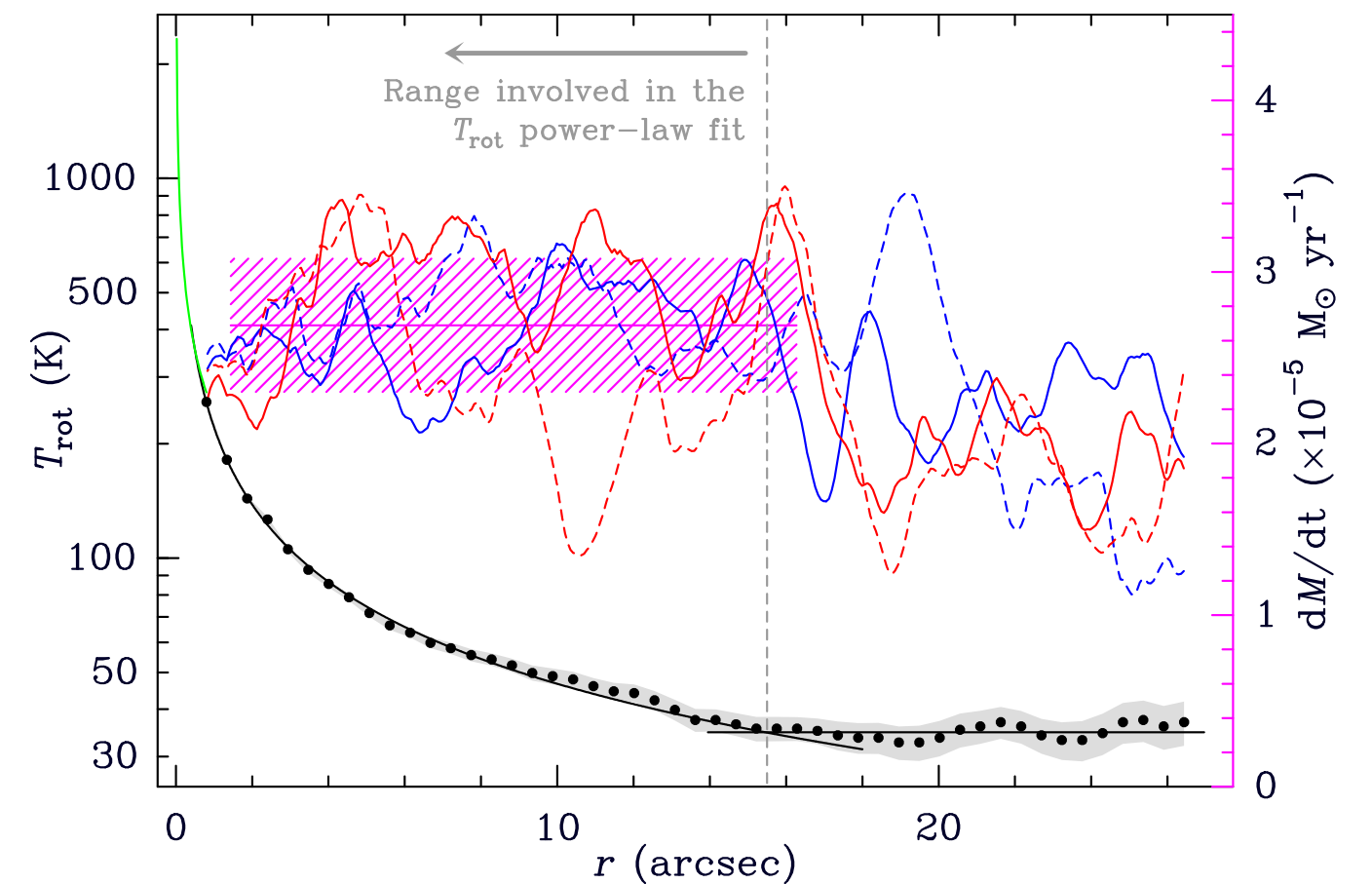
