



High Resolution Spectroscopy with EXES and GREAT

Adwin Boogert
SOFIA/USRA Support Scientist



20+21 May 2015

SOFIA Observers Workshop



1



Contents

1. High Spectral Resolution Capabilities SOFIA
2. **EXES:**
 - 2.1 Preparing EXES Observation of H₂O Ground-State Transition at 6.1 μm at High Spectral Resolution
 - 2.2 EXES Maps
 - 2.3 EXES versus TEXES
3. **GREAT:** Preparing High Spectral Resolution Observation of C⁺ (158 μm) and N⁺ (205 μm) toward Galactic Center Region (CMZ).
4. For Further Reading
5. EXES and GREAT as PSI Instruments



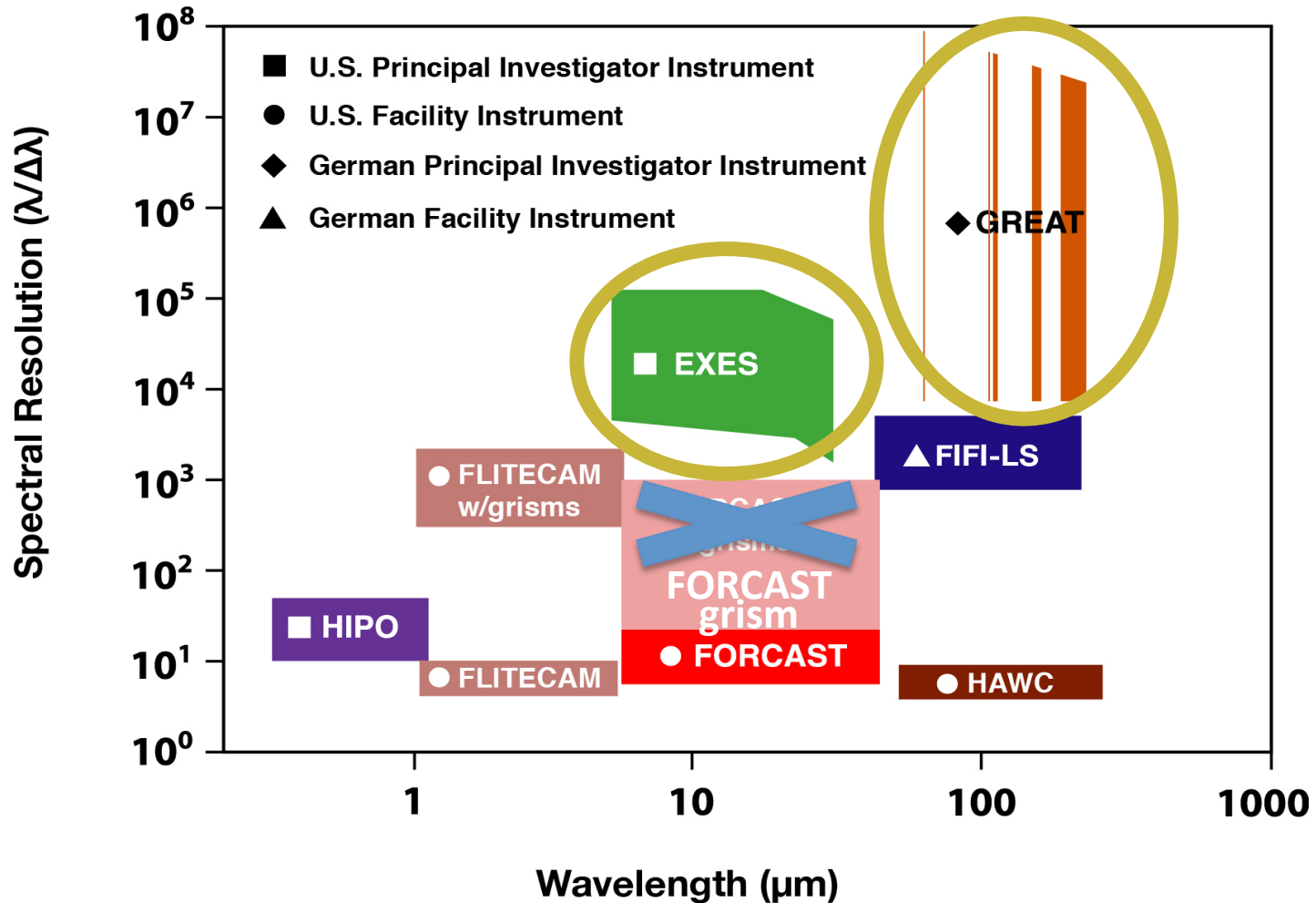
1. High Resolution Spectroscopy

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 Spectroscopy with SOFIA





1. High Resolution Spectroscopy with SOFIA



EXES (Echelon **C**ross **E**chelle Spectrograph):

