Concepcion – the university city of astronomical buses

Astrochemistry with the SOFIA Observatory

Hans Zinnecker
Deutsches SOFIA Institut
DSI Univ. Stuttgart & NASA Ames
(retired), Univ. Autonoma de Chile

Nov 28, 2018
KROME Astrochemistry School, UdeC, Chile

2014: SOFIA development phase → operations phase

http://www.sofia.usra.edu

SOFIA is doing Cycle 6 observations (~100 flights)

What is SOFIA?

SOFIA = Stratospheric Observatory for Infrared Astronomy

flying at ~12-14km

Boeing 747SP

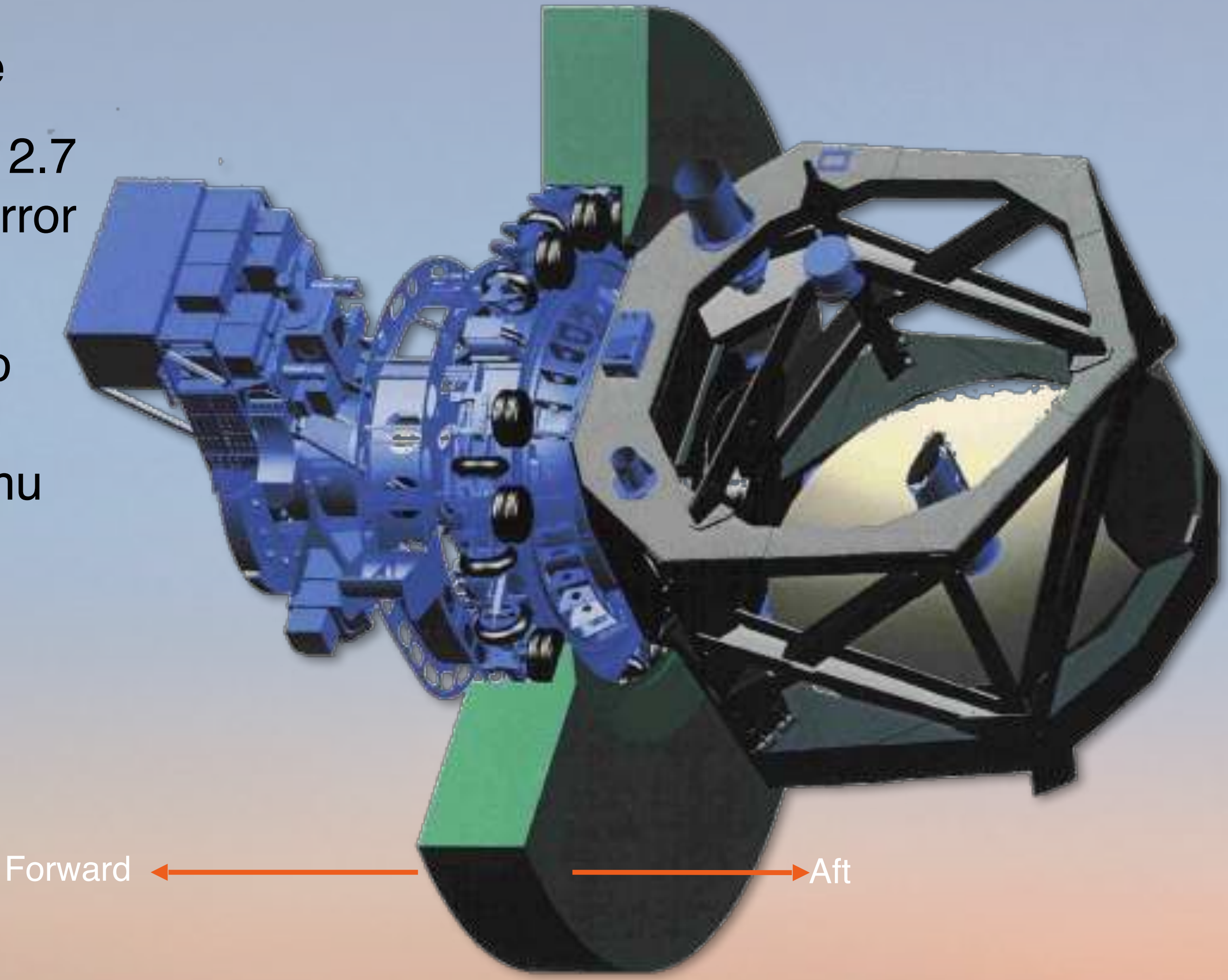
2.7-meter

- International partnership:
  - ➢ 80% -- NASA (US)
  - ➢ 20% -- DLR (Germany)
- Global deployments, incl. southern hemisphere (NZ)
- ~ 120 flights per year (goal) in full operation, ~250 staff.
- ~ 20 year projected lifetime, International Observatory

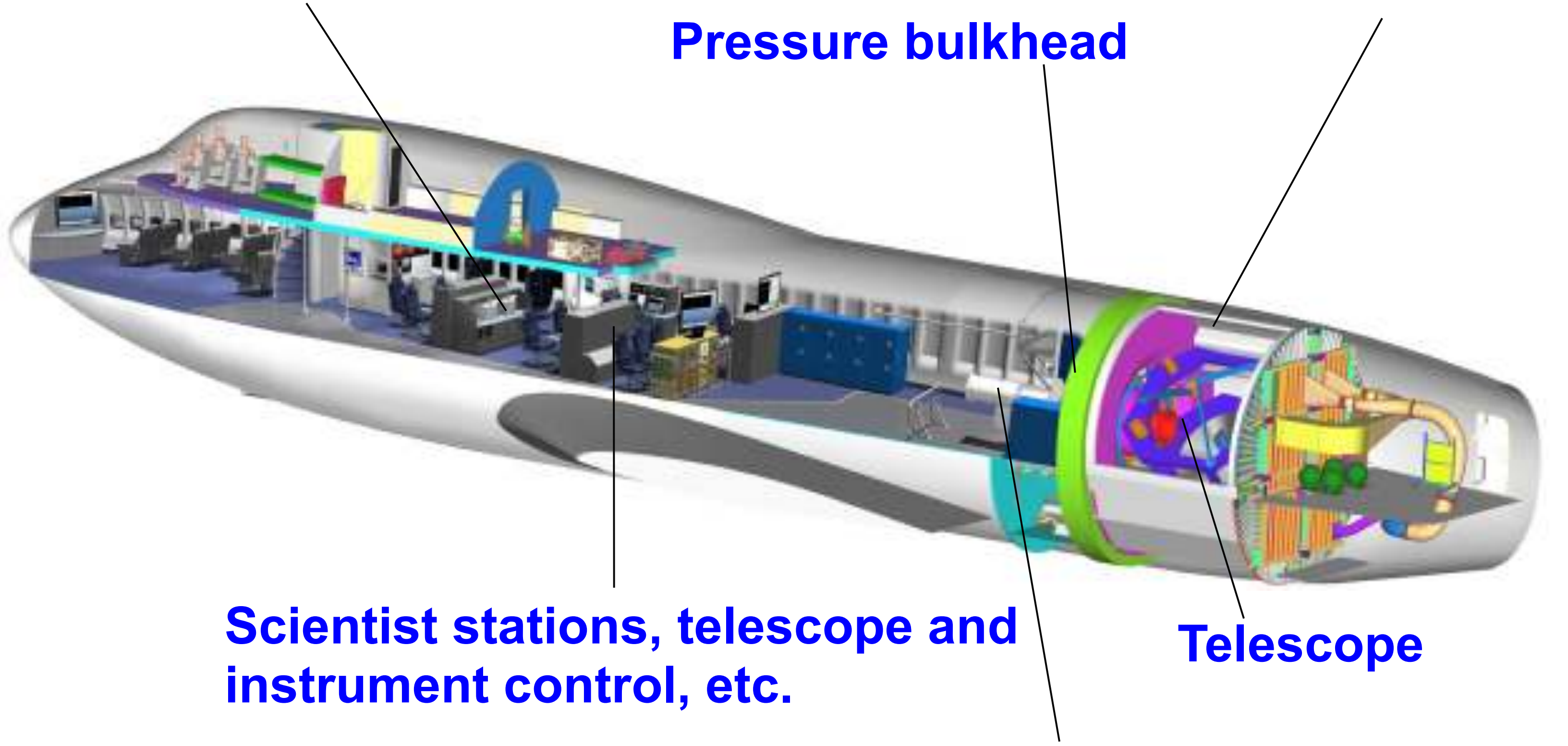
The SOFIA Telescope (DLR German contribution)

Onboard telescope

- Bent Cassegrain, 2.7 meter diameter mirror (~10 feet)
- Wavelength: 0.3 to 1,600 mu (mirror), effectively 1-250 mu
- Installed weight: 17 metric tons (mirror: 600 kg)



SOFIA – The Observatory



Educators work station

Open cavity (door not shown)

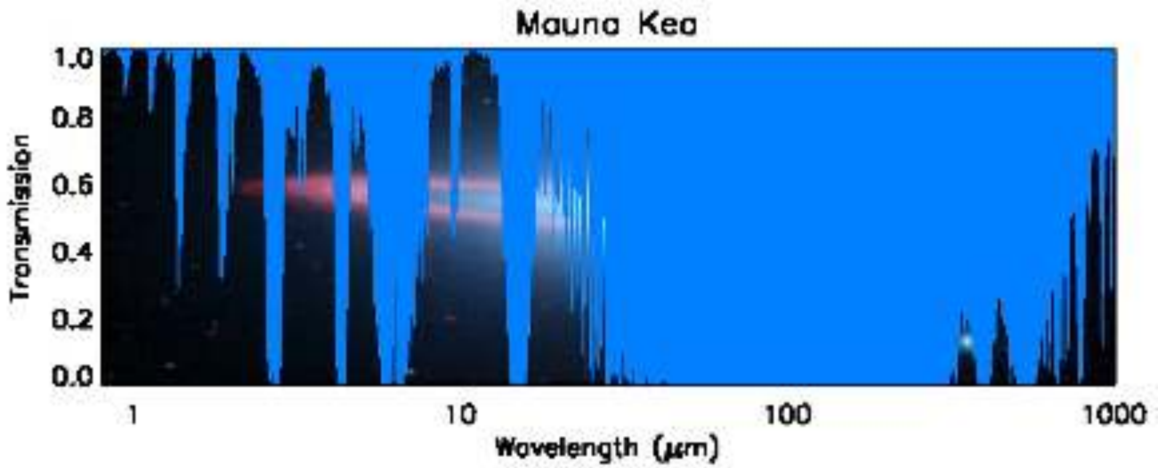
Pressure bulkhead

Scientist stations, telescope and instrument control, etc.

Telescope

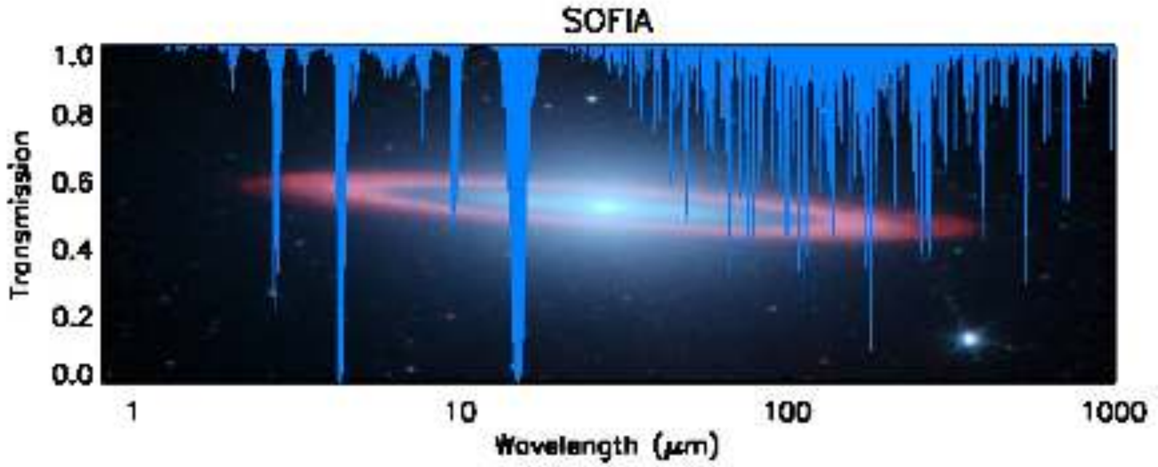
Scientific instrument

Why SOFIA: Motivation for Airborne Astronomy



For much of the infrared, the Earth’s atmosphere blocks all transmission.

- The problem is water vapor
- esp. 30-300 microns



If we can get above this water vapor, much more can be observed (average PWV is 10-20 mu, < 0.2%)

50x better than Mauna Kea
20x better than ALMA site

What is SOFIA’s science mission?

SOFIA is a primarily far-IR Observatory for studying interstellar matter cycle + feedback processes:

-atomic/molecular gas spectroscopy (high spectral res.)
collapse, outflows, shocks / heating, cooling, PDR

-dust emission broad-band, narrow-band, pol. imaging
mid-IR/far-IR sources, PAH spectroscopy, magn fields

ASTROPHYSICS → dynamics, FS line cooling (eg. C+)
ASTROCHEMISTRY→ molecules, fractionation (H2D+)

Continuing IRAS, ISO, Spitzer and Herschel observations

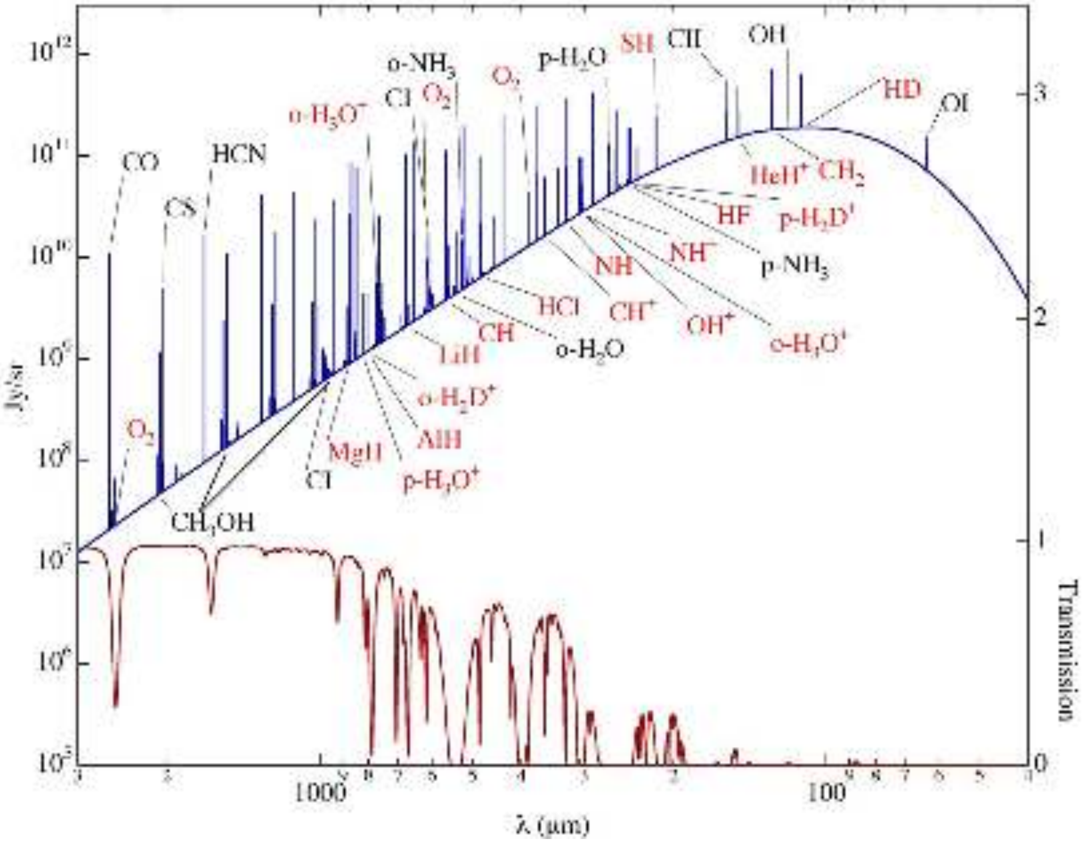
Astrochemistry (light molecules, hydrides)

- I will discuss 5 key examples: SH, OH, OD, H_2D^+, NH_3, all observed with the SOFIA GREAT instrument
- Rotational transitions in the THz range (cf. HIFI, but HIFI on Herschel could not cover those frequencies)
- mention: light hydrides as H_2 proxies, e.g. HD J=1-0 (also HF J=1-0, CH J=1-0, and C^+ for CO-dark gas)
- H20 ro-vib. transition at 6.1mu (Indriolo et al. 2015)