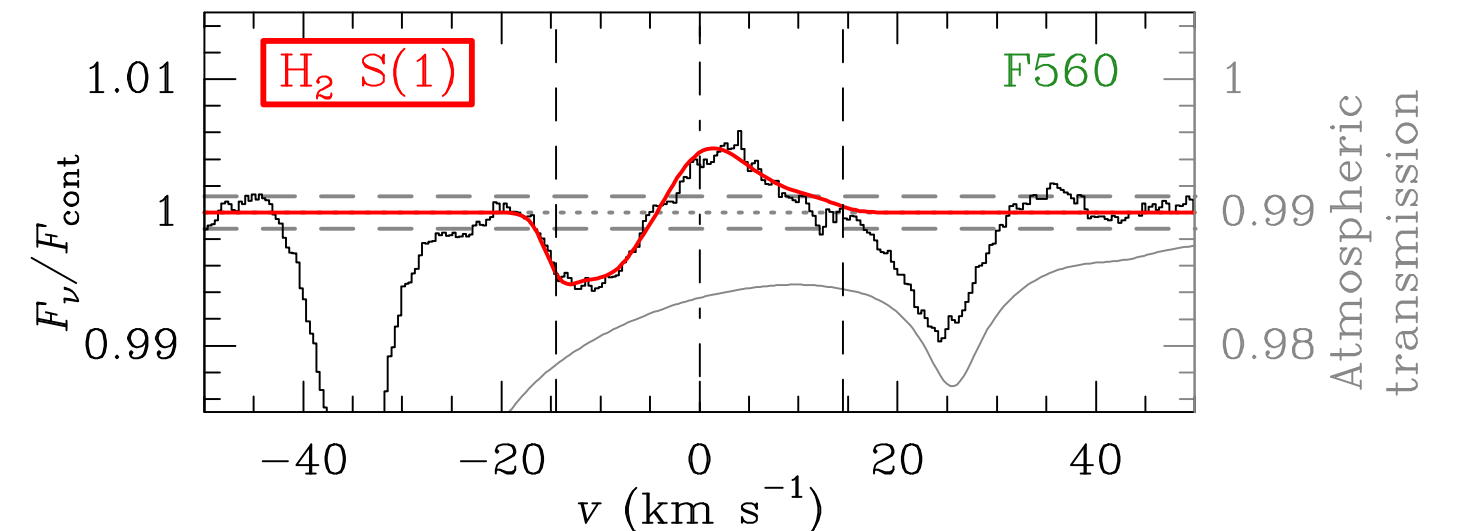