- Echelon (high resolution) + Echelle (cross dispersion+low resolution)
- $R=1000-100,000$, i.e., ≥ 3 km/s
- 4.5-28.3 μm
- spatial resolution $>\sim 3.5''$
- slit lengths: 1-180''
- slit widths: 1.4-3.2''
- array size 1024x1024 (same as JWST/MIRI)

GREAT (**G**erman **R**Eceiver for **A**stronomy at **T**erahertz Frequencies):

- Heterodyne receiver
- $R=10-50$ million, i.e., <0.1 km/s
- 63 μm , 197-240 μm , 157-165 μm
- spatial resolution: 6-24'' (15.9'' at C⁺)
- single pixel on sky (for 7-pixel array upGREAT, see talk by Randolph Klein)



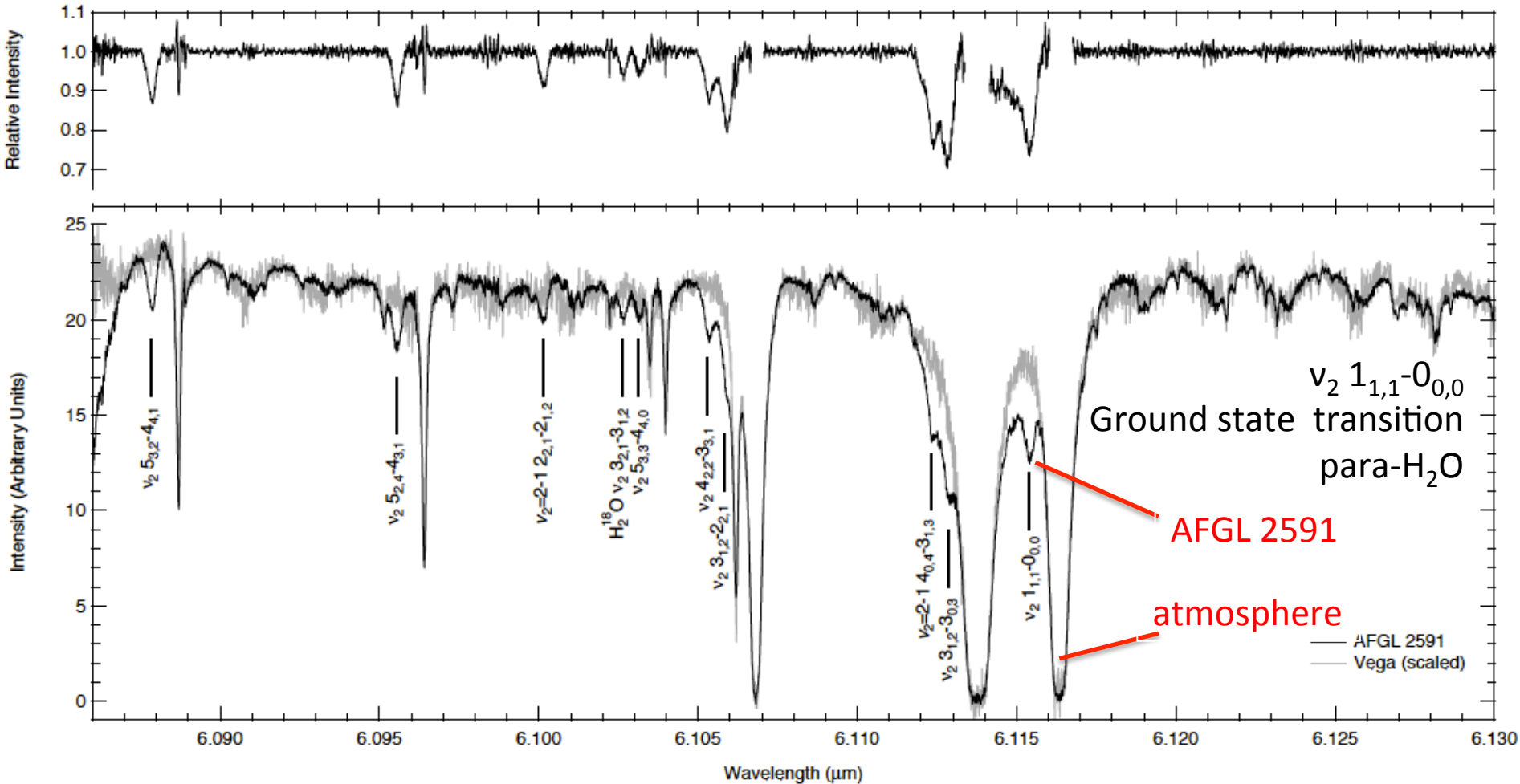
1. High Resolution Spectroscopy with SOFIA: Science Applications



