Spatial Variation in Temperature and Density in the IC 63 PDR from H_2 Spectroscopy

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New collabs.: Kyle Kaplan (SSC), Lars Bonne (SSC), Robert Minchin (NRAO), L N Tram (Max Planck) +…

SOFIA Teletalk

02/15/2023

The Astrophysical Journal, 923:107, 2021

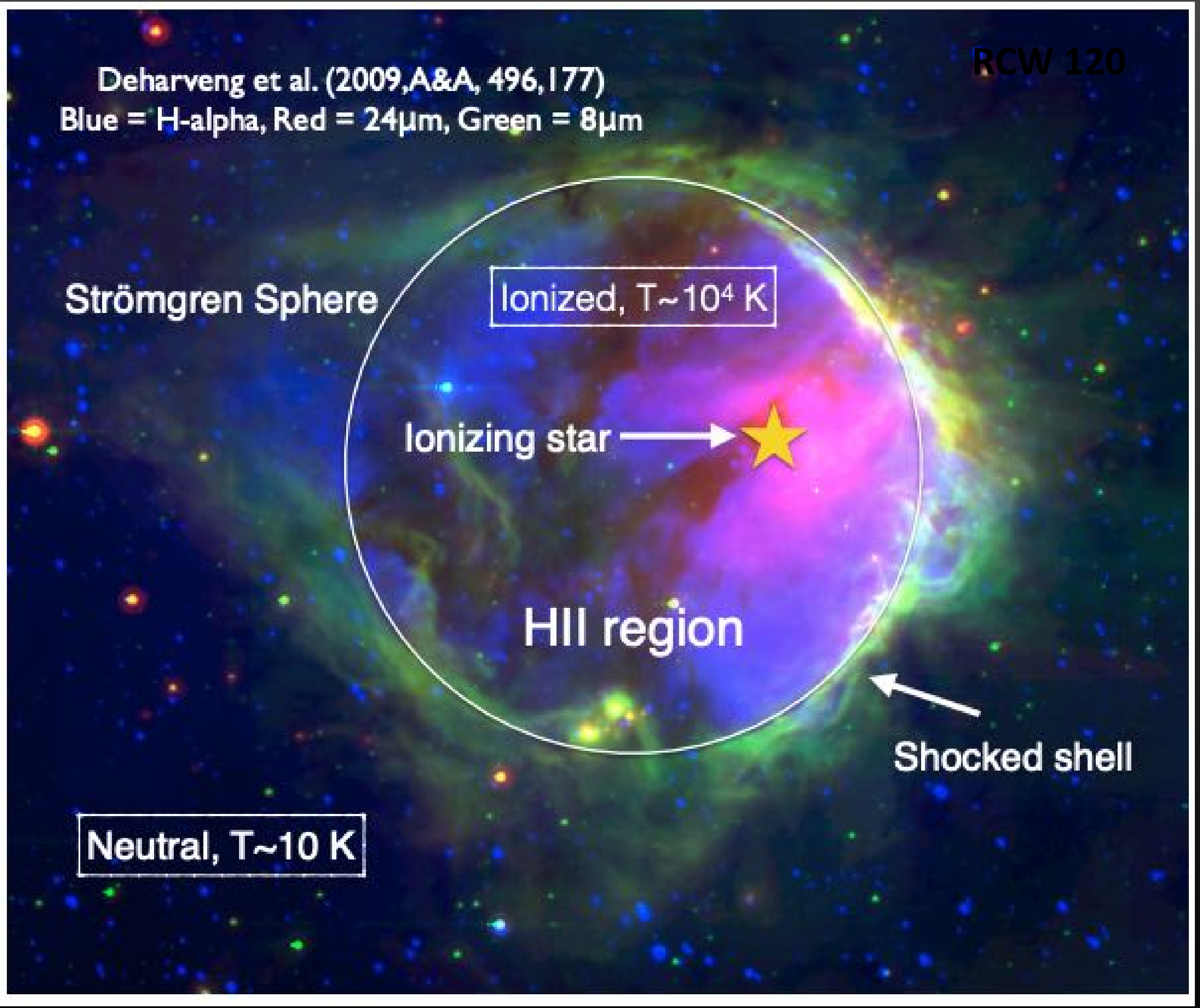
I had the best time of my academic life with SOFIA…….

Outline:

- Introduction on PDRs
- Our motivation towards PDR IC63
- EXES observations and data reduction
- Spectral lines and construction of rotation diagram
- PDR modeling
- Summary

Expanding HII regions

- Photoionization heats gas from 10-100K up to $\approx 10^4$ K.
- Creates overpressurised bubble.
- This drives expansion (usually supersonic), sweeps up dense shell.
- Carves out pillars, blisters, globules, etc.

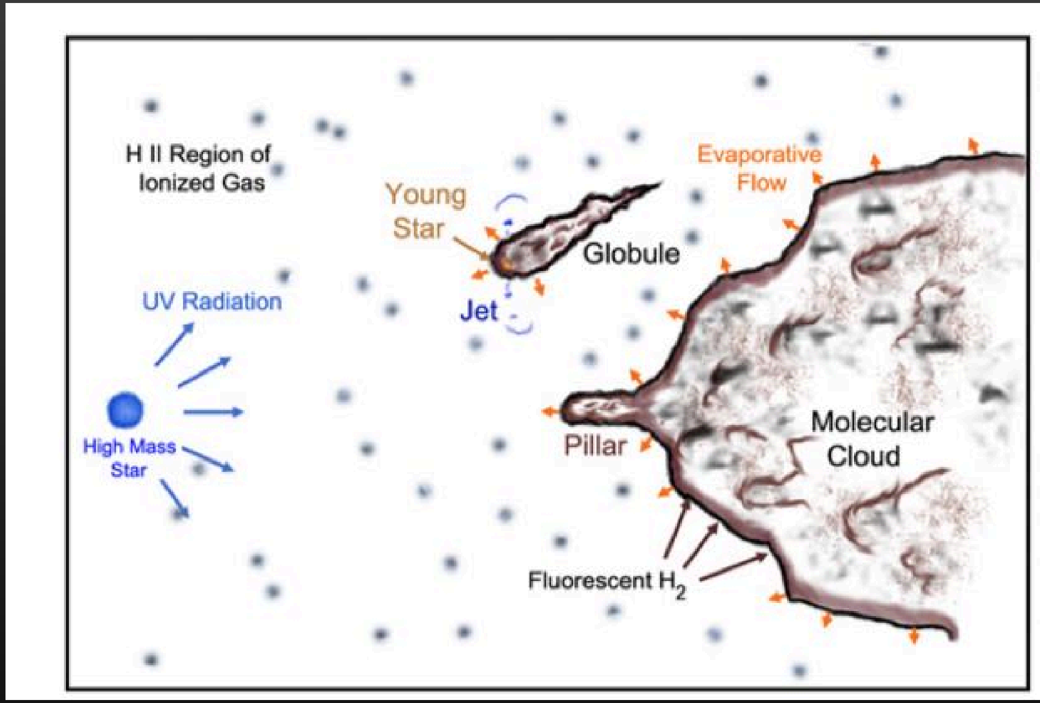


Credit: pic from Jonathan Mackey's slides, 15 February 2017, "6 years of ISM-SPP - what have we learned?", Cologne.

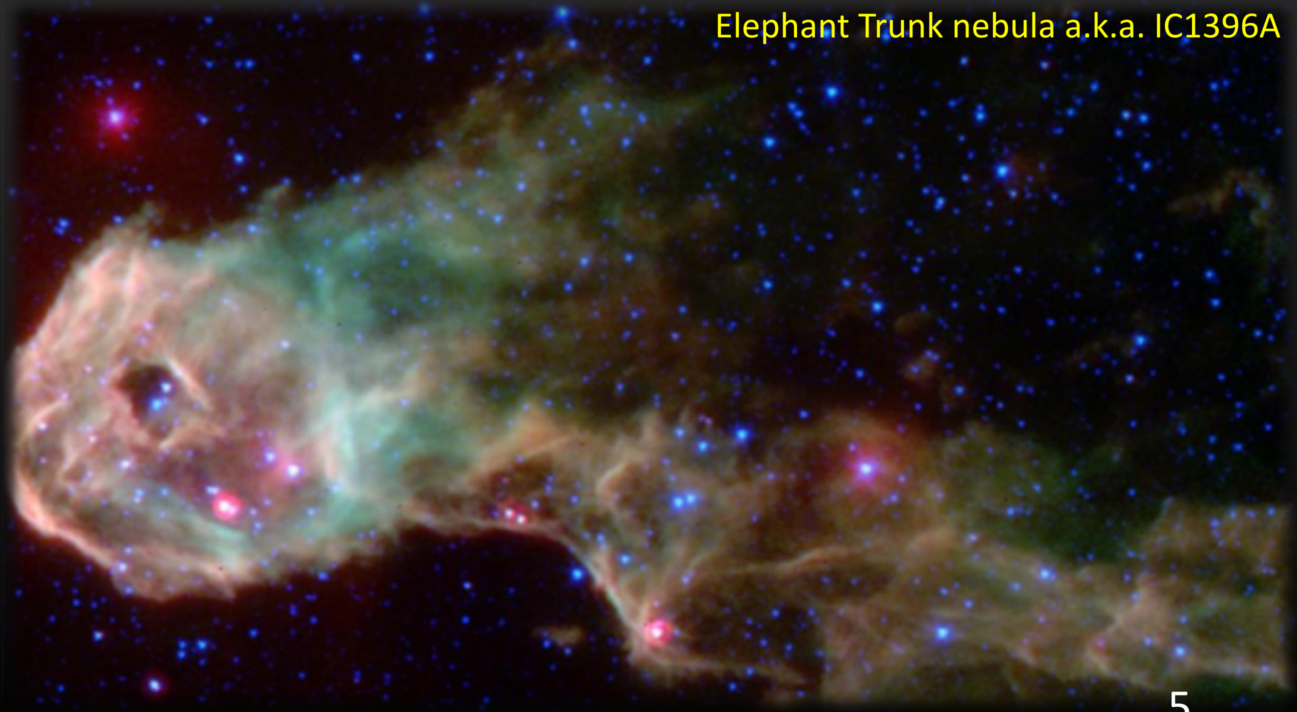
PDR geometry

Pillars: a column-like shape and a physical connection to the gas reservoir of the molecular cloud.

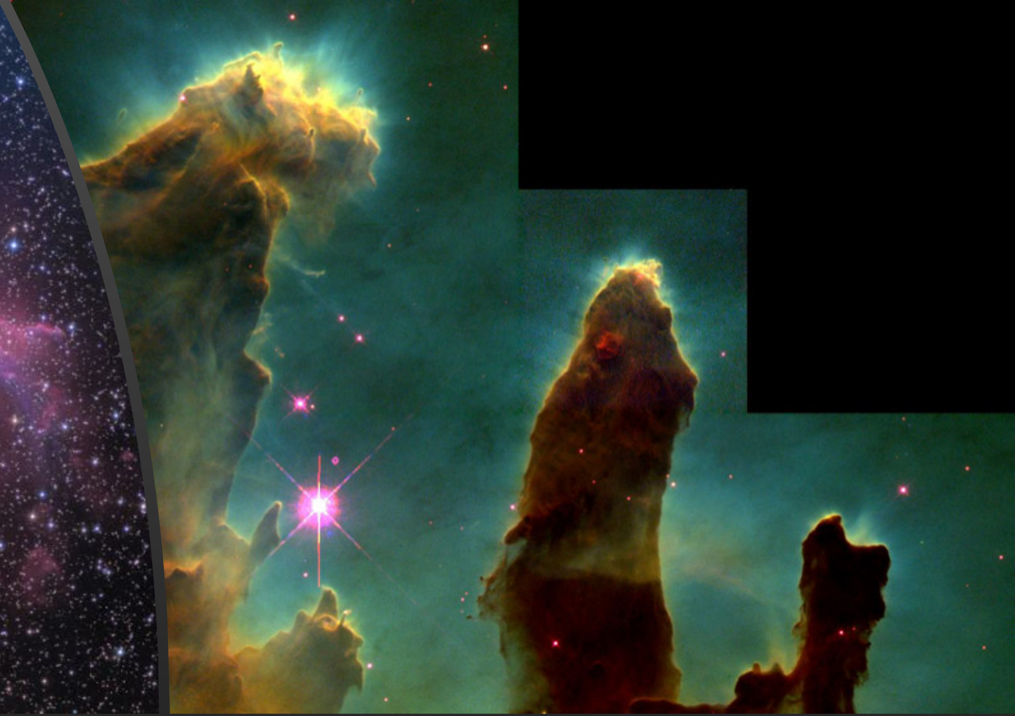
Globules: a head-tail structure pointing toward the illuminating source and isolated to the molecular cloud.