Results: Where are the high excitation H₂ rotational lines?



Results: Best fit – Mass-loss rate and CO abundance

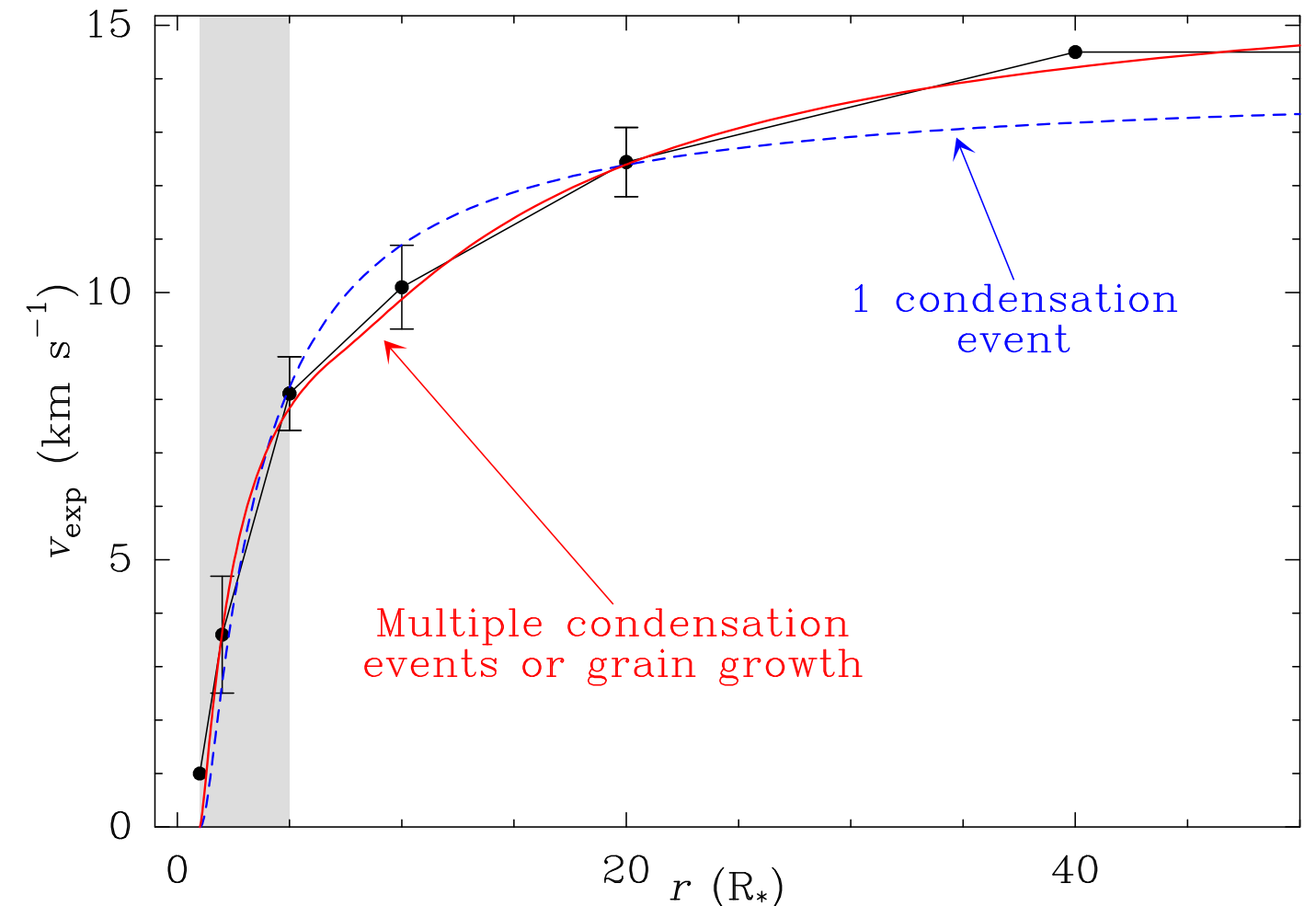
- Line fitting was done automatically (χ^2 minimization). It was repeated several times starting from different initial conditions
- The average minimum deviation was 1.5σ
- Previous mass-loss rates range from 1 to $5 \times 10^{-5} M_{\odot} \text{ yr}^{-1}$. We derive $(2.43 \pm 0.21) \times 10^{-5} M_{\odot} \text{ yr}^{-1}$
- Previous estimates of CO/H₂ range from 0.5 to 3×10^{-3} . We derive $(6.7 \pm 1.4) \times 10^{-4}$
- O/H = $(3.3 \pm 0.7) \times 10^{-4}$ and C/H = $(5.2 \pm 0.9) \times 10^{-4}$, which means [O/H] = -0.16 ± 0.10 and [C/H] = 0.28 ± 0.09 (solar values from [Asplund et al., 2009](#))
- The C/O for typical C-rich AGB stars is 1.2 – 2.0 ([Winters et al., 1994](#)). We derive $C/O > 1.5 \pm 0.4$



(Guélin et al. 2018)