Unique science applications with SOFIA:

- EXES:
 - ro-vibrational transitions molecules (**H₂O**, CH₄, CH₃, etc.)
 - rotational transitions H₂ (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**)

2.1 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)



2.1 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 H₂O
- Detect $v_2 1_{1,1}-0_{0,0}$ ground state transition para-H₂O at 6.1163311 micron (never detected before), for total 'cool' gas column.



2.1 Preparing EXES Observation



Key instrument/observation parameters:

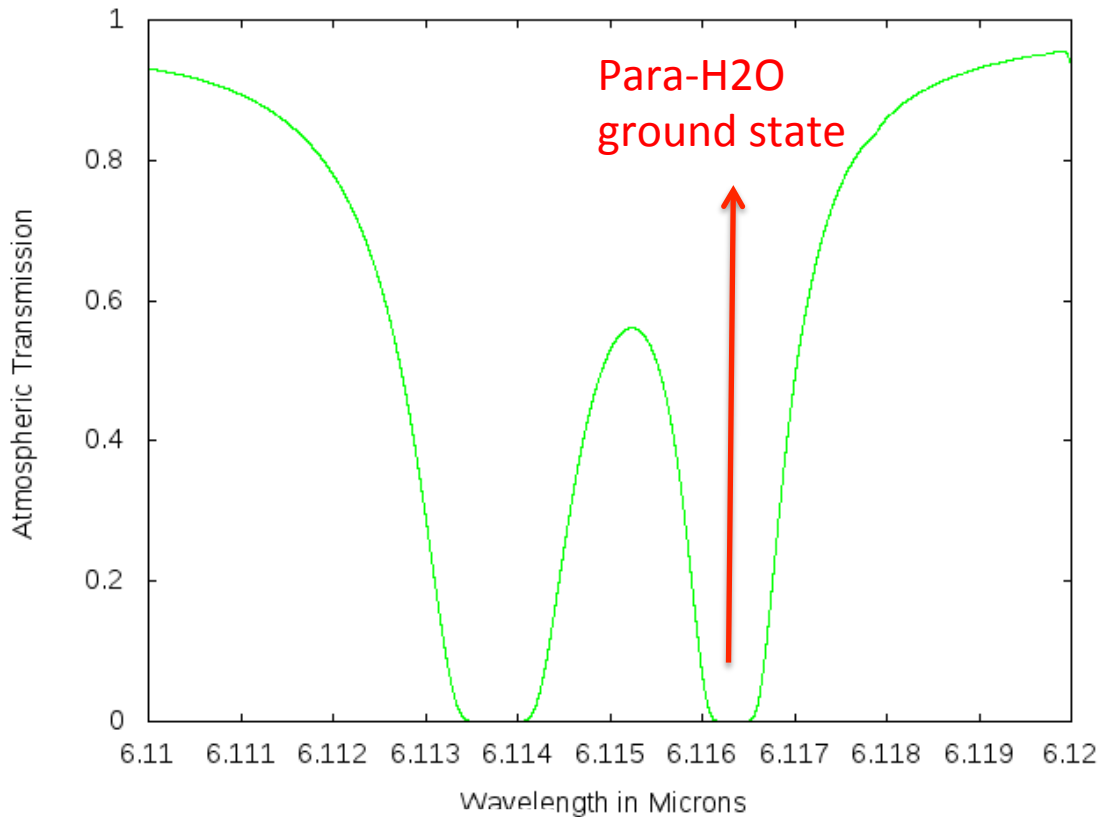
1. Atmospheric transmission and Doppler shifts [\[use ATRAN!\]](#)
2. Spectral resolution and instantaneous wavelength coverage needed: Instrument configuration, slit width, echelle order [\[use EXES ETC!\]](#)
3. Background emission subtraction: nodding mode [\[use EXES ETC!\]](#)
4. Clock time needed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



2.1 Preparing EXES Observation: Doppler Shifts



$v_2 1_{1,1}-0_{0,0}$ ground state transition para-H₂O at 6.1163311 micron: how deep and wide is this line in the Earth's atmosphere at typical SOFIA altitude of 41,000 feet? Use ATRAN: <https://atran.arc.nasa.gov/cgi-bin/atran/atran.cgi>



Seems hopeless?
Need Doppler shift!



