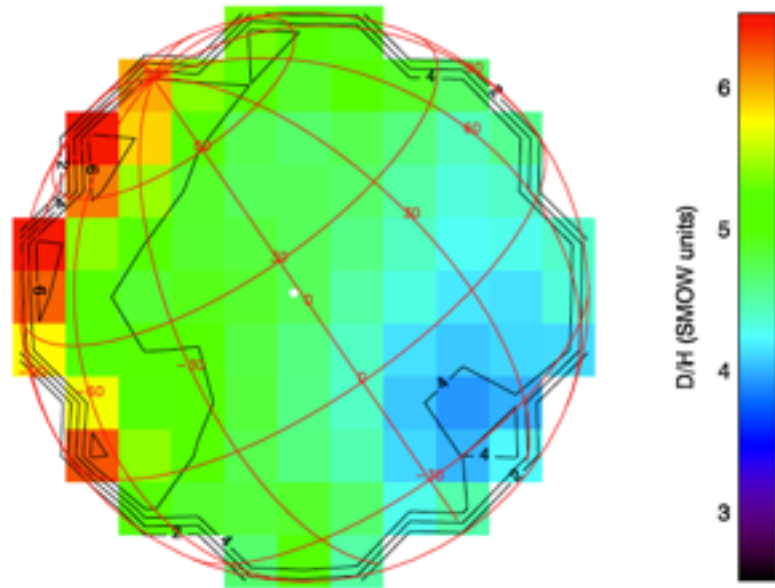




# High Resolution Spectroscopy with EXES



Mars HDO/H<sub>2</sub>O map, Encrenaz et al. (2016)

Adwin Boogert  
SOFIA/USRA  
Support Scientist

[thanks to the EXES Instrument  
Team: Matt Richter and  
Curtis DeWitt]

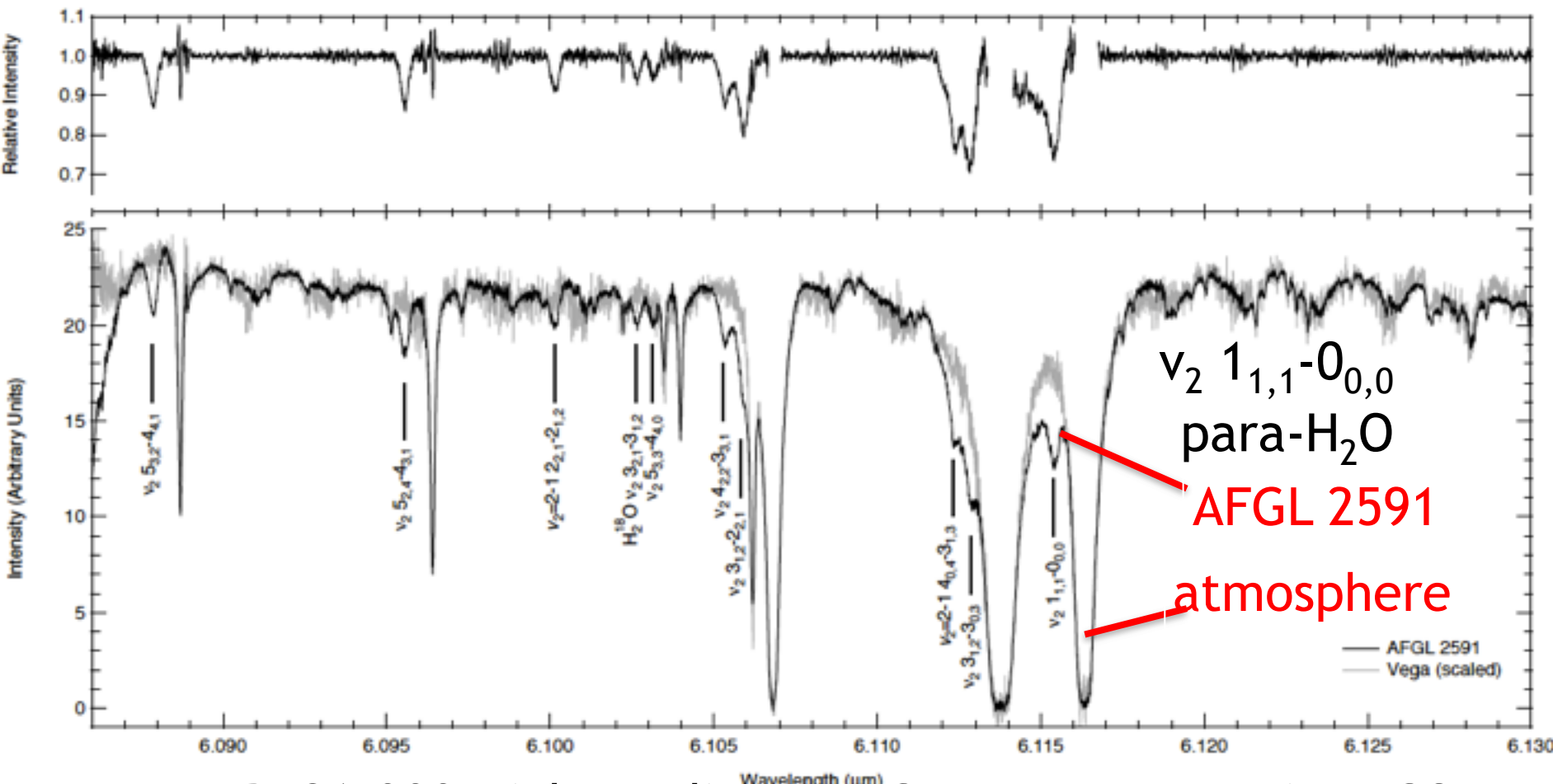


# Contents

1. Why High Resolution Infrared Spectroscopy?
2. Preparing EXES Observation of H<sub>2</sub>O Ground-State Transition at 6.1  $\mu\text{m}$  at High Spectral Resolution
3. EXES Maps
4. Limitations
5. EXES versus TEXES
6. For Further Reading
7. EXES as **PSI Instrument**



# 1. High Resolution Infrared Spectroscopy



R=86,000 High\_Medium EXES spectrum massive YSO  
 AFGL 2591 (Indriolo et al. [2015ApJ...802L..14I](https://doi.org/10.1086/151111))