Results: Best fit – Gas expansion velocity

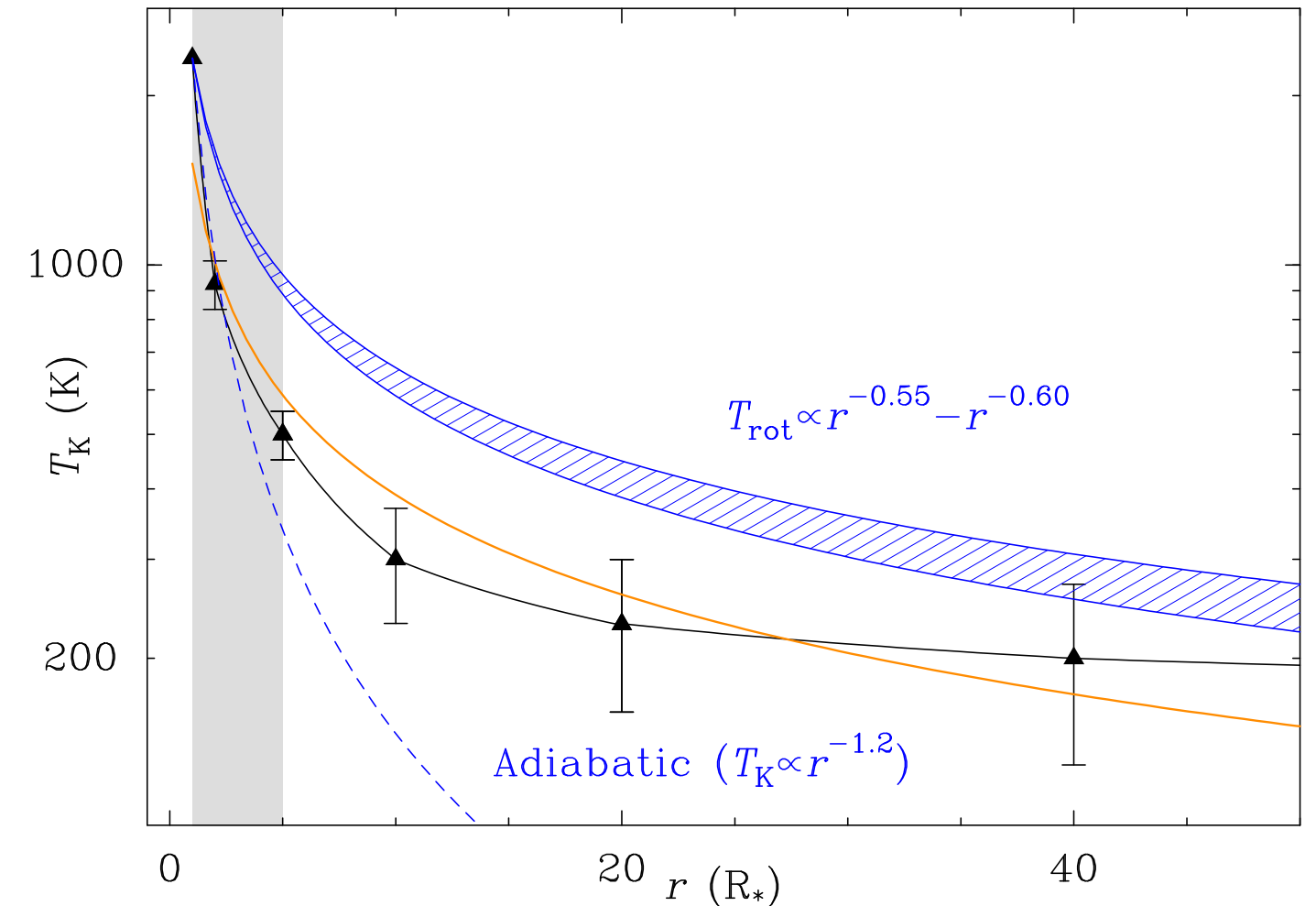
- Expansion velocity separates the contributions of layers expanding at different velocities
- The physical conditions at several distances from the star were derived from the fit to the S(1) line
- Gas seems to be **accelerated from the photosphere** \implies Dust forms at the photosphere
- The terminal expansion velocity is suggested to be reached at $\simeq 40R_*$. However, the S(1) line is not sensitive to this parameter as it is produced by gas up to $\simeq 150R_*$. Previous estimates are more reliable (e.g., [Fonfría et al., 2008, 2015](#); [Agúndez et al., 2012](#))
- v_{exp} cannot be explained by dust suddenly created at a given r and accelerated afterwards. Continuous dust **grain growth** or **multiple condensation** events are needed