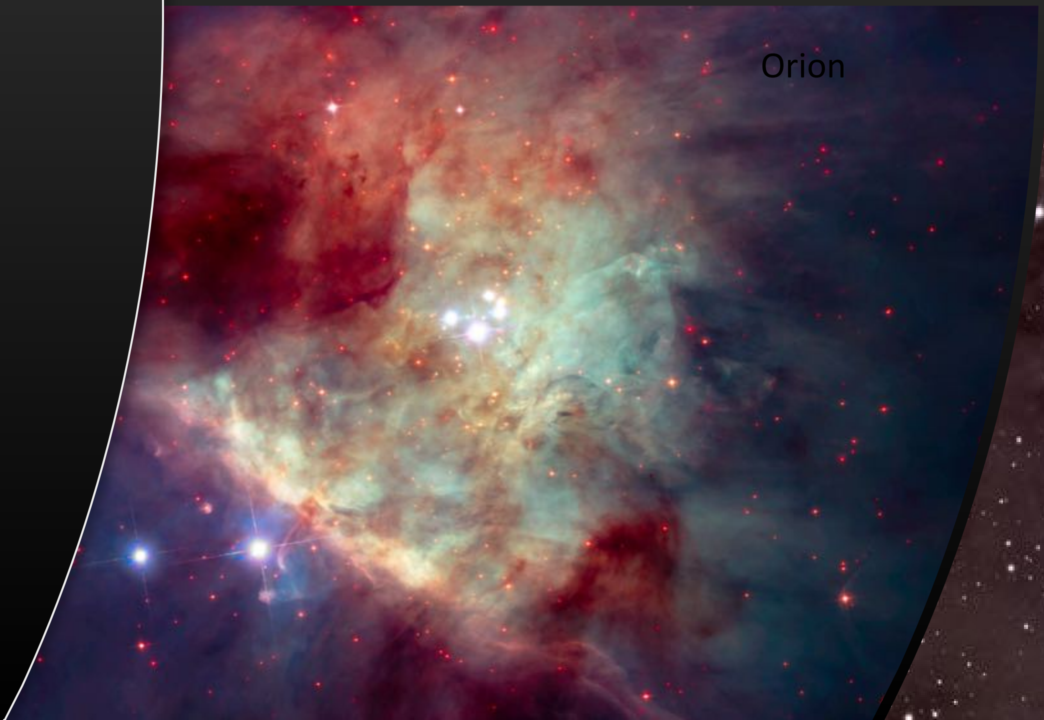


Sketch of a photodissociation region (PDR)
(Hartigan et al. 2015)



- ***Some examples of PDRs***





Credits: HST, NASA, ESA, APOD

Anatomy of Photodissociation Regions (PDRs)

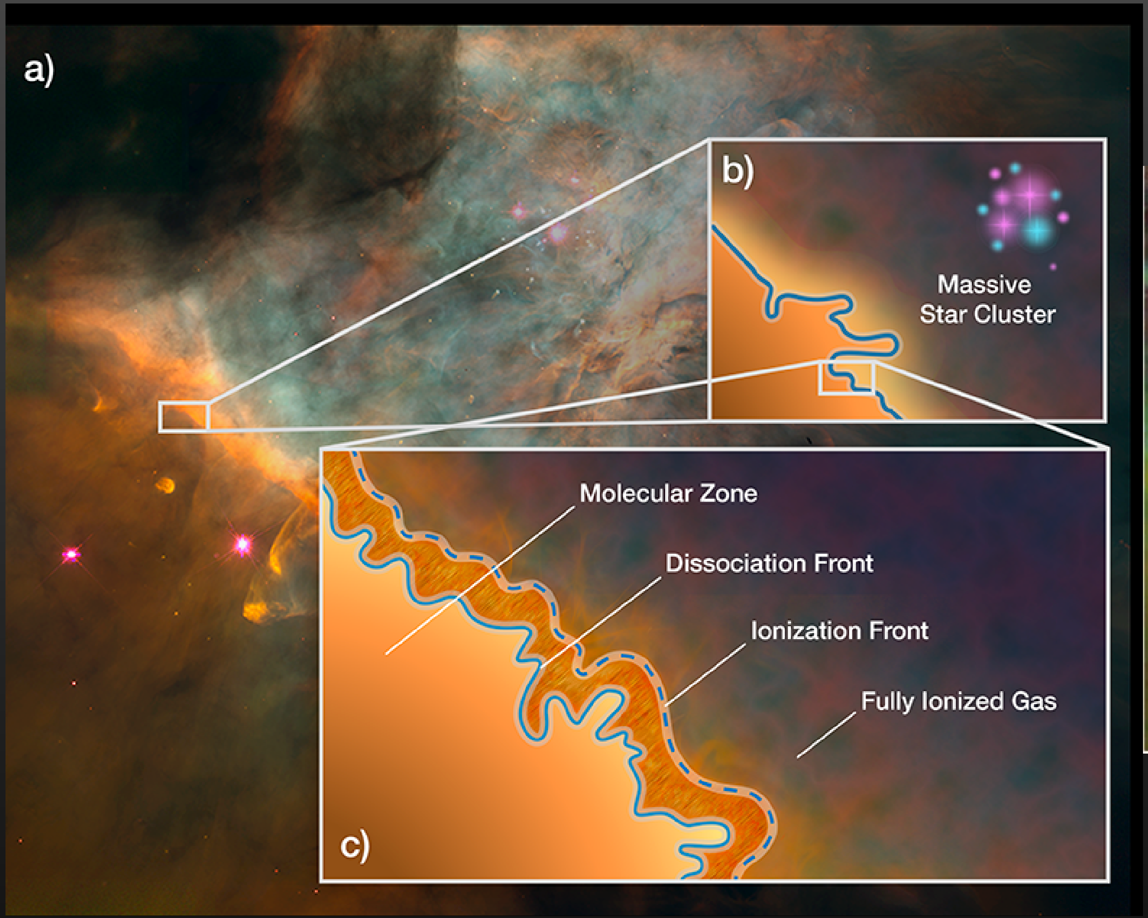
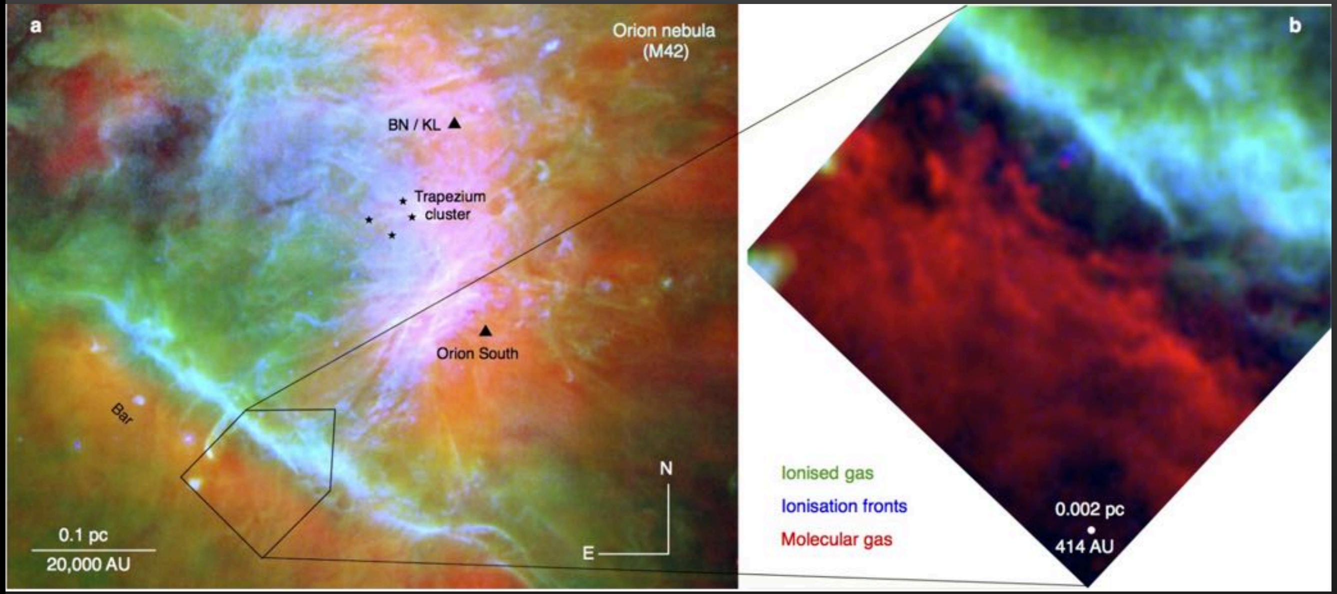


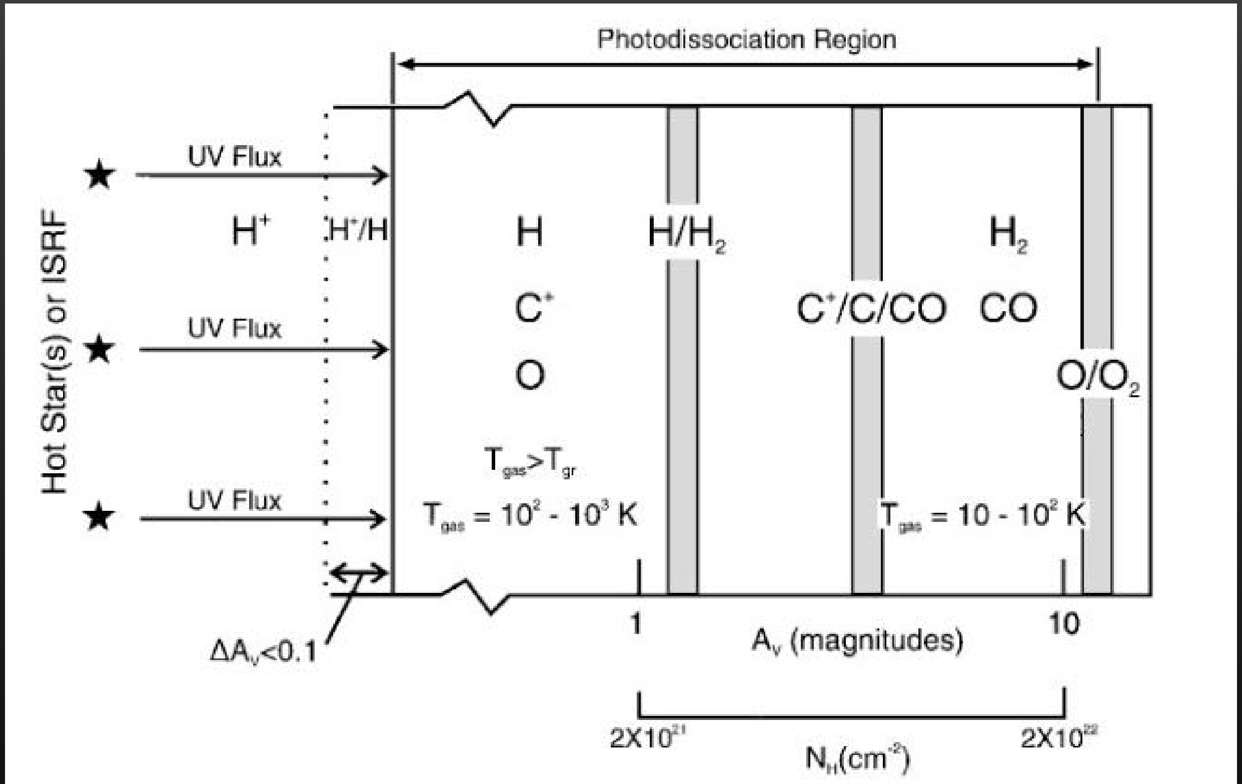
ILLUSTRATION: NASA, ESA, CSA, Jason Champion (CNRS), Pam Jeffries (STScI), PDRs4ALL ERS Team



Goicoechea et al., 2016

Goicoechea et al. 2016, *Nature*

PDR schematics



Hollenback & Tielens (1997), ARA&A, 35:179–215

- The PDR is illuminated from one side and extends from the predominantly atomic surface region to the point where O_2 is not appreciably photodissociated (≃10 visual magnitude).
- The PDR includes gas where hydrogen is mainly H_2 and where carbon is mostly CO.
- Large columns of warm O, C, C^+, and CO and vibrationally excited H_2 are produced in the PDR.
- The gas temperature T_{gas} generally exceeds the dust temperature T_{dust} in the surface layer.

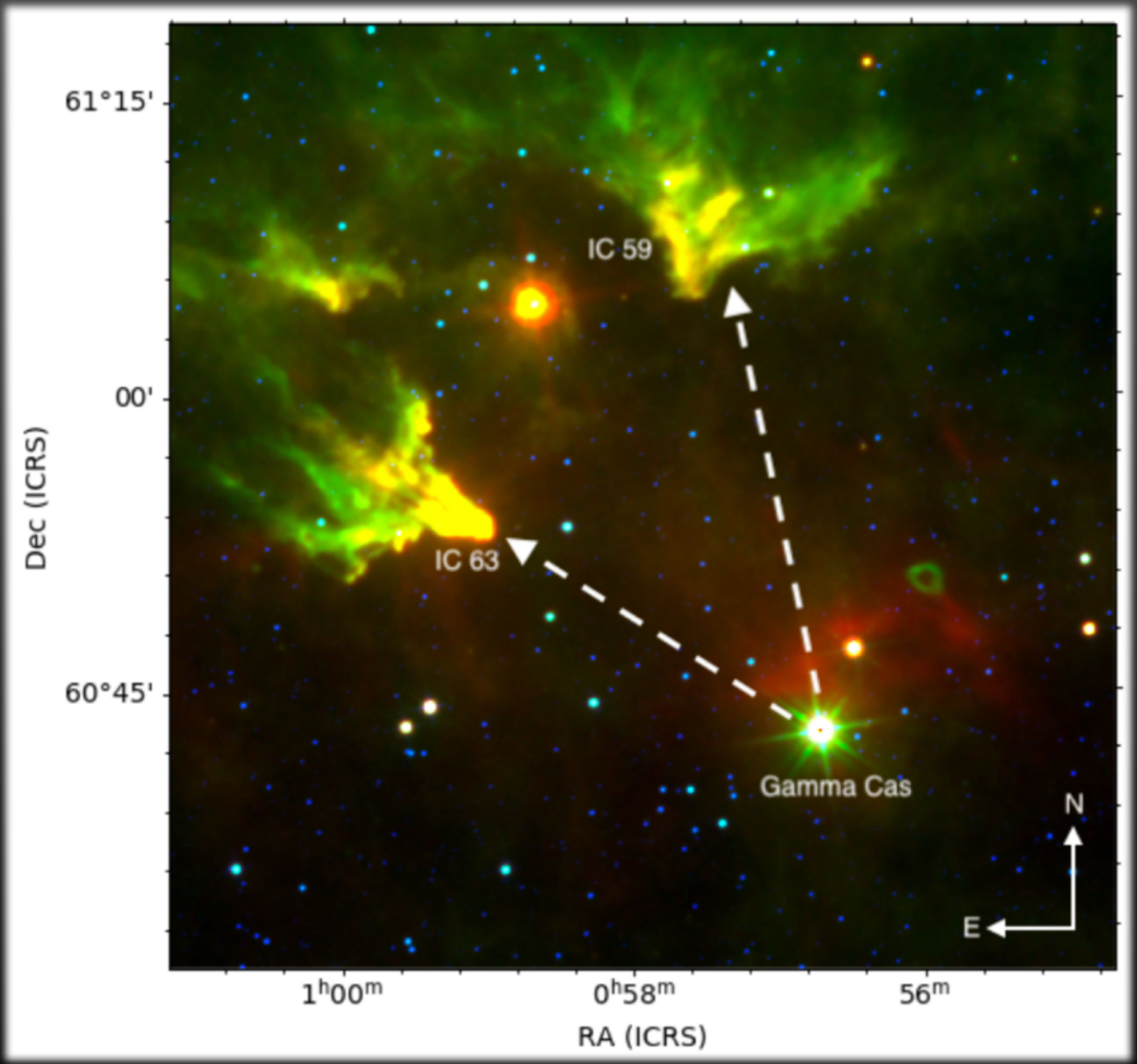
This work

System under investigation: Sh 185 HII region

- IC59 and IC63 reflection nebulae illuminated by FUV radiation from B0.5IVe star γ-Cas