2.1 Preparing EXES Observation: Doppler Shifts



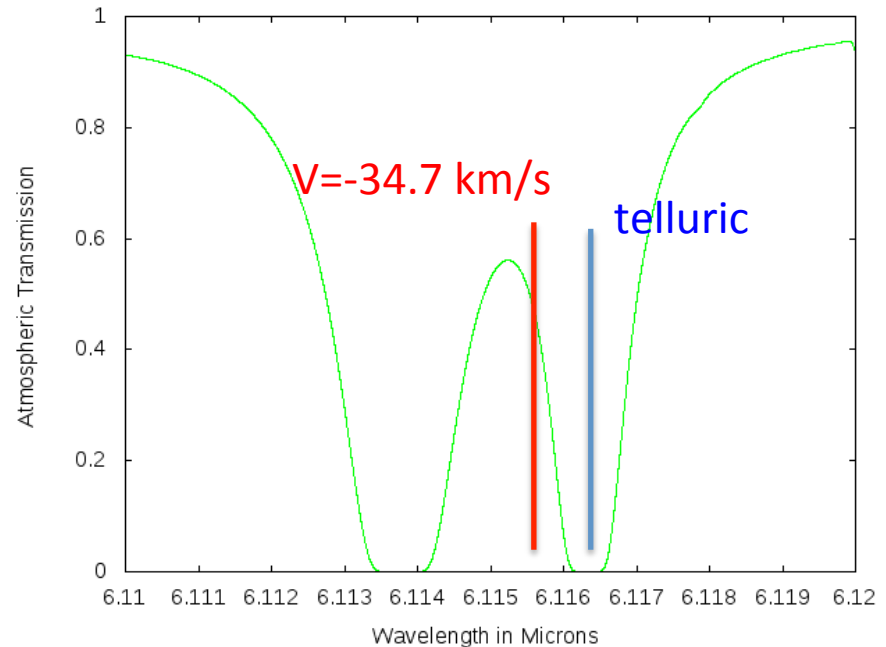
Velocity line absorption on given date, V_{DOP} , taking into account velocity AFGL 2591 (V_{LSR} or V_{HELIO}) as well as V_{EARTH} in LSR or HELIO reference frame toward position AFGL 2591. Earth rotates around sun at ~ 30 km/s. See details in next slide:

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





2.1 Preparing EXES Observation: Doppler Shifts



Easy way:

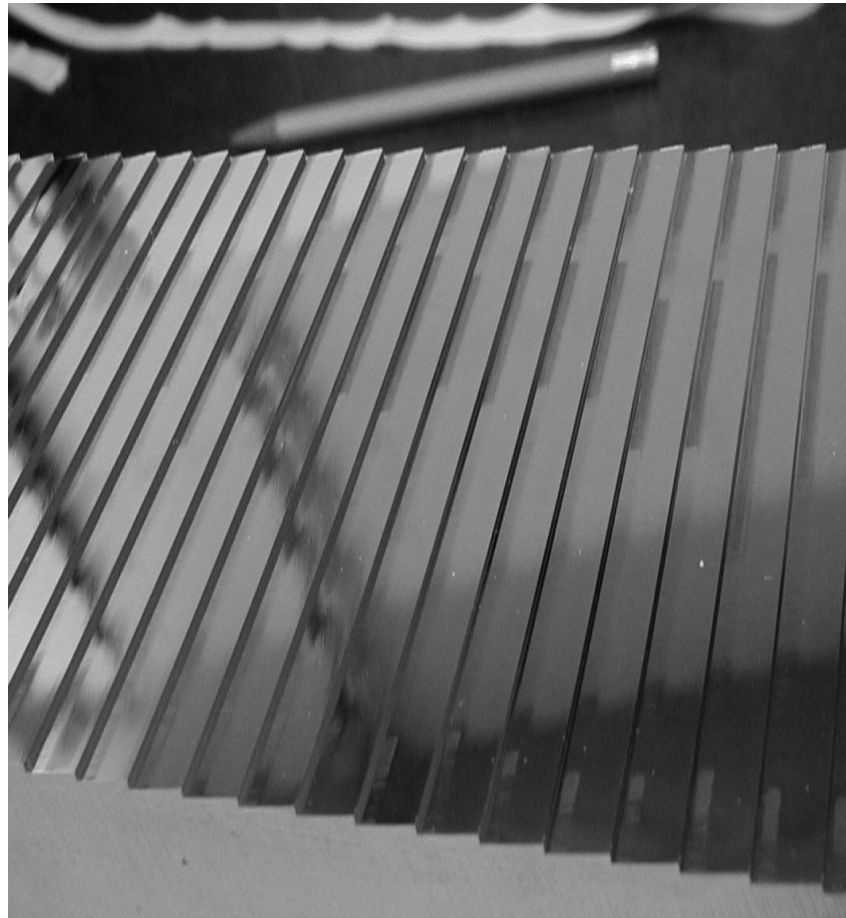
- calculate motion of earth in LSR frame w.r.t target on given date:
<http://www.astro.virginia.edu/~emm8x/utils/vlsr.html>
- add V_{LSR} target to that.