The parameters in the shaded region may be more uncertain than expected owing to our poor knowledge about dust at $r \lesssim 5R_$*

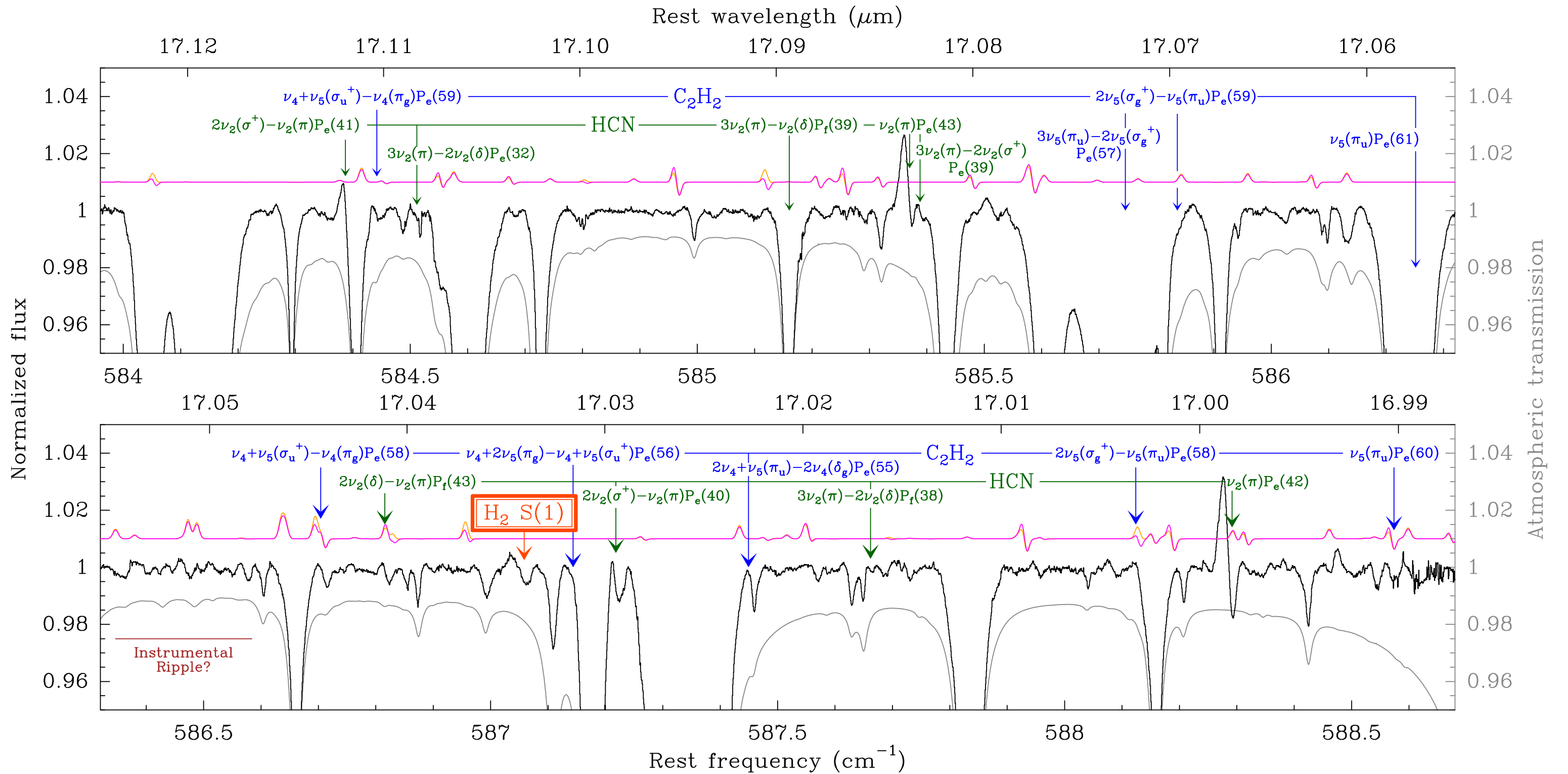
Results: Best fit – Kinetic temperature

- T_K was fixed to the effective temperature of the star ($\simeq 2300$ K; [Ridgway & Keady 1988](#))
- Fast decrease close to the photosphere is predicted by numerical calculations of Bladh & Freytag ([Freytag et al., 2017](#); [Agúndez et al., 2020](#))
- Beyond $5R_*$, T_K becomes less steeper
- Approximately, T_K can be described with the power-law $\propto r^{-0.6}$ (e.g., [Agúndez et al., 2012](#); [De Beck et al., 2012](#))