Importance of Far IR / Sub-mm

- Most of the key atomic/ionic and molecular tracers of the Interstellar Medium are in the far-infrared and sub-mm
- SH, OH, OD, HD
- o-NH3, p-H2D+
- CII, OI, OIII, NII

Molecular Cloud SED



Ted Bergin, 2008

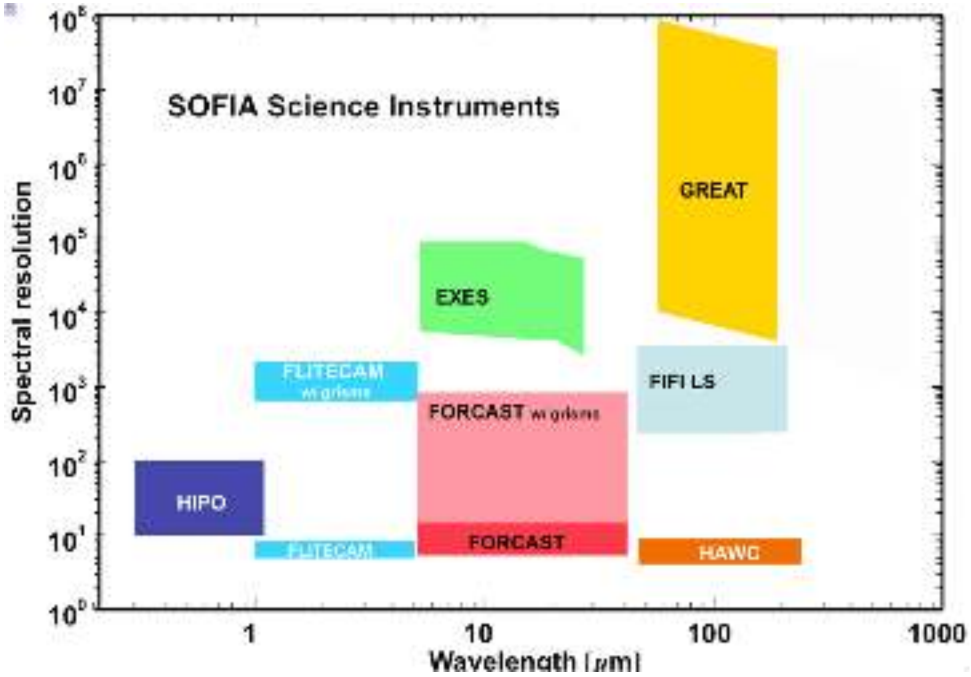
Multitude of mid-IR and far-IR instruments

SOFIA's suite of instruments comprehensively covers the wide range of wavelengths and spectral resolution (NIR, MIR, FIR; spectral resolution up to 10,000,000)

near-infrared: 1-5 micron
mid-infrared: 5-30 micron
far-infrared: 30-300 micron

SOFIA's Instrument Complement

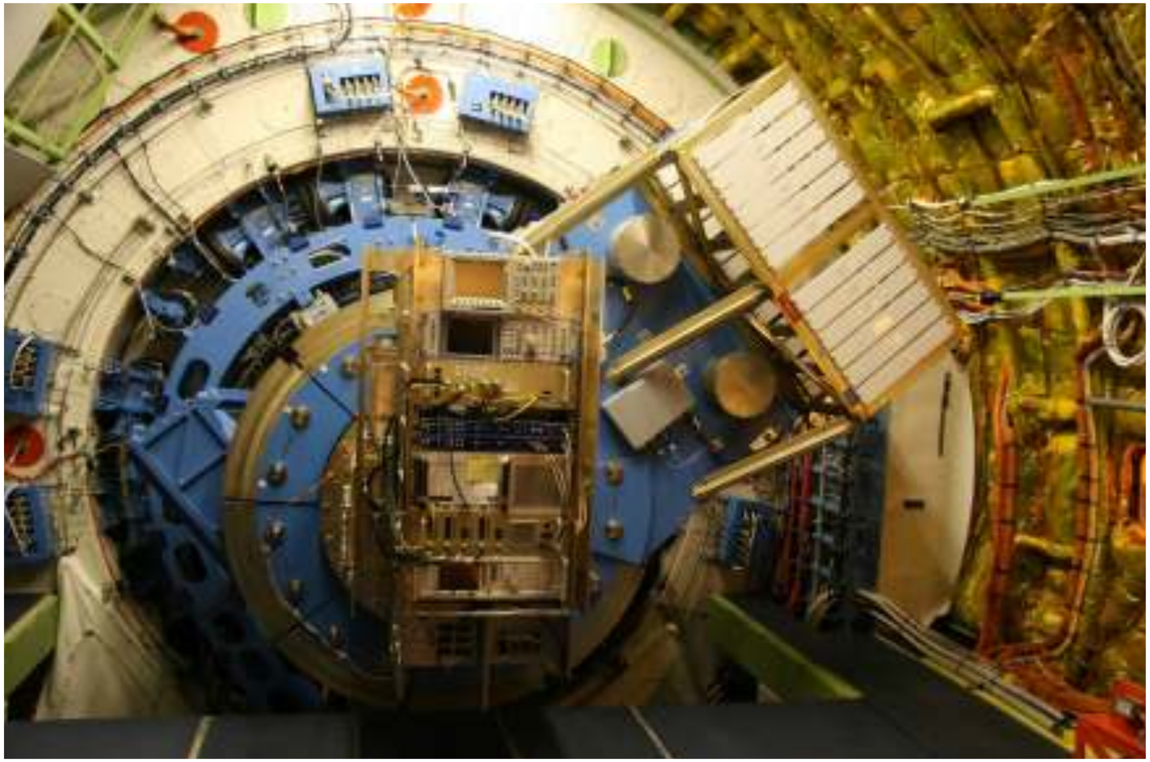
- FORCAST
- GREAT, upGREAT (LFA/HFA)
- FIFI-LS
- EXES
- FPI+
- HAWC+ (2nd gen, polarimetry)
- 3rd gen instrument selected
- (HIRMES, 25-122 microns)



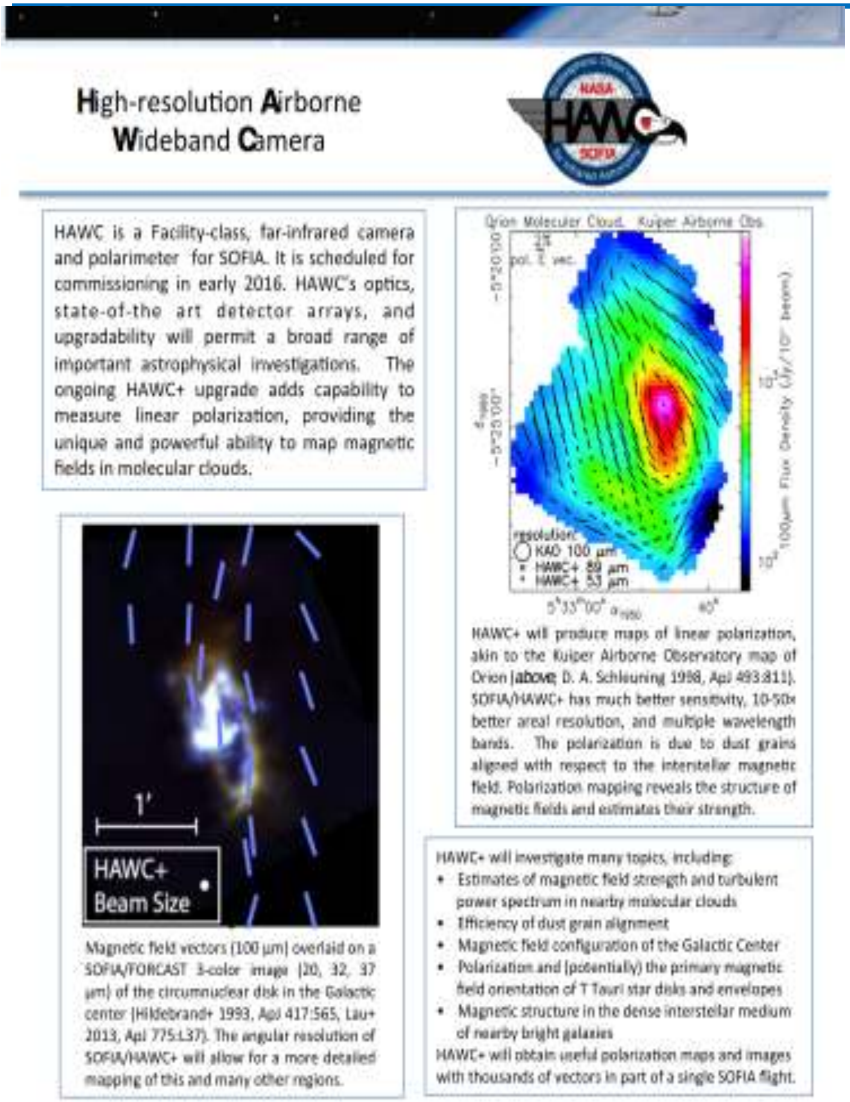
SOFIA First Science Flight (FORCAST, Dec 2010)

German REceiver for Astronomy at Terahertz frequ. (PI: R. Guesten, MPIfR/Bonn)

Channel	Frequencies [THz]	Astronomical lines of interest
low-frequency #1	1.25 – 1.50	[NII], CO(12-11), $^{(13)}$CO(13-12), HCN(17-16), H_2D^+
low-frequency #2	1.82 – 1.92	[CII], CO(16-15)
mid-frequency	2.4 – 2.7	HD, OH($^2\Pi_{3/2}$), CO(22-21), $^{(13)}$CO(23-22)
high-frequency	~ 4.7	[OI]



HAWC+ science and instrument sheet



High-resolution Airborne Wideband Camera

HAWC is a Facility-class, far-infrared camera and polarimeter for SOFIA. It is scheduled for commissioning in early 2016. HAWC's optics, state-of-the art detector arrays, and upgradability will permit a broad range of important astrophysical investigations. The ongoing HAWC+ upgrade adds capability to measure linear polarization, providing the unique and powerful ability to map magnetic fields in molecular clouds.

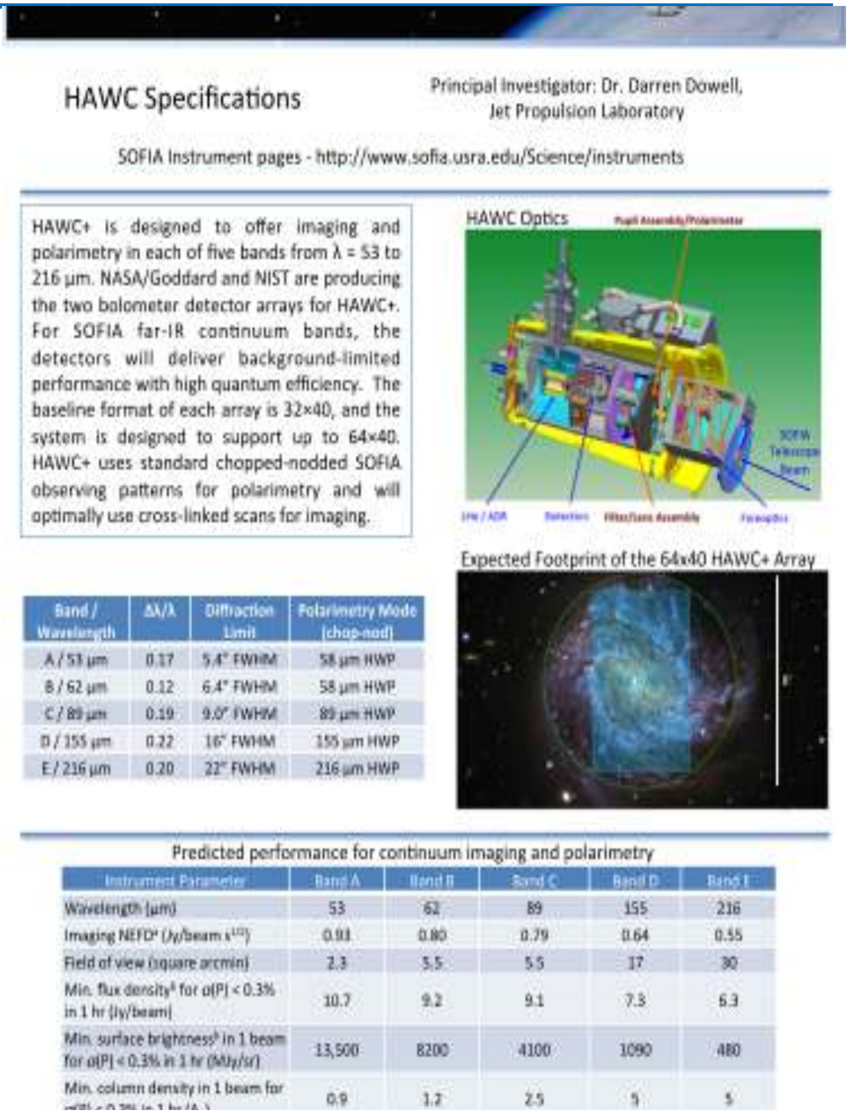
HAWC+ will produce maps of linear polarization, akin to the Kuiper Airborne Observatory map of Orion (**above**; D. A. Schleuning 1998, ApJ 493:811). SOFIA/HAWC+ has much better sensitivity, 10-50× better areal resolution, and multiple wavelength bands. The polarization is due to dust grains aligned with respect to the interstellar magnetic field. Polarization mapping reveals the structure of magnetic fields and estimates their strength.

Magnetic field vectors (100 μm) overlaid on a SOFIA/FORCAST 3-color image (20, 32, 37 μm) of the circumnuclear disk in the Galactic center (Hildebrand+ 1993, ApJ 417:565, Lau+ 2013, ApJ 775:L37). The angular resolution of SOFIA/HAWC+ will allow for a more detailed mapping of this and many other regions.

HAWC+ will investigate many topics, including:

- Estimates of magnetic field strength and turbulent power spectrum in nearby molecular clouds
- Efficiency of dust grain alignment
- Magnetic field configuration of the Galactic Center
- Polarization and (potentially) the primary magnetic field orientation of T Tauri star disks and envelopes
- Magnetic structure in the dense interstellar medium of nearby bright galaxies

HAWC+ will obtain useful polarization maps and images with thousands of vectors in part of a single SOFIA flight.



HAWC Specifications

Principal Investigator: Dr. Darren Dowell,
Jet Propulsion Laboratory

SOFIA Instrument pages - http://www.sofia.usra.edu/Science/instruments

HAWC+ is designed to offer imaging and polarimetry in each of five bands from λ = 53 to 216 μm. NASA/Goddard and NIST are producing the two bolometer detector arrays for HAWC+. For SOFIA far-IR continuum bands, the detectors will deliver background-limited performance with high quantum efficiency. The baseline format of each array is 32×40, and the system is designed to support up to 64×40. HAWC+ uses standard chopped-nodded SOFIA observing patterns for polarimetry and will optimally use cross-linked scans for imaging.