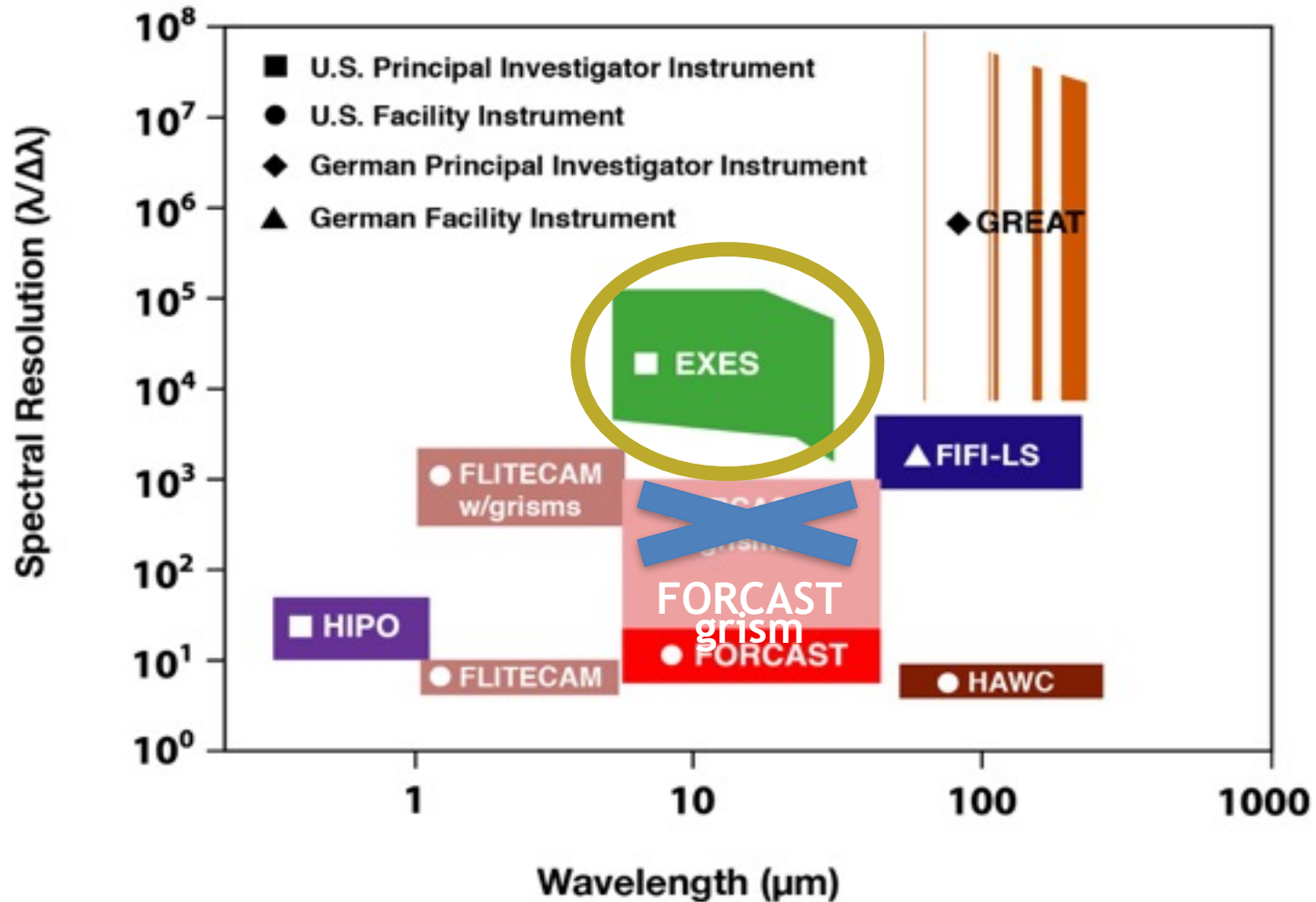
# 1. High Resolution Infrared Spectroscopy

High resolution spectroscopy powerful tool:

- Resolved line profiles yield **kinematic origin of line emission/absorption at scales not always spatially resolvable**, even with the largest telescopes, e.g.,
  - Infall
  - Outflow
  - Rotation
- Separation of spectroscopically crowded line regions
  - Emission line with foreground absorption
  - Closely spaced (ro-)vibrational transitions
- **Higher contrast** peak emission/absorption line increases detectability
- Separation telluric and astronomical line **improves sky correction**



# 1. High Resolution Infrared Spectroscopy with SOFIA





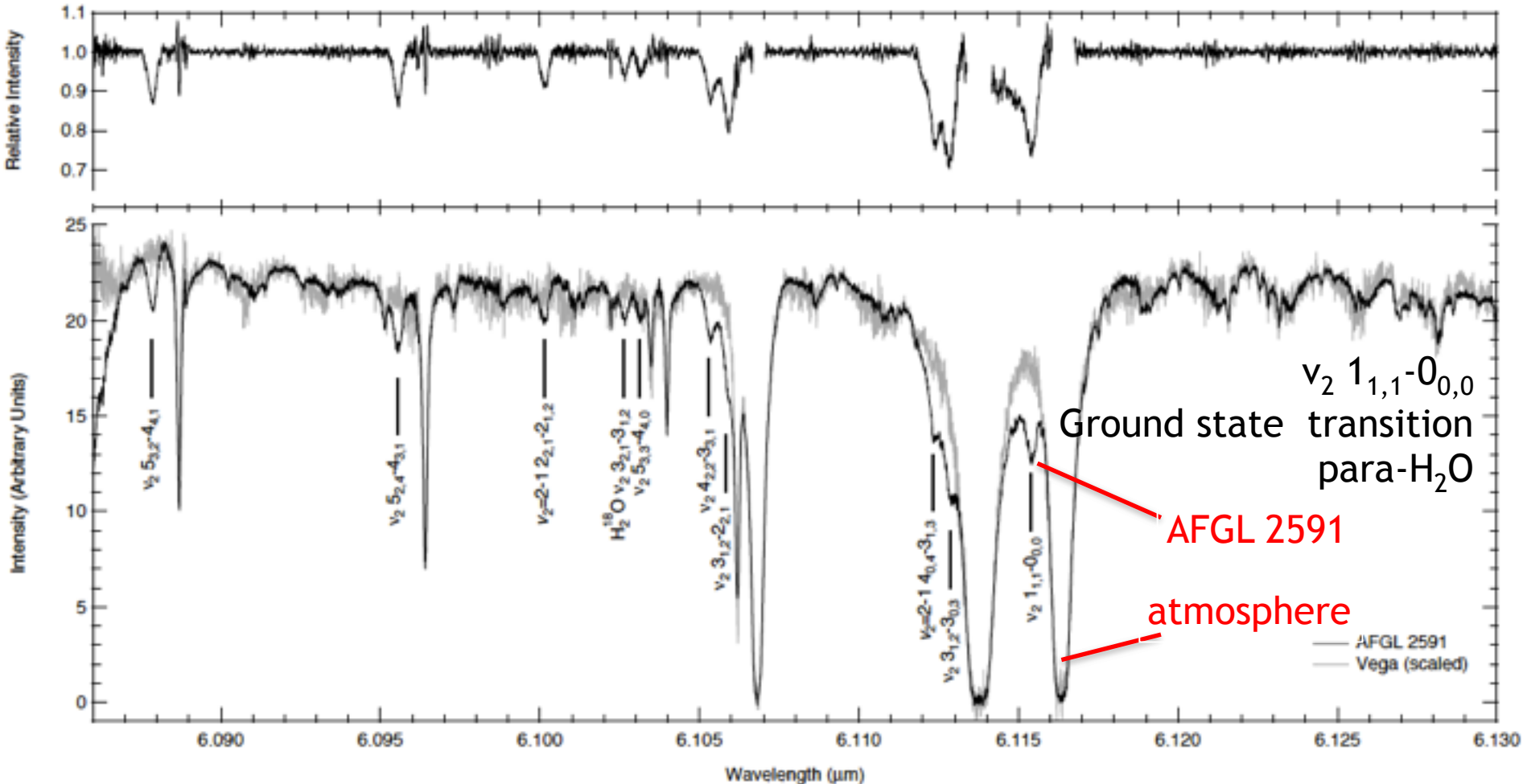
# 1. High Resolution Spectroscopy with SOFIA: EXES