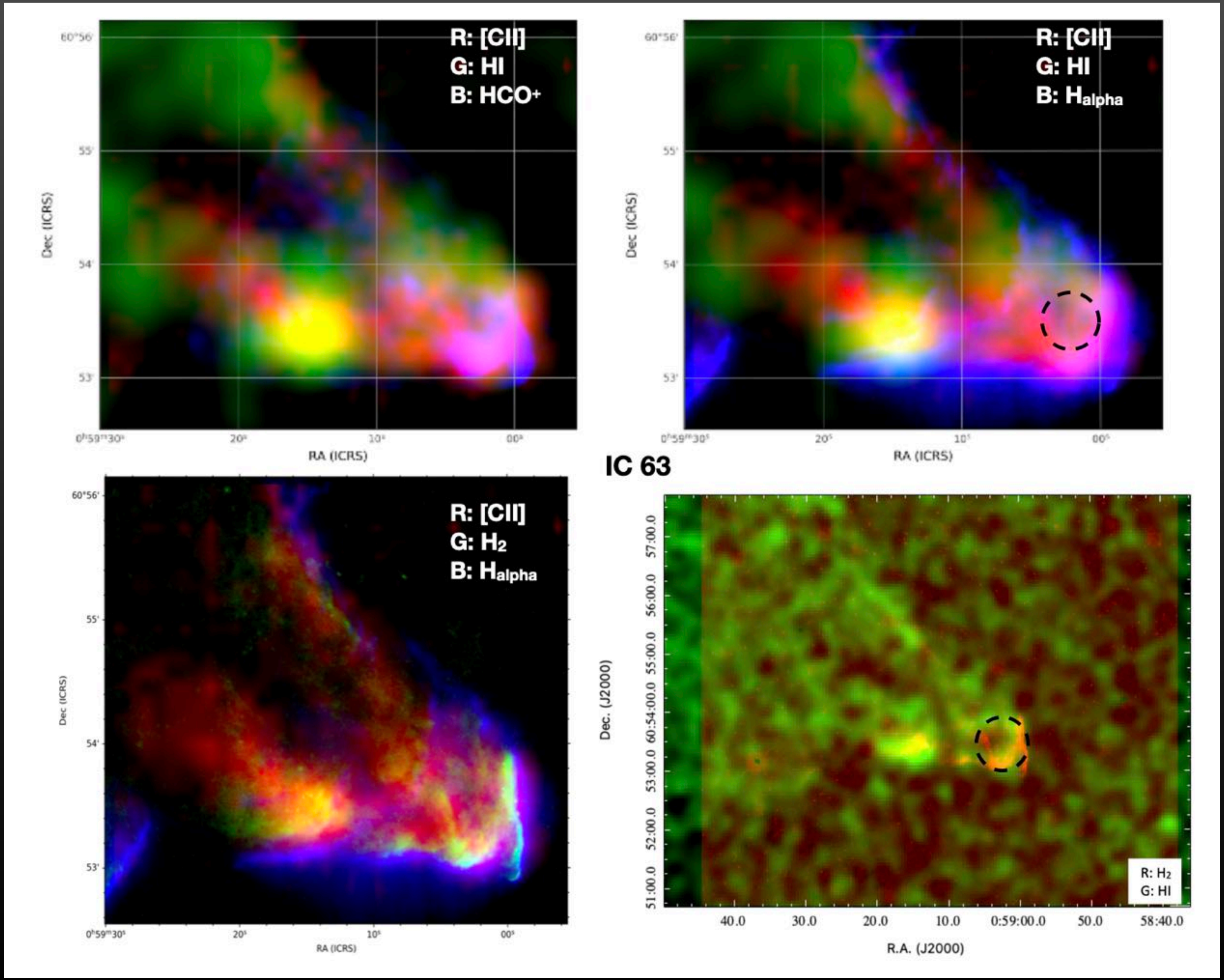
- Closest HII region with d~200 pc

- Projected distance IC63 from γ-Cas is ~1.5 pc



RGB image made from WISE W1 (3.4µm) in blue, W3 (12µm) in green, and W4 (22µm) in red (credit: Caputo et al. , in revision).

Ancillary data on IC63

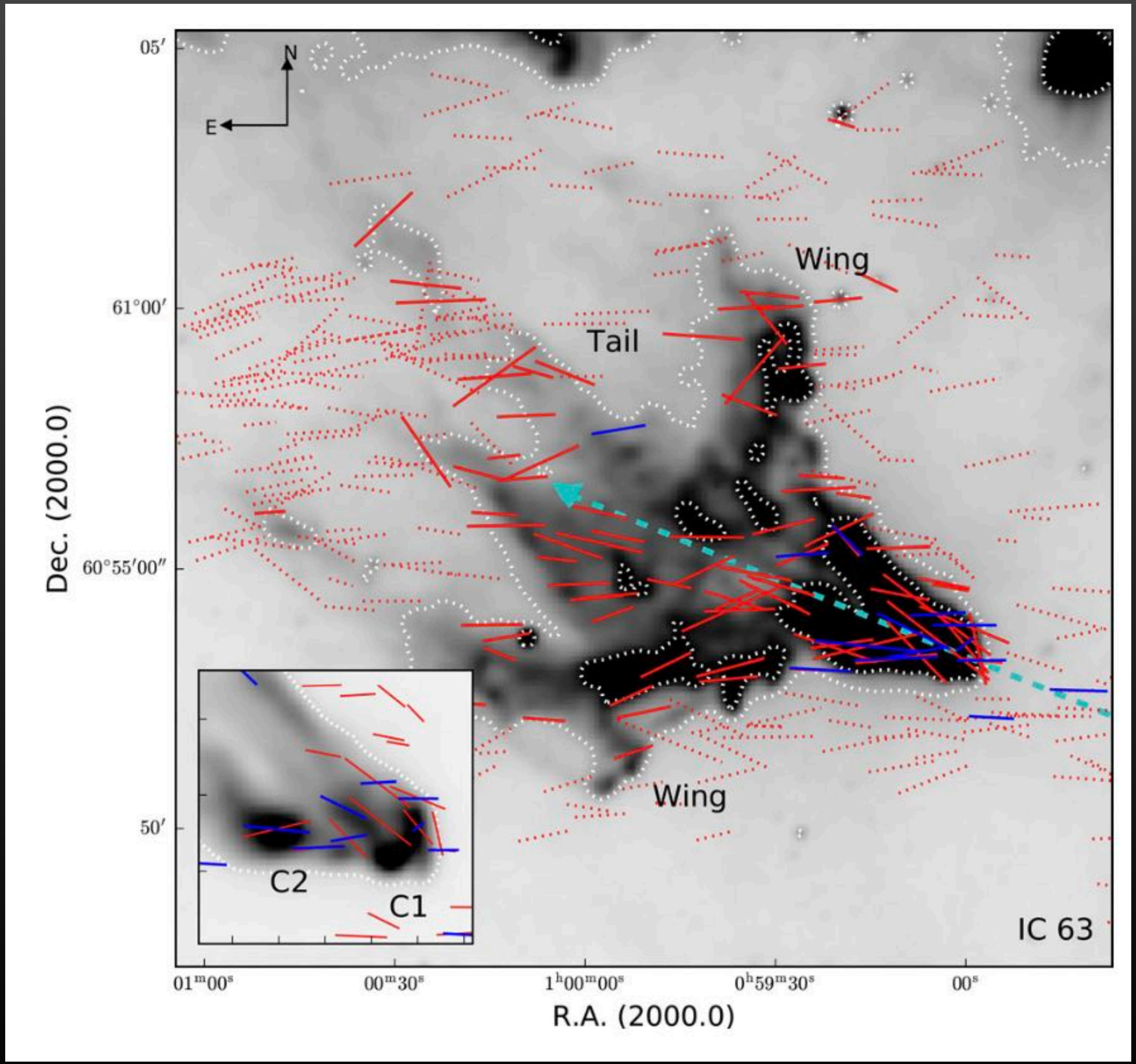


Andersson et al. (2013)

Caputo et al. (2023; under rev.)

Bonne et al. (2023; submitted)

Magnetic fields via. Optical polarization observations



Soam et al. (2017b)

Red solid lines: The vectors inside the outermost contour are shown using thick red lines.

Red dashed lines: The ones outside this contour

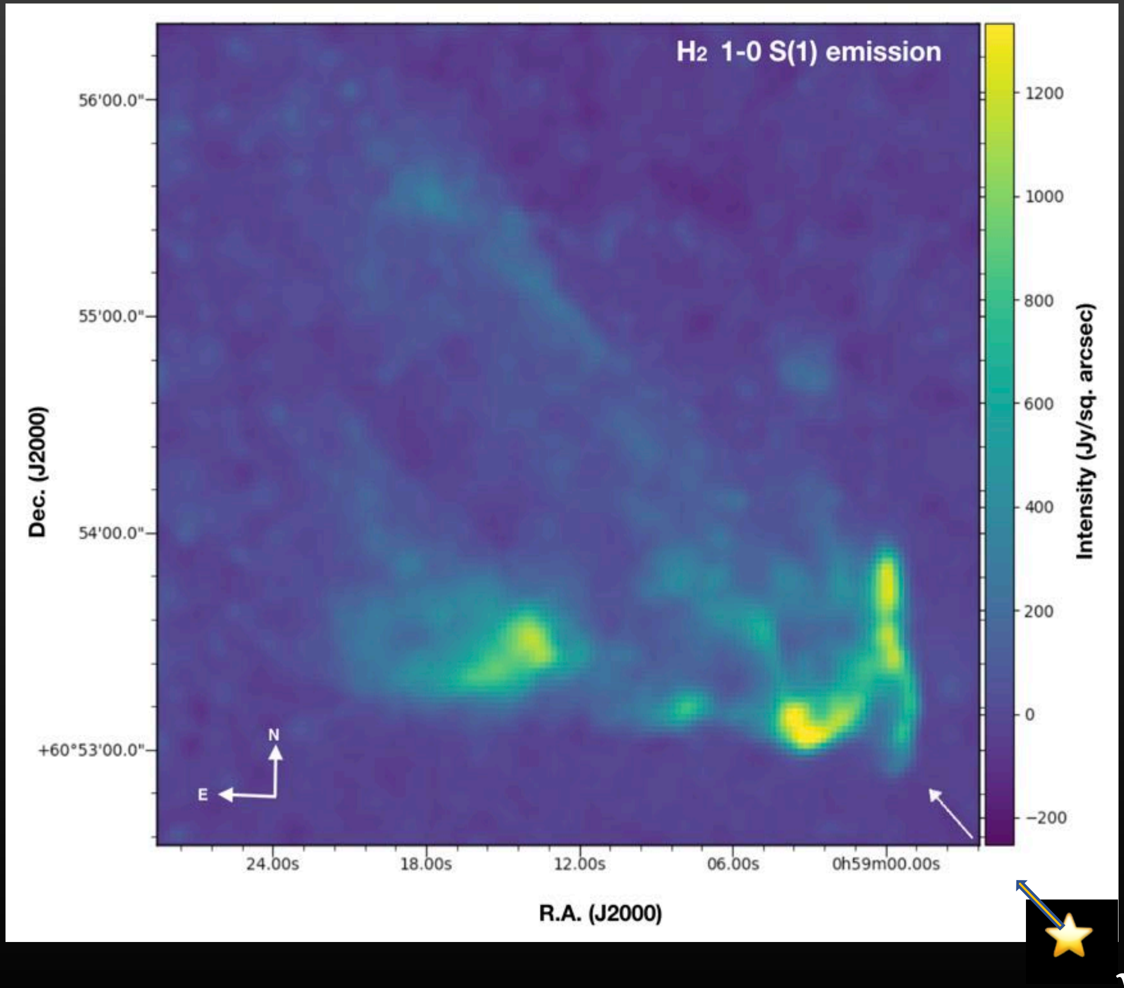
Blue solid lines: The vectors drawn in blue are from Andersson et al. (2013)

Cyan dashed arrow: direction of UV radiation from B type star gamma Cas

Field geometry along the direction of radiation

Motivation

- **Mapping pure-rotational molecular hydrogen in PDR IC 63**
- **Testing the two-temperature hypothesis of a previous study by Thi et al. (2009)**



2.12 µm 1-0 S(1) emission (Andersson et al. 2013)