HAWC Optics

Band / Wavelength	Δλ/λ	Diffraction Limit	Polarimetry Mode (chop-nod)
A / 53 μm	0.17	5.4" FWHM	58 μm HWP
B / 62 μm	0.12	6.4" FWHM	58 μm HWP
C / 89 μm	0.19	9.0" FWHM	89 μm HWP
D / 155 μm	0.22	16" FWHM	155 μm HWP
E / 216 μm	0.20	22" FWHM	216 μm HWP

Expected Footprint of the 64x40 HAWC+ Array

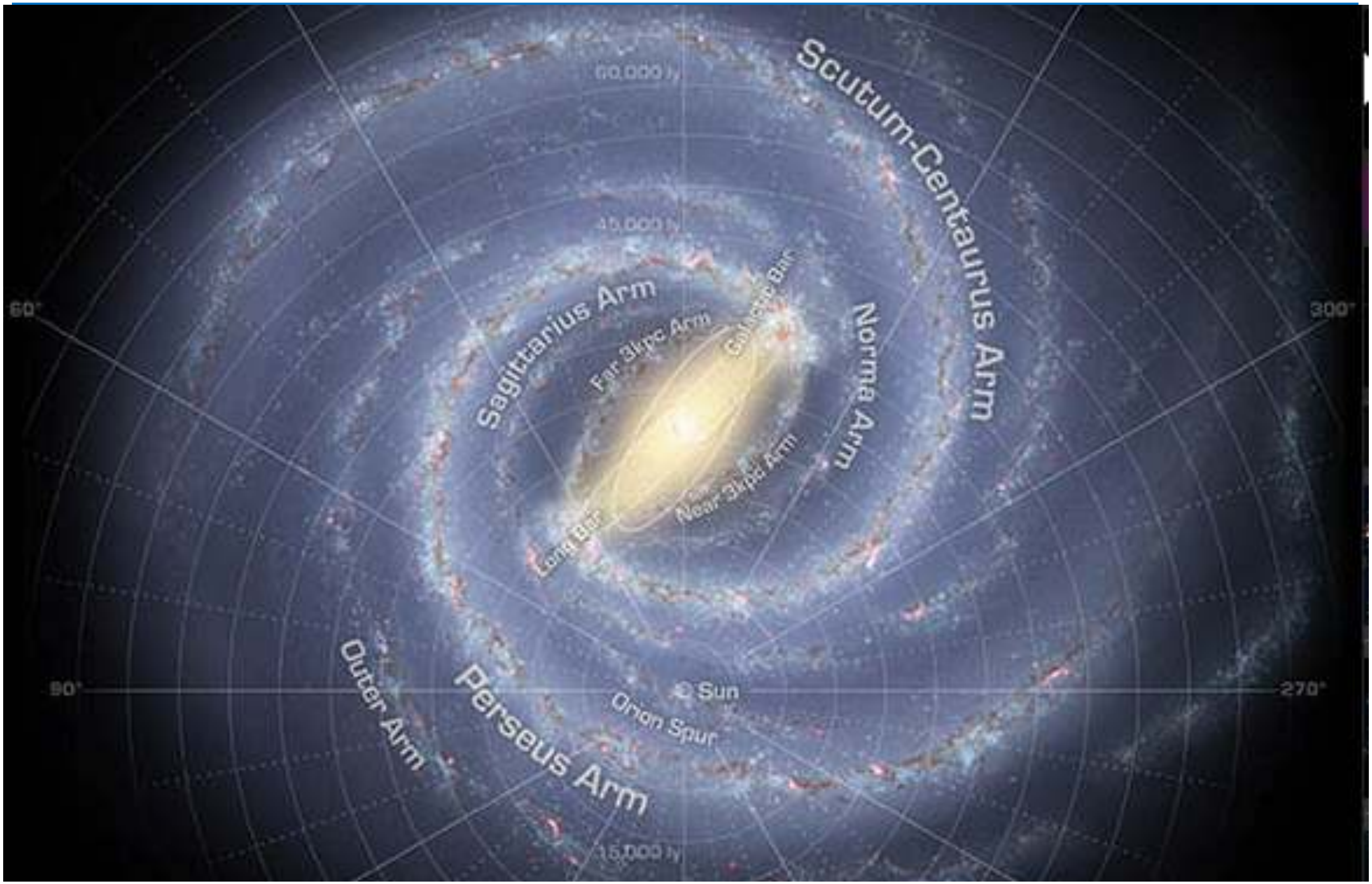
Predicted performance for continuum imaging and polarimetry

Instrument Parameter	Band A	Band B	Band C	Band D	Band E
Wavelength (μm)	53	62	89	155	216
Imaging NEFD[a] (Jy/beam $s^{1/2}$)	0.93	0.80	0.79	0.64	0.55
Field of view (square arcmin)	2.3	5.5	5.5	17	30
Min. flux density[b] for σ(P) < 0.3% in 1 hr (Jy/beam)	10.7	9.2	9.1	7.3	6.3
Min. surface brightness[b] in 1 beam for σ(P) < 0.3% in 1 hr (MJy/sr)	13,500	8200	4100	1090	480
Min. column density in 1 beam for	0.9	1.2	2.5	5	5

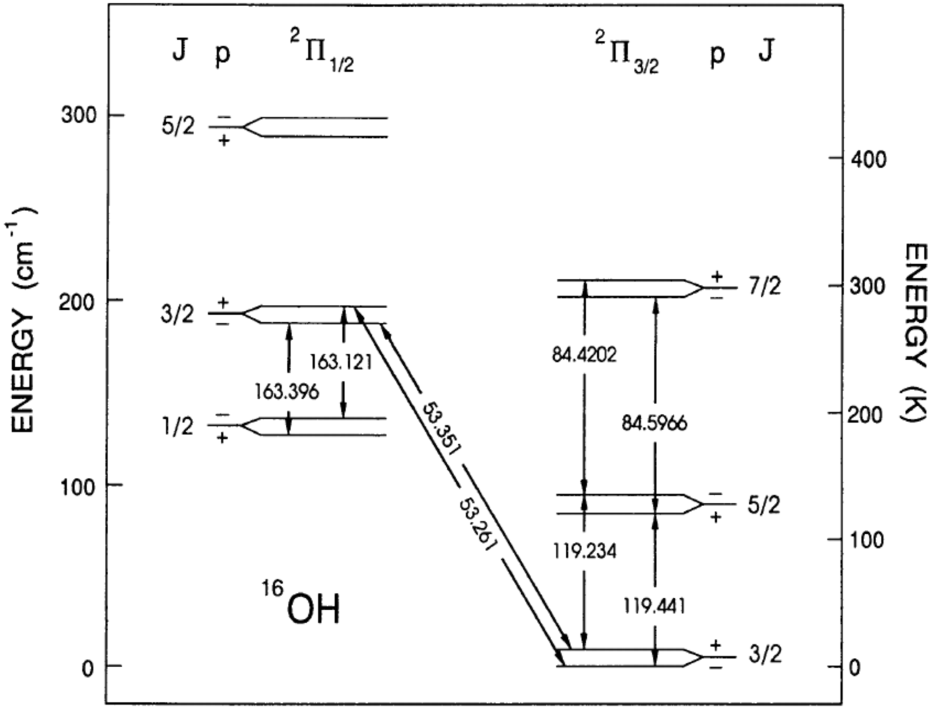
Instrument Overview

- HIRMES is a direct detection spectrometer covering the spectral range from 25 to 122 μm (H2 and HD)
- There are four spectroscopic modes to HIRMES
  - High-res mode (FPI) R ~ 100,000
  - Mid-res mode (FPI) R ~ 10,000
  - Low-res mode (grating) R ~ 600
  - Imaging spectroscopy mode (FPI): R ~ 2000
- The modes are optimized to deliver the maximum sensitivity achievable with SOFIA. HIRMES uses:
  - Background limited bolometers
  - Combination of Fabry-Perot Interferometers and gratings

face-on view of our Milky Way Galaxy

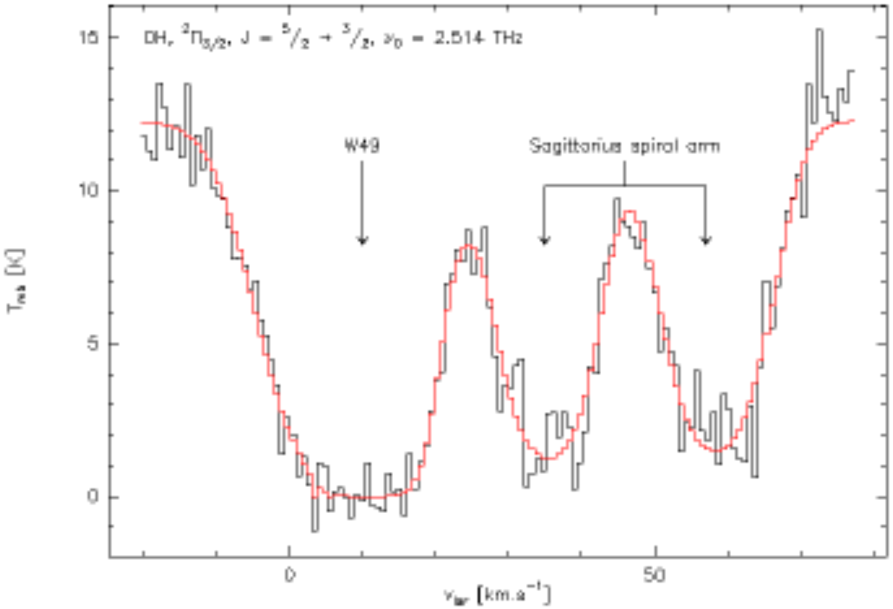


GREAT SOFIA Science beyond Herschel: 2.5 THz **OH absorption**



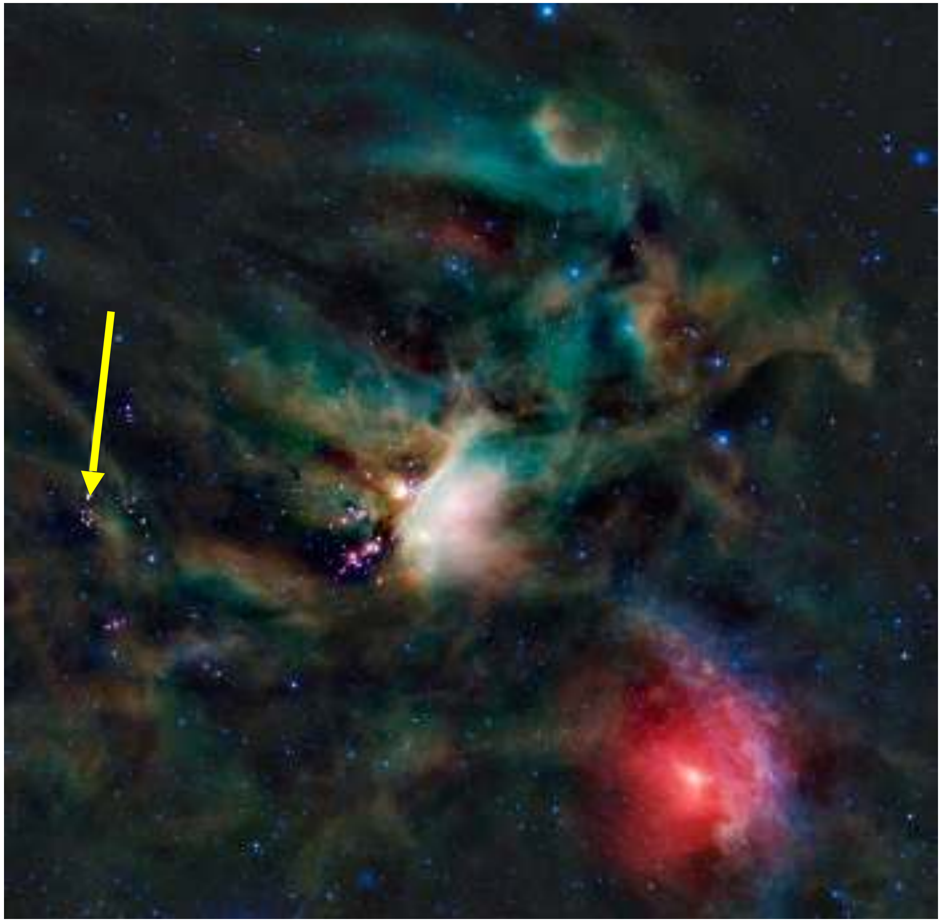
First >2 THz spectroscopy from SOFIA

- OH ground-state absorption against W49N
- spectral features of Sagittarius spiral arm
- Optically thick, but 18OH optically thin
- possibility to study oxygen gas abundance



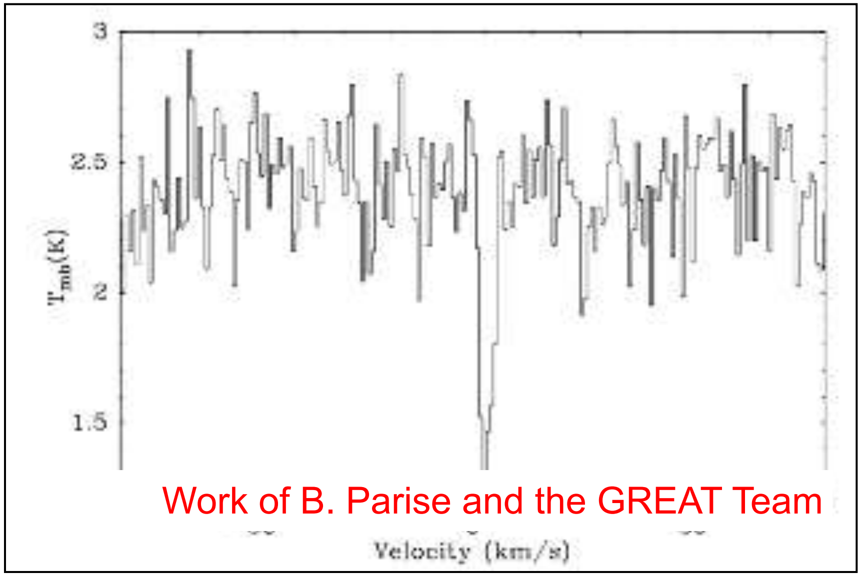
- discovery of ^{18}OH towards W49N core (Wiesemeyer et al. 2012, A&A 542, L7)

Detection of OD Toward the Low-Mass Protostar IRAS16293



Detection of the OD ground state line at 1.39 THz in absorption (inaccessible to Herschel HIFI) toward the line-of-sight of a low-mass protostar.

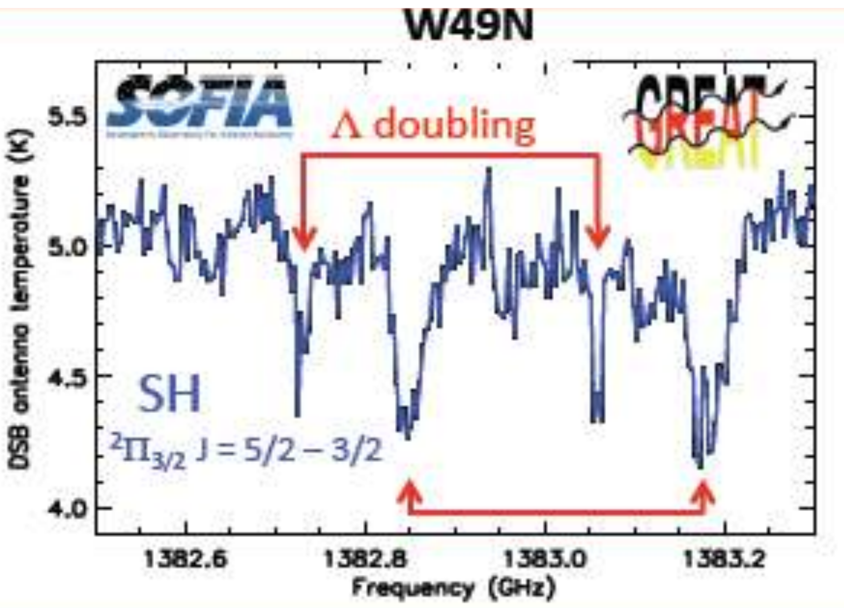
First detection of OD outside of the solar system.



Work of B. Parise and the GREAT Team

Analysis is ongoing, but high OD abundance suggests a higher than predicted OH fractionization

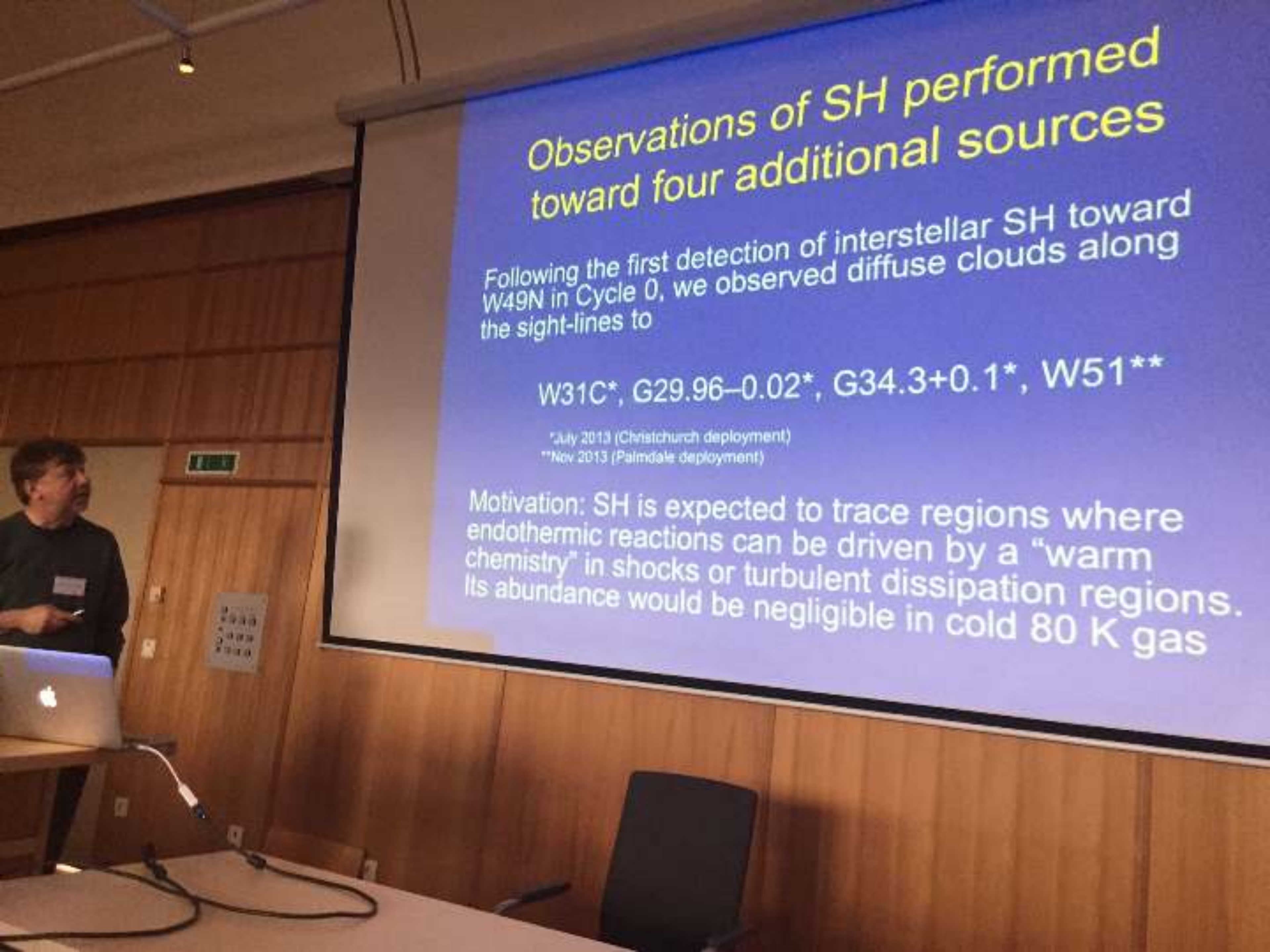
GREAT THz early science highlights



Neufeld 2012: discovery of interstellar mercapto radical in absorption against W49N.