## EXES (Echelon Cross Echelle Spectrograph):

- Echelon (high resolution) + Echelle (cross dispersion+low resolution)
- $R=1000-100,000$ , i.e.,  $\geq 3$  km/s
- 4.5-28.3  $\mu\text{m}$
- spatial resolution  $> \sim 3.5''$
- slit lengths: 1-180''
- slit widths: 1.4-3.2''
- array size 1024x1024 (same as JWST/MIRI)
- Roughly, observations very difficult for source brightnesses :  $< 1$  Jy (low resolution),  $< 10$  Jy (high resolution),  $< 100$  Jy (high resolution spectral survey)

# 2. Preparing EXES Observation



R=86,000 High\_Medium EXES spectrum massive YSO AFGL 2591  
 Indriolo et al. [2015ApJ...802L..14I](https://doi.org/10.1086/7000000)



## 2. Preparing EXES Observation



### Goals:

- obtain  $S/N=100$ ,  $R=80,000-100,000$  spectrum massive YSO AFGL 2591 between 6.085-6.130 micron.
- Line profiles will reveal location and perhaps chemical origin of H<sub>2</sub>O
- Detect  $v_2 1_{1,1}-0_{0,0}$  ground state transition para-H<sub>2</sub>O at 6.1163311 micron (never detected before), for total 'cool' gas column.





## 2. Preparing EXES Observation



Key instrument/observation parameters:

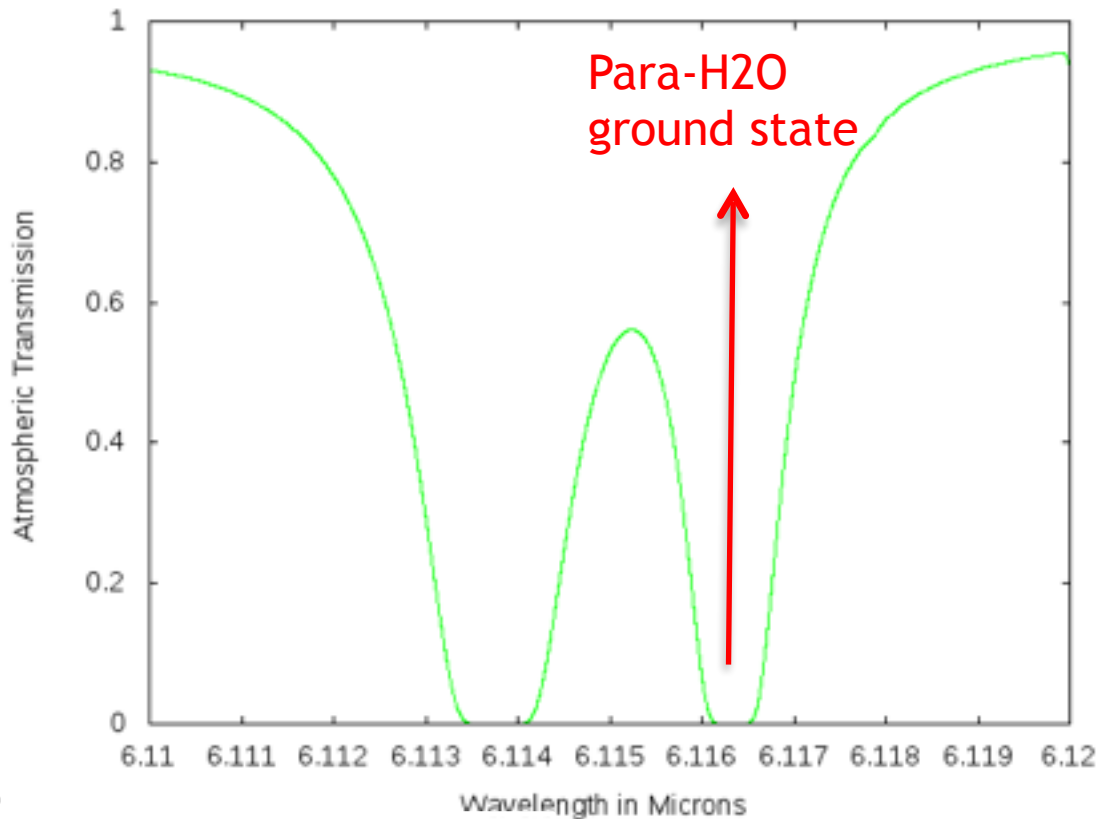
1. Atmospheric transmission and Doppler shifts [\[use ATRAN!\]](#)
2. Spectral resolution and instantaneous wavelength coverage needed: Instrument configuration, slit width, echelle order [\[use EXES ETC!\]](#)
3. Background emission subtraction: nodding mode [\[use EXES ETC!\]](#)
4. Clock time needed [\[use EXES ETC!\]](#)
5. Atmospheric absorption line correction: telluric standards
6. Photometric Calibration



## 2. Preparing EXES Observation: Doppler Shifts



$v_2 1_{1,1}-0_{0,0}$  ground state transition para-H<sub>2</sub>O at 6.1163311 micron: **how deep and wide is this line in the Earth's atmosphere at typical SOFIA altitude of 41,000 feet?**



[ran/atran.cgi](http://ran/atran.cgi)

Seems hopeless?