Scriptable way (IDL):

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



2.1 Preparing EXES Observation: Instrument Configuration



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)

EXES Echelon

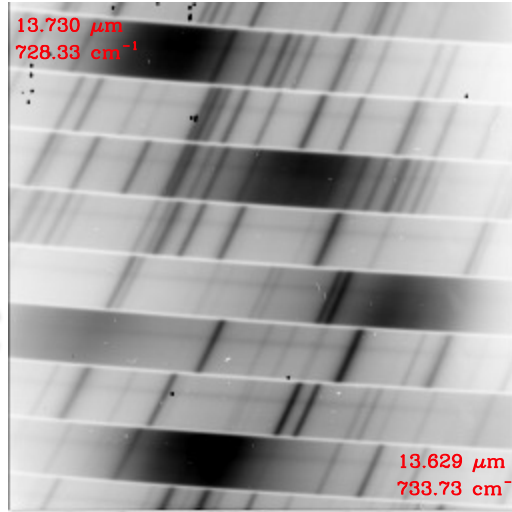


2.1 Preparing EXES Observation: Instrument Configuration



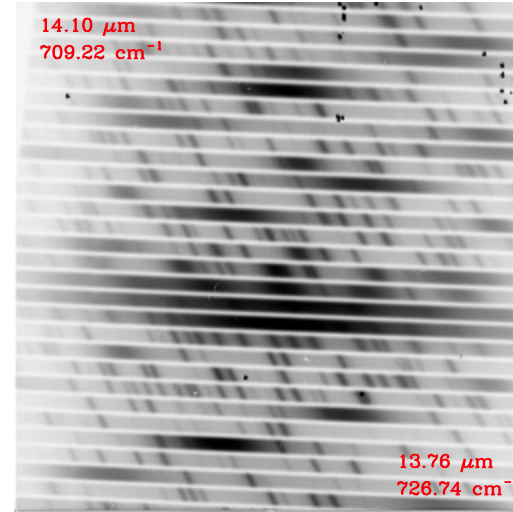
[Raw data, showing standing waves and sky emission lines]