SH is endothermic (9800 K): Evidence for warm chemistry

(more detections of SH, e.g. in abs. against G34.3, W51)



Observations of SH performed toward four additional sources

Following the first detection of interstellar SH toward W49N in Cycle 0, we observed diffuse clouds along the sight-lines to

W31C*, G29.96–0.02*, G34.3+0.1*, W51**

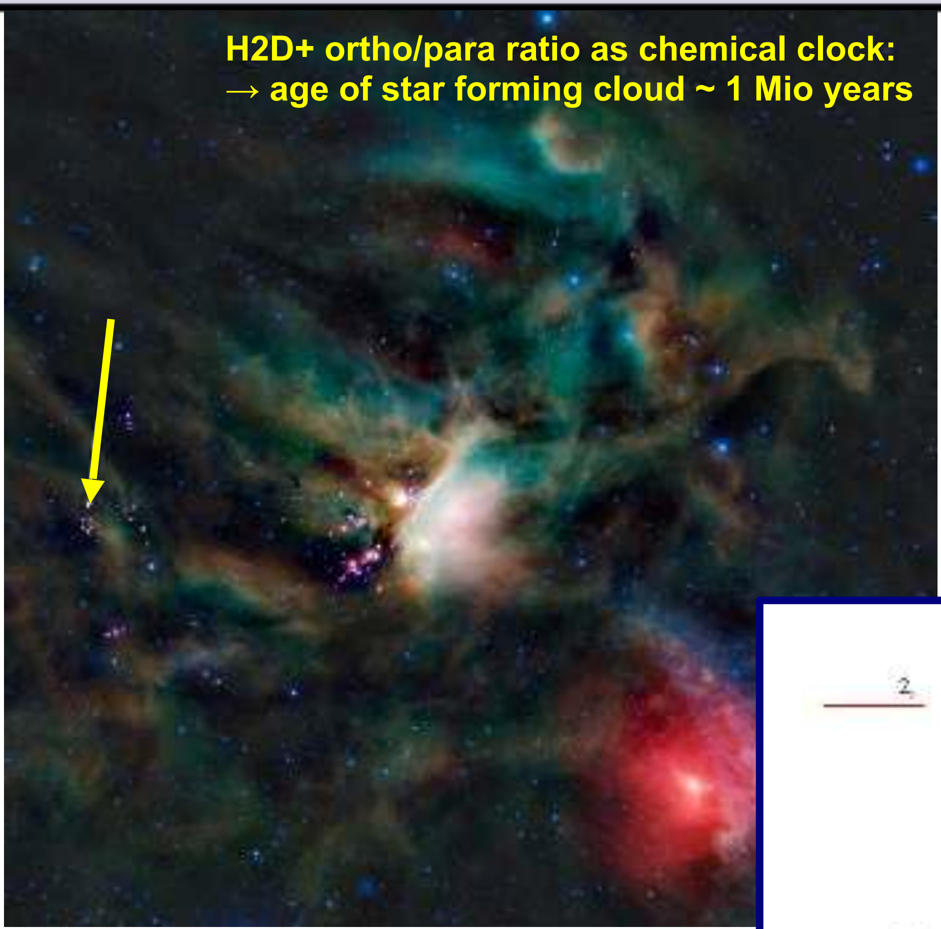
*July 2013 (Christchurch deployment)
**Nov 2013 (Palmdale deployment)

Motivation: SH is expected to trace regions where endothermic reactions can be driven by a "warm chemistry" in shocks or turbulent dissipation regions. Its abundance would be negligible in cold 80 K gas

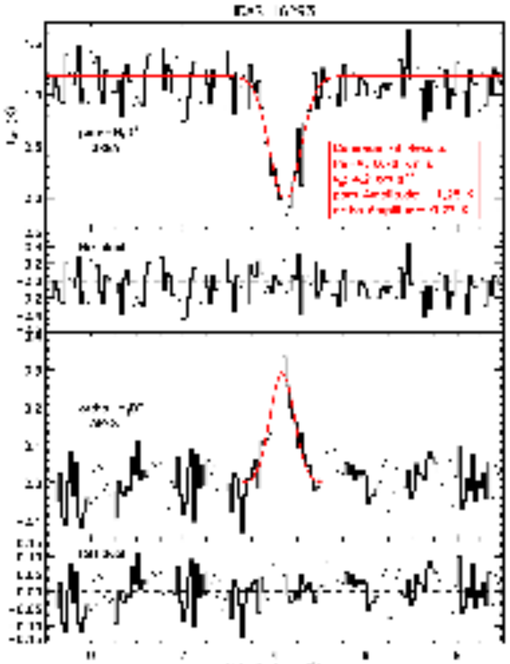
What is lambda doubling?

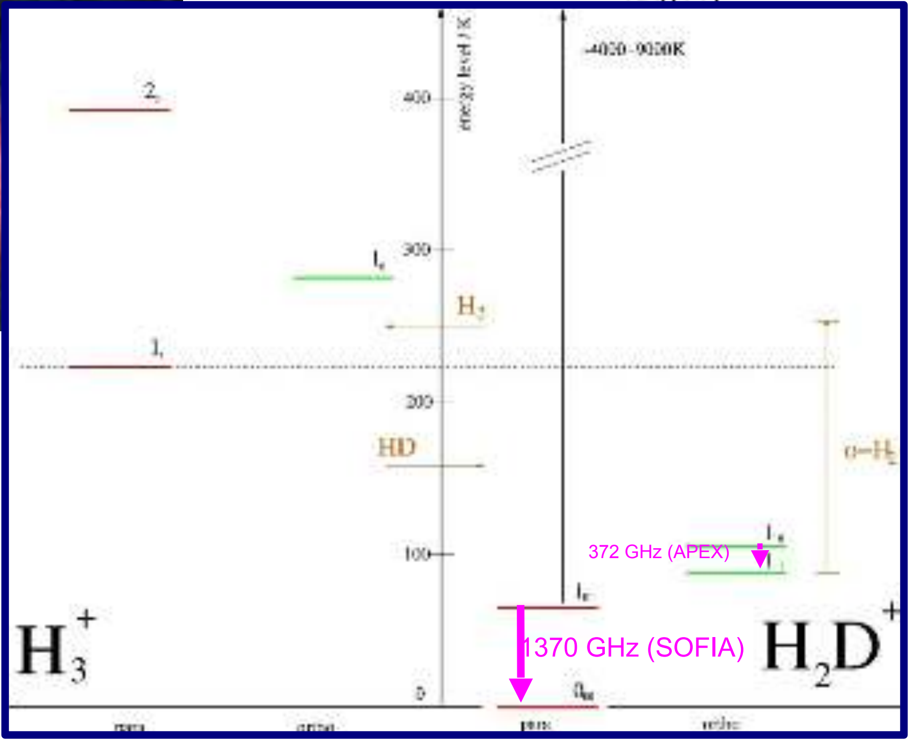
- Total electronic orbital angular momentum L and spin S projected along intermolecular axis
- CH, OH, SH hetero-nuclear molecules: L = 1, S=1/2
- Slight difference in energy, symmetry broken
- Hyperfine structure on top of lambda doubling
- SH: lambda doubling gs/1st amounts to 72 km/s
- OH: gs lambda doubling yields 18 cm radio lines
- Note the case of HF: S=0, no lambda doubling

GREAT: first firm detection of para H_2D^+ 1370 GHz



H2D+ ortho/para ratio as chemical clock:
→ age of star forming cloud ~ 1 Mio years





$$
\begin{aligned}
H + H &\xrightarrow{\text{dust}} H_2 \\
H + \text{cr}/\gamma &\longrightarrow H^+ + e \\
C + \text{cr}/\gamma &\longrightarrow C^+ + e \\
\\
H_2 + H^+ &\longrightarrow H_3^+ \\
&\longrightarrow H + H + H^+ \\
H_3^+ + HD &\longrightarrow \boxed{H_2D^+} + H_2 \\
\\
H_2 + C^+ &\longrightarrow CH^+ + H \\
CH^+ + O &\longrightarrow CO + H^+ \\
OH + C &\longrightarrow CO + H
\end{aligned}
$$

Nature paper:
Brünken et al, 2014

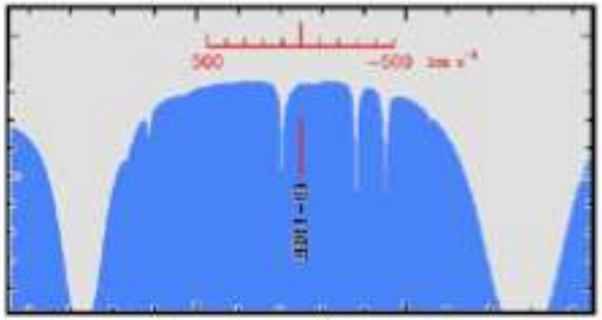
NOTE:
KAO Betz et al.
tentative detection Orion
T_{rec}=30000 K

ortho/para (parallel/antiparallel spins)
ortho-para ratio of H_2 from H_2D^+
can be used as a chemical clock:
more and more para from initial ortho
due do collisional exchange reactions

meanwhile, even HD_2^+ detected !
likely an even better chemical clock
new way to calibrate cloud core ages

Cold Molecular Hydrogen using HD

SOFIA will study deuterium in the galaxy using the ground state HD line at 112 microns. This will allow determination the cold molecular hydrogen abundance.



Atmospheric transmission around the HD line at 40,000 fe

Deuterium in the universe is created in the Big Bang.

Measuring the amount of cold HD (T<50K) can best be done with the ground sta rotational line at 112 microns accessible with SOFIA (HD in emssion and in absorptior

.

Detections with ISO means that GREAT high resolution spectroscopic study is possible

HD has a much lower excitation temperature and a dipole moment that almo compensates for the higher abundance of molecular hydrogen.

As pointed out by Bergin and Hollenbach, HD traces the cold molecular hydrogen

Summary

- Light hydrides are beginning of astrochemistry including warm chemistry (SH) and deuterium fractionation (OD) and chemical clocks (H2D+)
- light hydrides to study astrophysical processes eg. protostellar infall (NH3), protopl disks (HD)
- Light hydrides trace atomic and molecular gas, including the amount of H2 via proxies like HD, HF
- SOFIA plays a key role in this (GREAT, HIRMES)
- Astrochemistry and Astrophysics often intertwined

EXES Commissioning : Water in abs. in AFGL 2591

10 Mo protostar in Cygnus

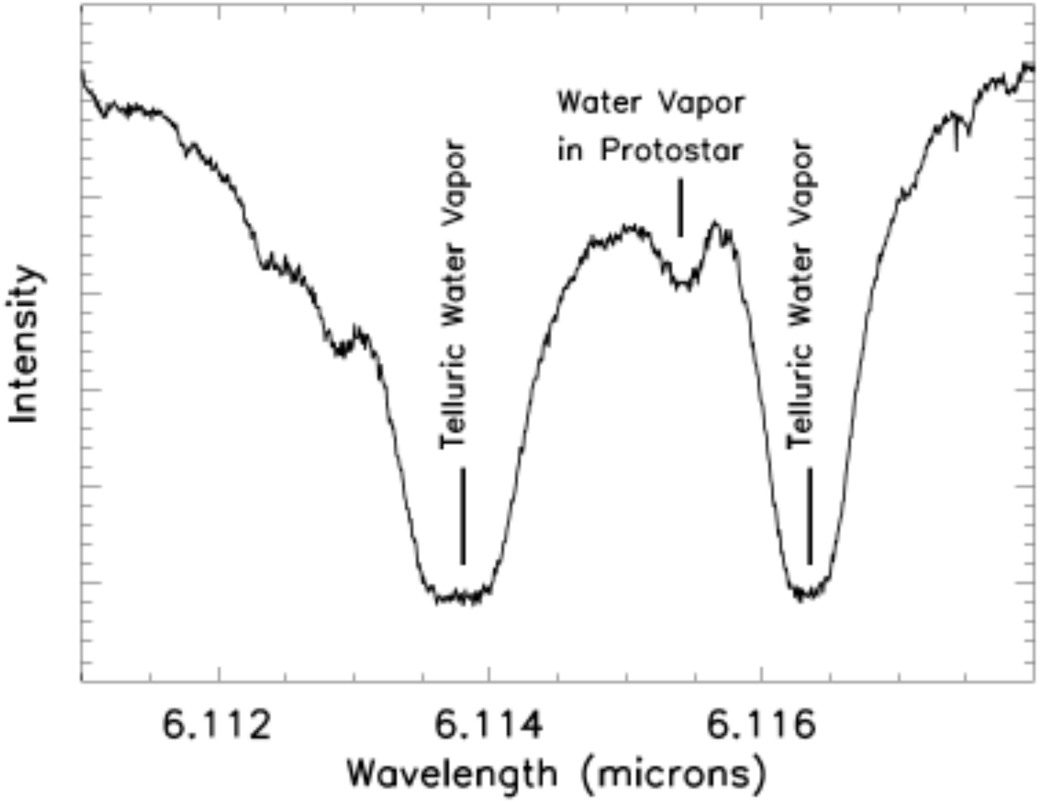
0(0,0)→1(1,1) H2O transition
and other ro-vib. water lines

unobservable from ground

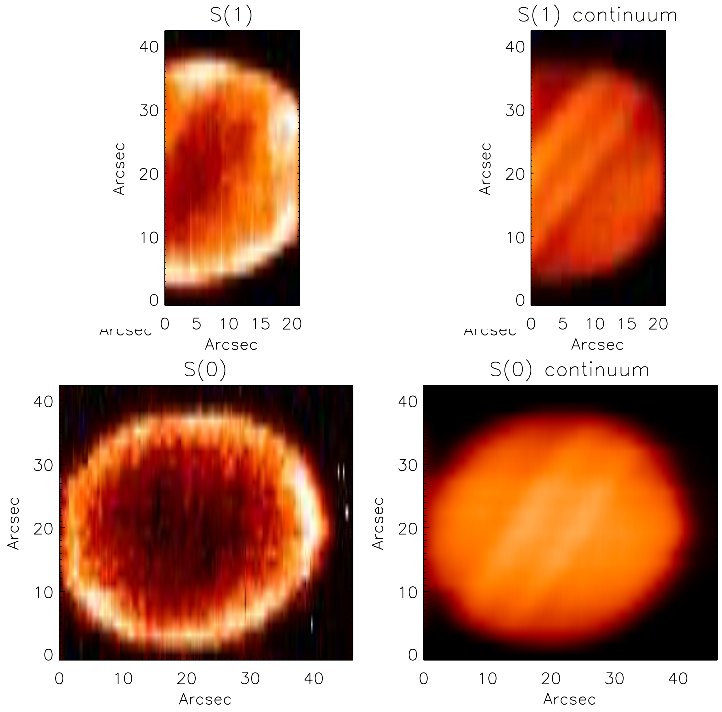
T ~ 500 K, likely produced by
evaporation of grain mantles
(base of molecular outflow)