Need Doppler shift!



## 2. Preparing EXES Observation: Doppler Shifts

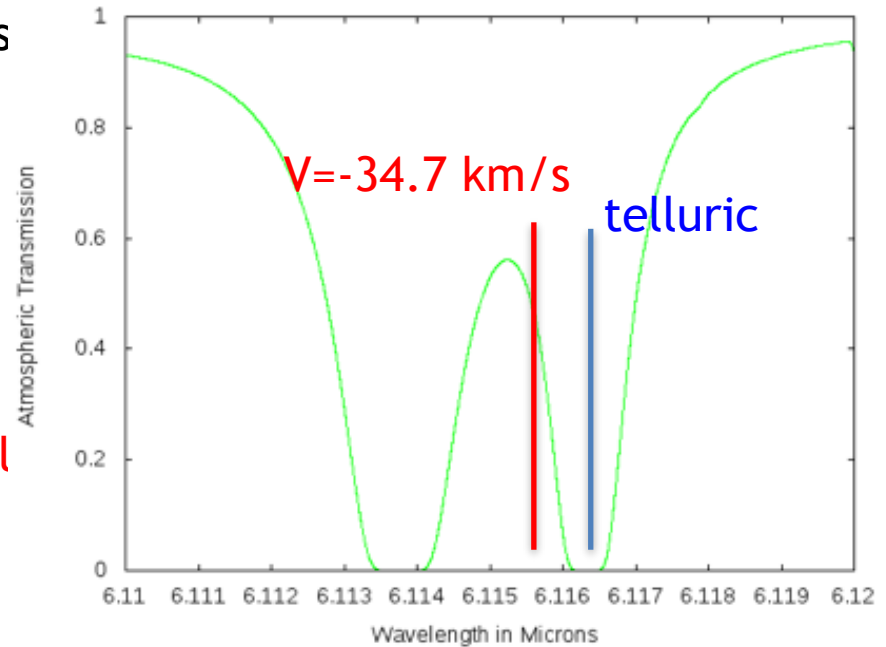


Velocity line absorption on given date,  $V_{DOP}$ , taking into account velocity AFGL 2591 ( $V_{LSR}$  or  $V_{HELIO}$ ) as well as  $V_{EARTH}$  in LSR or HELIO reference frame toward position AFGL 2591. Earth rotates around sun at  $\sim 30$  km/s. See details in next slide:

AFGL 2591:  $V_{LSR} = -5.5$  km/s (submm CO lines)  
 $V_{HEL} = -23.5$  km/s

$V_{DOP} = -34.7$  km/s on April 1 ( $= 0.0007 \mu\text{m}$ )  
 $= -12.6$  km/s on Oct 1

Derive acceptable Doppler shift and set time constraints for observation in proposal  
Tight constraints limit chances for observation to be scheduled!



Note: if line entirely free of telluric absorption, it may be better done from ground!



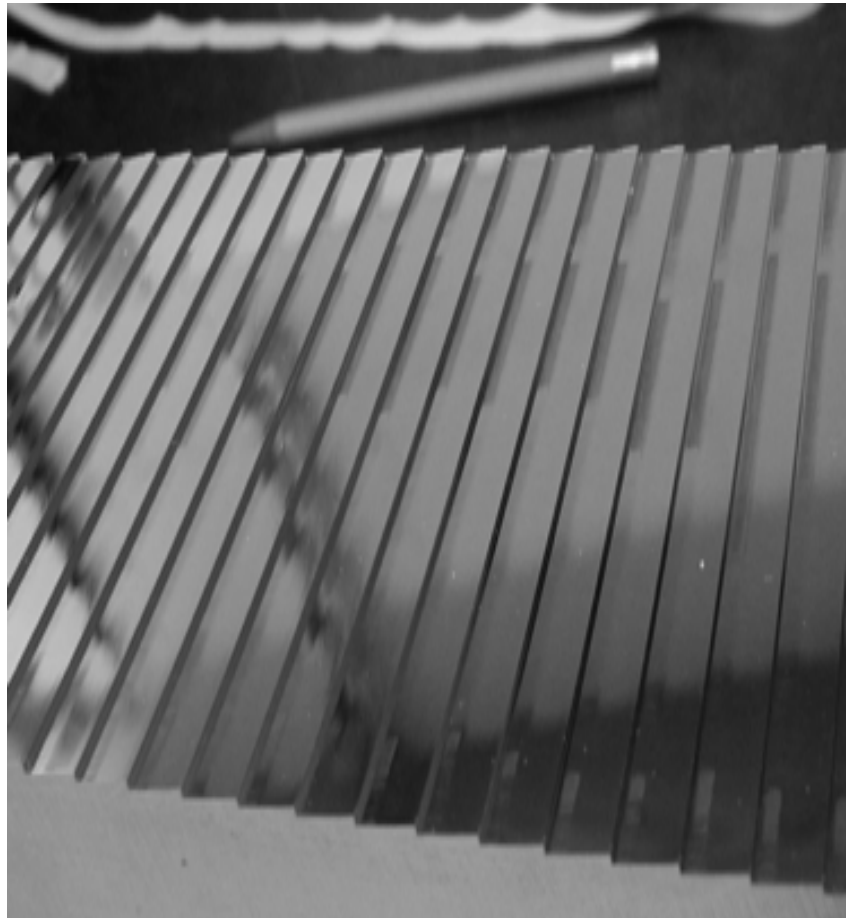
## 2. Preparing EXES Observation: Doppler Shifts



Scriptable way (IDL):

- Example given in baryvel.pro in IDL astronomy library:  
jdcnv, year, month, day, hour, jd ;convert to julian date  
baryvel, jd, epoch, vh, vb ;heliocentric velocity of earth for give date in km/s
- project earth velocity toward star. RA and Dec stellar position in radians  
 $V_{\text{EARTH}} = \text{vh}[0] * \cos(\text{Dec}) * \cos(\text{RA}) + \text{vh}[1] * \cos(\text{Dec}) * \sin(\text{RA}) + \text{vh}[2] * \sin(\text{Dec})$
- add radial heliocentric velocity of star to radial heliocentric velocity of the earth at that date. The sign of  $V_{\text{EARTH}}$  is negative!  $V_{\text{DOP}} = V_{\text{HELIO}} - V_{\text{EARTH}}$
- Note: to convert  $V_{\text{LSR}}$  to  $V_{\text{HEL}}$  use helio2lsr.pro (Erik Rosolowsky; <https://people.ok.ubc.ca/erosolo/idl/lib/helio2lsr.pro>)