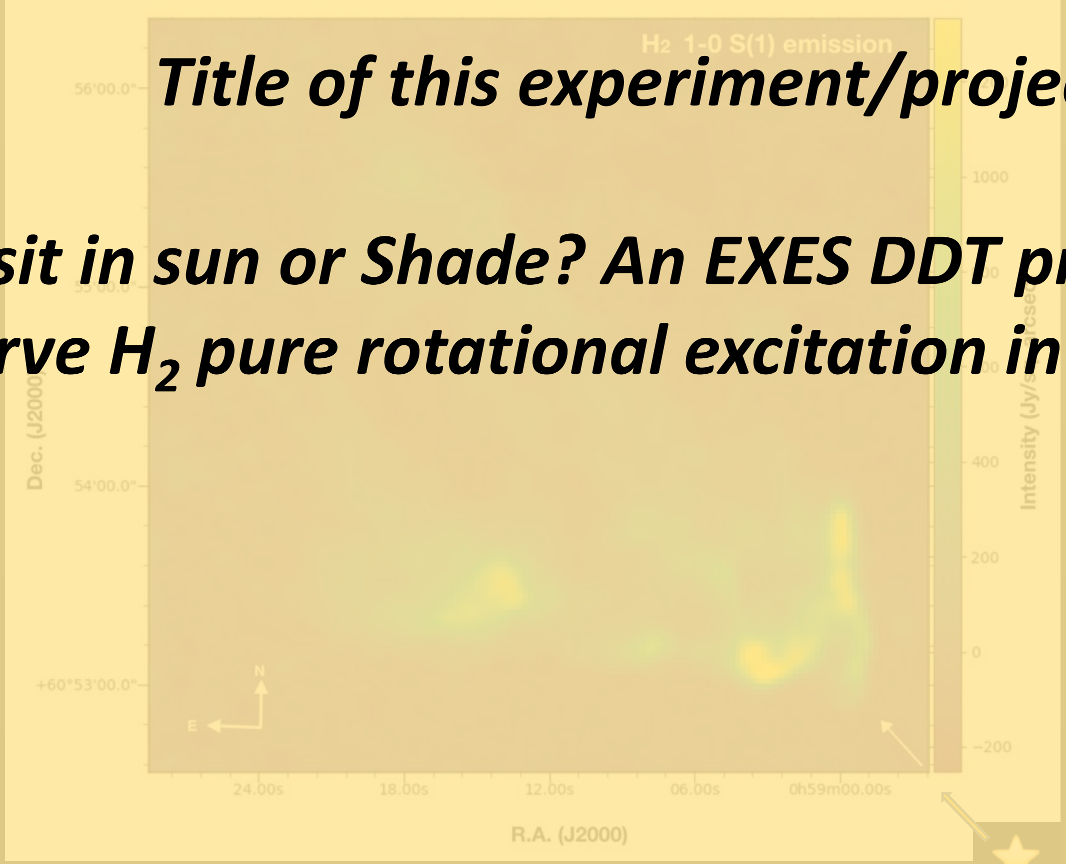
γ Cas (B0.5 IV)

Motivation

- Mapping pure-rotational molecular hydrogen in nearby (~200 pc) PDR IC 63
- Testing the two-temperature hypothesis of a previous study by Thi et al. (2009)

Title of this experiment/project:

Do I sit in sun or Shade? An EXES DDT proposal to observe H_2 pure rotational excitation in IC 63



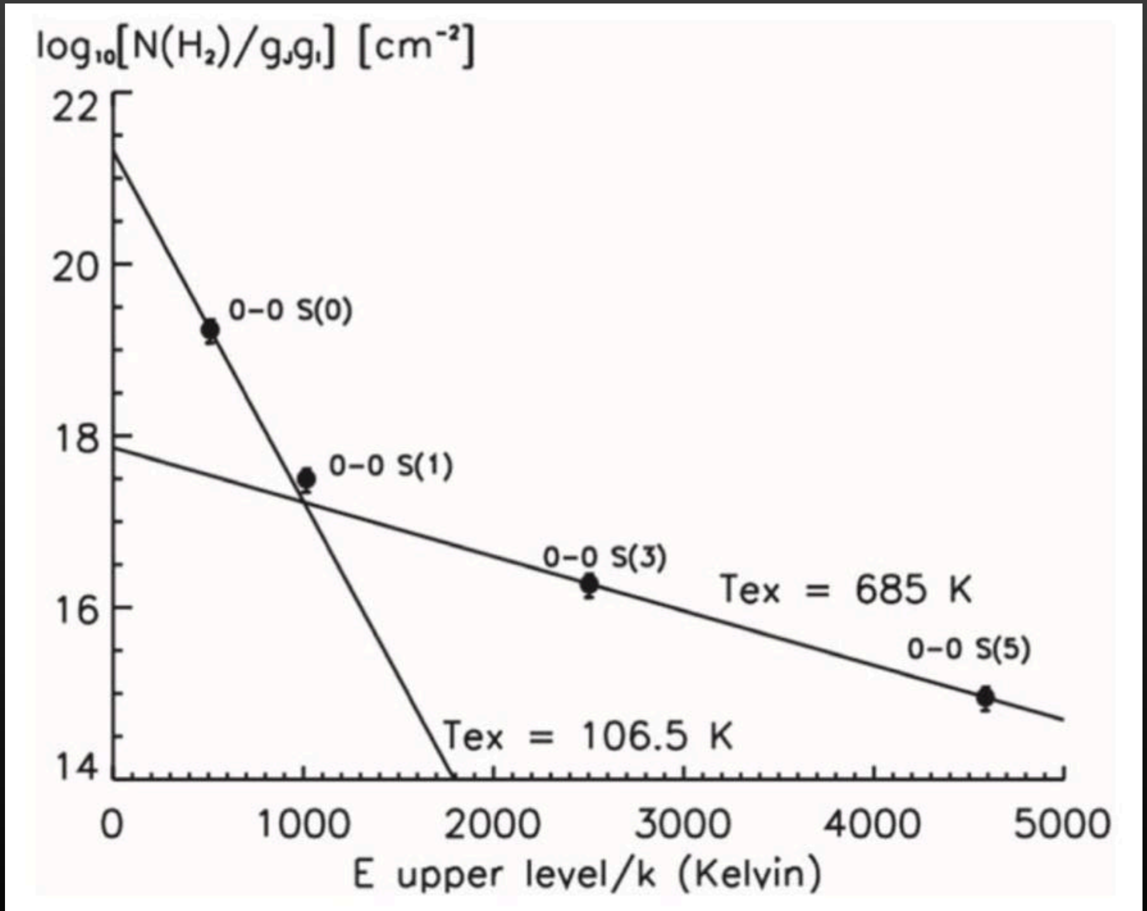
2.12 μm 1-0 S(1) emission (Andersson et al. 2013)

γ Cas (B0.5 IV)

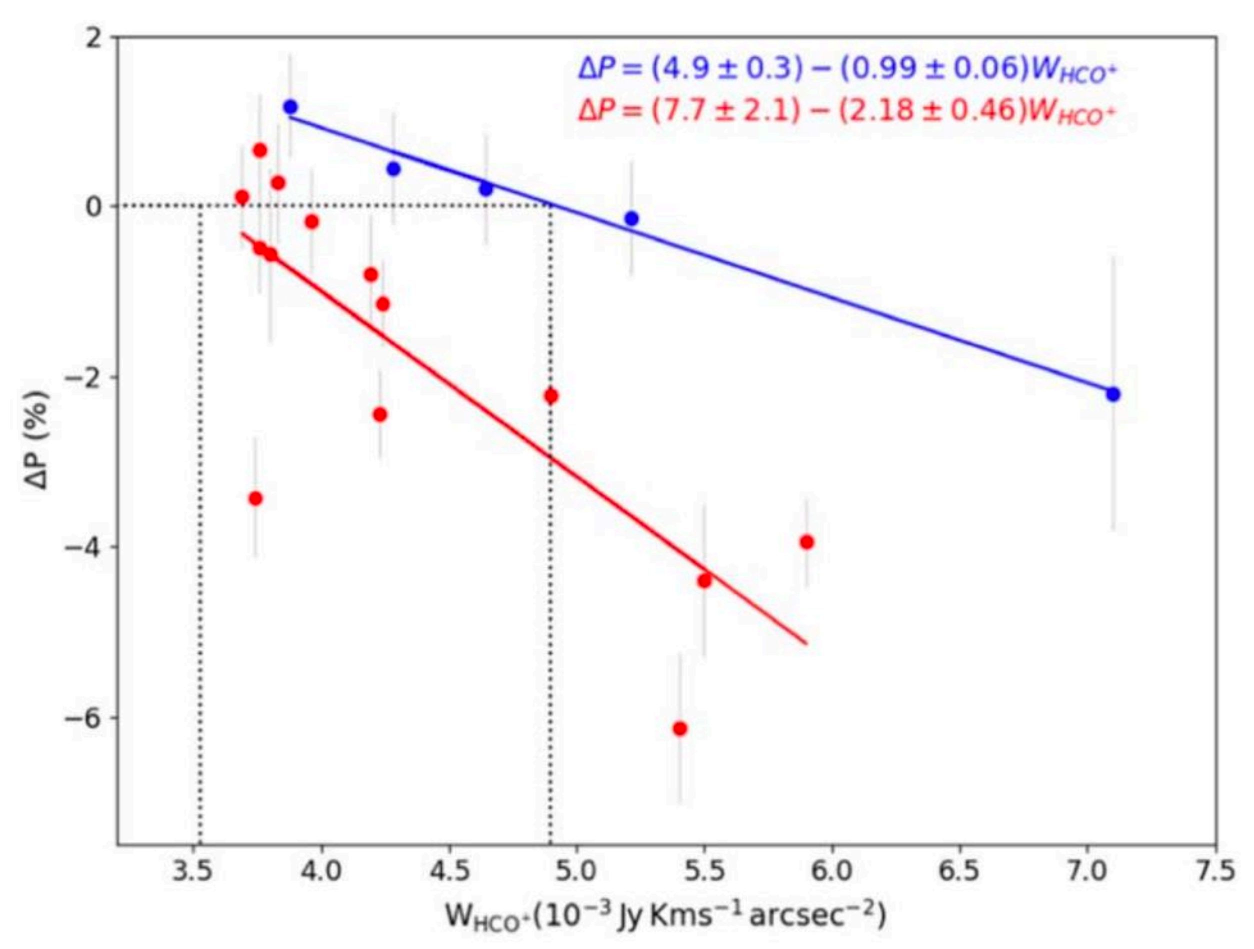
Two temperature hypothesis: support from our polarization study on IC 63

Story begins with two temperature regions seen by Thi et al. (2009) using ISO/SWS

We used polarization and gas densities presenting different gas-dust collision rates in regions with different temperatures



Thi et al. (2009)



Soam & Andersson et al. (2021a)