HIGH_MED Configuration



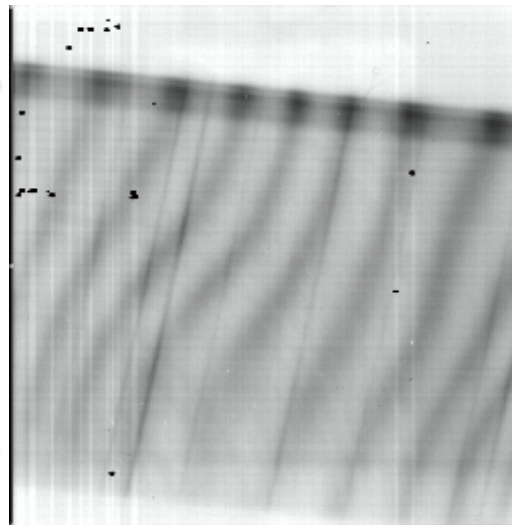
23" slit length

HIGH_LOW Configuration



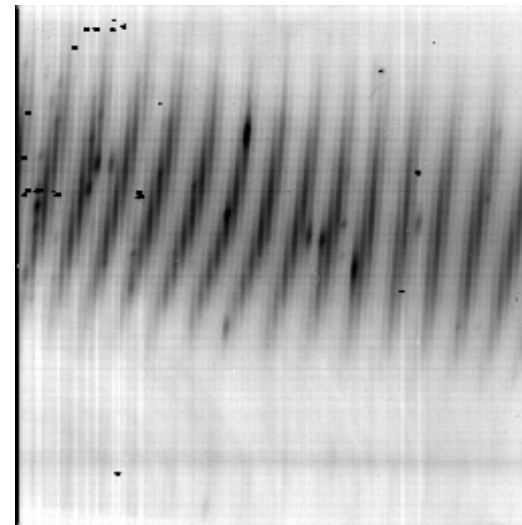
5.5" slit length

MEDIUM Configuration



180" slit length

LOW Configuration



20+21 May 2015

SOFIA Observers Workshop





2.1 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)



2.1 Preparing EXES Observation: Instrument Configuration



- **MEDIUM:**
 - Echelle only, at medium resolution
 - $R \sim 4,000-18,000$ 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
 - $R \sim 1,000-5,000$ depending on slit width
 - Same wavelength coverage as High_Low, at longer slits and higher sensitivity
 - Application: e.g., narrow ice or dust features?
 - **Use in shared risk mode; please contact team for more information!**



2.1 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.arc.nasa.gov/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⁻¹]

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:





2.1 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 ²)	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



2.1 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. ETC updated June 8. 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 ⁻¹)	(cm ⁻¹)	(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.





2.1 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 ⁻¹)	Maximum Wavenumber (cm ⁻¹)	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.





2.1 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



2.1 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

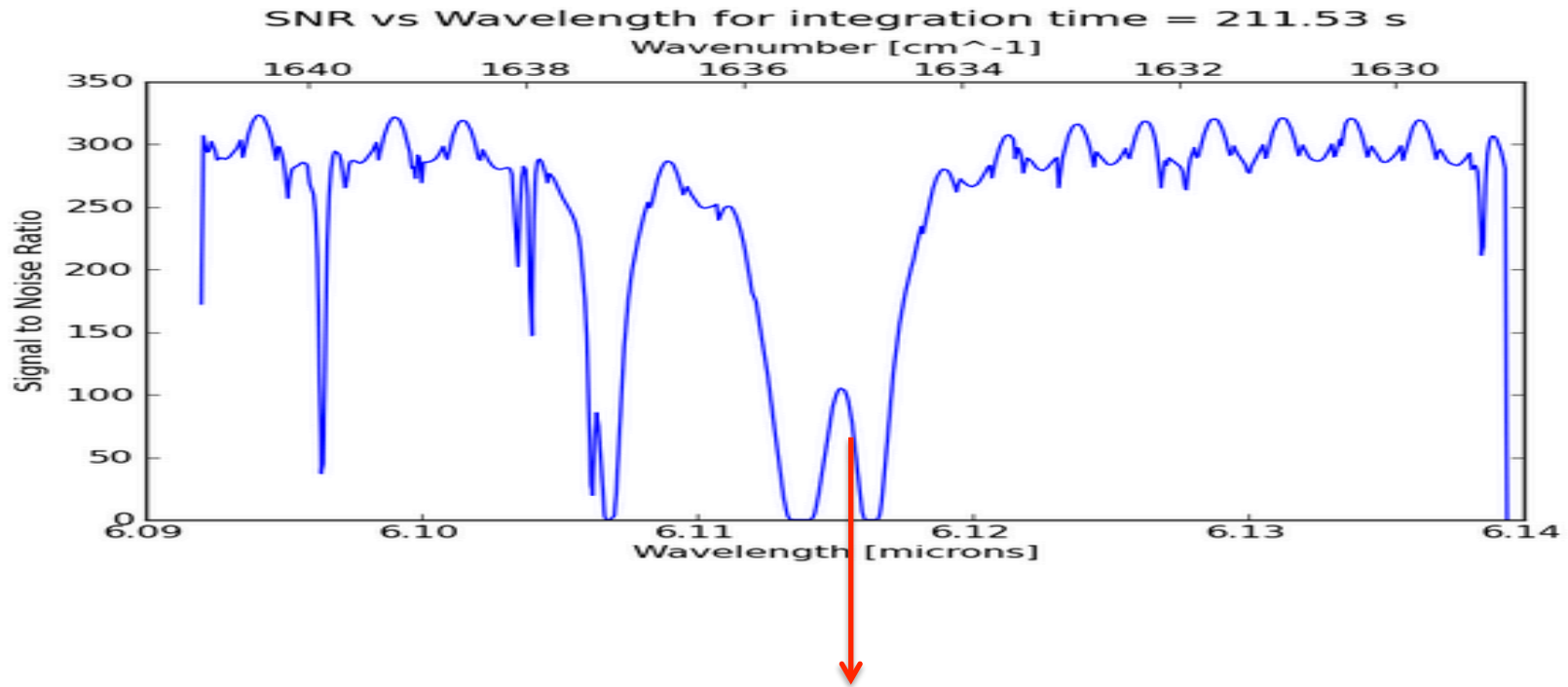
Integration time:	211.53 seconds	Total EXES Clock time:	846.14 seconds
Source count rate (e-/s):	1695	Background count rate (e-/s):	44517
Read noise counts (e-/readout):	451584	Number of readouts (to avoid nonlinearity):	1