## 2. Preparing EXES Observation: Instrument Configuration



EXES Echelon

Two dispersive elements set the instrument configuration:

1. **Echelon**: provides high spectral resolution
2. **Echelle**:
  - **Either ...** medium or low resolution cross dispersion of echelon orders
  - **Or ...** medium or low resolution spectroscopy (echelon bypassed)



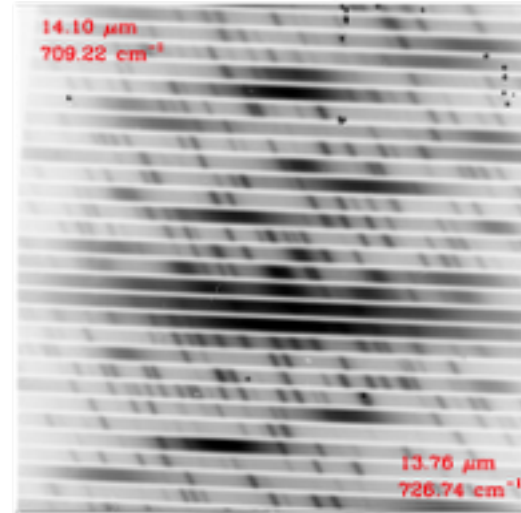
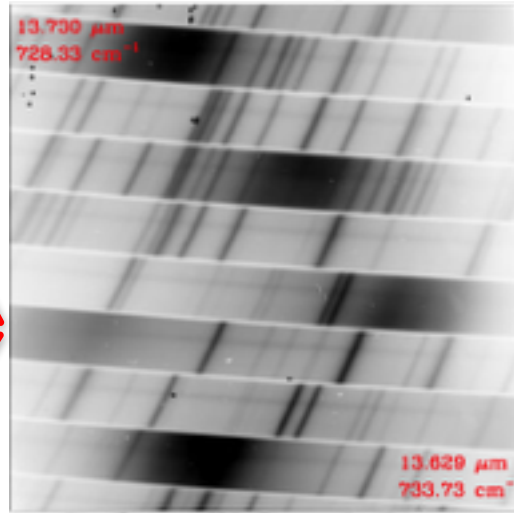
# 2. Preparing EXES Observation: Instrument Configuration



[Raw data, showing standing waves and sky emission lines]

HIGH\_MED Configuration

HIGH\_LOW Configuration

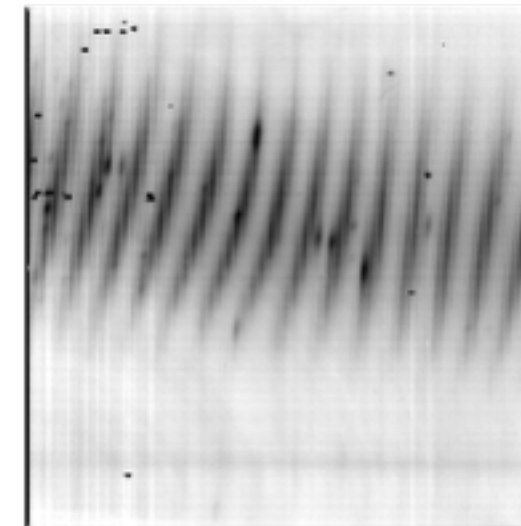
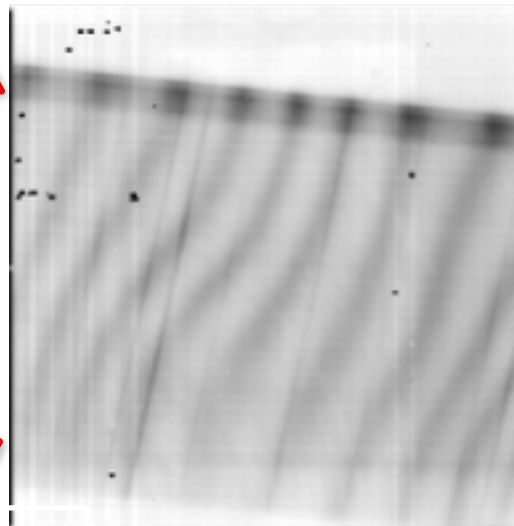


23" slit length

5.5" slit length

MEDIUM Configuration

LOW Configuration



180" slit length



10 May 2016

SOFIA Observers Workshop Tucson: EXES





## 2. Preparing EXES Observation: Instrument Configuration



- **HIGH\_MEDIUM:**
  - Echelon at high resolution+cross disperser echelle at medium resolution
  - $R=50,000-100,000$  (depending on slit width)
  - Application: high spectral resolution observation of single or a few lines
- **HIGH\_LOW:**
  - Echelon at high resolution+cross disperser echelle at low resolution
  - $R=50,000-100,000$  (depending on slit width)
  - Larger wavelength coverage than High\_Medium, at same resolution and shorter slits
  - Application: e.g., high spectral resolution line surveys of very bright targets (short slits: no on-slit nodding, slit loss)



## 2. Preparing EXES Observation: Instrument Configuration



- **MEDIUM:**
  - Echelle only, at medium resolution
  - R~4,000-18,000 depending on slit width and echelle order
  - Same wavelength coverage as High\_Medium, at medium resolution, higher sensitivity, and longer slit.
  - Application: e.g., sensitive spatial mapping lines at medium resolution
- **LOW:**
  - Echelle only, at low resolution
  - R~1,000-5,000 depending on slit width
  - Same wavelength coverage as High\_Low, at longer slits and higher sensitivity
  - Application: e.g., narrow ice or dust features?
  - Limitations (please contact team for more information! ):
    - Strong standing waves
    - Saturation issues at longer wavelengths ( $> \sim 8 \mu\text{m}$ )





# 2. Preparing EXES Observation: Exposure Time Calculator

The EXES “Exposure Time Calculator” (ETC) is **more than an exposure time calculator**. It shows many more instrument setup options. <https://dcs.sofia.usra.edu/proposalDevelopment/SITE/index.jsp>  
<http://irastro.physics.ucdavis.edu/exes/etc/>

## Welcome to the SOFIA - EXES Exposure Time Calculator

### Step 1

Enter either the rest-frame wavelength OR the rest-frame wavenumber to be observed:  [4.5 - 28.5 micron, or 350 - 2220 cm<sup>-1</sup>]

6.1163311 um

Check here if the source is Doppler shifted:  and enter its radial velocity:  [km/s, negative if the source is approaching]

-34.7 km/s

### Step 2

Next, select the instrument mode from the options below:

- Cross-dispersed High-Medium
- Cross-dispersed High-Low
- Single-order Long Slit Medium
- Single-order Long Slit Low

Configuration: High\_Medium

Click the submit button to continue on to the next step:



# 2. Preparing EXES Observation: Exposure Time Calculator

Slit width sets the resolution. Narrower slits block more star light (SOFIA PSF ~3.5"). Trade off between resolving power and S/N! Is highest resolution really necessary?