Two temperature hypothesis: support from our polarization study on IC 63

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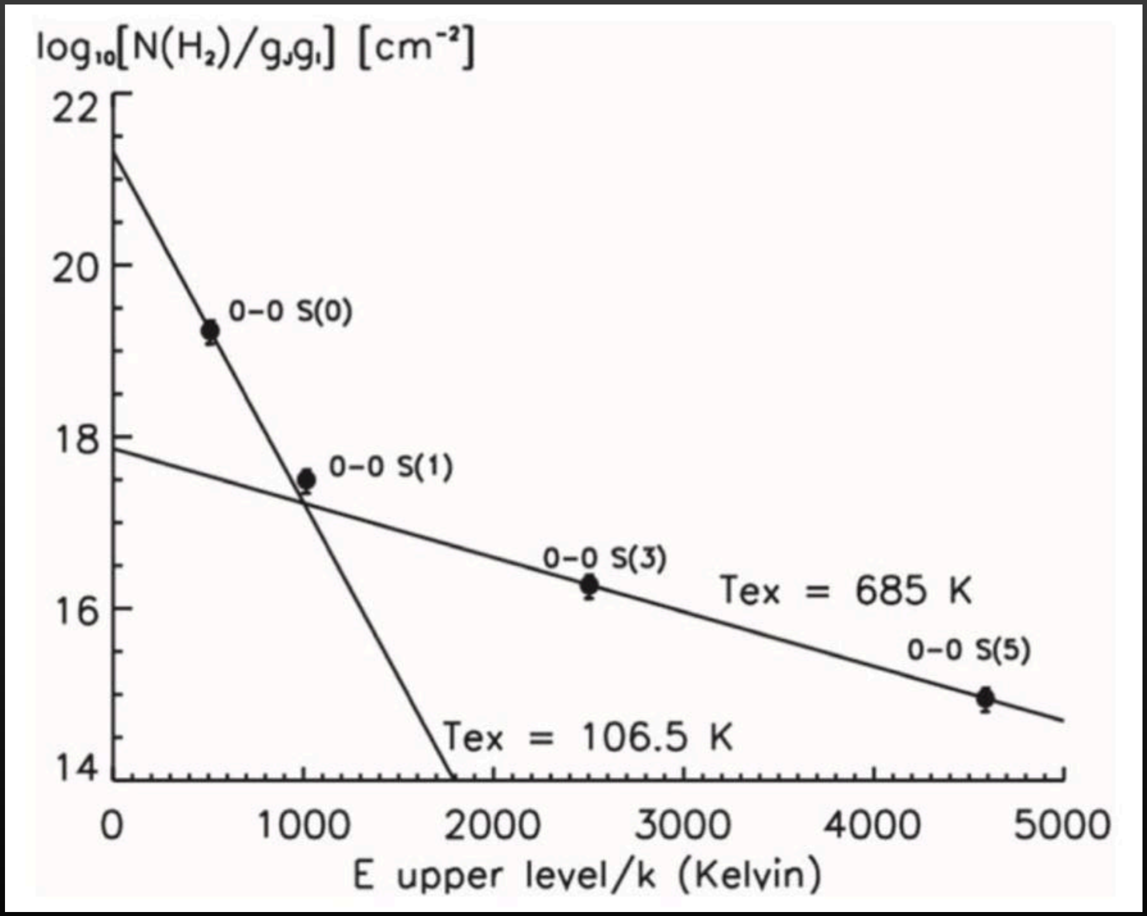
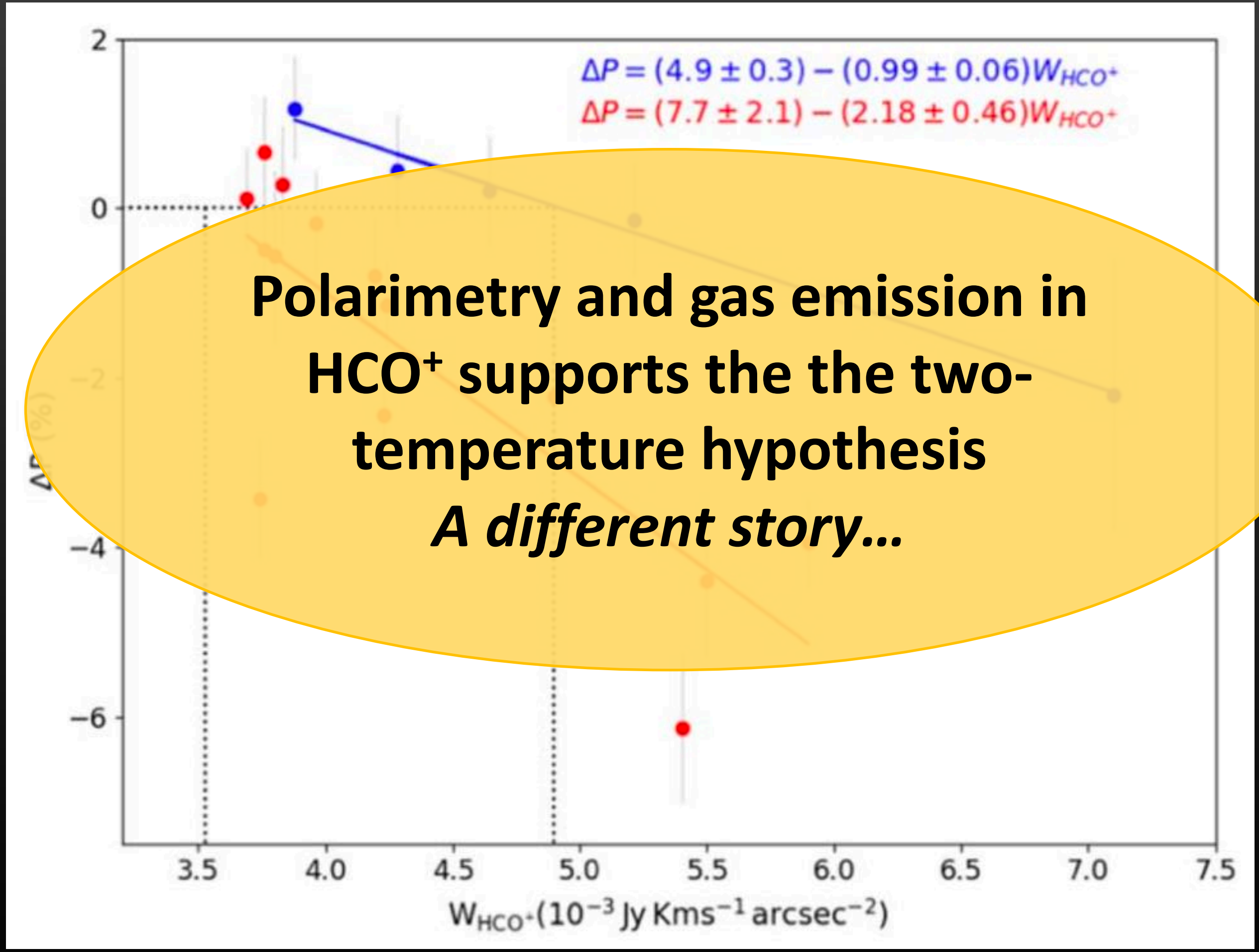


Thi et al. (2009)

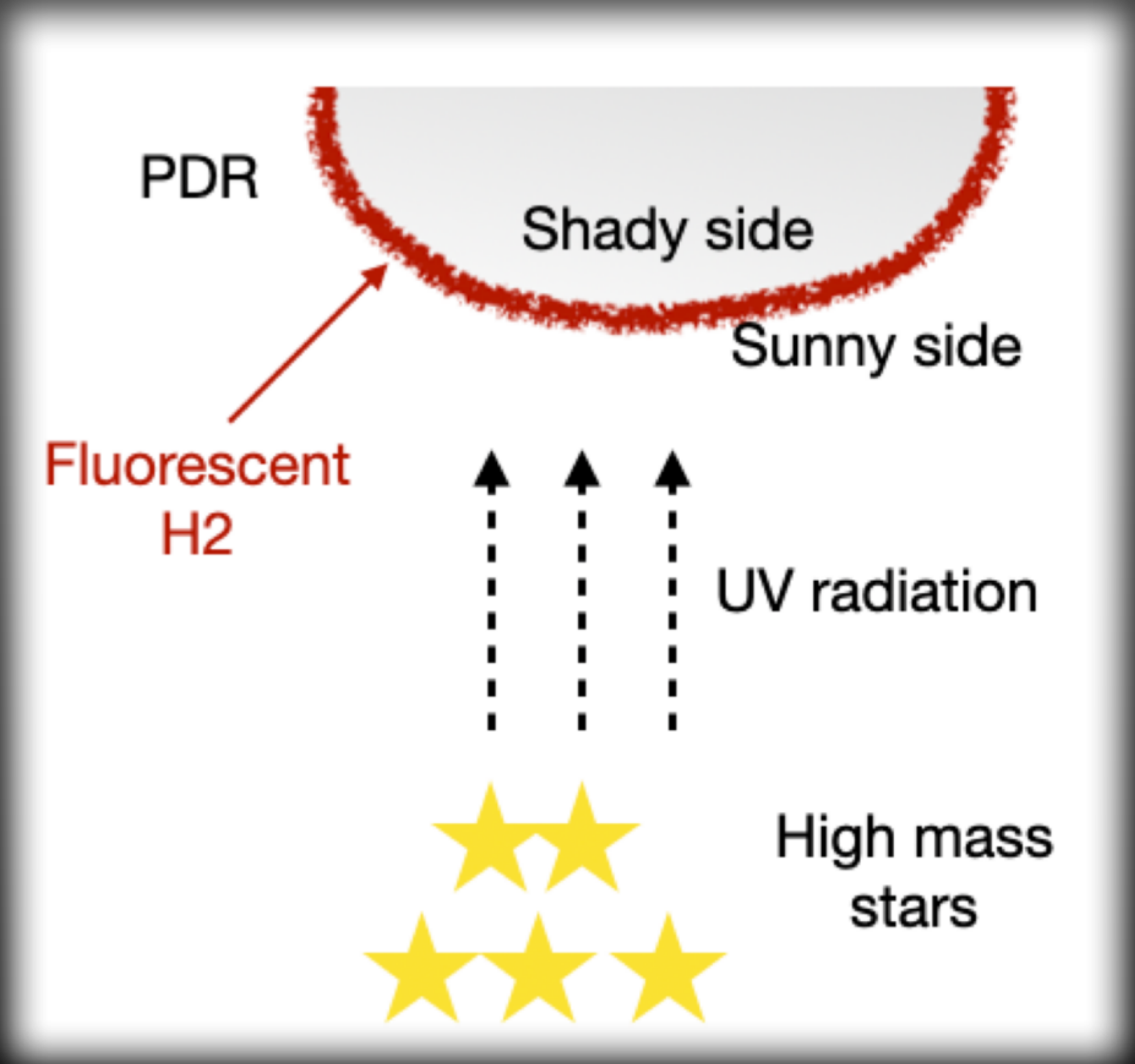


Polarimetry and gas emission in HCO^+ supports the the two-temperature hypothesis

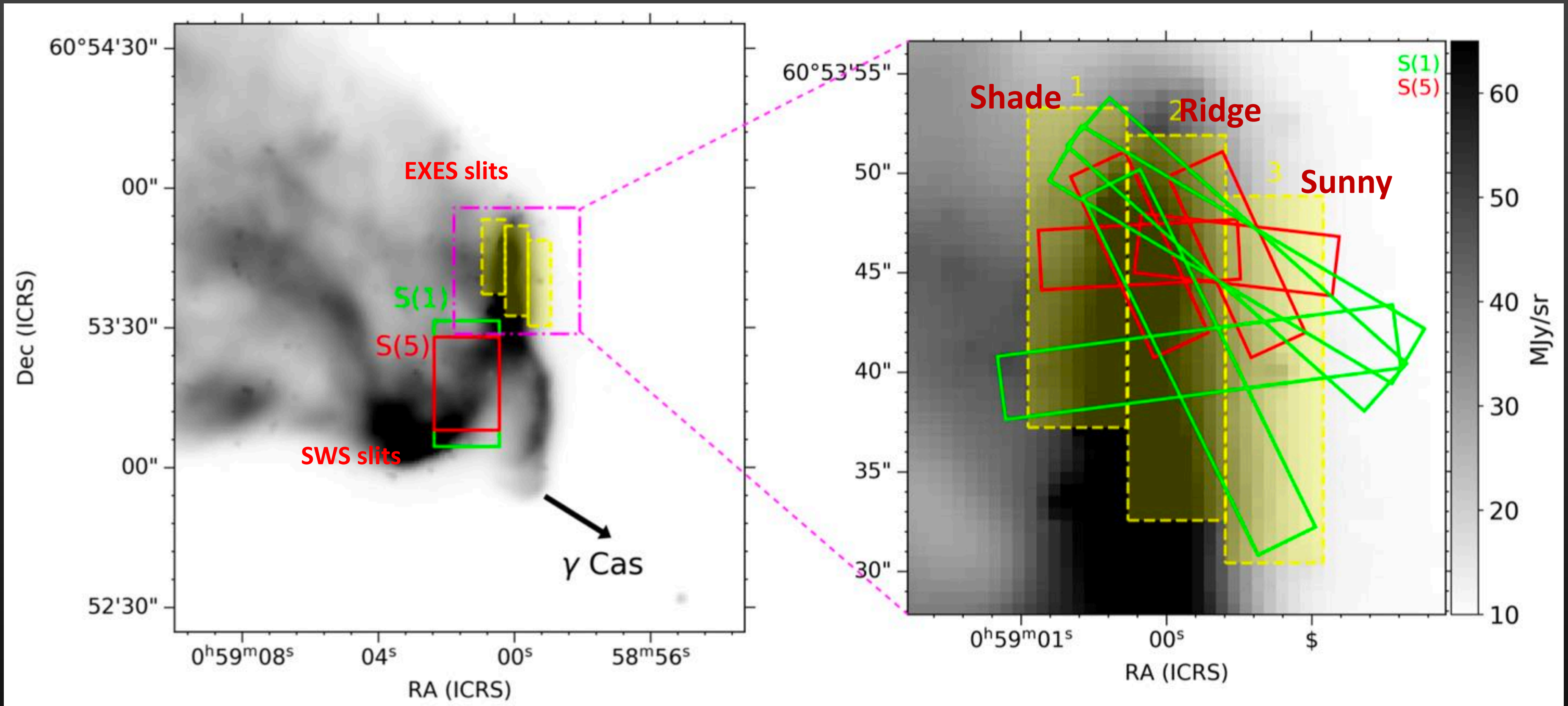
A different story…

Soam & Andersson et al. (2021a)

Naming regions



ISO/SWS and SOFIA/EXES observations: positioning of the slits



EXES slit rotation pattern and actual extraction regions of S(1) and S(5) emission shown with green and red rectangles, respectively.

Soam et al. (2021d)

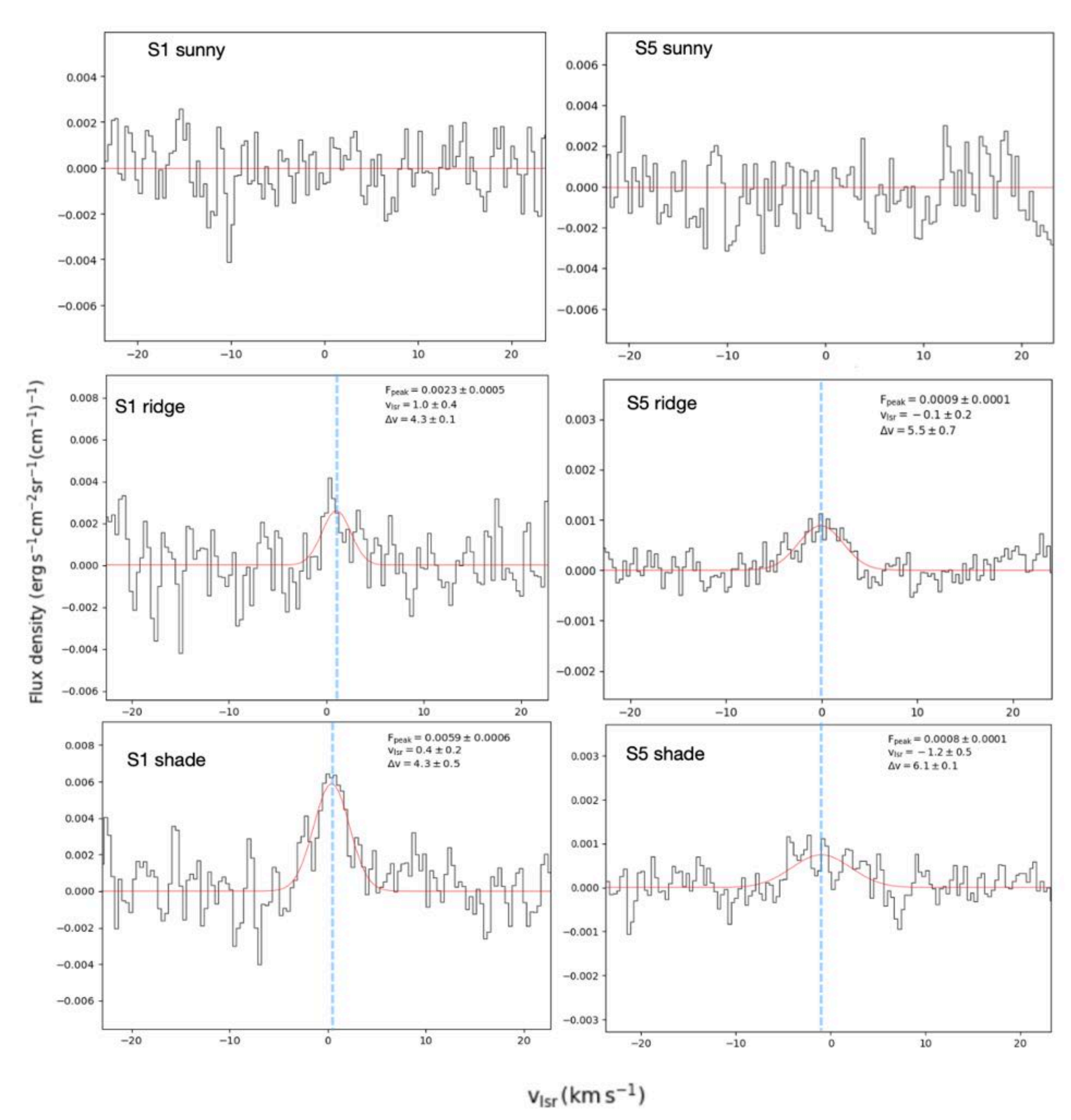
Locations of ISO/SWS slits (bigger area and lower resolution) and EXES slits (smaller area and higher resolution)