improves on R=2000 ISO studies

paper: Indriolo et al. 2015, ApJ



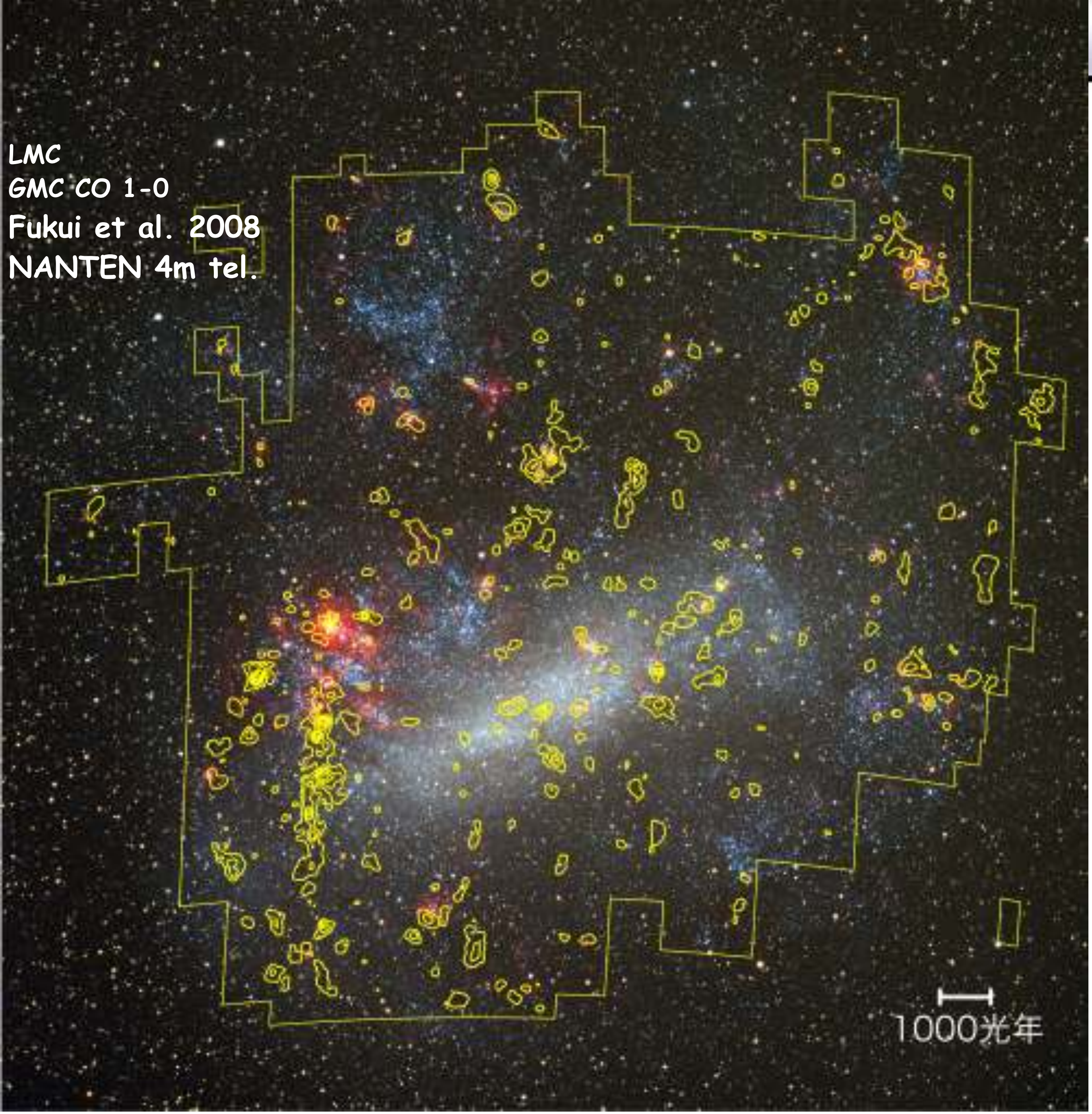
EXES Commissioning Science: Ortho/para H_2 maps on Jupiter



- spectral maps by stepping slit position across extended source
- Jupiter stratospheric H2 emission: limb brightening
- S(0) at 28.3 mu unobservable from ground
- S(1)//S(0) gives temperature, with long latency
- Combined with other temperatiure measurements, implies convective motion into the stratosphere and circulation

unpublished

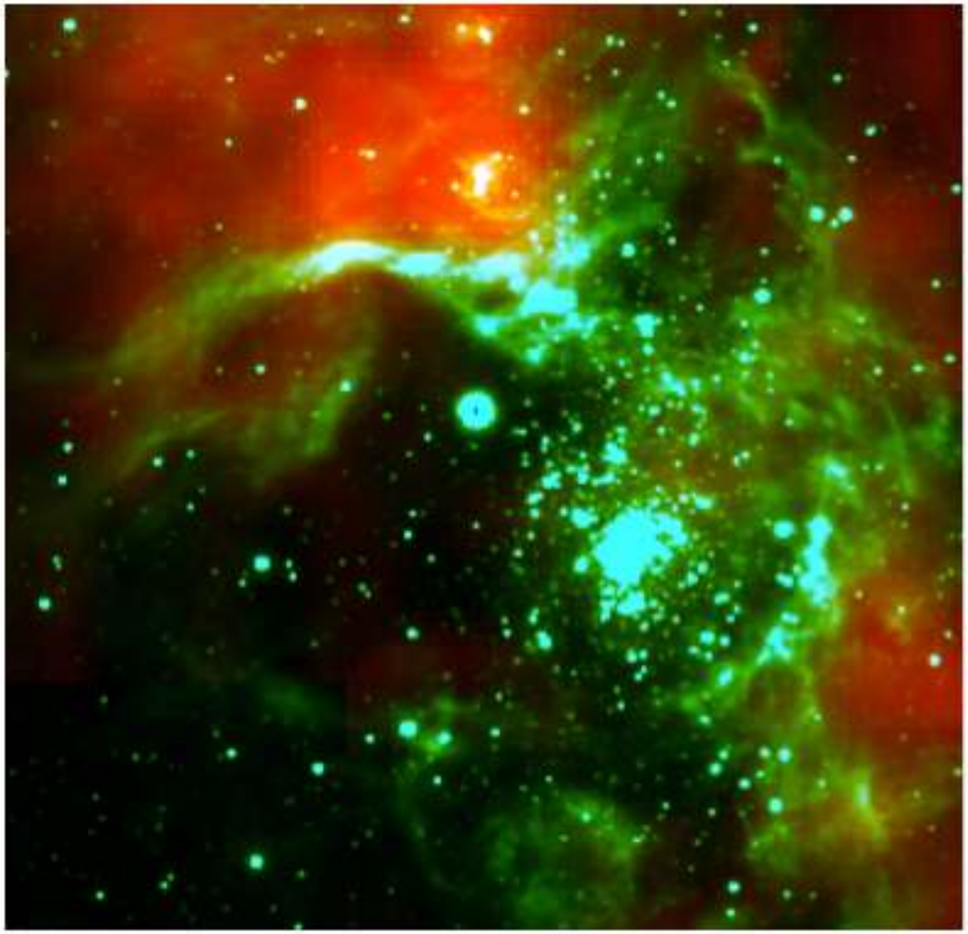
convective motion into the Stratospheric emission from H_2; limb brightening



The question
of CO-dark H2 gas

C+ is a key tracer

CII (red) in 30 Dor in LMC



www.sofia.usra.edu

Next SOFIA event:
Ringberg Workshop
Jan 20-23, 2019

Gracias!
Questions?

On the SOFIA plane in flight

HIRMES

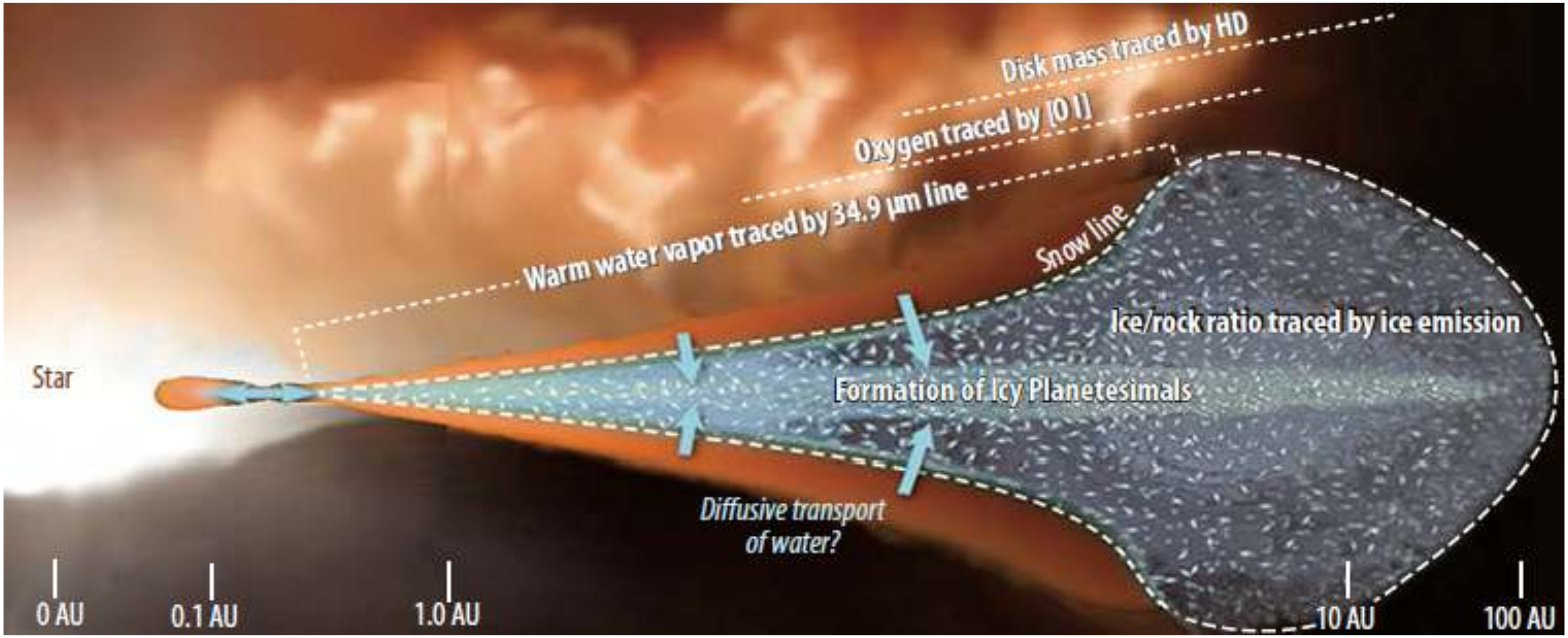
HIgh Resolution Mid-infrarEd Spectrometer

PI: Harvey Moseley (GSFC)
Deputy PI: Alexander Kutyrev (GSFC)
Project Manager: Wen-Ting Hsieh (GSFC)

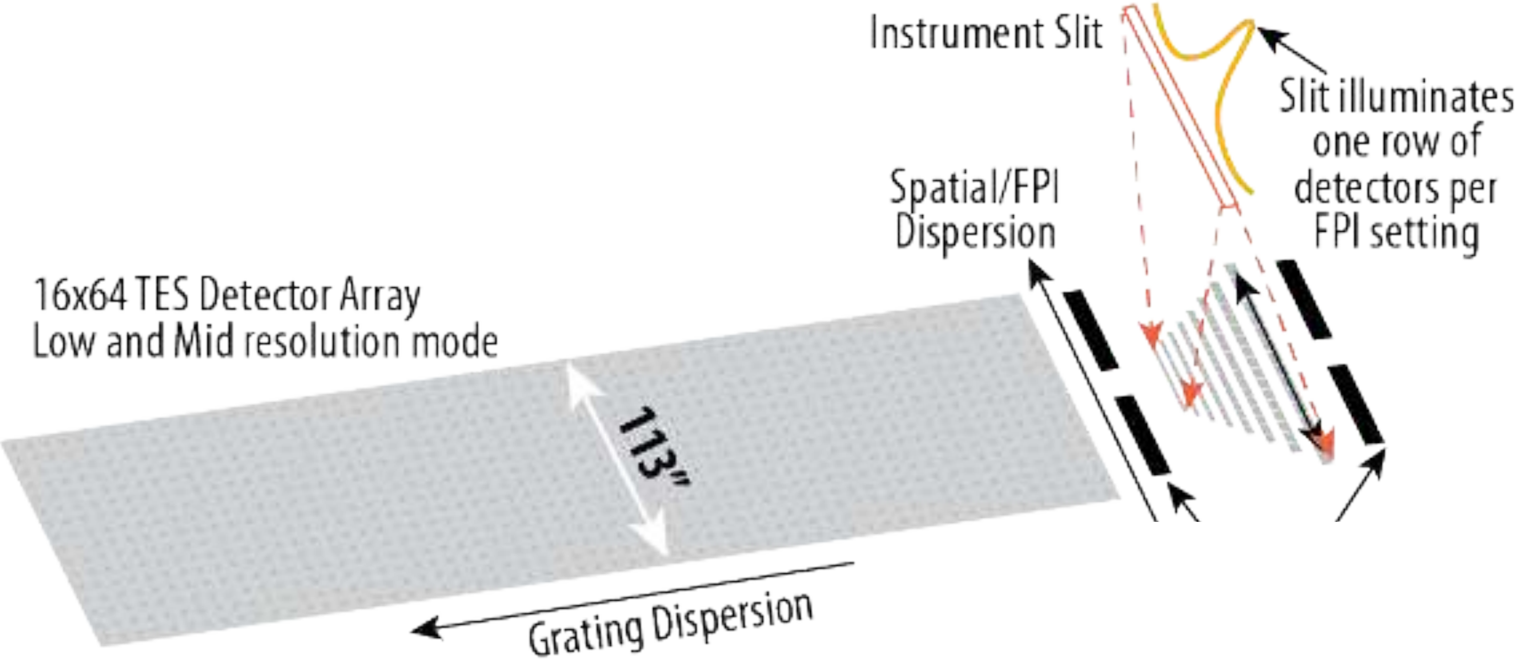
Science team
D. Neufeld (JHU)
G. Melnick (SAO)
D. Watson (Rochester)
G. Stacey (Cornell University)
K. Pontoppidan (JHU)
E. Bergin (Univ. of Michigan)
J. Staguhn (JHU/GSFC)
S. Rinehart (GSFC)

In 2019: HIRMES (High Resolution Mid-InfrarEd Spectrometer)

- Wavelength range: 25µm – 122µm; diffraction limited
- Variety of observing modes
  - Spectroscopy with R=600 to R=100,000
  - Spectral imaging capabilities for a few selected emission lines



The HIRMES Focal Plane



Instrument Slit

Slit illuminates one row of detectors per FPI setting

Spatial/FPI Dispersion

16x64 TES Detector Array
Low and Mid resolution mode

113"