## Step 4 - Select a slit width

	Slit Width	Ext. Source Aperture	R	R	R	R
	(arcsec)	(Slit Width x IQ, arcsec <sup>2</sup> )	6th order	7th order	8th order	9th order
<input type="radio"/>	1.44	4.77	112000	112000	112000	112000
<input checked="" type="radio"/>	1.89	6.24	85590	85590	85590	85590
<input type="radio"/>	2.43	8.01	66667	66667	66667	66667
<input type="radio"/>	3.23	10.68	50000	50000	50000	50000



# 2. Preparing EXES Observation: Exposure Time Calculator

Cross disperser grating order sets the echelon order separation, and thus the number of echelon orders (i.e., wavelength coverage) that fit on the array. Not all orders as sensitive as expected. Slit length is matched to the echelon order separation:

## Step 3 - Select an observing order

Order	Grating Angle (alpha)	R	Minimum Wavelength	Maximum Wavelength	Minimum Wavenumber	Maximum Wavenumber	Slit Length	Point Source Nodding
	(Degrees)	(with default slit)	(micron)	(micron)	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(arcsec)	
<input type="radio"/>	6	112000	6.06134	6.17088	1620.51	1649.8	3.75	Must be off-slit.
<input type="radio"/>	7	112000	6.07295	6.15889	1623.67	1646.65	5.06	Must be off-slit.
<input type="radio"/>	8	112000	6.08283	6.14877	1626.34	1643.97	6.9	Must be off-slit.
<input checked="" type="radio"/>	9	112000	6.09202	6.1394	1628.82	1641.49	10.01	Must be off-slit.





# 2. Preparing EXES Observation: Exposure Time Calculator

Cross disperser grating order sets the echelon order separation, and thus the number of echelon orders (i.e., wavelength coverage) that fit on the array. Slit length is matched to the echelon order separation **and thus whether on-slit nodding is possible:**

## Step 3 - Select an observing order

Order	Grating Angle (alpha) (Degrees)	R (with default slit)	Minimum Wavelength (micron)	Maximum Wavelength (micron)	Minimum Wavenumber (cm <sup>-1</sup> )	Maximum Wavenumber (cm <sup>-1</sup> )	Slit Length (arcsec)	Point Source Nodding	
<input type="radio"/>	6	32.854	112000	6.06134	6.17088	1620.51	1649.8	3.75	Must be off-slit.
<input type="radio"/>	7	39.63	112000	6.07295	6.15889	1623.67	1646.65	5.06	Must be off-slit.
<input type="radio"/>	8	47.192	112000	6.08283	6.14877	1626.34	1643.97	6.9	Must be off-slit.
<input checked="" type="radio"/>	9	56.118	112000	6.09202	6.1394	1628.82	1641.49	10.01	Must be off-slit.



## 2. Preparing EXES Observation: Mode

EXES does not use the chopper. Its observing modes are

- **nod\_on\_slit**: compact sources, if the slit is long enough (typically longer than 4 times PSF FWHM) → see ETC (previous slide). Note that slit length is a strong function of wavelength
- **nod\_off\_slit**: extended sources and if slit is too short
- **mapping** (i.e., slit scan): see later slides





# 2. Preparing EXES Observation: Clock Time and S/N



## Observation Summary

Signal to noise ratio:	80
Source type:	Point source
Source flux:	400 Jy
Atmosphere:	39,000 ft altitude, 45 degrees elevation angle

## Exposure Time Calculation

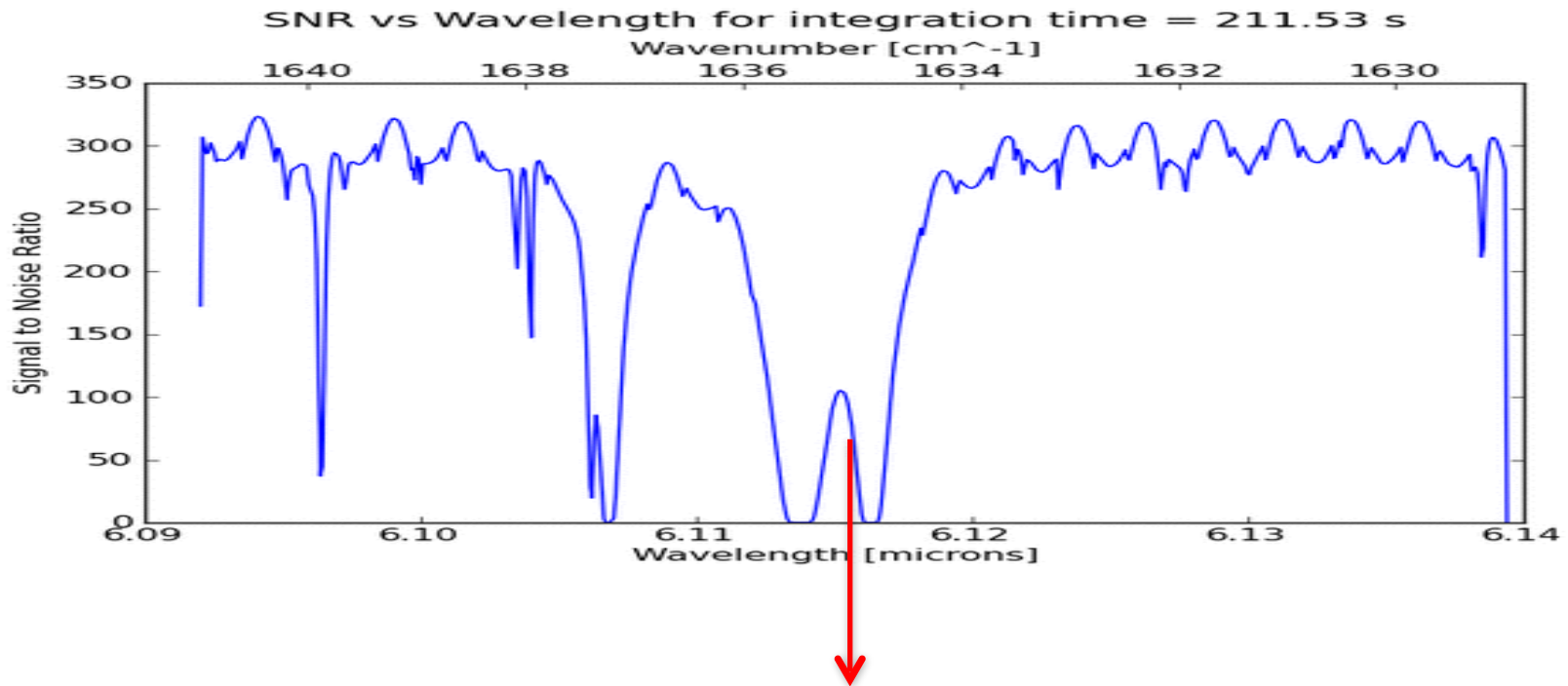
Integration time:	211.53 seconds	Total EXES Clock time:	846.14 seconds
Source count rate (e-/s):	1695	Background count rate (e-/s):	44517
Read noise counts (e-/readout):	451584	Number of readouts (to avoid nonlinearity):	1