Observations and data reduction

- Pure rotational lines S(1) [v=0-0 H_2 (J=3-1)] and S(5) [v=0-0 H_2 (J=7-5)] were observed with EXES using 19" and 10" slits, respectively with a resolution of 60,000.
- For the H_2 S(1) observations, we observed at 587 cm^{-1} in third order, with a slit length of 19" (0.0184 pc assuming a distance of ≈200 pc).
- For H_2 S(5), we observed at 1447 cm^{-1} in eighth order, with a slit length of 10" (0.0097 pc).
- The spatial resolution of the observations is approximately 3".7 for both wavelengths.
- Data were reduced using with the SOFIA Redux pipeline (Clarke et al. 2015), including steps for spike removal, nod- subtraction, flat-fielding, flux calibration, order rectification, and coadding of nodded pairs.
- The wavelength scales were calibrated by matching the sky emission lines within the spectral settings to their values in the HITRAN database (Gordon et al. 2017).
- The uncertainty in the wavelength solution is estimated to be ~0.3 km s^{-1}.

Thanks to EXES instrument scientist Curtis DeWitt and team

Flux extraction and line plotting



Soam et al. (2021d)

Gaussian fitted spectra

- We calculated the flux values by calculating the area of the Gaussian fits.
- Used pyspeckit and matplotlib packages from python to draw spectrum and fit Gaussian.
- The Gaussian fitted parameters were used as mean flux, line width a.k.a. velocity dispersion and LSR velocity.
- No detection of S(1) and S(5) in sunny sides
- *The signal is better detected in shade*

Observed fluxes

Properties of Observed H_2 Transitions in IC 63 PDR

Line	Reg[a]	λ (μm)	I_{ul} 10^{-5} erg cm^{-2} s^{-1} sr^{-1}	E_{up}/k_B (K)	A_{ul}[b] (s^{-1})	Δv[c] (km s^{-1})
S(1) 3–1	Shady	17.035	5.3 ± 0.8	1015.12	4.8×10^{-10}	4.3 ± 0.5
S(1) 3–1	Ridge	17.035	2.2 ± 0.8	1015.12	4.8×10^{-10}	5.1 ± 1.5
S(1) 3–1	Sunny	17.035	…	1015.12	4.8×10^{-10}	…
S(5) 7–5	Shady	6.901	2.5 ± 0.6	4586.30	5.9×10^{-8}	6.1 ± 1.2
S(5) 7–5	Ridge	6.901	2.6 ± 0.4	4586.30	5.9×10^{-8}	5.5 ± 0.7
S(5) 7–5	Sunny	6.901	…	4586.30	5.9×10^{-8}	…

Notes.
[a] See Figure 1 for explanation of regions.
[b] Einstein *A*-coefficients from Wolniewicz et al. (1998).
[c] Line width values were calculated from inspection of each line profile individually and may differ from values given by the fits in Figure 2.

Construction of rotation diagram

Constructing Rotation Diagram

$$I_{ul} = N_u A_{ul} h\upsilon_{ul}/4\pi$$

I_{ul} - **Intensity of the transition between upper level (u) and lower level (l)**
A_{ul}- **Einstein coefficient of the transition (Hz)**
υ_{ul} - **Frequency of the transition (Hz)**
N_u - **Population of the upper level (cm^{-2})**

For our H_2 pure rotational lines:
S(1) (J = 3-1):
A_{ul} **= 4.8×10^{-10}**
υ_{ul} **= 17.6 THz**
S(5) (J = 7-5):
A_{ul} **= 5.9×10^{-8}**
υ_{ul} **= 43.4 THz**

$$N_u = I_{ul} 4\pi / A_{ul} h\upsilon_{ul}$$

Two methods to obtain total intensity:

1. Calculate area of Gaussian fit

$$Area = a * \sqrt{2\pi c^2}$$

$$I_{ul} = F_{peak}\sqrt{2\pi}\,\frac{\Delta k}{2.355}$$

Note: Δv from fits is a velocity but we need in wavenumber (k)

$$\Delta k = \upsilon_{ul}\Delta v / c^2$$

2. Direct line integration
   - Integrate total area of spectra from +/-10 km/s on either side of v_{lsr} = 0
   - Multiply the intensity value by the wavenumber width (Δk)

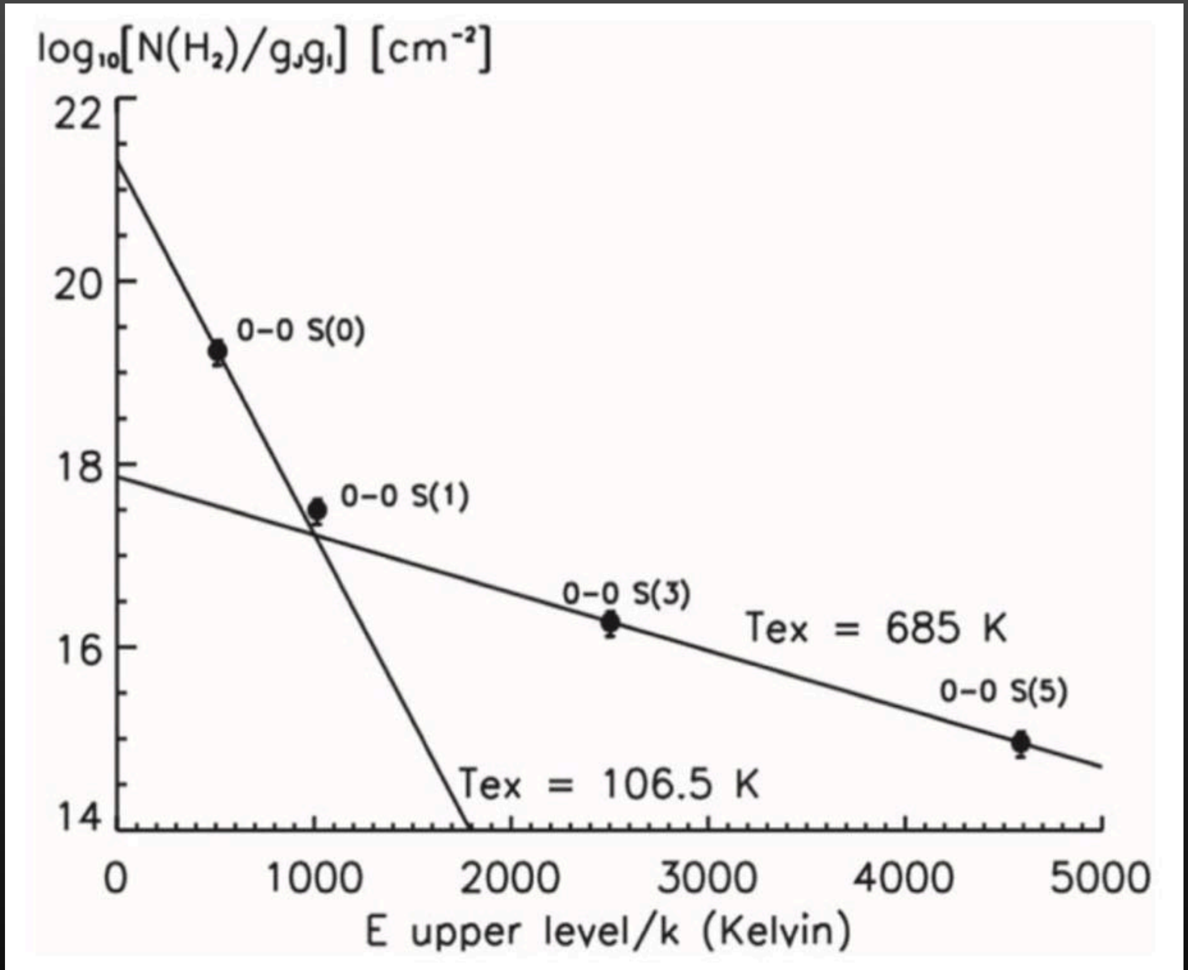
Constructing Rotation Diagram

$$N_u = I_{ul} 4\pi / A_{ul} h\upsilon_{ul}$$

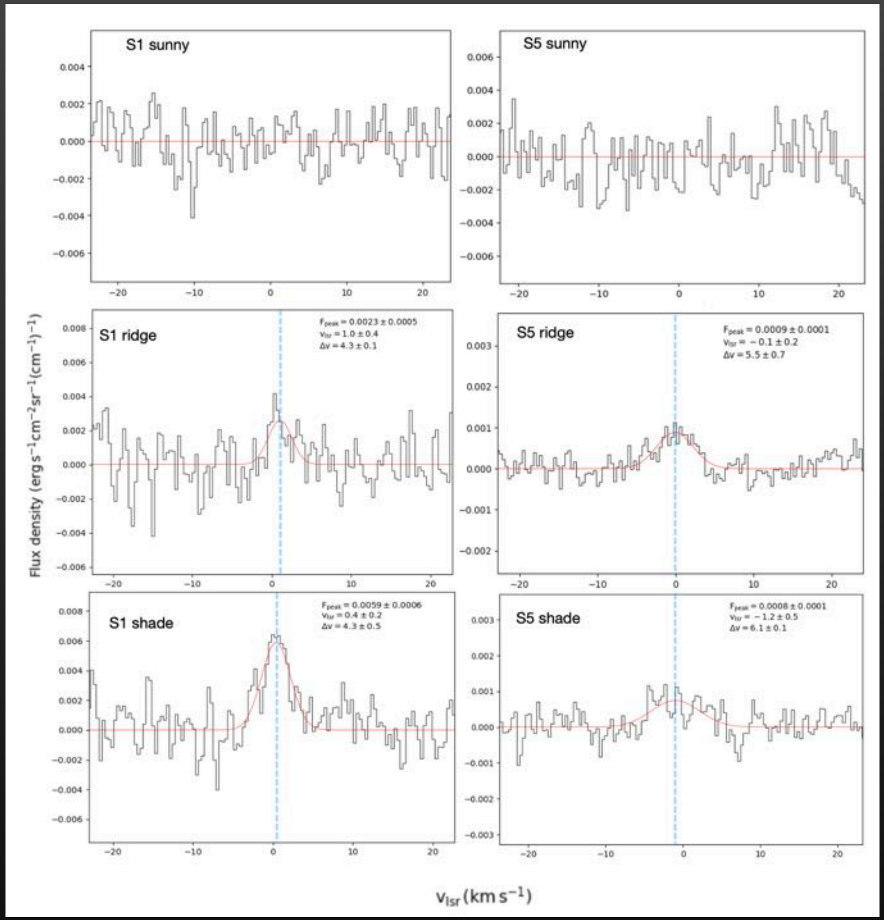
$$N_u = \mathrm{N}(H_2) g_I g_u e^{-E_{ul}/T_{ex}} / Q(T_{ex})$$