- Beyond $\simeq 60R_*$ we adopt the T_K derived by [Guélin et al. \(2018\)](#): $T_K = 256.9(40R_*/r)^{0.68}$ K
- Previous estimates of T_K throughout the acceleration zone are significantly higher than our results suggest. These differences are likely related to the effect of the ro-vibrational transitions on the rotational temperature owing to the strong infrared radiation field



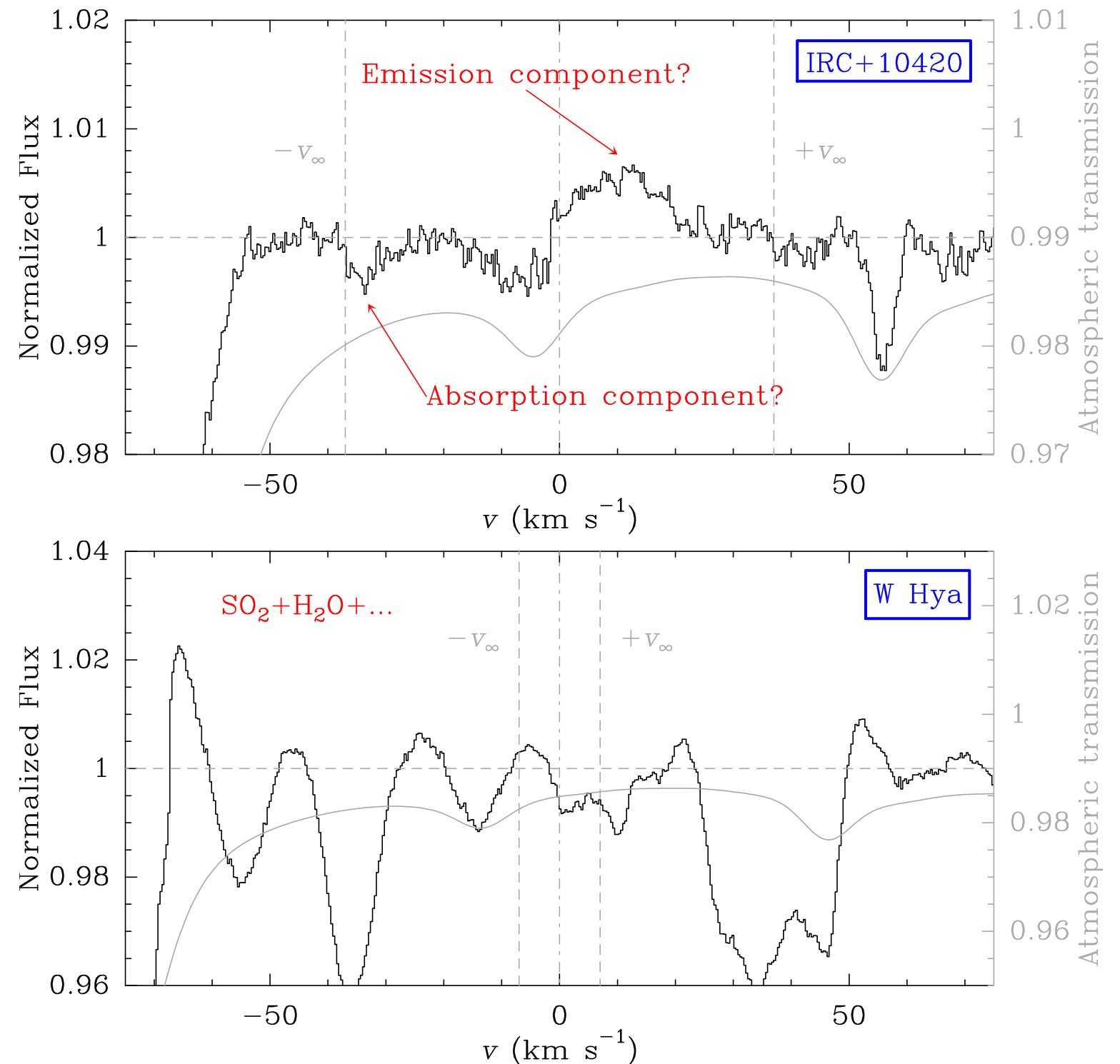
The parameters in the shaded region may be more uncertain than expected owing to our poor knowledge about dust at $r \lesssim 5R_$*