In SPT and SSPOT, always use “**clock time**”, which includes all overheads, and time on and off source, except acquisition and instrument setup. *This is different from on-target time that other SOFIA instruments use.*

Note: The integration refers to the time on target - overhead time and nodding are included in calculating the clock time.



## 2. Preparing EXES Observation: Clock Time and S/N



At expected line position,  $S/N=80$ ; much better elsewhere.



## 2. Preparing EXES Observation: Telluric Absorption



For each EXES observation of a given target and wavelength, a blackbody source and the sky are observed:

In theory, this can be used to remove telluric absorption lines:

$$I_\nu(\text{obj}) \approx S_\nu(\text{obj} - \text{sky}) \frac{B_\nu(T_{\text{tel}})}{S_\nu(\text{black} - \text{sky})}$$

For lines overlapping with strong telluric lines, **a telluric standard may need to be observed**: a bright star <10 um, or an asteroid or Galilean moon at longer wavelengths.

**Time on the telluric standard needs to be taken into account in the time request.**  
The actual standard is selected in the flight planning process (see call for proposals and handbook).

Note: application of models of the Earth's transmission may reduce/eliminate the need for telluric standards (this is under investigation).





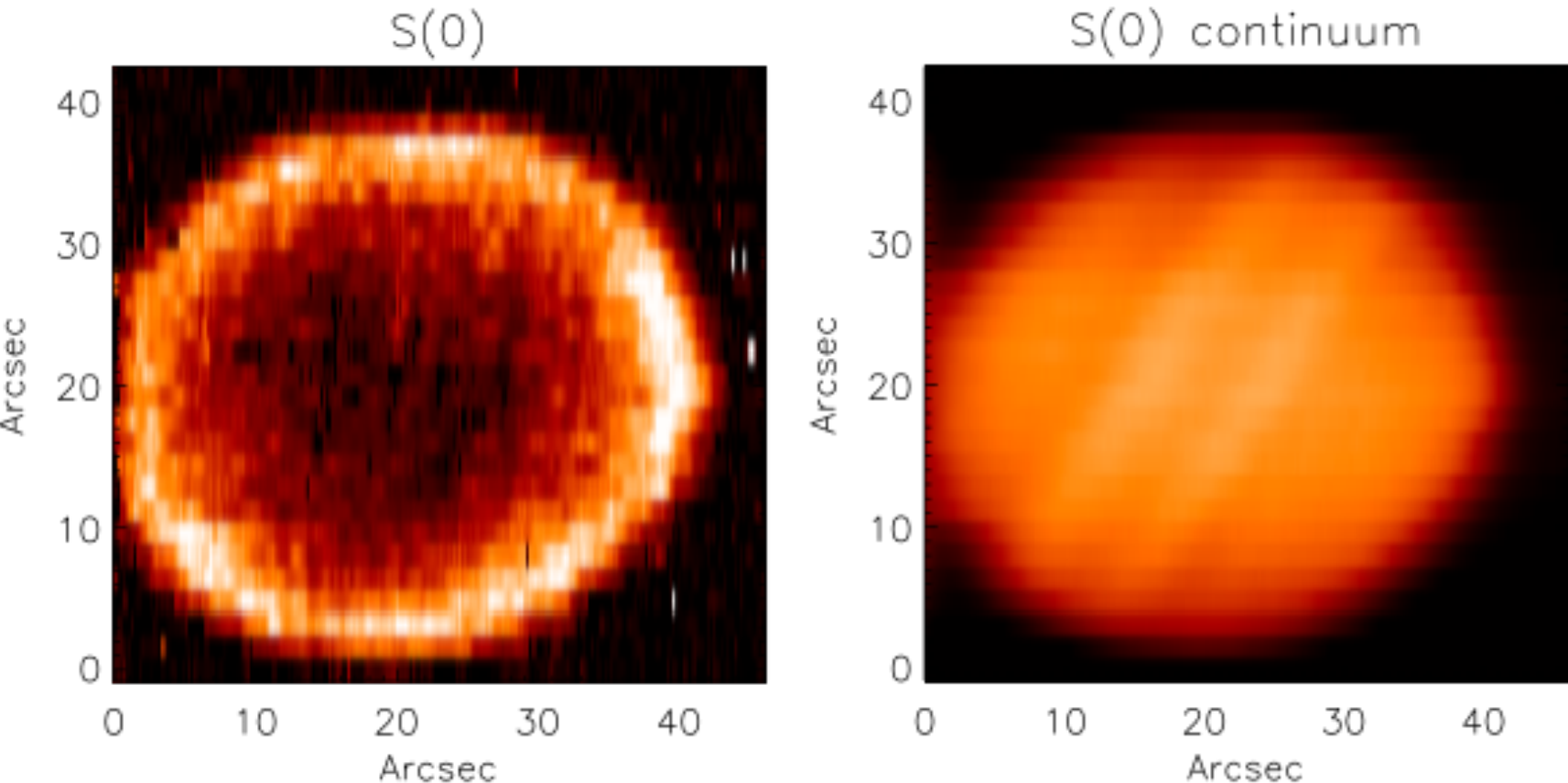
## 2. Preparing EXES Observation: Photometric Calibration

The blackbody integration also takes care of the flux calibration at an accuracy of, generally, <20%.

$$I_{\nu}(\text{obj}) \approx S_{\nu}(\text{obj} - \text{sky}) \frac{B_{\nu}(T_{\text{tel}})}{S_{\nu}(\text{black} - \text{sky})}$$

If more accurate flux calibration is important, time on a calibrator must be separately requested in the proposal!