Grating Dispersion

MDLF: High Resolution – R = 10^5

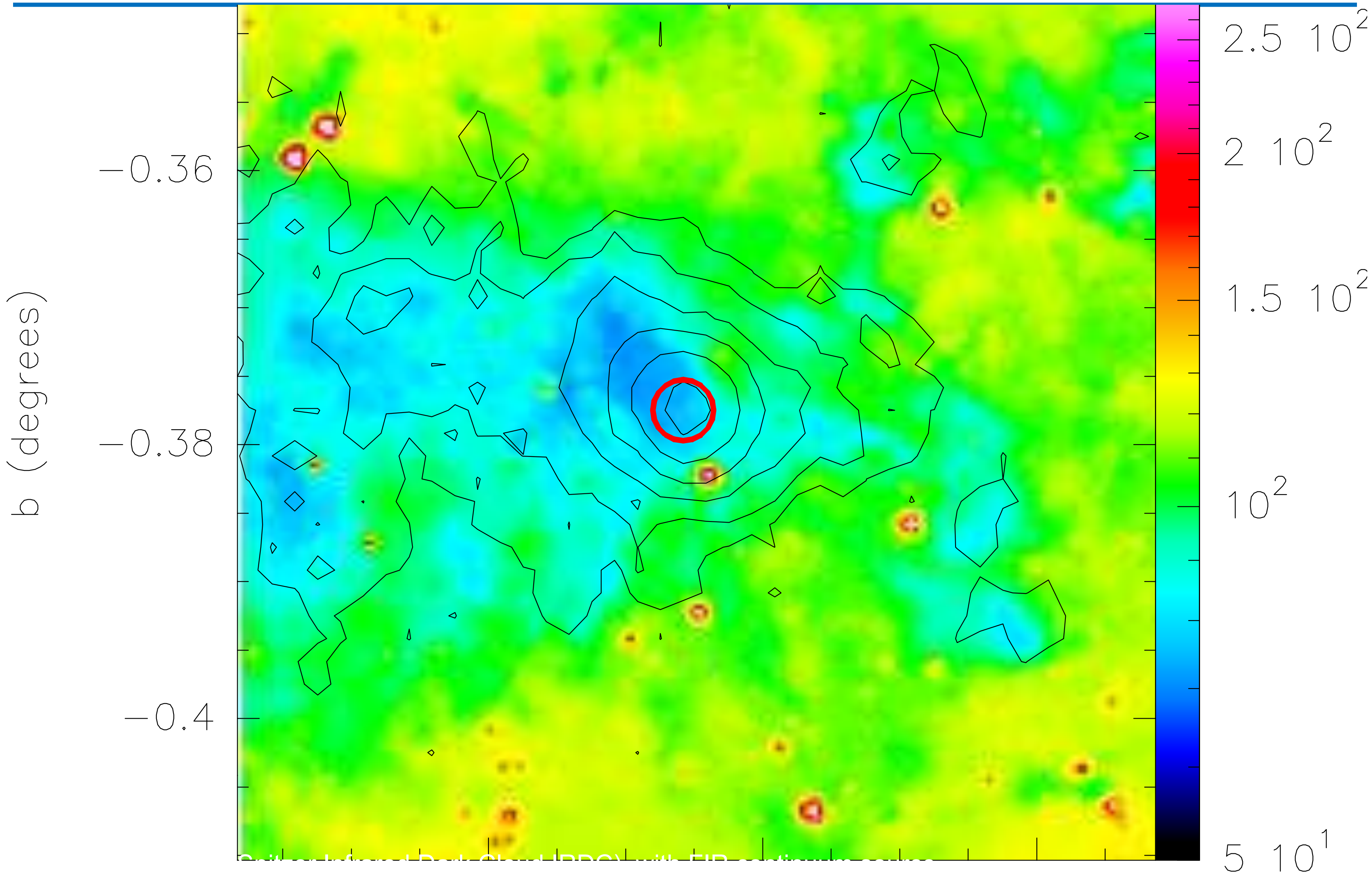
Line/ wavelength (μm)	V_{obs} (km/s)	Pixel	η_{atm} (%)	ε_{warm} (%)	η_{cold} (%)	P_{pixel} (Watts)	NEP ($W/Hz^{1/2}$)	η_{pix} (%)	NEF ($W/m^2/Hz^{1/2}$)	MDLF (W/m^2, 5σ/hr)
H_2O 34.9823	-40	2.9	94	20	35	8.4E-15	1.34E-17	60	2.4E-17	1.4E-18
	+20		84	28		2.4E-14	2.22E-17		4.4E-17	2.6E-18
	+40		93	20		8.5E-15	1.34E-17		2.4E-17	1.4E-18
[OI] 63.1837	-40	5.2	65	43	32	1.4E-14	1.33E-17	60	3.7E-17	2.2E-18
	0		62	45		1.5E-14	1.36E-17		4.0E-17	2.4E-18
	+40		59	48		1.6E-14	1.40E-17		4.4E-17	2.6E-18
HD 112.0725	-40	9.2	58	48	37	1.3E-14	1.00E-17	60	2.8E-17	1.6E-18
	0		58	48		1.3E-15	1.01E-17		2.8E-17	1.6E-18
	+40		56	50		1.4E-15	1.02E-17		3.0E-17	1.7E-18

These are for point sources!

Astrophysics (star formation, collapse, outflows)

Part 2

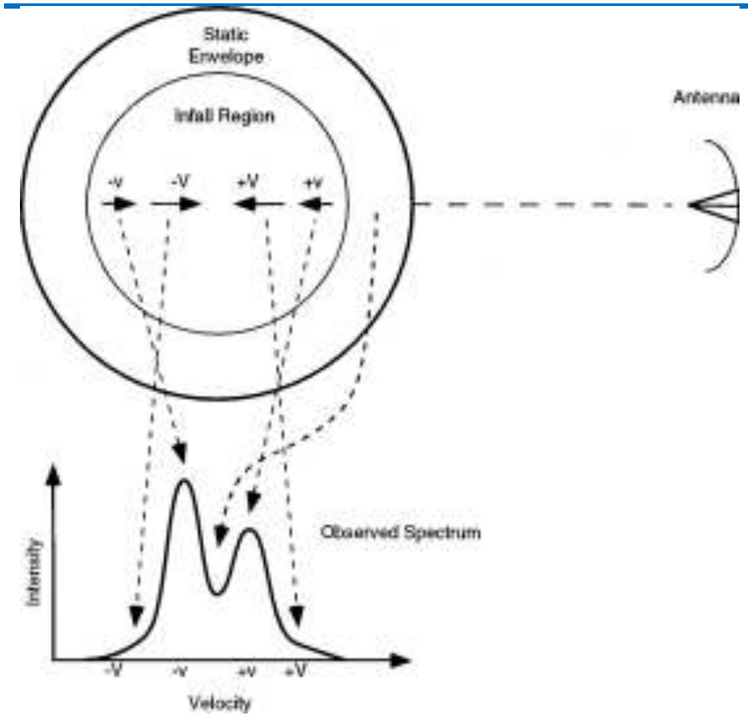
ATLASGAL submm clump G23.21 (Spitzer IRDC)

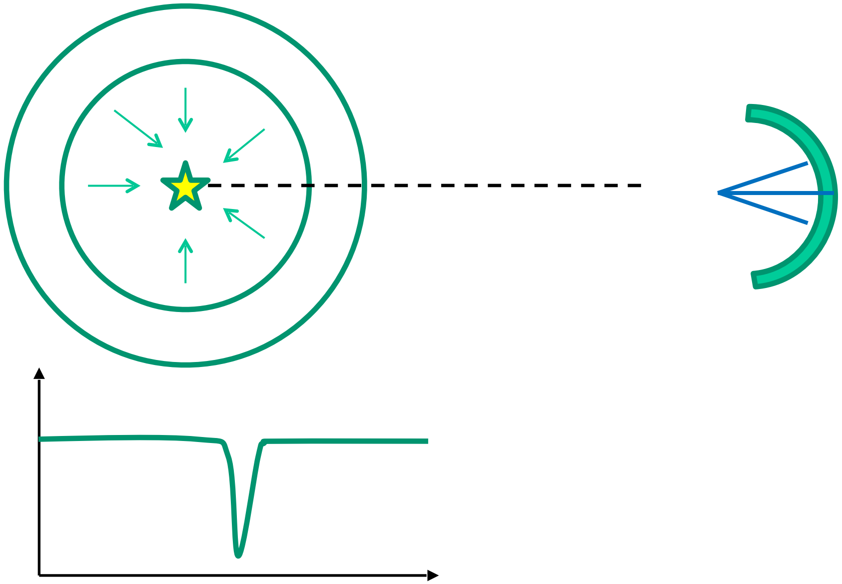


Spitzer Infrared Dark Cloud (IRDC) with FIR continuum source

Using THz Lines probing collapse

esp. NH3 at 1.81 THz, Wyrowski 2015

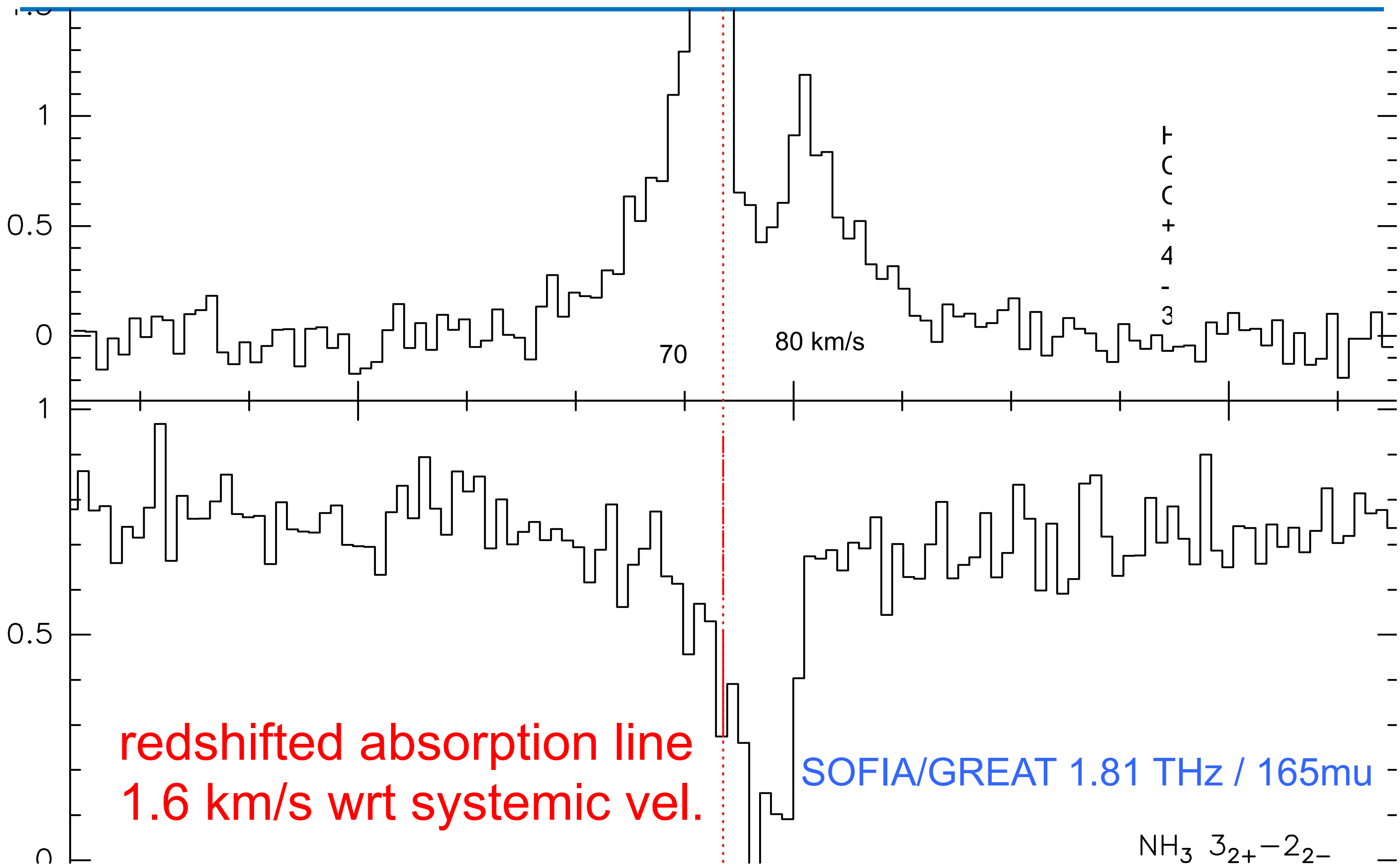




Interpretation of infall using optically thick emission lines is difficult, due to complicated radiative transfer and possible contributions from outflowing molecular gas.

Absorption measurements against a FIR continuum source are much more strainghtforward to interpret. Infall (“collapse”) is the Holy Grail of star formation, and SOFIA THz absorption allows us to measure the gas infall rate (“accretion rate”) and infall speed (in units of free-fall)

G23.21 gas clump: protocluster infall



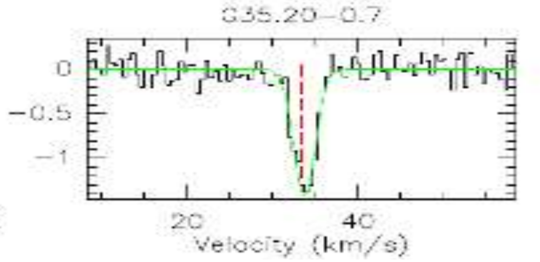
redshifted absorption line
1.6 km/s wrt systemic vel.

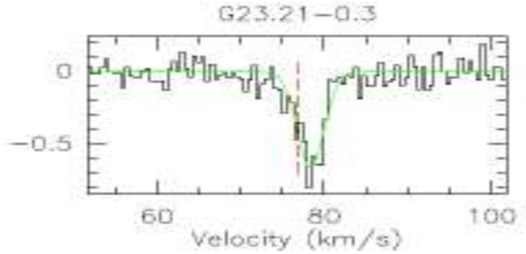
SOFIA/GREAT 1.81 THz / 165mu

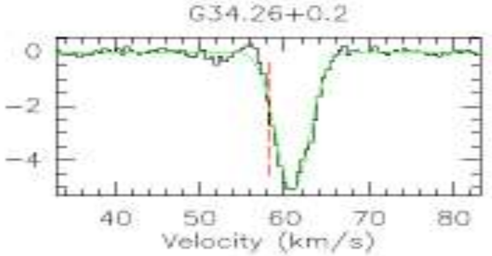
1.8 THz Detection of Infall. . .

H. Zinnecker, SOFIA, Stuttgart, Germany

More examples of 1.81 THz absorption lines
against bright FIR continuum sources (infall)