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.



2.1 Preparing EXES Observation: Clock Time and S/N



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



2.1 Preparing EXES Observation: Telluric Absorption



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

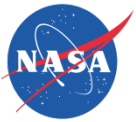
In theory, this can be used to remove telluric absorption lines:

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

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).



2.1 Preparing EXES Observation: Photometric Calibration

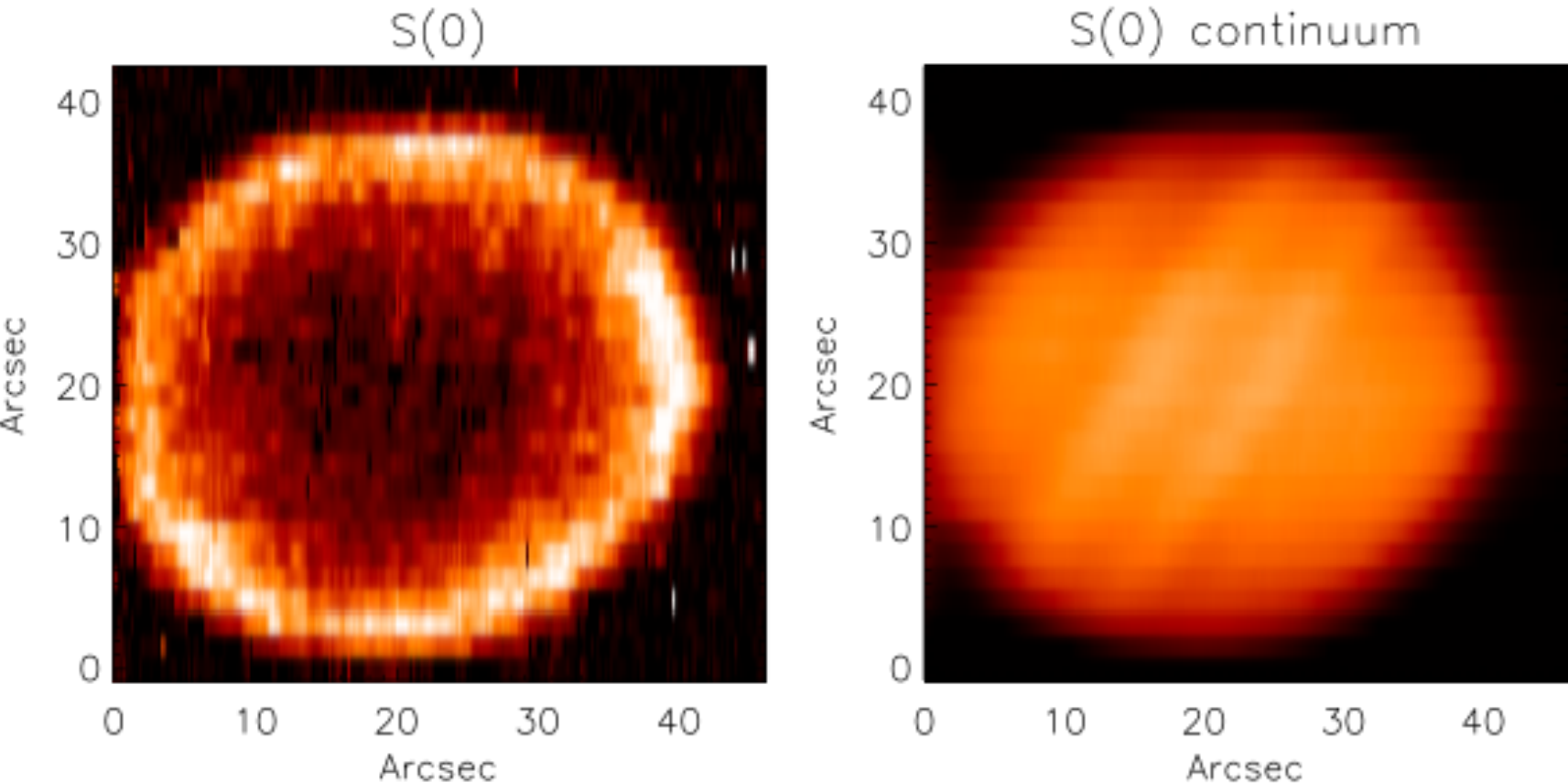


The blackbody integration also takes care of the flux calibration at an accuracy of, generally, <20%.