Results: Line identification at 17 μm



On-going work: (Very) preliminary results

- New proposal for Cycle 10: survey of AGB, RSG, and YHG stars to observe the H₂ rotational lines S(1) and S(5)
- Two sources observed: IRC+10420 (YHG; S(1) line) and W Hya (AGB; S(1) and S(5) lines)
- **IRC+10420**: the S(1) line **might** be strong enough to be detected. Possible emission and absorption components
- **W Hya**: the spectral range around the S(1) is crowded with lines. Some of them are of SO₂ and H₂O but there still are unidentified lines. The range around the S(5) line remains to be explored



Conclusions and Final remarks

- A rotational line of H₂ was detected for first time in an AGB star (IRC+10216) thanks to the ability of SOFIA to avoid most of the atmosphere and the high capabilities of EXES.
- The H₂ lines (S(1), S(5), and S(7)) were observed using three settings at 17, 6.9, and 5.5 μm. The rms noise was very low for the three settings, particularly at 17 μm (0.04 % of the continuum). The resolving power ranged from 88,000 to 95,000, providing us with spectral resolutions of $\simeq 3.1 - 3.4 \text{ km s}^{-1}$.
- The S(1) line was detected with a good S/N $\simeq 12$. The S(5) and S(7) lines were not detected. We interpret the absence of these lines as an effect of dust opacity, which is higher than expected close to the star. This opacity has a limited impact on the SED.
- We derive a mass-loss rate of $(2.43 \pm 0.21) \times 10^{-5} M_{\odot} \text{ yr}^{-1}$, the CO abundance relative to H₂ is $(6.7 \pm 1.4) \times 10^{-4}$, and the C/O ratio is $> 1.5 \pm 0.4$.
- The gas is accelerated from the photosphere. The velocity profile is compatible with dust grain growth over several stellar radii or multiple sudden condensations.
- The kinetic temperature decreases about 1500 K in the first $5R_{\star}$ and only a few hundreds of K over the next $50R_{\star}$. Approximately, $T_{\text{K}} \propto r^{-0.6}$ throughout the acceleration zone.
- We estimate the abundance of HNC is $\lesssim 0.5 - 1.0 \times 10^{-7}$.