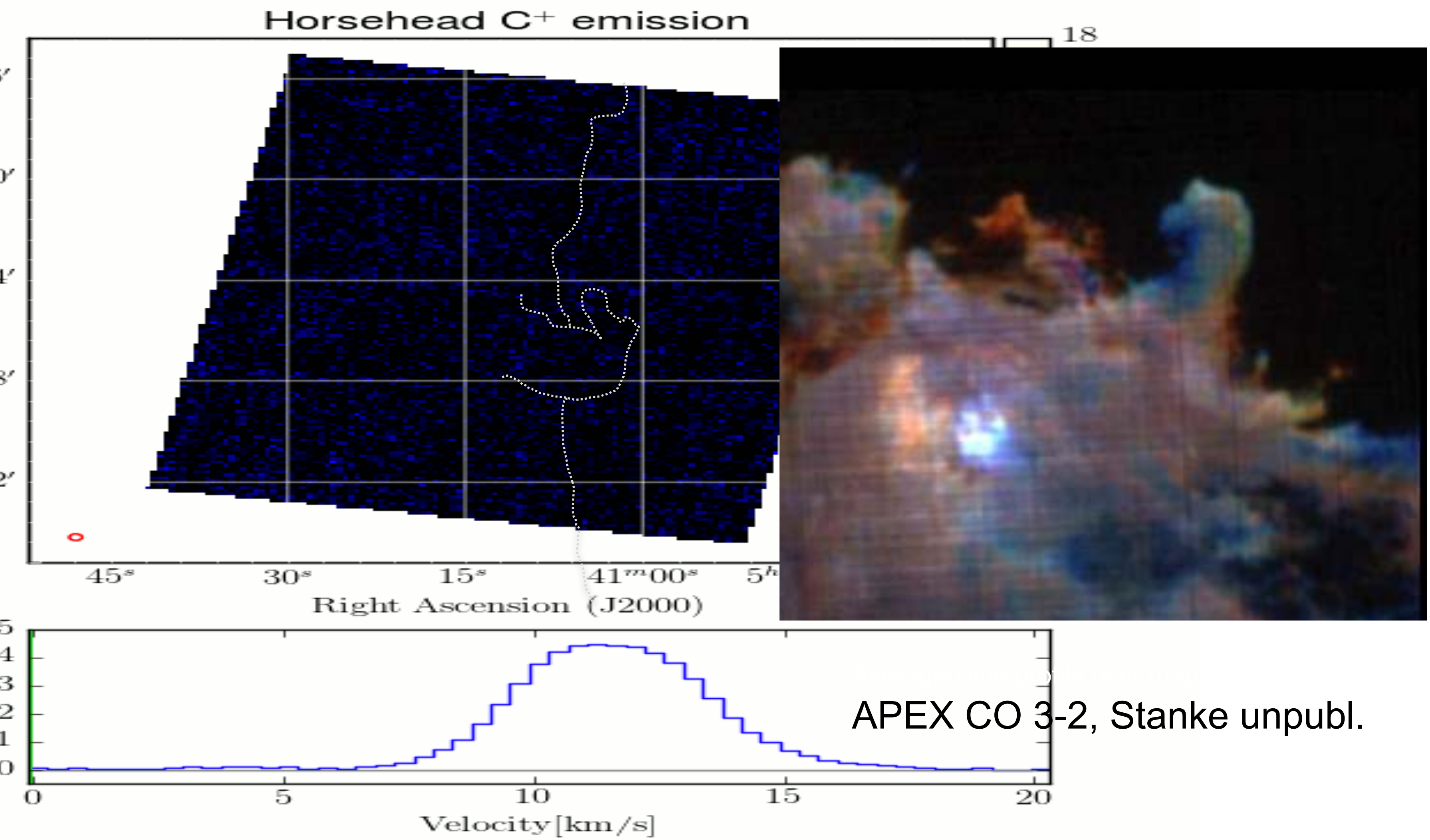






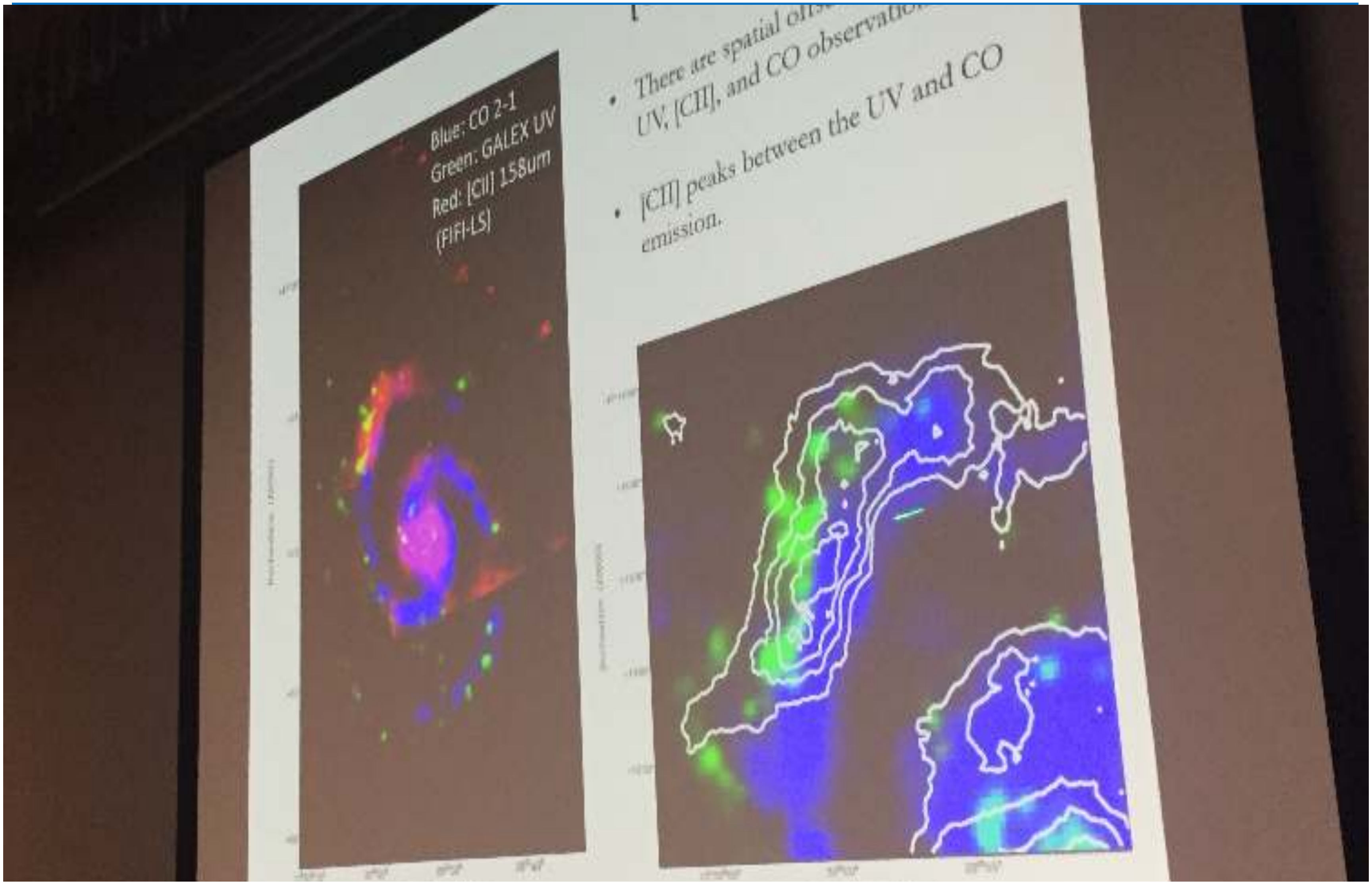
DDT Demo Observation

upGREAT [C II] map vs. APEX CO 3-2 map



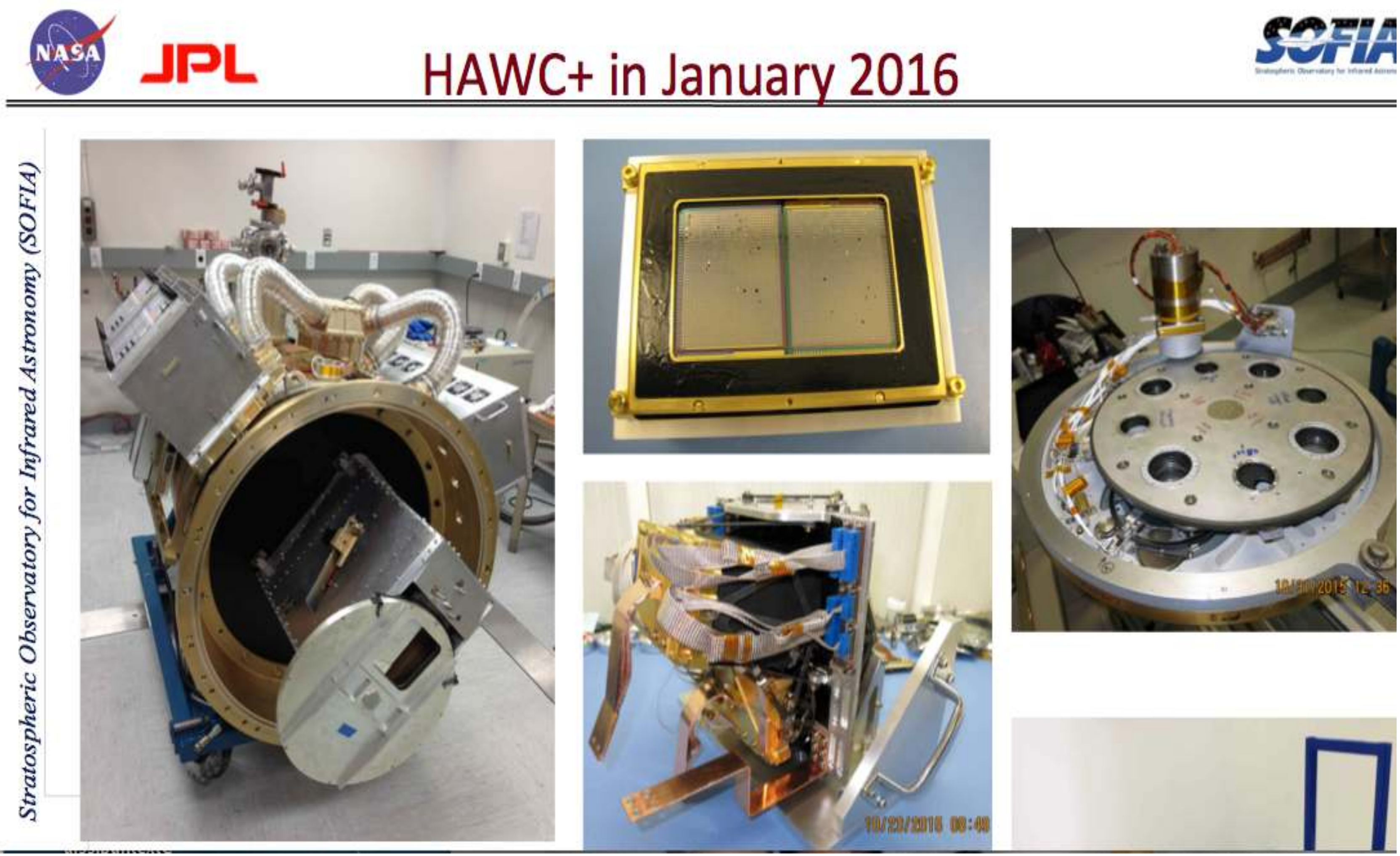
APEX CO 3-2, Stanke unpubl.

M51: CII peaks between UV and CO



- There are spatial o UV, [CII], and CO observatio
- [CII] peaks between the UV and CO emission.

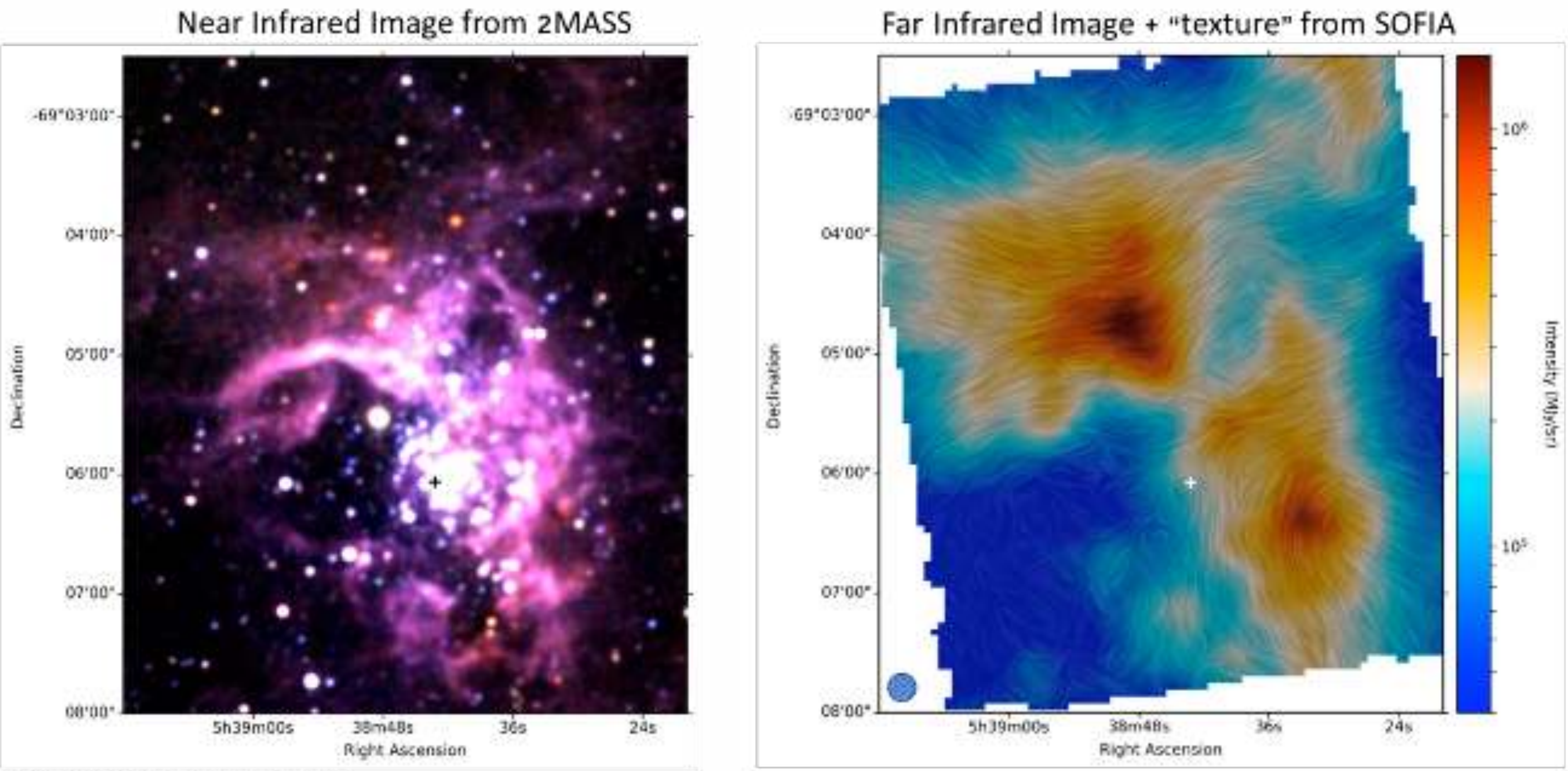
HAWC+ hardware



HAWC+ in January 2016

Stratospheric Observatory for Infrared Astronomy (SOFIA)

30 Dor: Far-IR polarimetric image



+ location of R136a, a starburst region

30 Doradus is one of the nearest laboratories to test the laws of star formation under extreme conditions. Near-IR shows older stars. Far-IR photometry reveals newer star forming regions. Never before seen magnetic fields structure (shown by "texture") at this scale.

SOFIA in Context with Other Observatories

- Herschel ran out of cryogens in Spring 2013: SOFIA natural successor, Herschel community using SOFIA
- SOFIA will provide the only regular access for you to the far-IR (30 to 300 micron) for quite some time
- JWST (MIRI 5-28 micron) not really a competition …
- Synergies with ALMA/APEX, IRAM/NOEMA, SMA, alas CCAT cancelled (spatial res. similar to SOFIA)

Brief summary of SOFIA ISM science highlights

FORCAST (5-40 mu) :
A new mid-IR self-luminous source in Orion BN-KL (IRc4, brighter than BN)
Young star clusters embedded in HII regions (e.g. W43, Wd1;Spitzer saturated)
A mid-IR dusty circumnuclear ring (CNR) in the Galactic Center (3pc diameter)
Dust emission in Sgr A East supernova remnant(dust surviving reverse shock)

GREAT (dual channel 1-5 THz spectrometer) [for upGREAT → R. Guesten talk]
Detection of two new molecules: SH, OD (THz rot transitions in Herschel gaps)
Detection of the ground-state OH absorption towards W49N at 2.5 THz (strong)
Detection of the ground-state HD emission towards SgrB2 at 2.7 THz (v. weak)
Detection of protocluster infall in absorption against ATLASGAL cont. sources
Detection of para-H2D+ in absorption towards IRAS 16293 (strong continuum)
High-res velocity-resolved spectroscopy of [OI] 63mu line in planetary nebulae
High-res velocity-resolved spectroscopy of [OI] 63mu line in outflow sources
Tracing MHD-shocks in supernova remnants via CO high J ladder (eg. IC433)
[CII] in 30 Dor and N11/LMC massive photodissociation regions (CO-dark H2)
Optically thick [CII] and optically thin [13CII] in NGC 2024, extragal. implication

Brief summary of SOFIA ISM science highlights

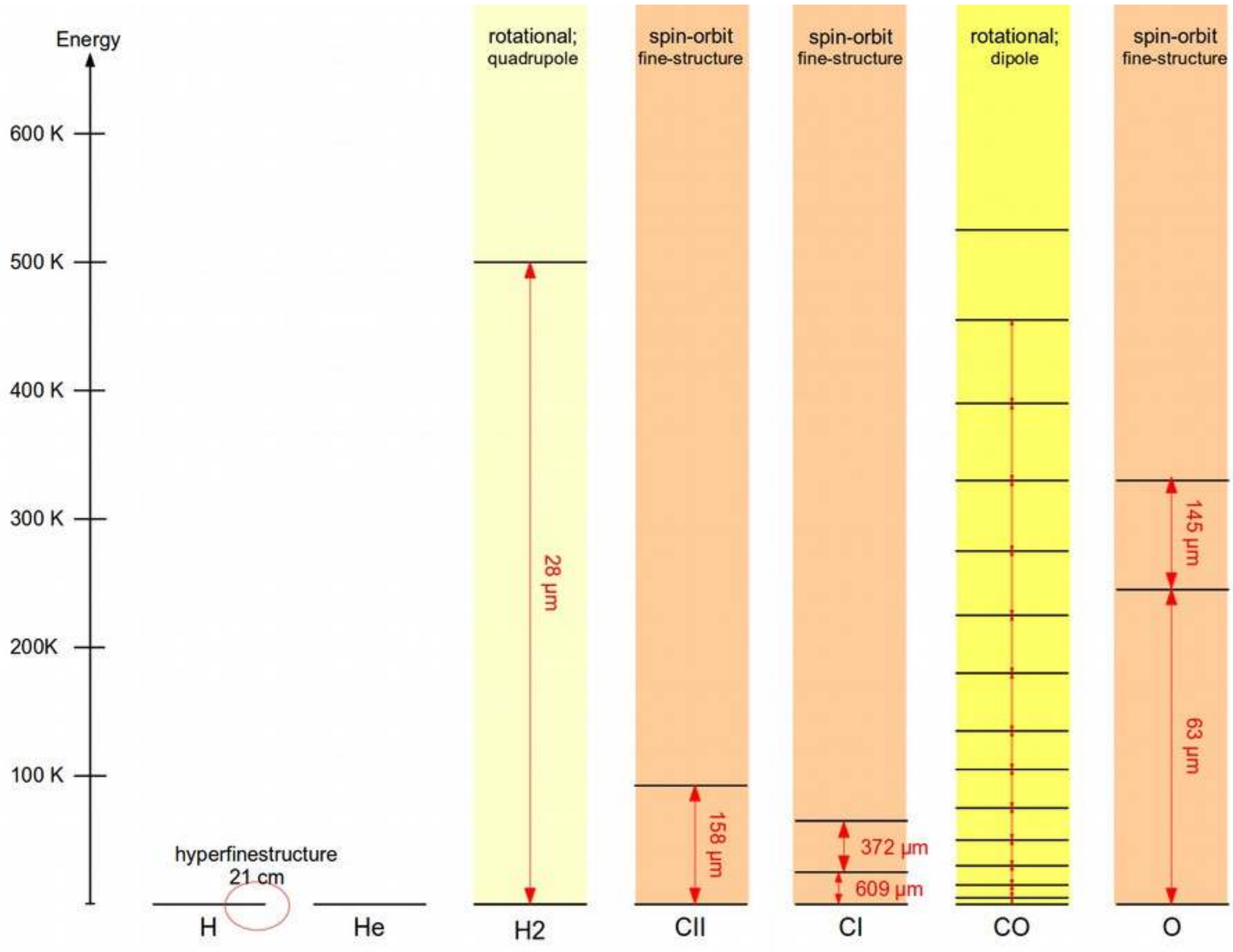
EXES (5-28mu, high-res. long-slit spectrometer)
28mu J=2-0 para-H_2 emission, also 17mu J=3-1 ortho-H_2 emission (on Jupiter)
6.1 mu high-res. ro-vib H_2O absorption in AFGL 2591: outflow vs. disk origin?