# 3. EXES Maps



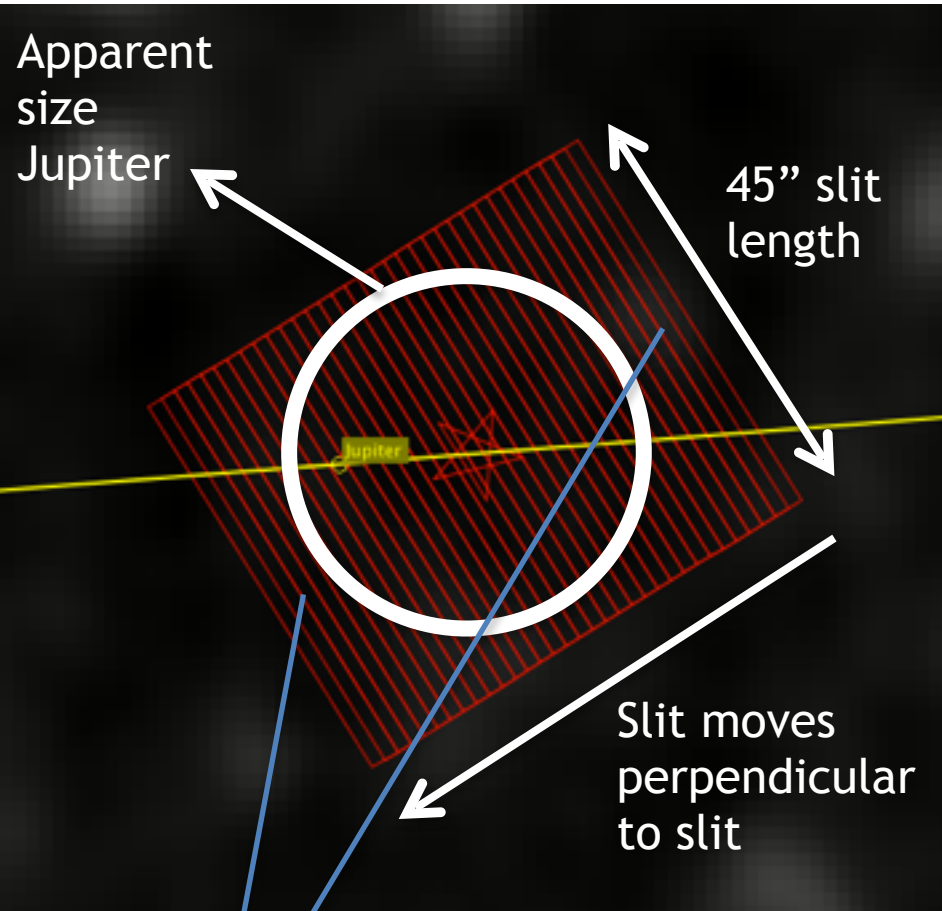
Map H<sub>2</sub> S(0) line and continuum 28.2 μm obtained in first EXES flight (08 April 2014).

Configuration (parameters from ETC): HIGH\_MEDIUM, 3.2" slit, echelle order 2, R=50,000, slit length=45", step size=1.6", 32 points "slit scan".



# 3. EXES Maps

SSPOT visualization:



EXES maps produced by moving slit perpendicular to slit (default). This is called a "stripe". Each stripe is one AOR.

Other options: parallel to slit or at an angle.

Default move is half a slit width.

Stripe orientation not known until AOR is scheduled.

First and last slit positions used for background subtraction. Dedicated off possible too.

First and last pointings used for background

EXES ETC gives extended source sensitivity, and clock time for entire map assuming half slit width sampling.



# 4. Limitations

- EXES is optimized for high S/N observations of narrow spectral features in the high spectral resolution configurations. Broad spectral features ( $> \sim 50$  km/s) suffer from contamination by standing wave residuals in all configurations. Please contact the instrument team if you expect to propose for such observations.
- Observations of spectral lines overlapping with telluric lines require a standard star observation, which must be accounted for in the proposal.
- Slit orientation on the sky not known until date and time of observation
- In the Low configuration, detector saturation may occur at wavelengths above  $\sim 8 \mu\text{m}$ .



## 5. EXES versus TEXES



For observations in **wavelength regions possible from the ground**, EXES sister instrument **TEXES** may be used. It is offered alternately at **Gemini-North and IRTF**. Differences with EXES:

- TEXES has smaller array ( $256^2$  versus  $1024^2$ ), hurting spectral coverage and spectral survey speed
- Ground-based telescopes have much better PSF at wavelengths  $<20 \mu\text{m}$ , and **TEXES is more sensitive than EXES/SOFIA, atmosphere permitting.**



## 6. For Further Reading



- “TEXES: A Sensitive High-Resolution Grating Spectrograph for the Mid-Infrared”; Lacy et al. <http://adsabs.harvard.edu/abs/2002PASP..114..153L> . About sister-instrument TEXES. Much applies to EXES; e.g., configurations, calibration procedures.
- PI page at UC Davis: <http://irastro.physics.ucdavis.edu/exes/>



# 7. EXES as PSI Instrument

EXES is Principal Investigator-class Science Instruments (PSI):

It is highly encouraged (not required) to contact the instrument team (EXES: Matt Richter, [mjrichter@ucdavis.edu](mailto:mjrichter@ucdavis.edu) ) when preparing observing proposals:

Best to do this early on to ensure the project is feasible!

## Call for proposals:

“Guest Investigators will receive calibrated data from the EXES team”

“Encouraged but not required to work closely with EXES team and include members on their papers.”





# Backup Slides





# 1. High Resolution Spectroscopy with SOFIA: Science Applications



Unique science applications with SOFIA:

- EXES:
  - ro-vibrational transitions molecules (**H<sub>2</sub>O**, CH<sub>4</sub>, CH<sub>3</sub>, etc.)
  - rotational transitions H<sub>2</sub> (**S(0)**, S(5)-S(8)). Note: S(1), S(2), and S(4) can be done from the ground (TEXES)
  - electronic transitions atoms (Fe, Ar)
- GREAT:
  - rotational transitions molecules (e.g., hydrides)
  - important fine structure (cooling) lines (OI, **CII**, **NII**)