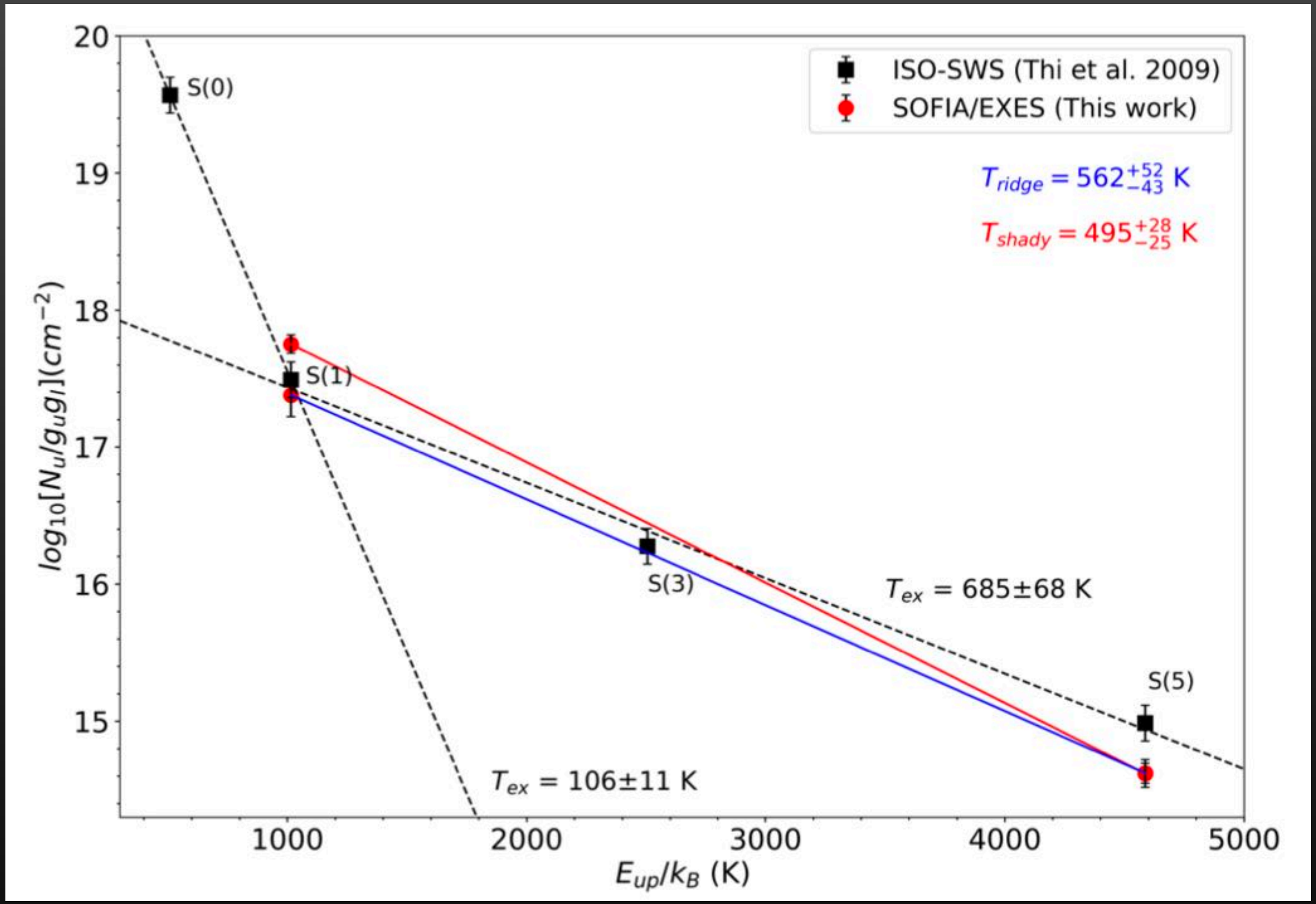
$$\log\left[\frac{N_u}{g_I g_u}\right] = -\frac{E_{ul}}{T_{ex}} + \log\left[\frac{N(H_2)}{Q(T_{ex})}\right]$$

N_u - Population of the upper level (cm^{-2})
g_I - nuclear spin degeneracy (g_I = 3 for H_2 when J is odd)
g_u - degeneracy of the upper level (2J+1)
E_{ul} - Energy of the transition
T_{ex} - Excitation temperature (K)
$Q(T_{ex})$ - Partition function at excitation temperature



Constructing Rotation Diagram





Soam et al. (2021d)

$$N_u = I_{ul} 4\pi / A_{ul} h \upsilon_{ul}$$

$$N_u = \mathrm{N}(H_2) g_I g_u e^{-E_{ul}/T_{ex}} / Q(T_{ex})$$

PDR Modeling

http://dustem.astro.umd.edu/

- Using observed spectral fluxes, PDR Toolbox can compute best-fit FUV incident intensity (G0) and cloud density (n).

- One can also fit H_2 rovibrational emission excitation diagrams to determine temperature and column density.

dustem.astro.umd.edu

PhotoDissociation Region Toolbox

TOOLS+ ABOUT CONTACT

Ultraviolet photons from O and B stars strongly influence the structure and emission spectra of the interstellar medium. The UV photons energetic enough to ionize hydrogen $h\nu > 13.6\mathrm{eV}$ will create the H II region around the star, but lower energy UV photons escape. These far-UV photons ($6\ \mathrm{eV} < h\nu < 13.6\ \mathrm{eV}$) are still energetic enough to photodissociate molecules and to ionize low ionization-potential atoms such as carbon, silicon, and sulfur. They thus create a ***photodissociation region*** (PDR) just outside the H II region. In aggregate, these PDRs dominates the heating and cooling of the neutral interstellar medium. The gas is heated by photo-electrons from grains and cools mostly through far-infrared fine structure lines like [O I] and [C II].

The **PDR Toolbox** is a science-enabling tool for the community, designed to help astronomers determine the physical parameters of photodissociation regions from observations. Typical observations of both Galactic and extragalactic PDRs come from ground- and space-based millimeter, submillimeter, and far-infrared telescopes such as ALMA, SOFIA, JWST, Spitzer, and Herschel. Given a set of observations of spectral line or continuum intensities, PDR Toolbox can compute best-fit FUV incident intensity and cloud density based on our models of PDR emission. One can also fit H_2 rovibrational emission excitation diagrams to determine temperature and column density.

The current version is 2.2.3 (released Feb 1, 2022)

- Pound & Wolfire (2008)
- Kaufman, Wolfire, & Hollenbach (2006)

Documents & Presentations

Below are links to relevant papers and to presentations we have made.

- *The PhotoDissociation Region Toolbox: Past & Future*, Marc W. Pound & Mark G. Wolfire. Poster presented at Celebrating the First 40 Years of Alexander Tielens' Contribution to Science: The Physics and Chemistry of the ISM., 2019
- *The Physics of PDRs*, Mark G. Wolfire, Invited Talk at 30 Years of Photodissociation Regions: A Symposium to Honor David Hollenbach's Lifetime in Science, 2015
- *Observational and Theoretical Review of the Multiphase ISM*, Mark G. Wolfire
- *The Photo Dissociation Region Toolbox*, Marc W. Pound & Mark G. Wolfire, 2008
- *[Si II], [Fe II], [C II], and H_2 Emission from Massive Star-forming Regions* Michael J. Kaufman, Mark G. Wolfire, & David J. Hollenbach, 2006
- BibTeX file of papers you should cite if you used the PDR Toolbox.

Lines and line ratios in the model

25	CO(J=7-6) / CO(J=6-5)	CO_65	CO_76/CO_65
26	CO(J=8-7) / CO(J=5-4)	CO_54	CO_87/CO_54
27	CO(J=8-7) / CO(J=6-5)	CO_65	CO_87/CO_65
28	CO(J=9-8) / CO(J=5-4)	CO_54	CO_98/CO_54
29	CO(J=9-8) / CO(J=6-5)	CO_65	CO_98/CO_65
30	CO(J=10-9) / CO(J=5-4)	CO_54	CO_109/CO_54
31	CO(J=10-9) / CO(J=6-5)	CO_65	CO_109/CO_65
32	CO(J=10-9) / CO(J=7-6)	CO_76	CO_109/CO_76
33	CO(J=11-10) / CO(J=5-4)	CO_54	CO_1110/CO_54
34	CO(J=11-10) / CO(J=6-5)	CO_65	CO_1110/CO_65
35	CO(J=12-11) / CO(J=5-4)	CO_54	CO_1211/CO_54
36	CO(J=12-11) / CO(J=6-5)	CO_65	CO_1211/CO_65
37	CO(J=13-12) / CO(J=5-4)	CO_54	CO_1312/CO_54
38	CO(J=13-12) / CO(J=6-5)	CO_65	CO_1312/CO_65
39	CO(J=14-13) / CO(J=5-4)	CO_54	CO_1413/CO_54
40	CO(J=14-13) / CO(J=6-5)	CO_65	CO_1413/CO_65
41	[C I] 609 μm / I_{FIR}	FIR	CI_609/FIR
42	([O I] 63 μm + [C II] 158 μm) / I_{FIR}	FIR	OI_63+CII_158/FIR
43	([O I] 145 μm + [C II] 158 μm) / I_{FIR}	FIR	OI_145+CII_158/FIR
44	[S III] 35 μm / [Fe II] 26 μm	FEII_26	SIII_35/FEII_26
45	H_2 0-0S(1) 17 μm / H_2 0-0S(0) 28.2μm	H200S0	H200S1/H200S0
46	H_2 0-0S(2) 12.3 μm / H_2 0-0S(0) 28.2μm	H200S0	H200S2/H200S0
47	H_2 0-0S(2) 12.3 μm / H_2 0-0S(1) 17μm	H200S1	H200S2/H200S1
48	H_2 0-0S(3) 9.7 μm / H_2 0-0S(1) 17μm	H200S1	H200S3/H200S1
49	H_2 0-0S(1) 17 μm / [S III] 35 μm	SIII_35	H200S1/SIII_35
50	H_2 0-0S(2) 12.3 μm / [S III] 35 μm	SIII_35	H200S2/SIII_35
51	H_2 6-5Q(1) 1.6 μm / H_2 1-0S(1) 2.12 μm	H210S1	H264Q11/H210S1

First, load up a set of models. Here we use the Wolfire/Kaufman 2006 models.

```
m = ModelSet(name="wk2006",z=1)
# Display all the available ratio and intensity model files. Files that have denominator = 1 are intensities.
m.table.show_in_notebook()
```

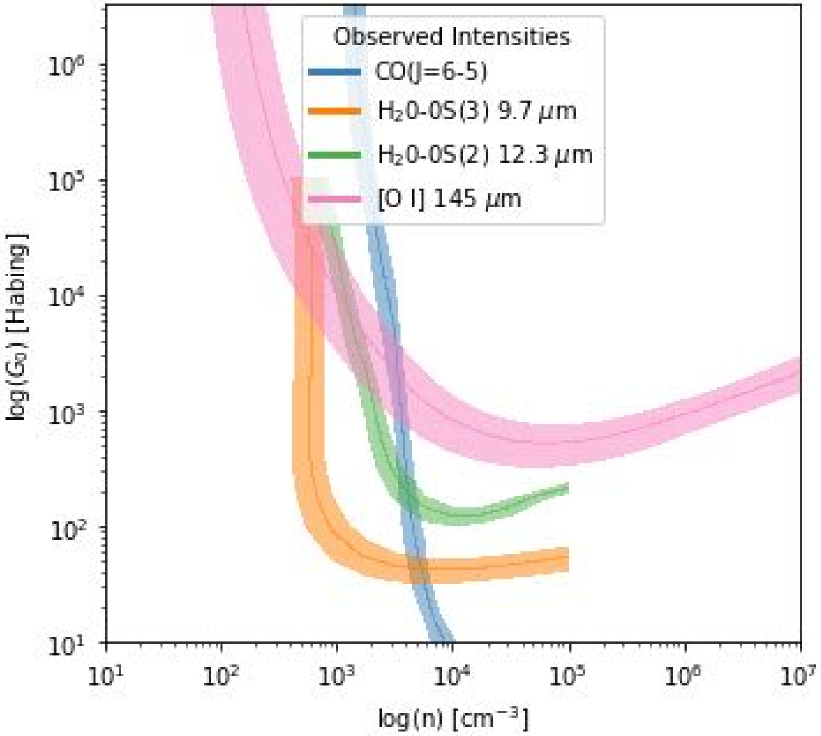
2	OI_63	CII_158	OI_63/CII_158	oicpweb	1.0	[O I] 63 μm / [C II] 158 μm
3	CII_158	CI_609	CII_158/CI_609	ciici609web	1.0	[C II] 158 μm / [C I] 609 μm
4	CI_370	CI_609	CI_370/CI_609	ciciweb	1.0	[C I] 370 μm / [C I] 609 μm
5	CII_158	CO_10	CII_158/CO_10	ciicoweb	1.0	[C II] 158 μm / CO(J=1-0)
6	CII_158	CO_32	CII_158/CO_32	ciico32web	1.0	[C II] 158 μm / CO(J=3-2)
7	CI_609	CO_10	CI_609/CO_10	cicoweb	1.0	[C I] 609 μm / CO(J=1-0)
8	CI_609	CO_21	CI_609/CO_21	cico21web	1.0	[C I] 609 μm / CO(J=2-1)
9	CI_609	CO_32	CI_609/CO_32	cico32web	1.0	[C I] 609 μm / CO(J=3-2)
10	CI_609	CO_43	CI_609/CO_43	cico43web	1.0	[C I] 609 μm / CO(J=4-3)
11	CI_609	CO_54	CI_609/CO_54	cico54web	1.0	[C I] 609 μm / CO(J=5-4)
12	CI_609	CO_65	CI_609/CO_65	cico65web	1.0	[C I] 609 μm / CO(J=6-5)
13	CO_21	CO_10	CO_21/CO_10	co2110web	1.0	CO(J=2-1) / CO(J=1-0)
14	CO_32	CO_10	CO_32/CO_10	co3210web	1.0	CO(J=3-2) / CO(J=1-0)

Here is an example plotting only intensities.