FIFI-LS (FIR integral field spectrometer)
[CII] 158mu and [OI] 63mu and 145mu emission in the Orion Nebula+Bar (PDR)
[CII] 158mu, [OIII] 52mu and 88mu emission in M82 (rotation + starburst wind)
[CII] and [OI] mapping of GC CND, and nearby spiral galaxies (e.g. NGC6946)
CO J=16-15 emission in He2-10: XDR vs. PDR (BH), cf. A. Krabbe poster

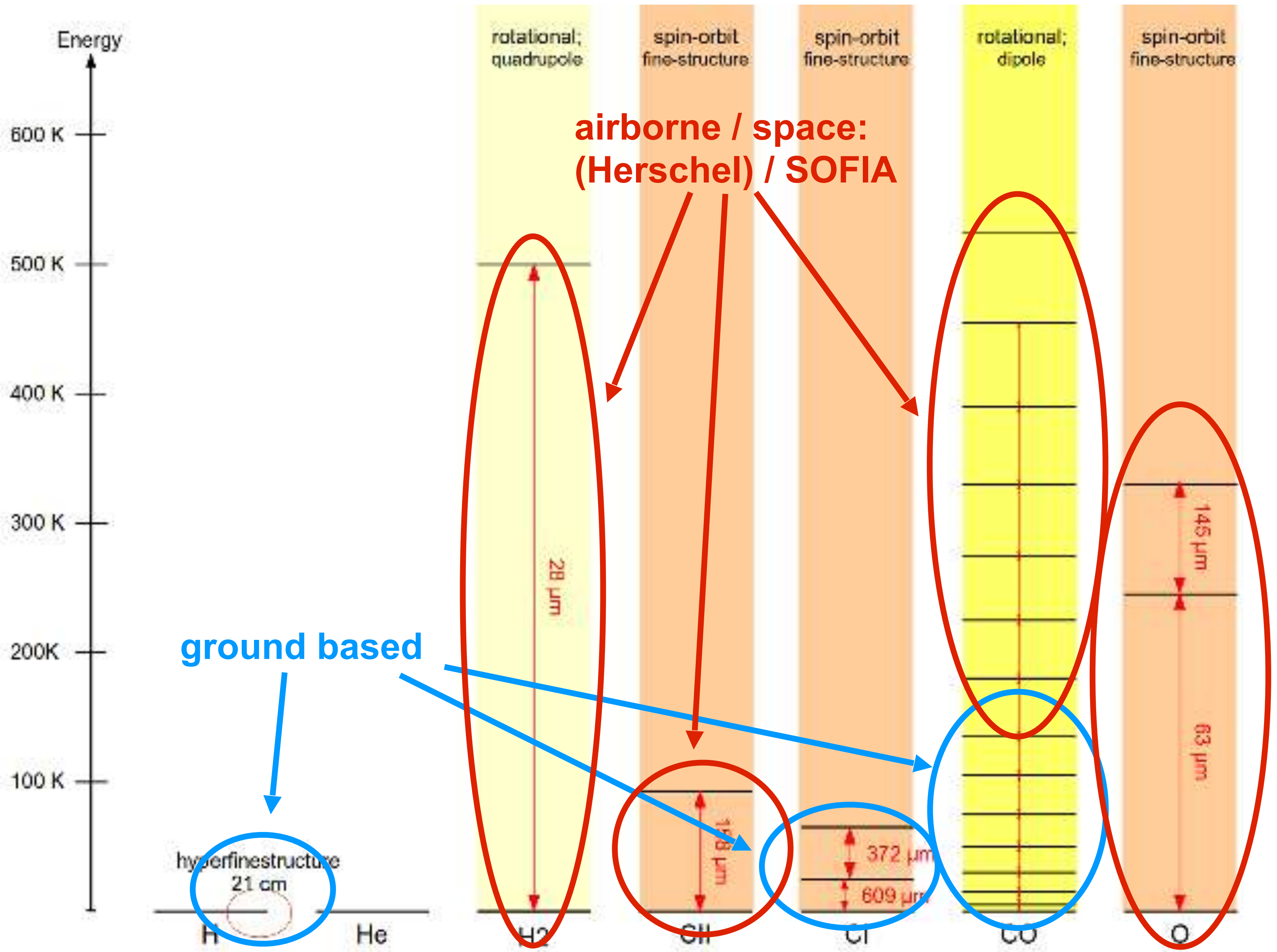
FLITECAM (1-5mu) and HIPO (FPI+) highlights
SN 2014J (M82) near-IR spectrum, evolving with time (ionised Cobalt lines)
Pluto occultation (June 29, 2015) in support of NASA’s New Horizons Mission

SOFIA publications from Early Science, Cycle 1 and Cycle 2+3 approaching 100

atomic / molecular physics: energy levels and spectral lines (H,He,C,O)



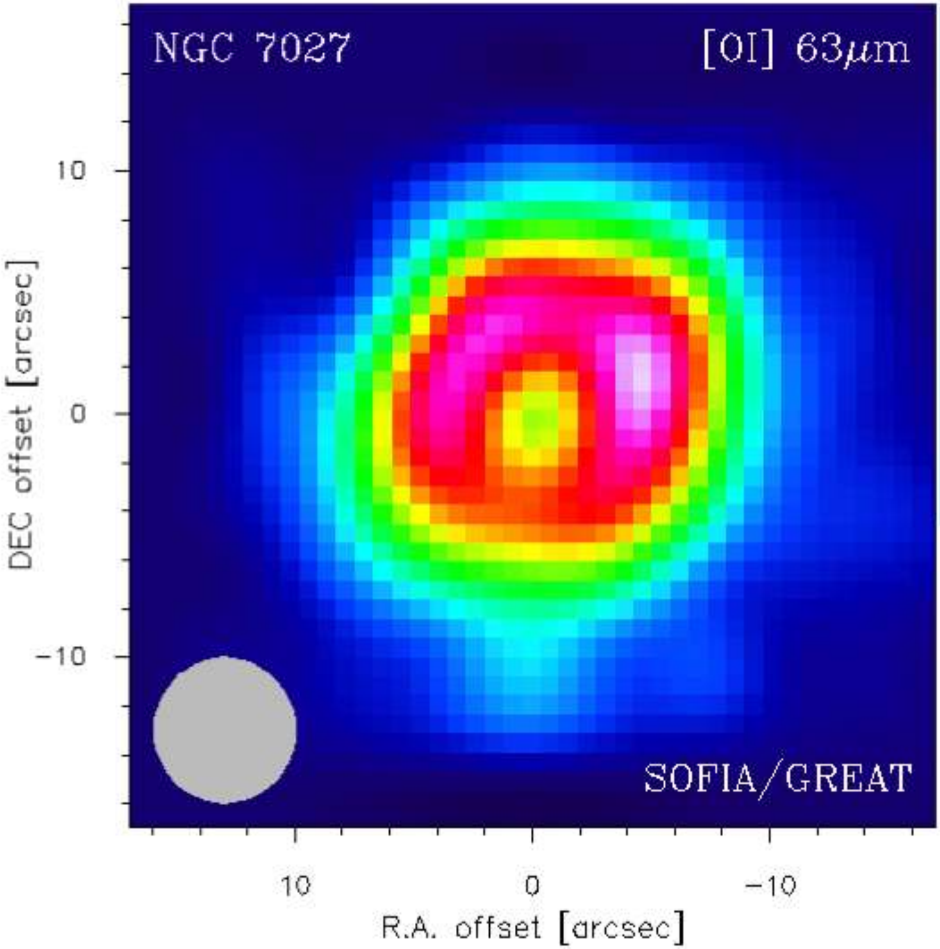
atomic / molecular physics: energy levels and spectral lines (H,He,C,O)

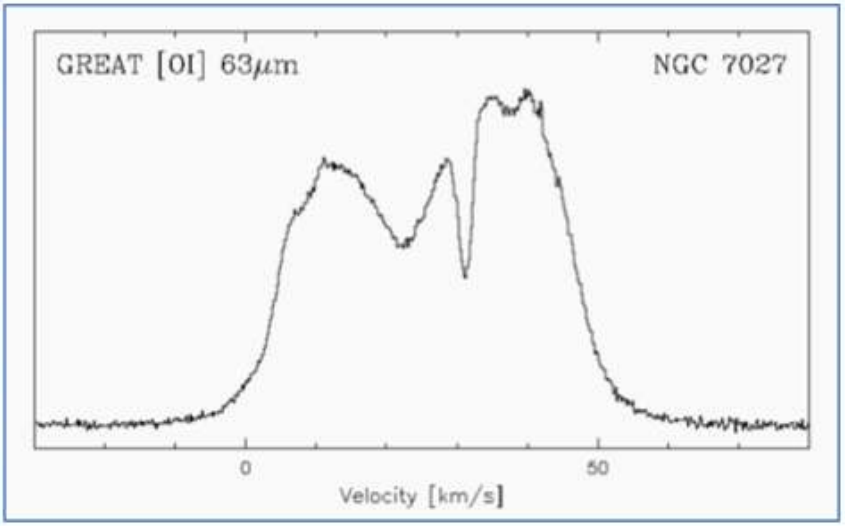


airborne / space: (Herschel) / SOFIA

ground based

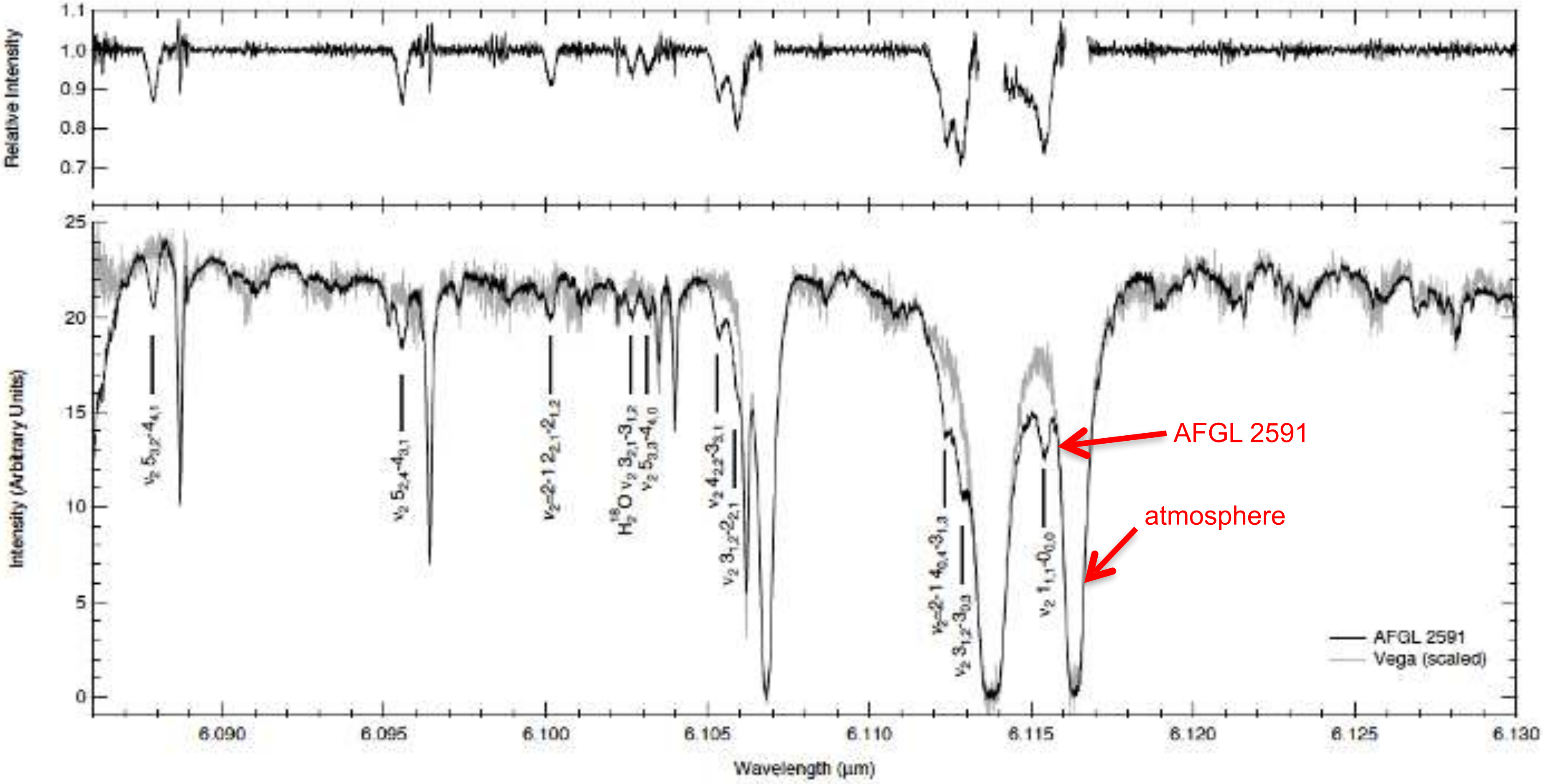
GREAT 4.7 THz First Light





Tomography of a planetary nebula

EXES Observations of Water in AFGL 2591



AFGL 2591

atmosphere

Indriolo, N. et al. 2015, ApJL, 802, L14.

Airborne Astronomy Ambassadors "Pilot" Program

Mary Blessing, Herndon, Va.; Cris DeWolf, Remus, Mich.; and Dana Backman (SETI)

Cecilia Scorza (DSI); Wolfgang Vieser, Munich, Germany; and Jörg Trebs, Berlin, Germany

Terry Herter (Cornell); Jim De Buizer (USRA); Theresa Paulsen, Mellen, Wis.; and Marita Beard, San Jose, Calif.

Pamela Harman (SETI); Margaret Piper, Frankfort, Ill.; and Kathleen Fredette, Palmdale, Calif.

Airborne Astronomy Ambassadors (AAA) Program

- The initial Airborne Ambassadors Pilot Program has proven the responsive chord that SOFIA provides to students
- Dozens of educators from all over the US are selected since 2012 to participate in AAS competitive program (and some teachers from Germany, too)

SOFIA's ISM POTENTIAL
ISM cycle, feedback

cycle: gas → stars → gas (molecules, dust)
feedback: ionis. radiation, winds, SN remnants

chemical enrichment (heavy elements, dust)
cooling, condensation, fragmentation, protostars

collapse, outflows, turbulence, mag. fields
shocks (dissipation, cooling), PDR/XDR (heating)

how much gas does not get recycled? (→D/H ratio)

some SOFIA publications

- SOFIA early science published in two 2012 special issues that highlight the science accomplished then
- Many more results by now, 2016 (new A&A special issue coming)
- HZ SOFIA AG review AN 334, 558 (2013)
- HZ SOFIA highlights 5th Zermatt-Symp 2015

Our house (LaAurora #72) in Curacavi/Chile

Hans at Universidad Autonoma de Chile

Flight Paths

Geographic Distribution of SOFIA Science Flights (2010-2011)

Take home messages

- SOFIA is in good shape (Cy6 in 2018, ~100 flights)
- SOFIA is a SF/ISM machine, with unique potential including astrochemistry/disks (simple molecules) & astrophysics (cloud collapse, shocks, heating/cooling)

- SOFIA is testing “local universe” and “local truth”.
- SOFIA is currently YOUR only far-IR observatory & fully supported by NASA/DLR for the next few years.
- NASA provides substantial $$ support for US PIs.
- As of Cycle 7, there are SOFIA legacy proposals