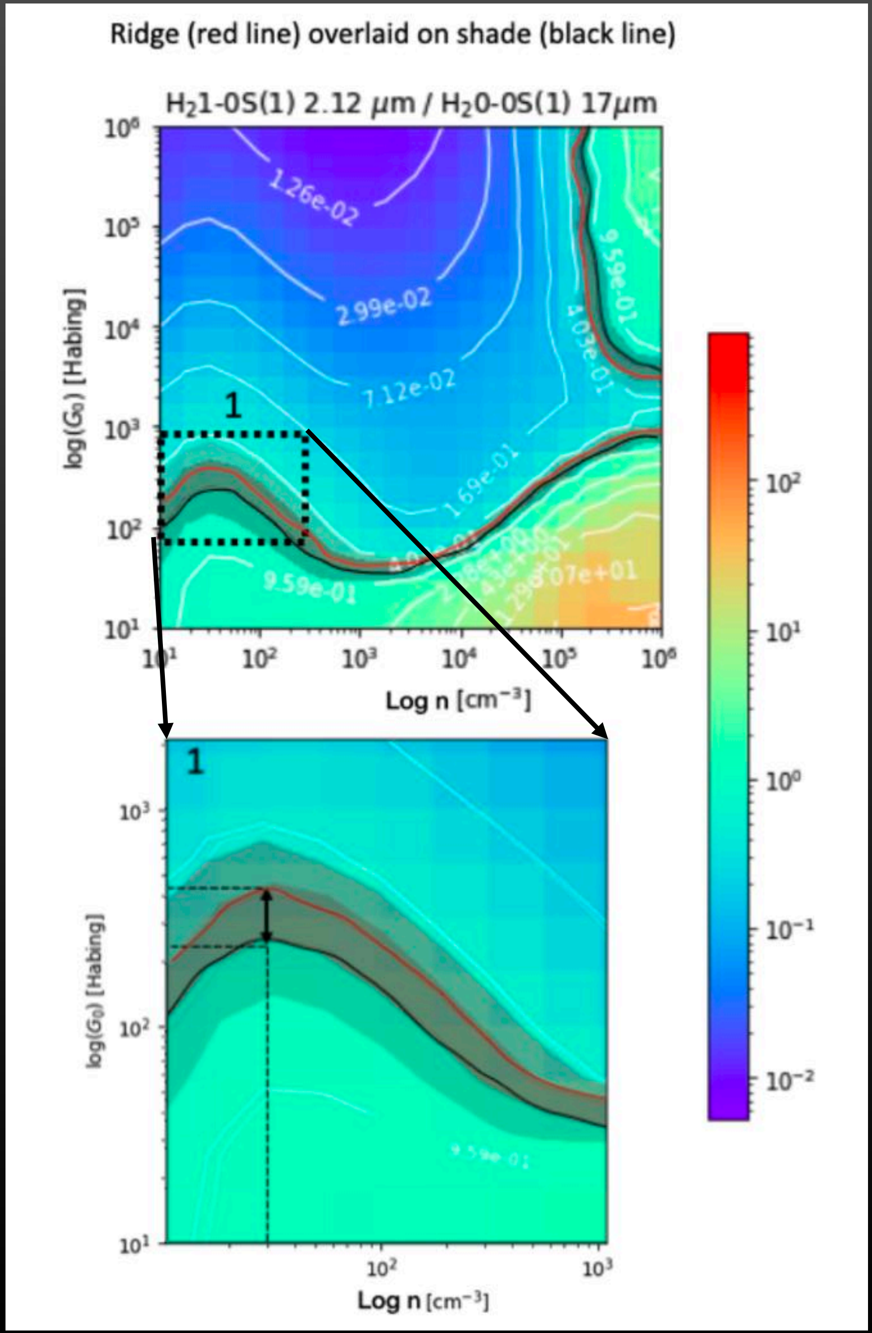
The code is smart enough to convert $K\ km\ s^{-1}$ to intensity units (as long as the Measurement has a RESTFREQ in the FITS header or given during creation) and change the legend label as appropriate.

```
ma=Measurement(data=[0.75],uncertainty = StdDevUncertainty(0.3),identifier="CO_65",unit="K km s-1",restfreq=692*u.GHz)
mb=Measurement(data=[1E-6],uncertainty = StdDevUncertainty(0.25E-6),identifier="H200S3",unit=myunit)
mc=Measurement(data=[2E-6],uncertainty = StdDevUncertainty(0.5E-6),identifier="H200S2",unit=myunit)
md=Measurement(data=[1.25E-4],uncertainty = StdDevUncertainty(0.5E-4),identifier="OI_145",unit=myunit)
a = [ma,mb,mc,md]
mp.overlay(measurements=a,shading=0.5)
```

```
Converting K km/s to erg / (cm2 s sr) using Factor = +3.396E-07 g / (cm K s2)
```



Application on IC63 using H_2 1-0 S(1) and $H_2$0-0 S(1) intensities



- Used PDR toolbox to estimate G0 and densities in ridge and shade sides.
- Difference in G0 values (“attenuation in G0”) in ridge and shade is used to estimate densities.

$$G_{0_{shade}} = e^{-\tau} G_{0_{ridge}}$$

- Av estimated from ‘Tau’ [relations in Whittet 2003]
- Av further gives column density and hence volume density
- We derived space densities of 6.2×10^3 cm^{-3} and 1.7×10^3 cm^{-3} in shade and ridge sides
- Densities are consistent to those obtained with rotation diagram.

Soam et al. (2021d)

Summary

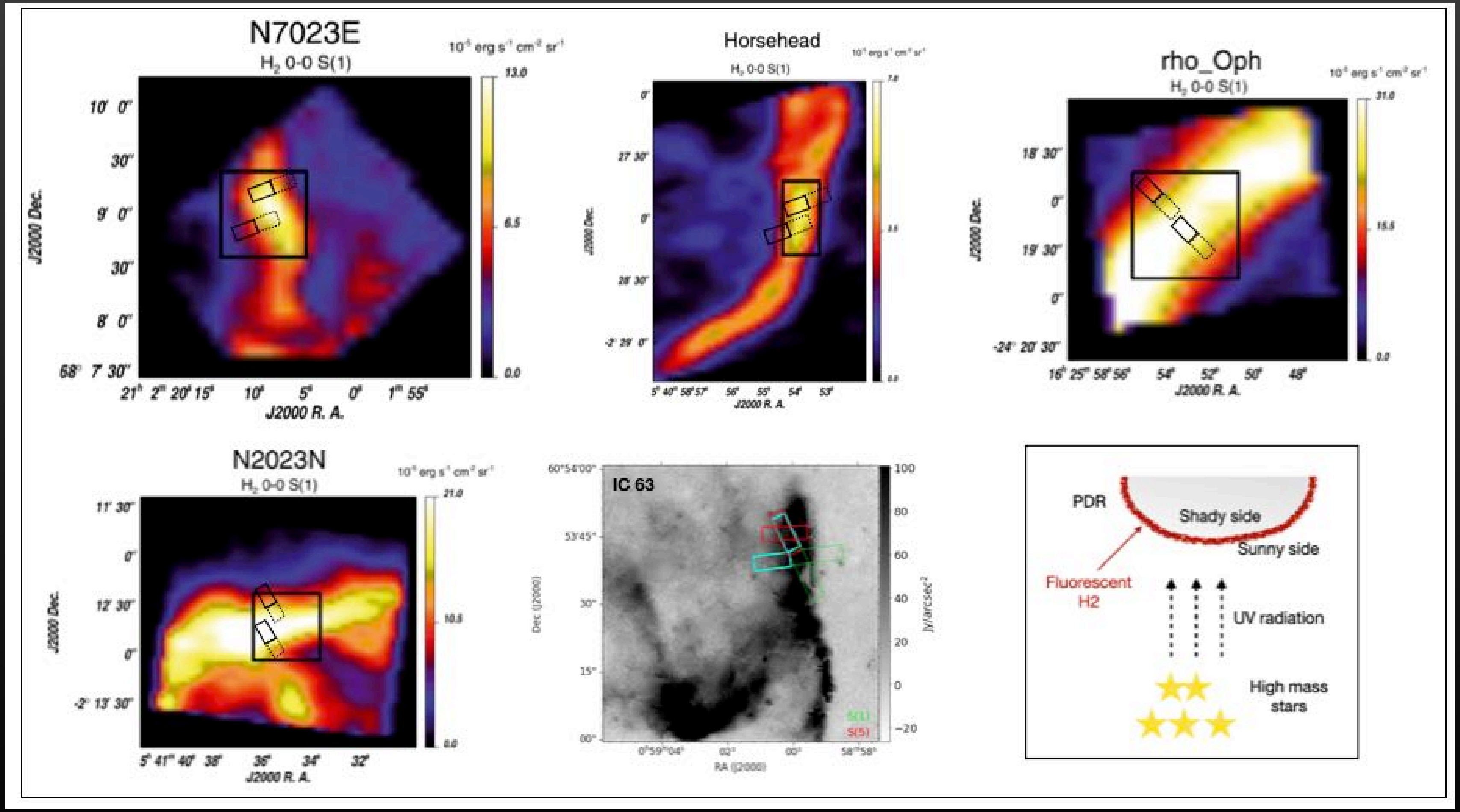
- We re-investigated the two-temperature hypothesis in IC 63 using pure rotational hydrogen lines.
- Earlier hypothesis was based on ISO/SWS observations.
- EXES has the capability of spatially resolving the subregions in PDRs like IC63.
- ISO observations of Thi et al. showed the warm component at T_{ex}=106±11K and the hot gas component seen at T_{ex} = 685 ± 68 K.
- We divided IC 63 PDR into shady, ridge, and sunny sides for our investigation.
- By constructing a rotation diagram using S(1) and S(5) line data from EXES, we obtained a temperature of T = 562+52 K toward the ridge and T = 495+28 K in the shady side.
- Our model suggests a lower value of FUV radiation (G0) in the shade as compared to the one in the ridge. We used this damping in FUV radiation to estimate the optical depth of the PDR.
- Optical depth led us to estimate extinction and hence column densities of different regions.

After IC63….

A pilot program accepted in cy9 (09_0211) and cy10 (but .. ☹)

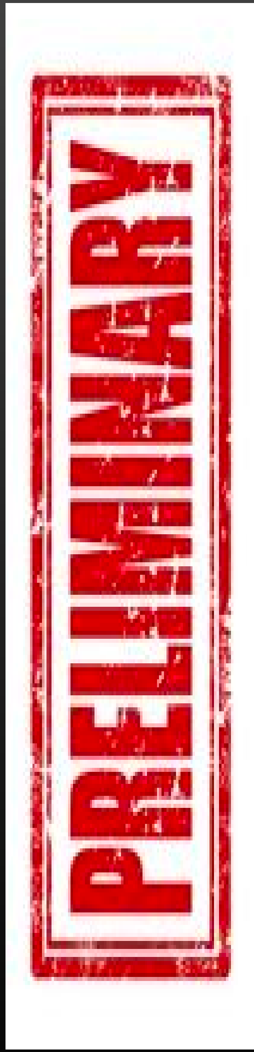
INSPIRE: INvestigating Spatially varying temperatures in PDRs from pure rotational excItation of moleculaR hydrogEn

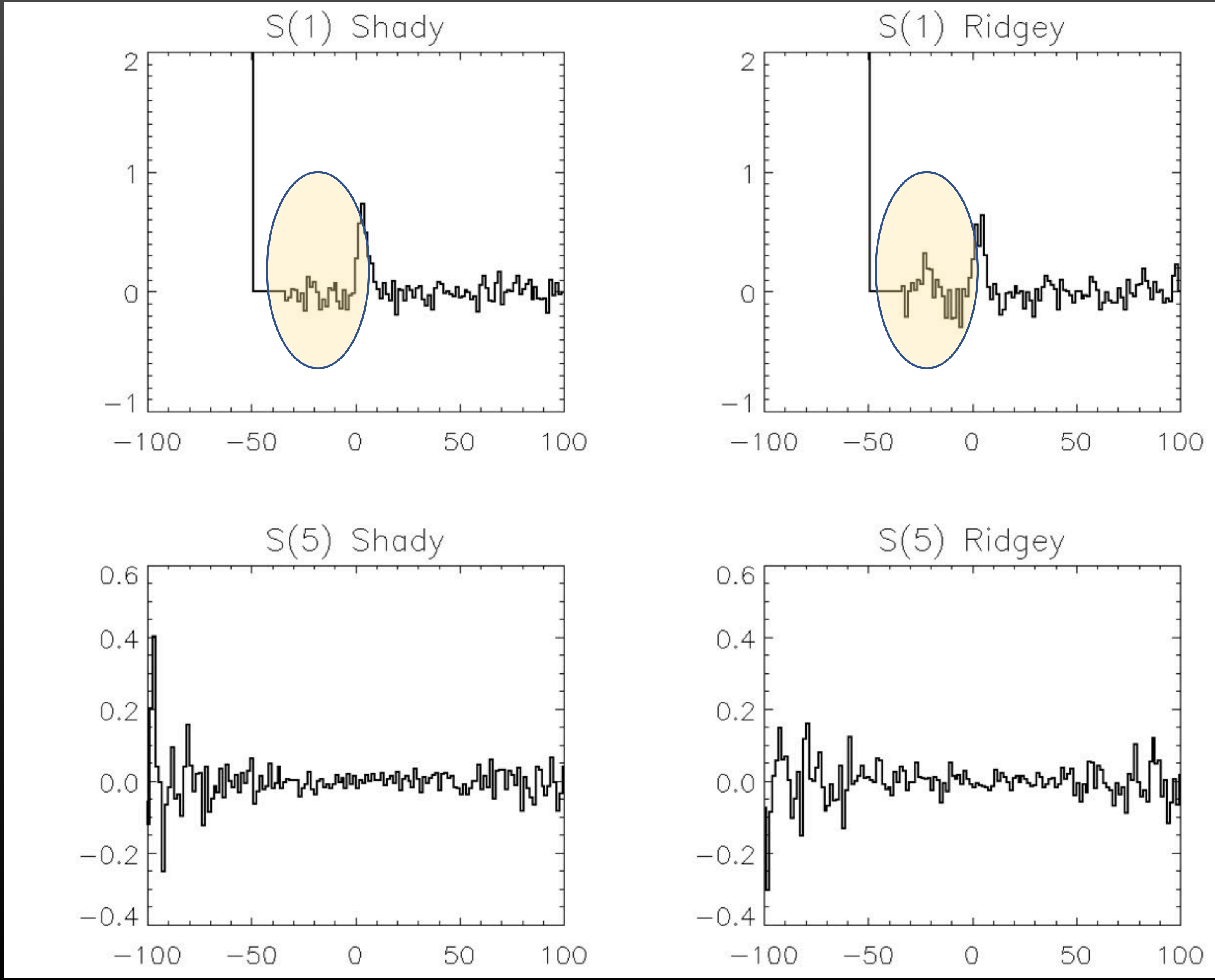
Team: Archana Soam, B-G Andersson, Curtis DeWitt, Matthew Richter, Janik Karoly, Kyle Kaplan



Planning to run this program at IRTF/TEXES

<u>NGC7023</u> was observed before SOFIA was closed. ☹





Integration time was not enough for S(5).

Some data on Rho Oph has also been obtained

Thank you!