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

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

2.2 EXES Maps



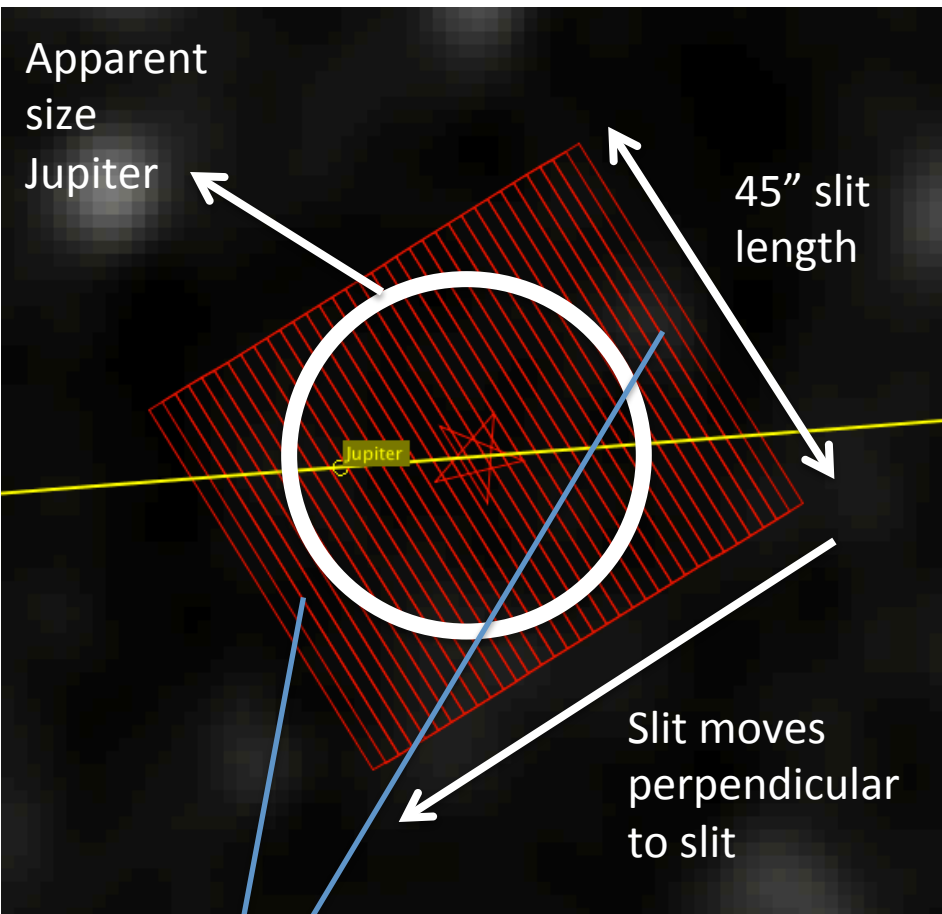
Map H₂ S(0) line and continuum 28.2 μm obtained in first EXES flight (08 April 2014). Configuration: HIGH_MEDIUM, 3.2" slit, echelle order 2, R=50,000, slit length=45", step size=1.6", 32 points "slit scan".



2.2 EXES Maps



SSPOT visualization:



First and last pointings used for background

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.

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





2.3 EXES versus TEXES

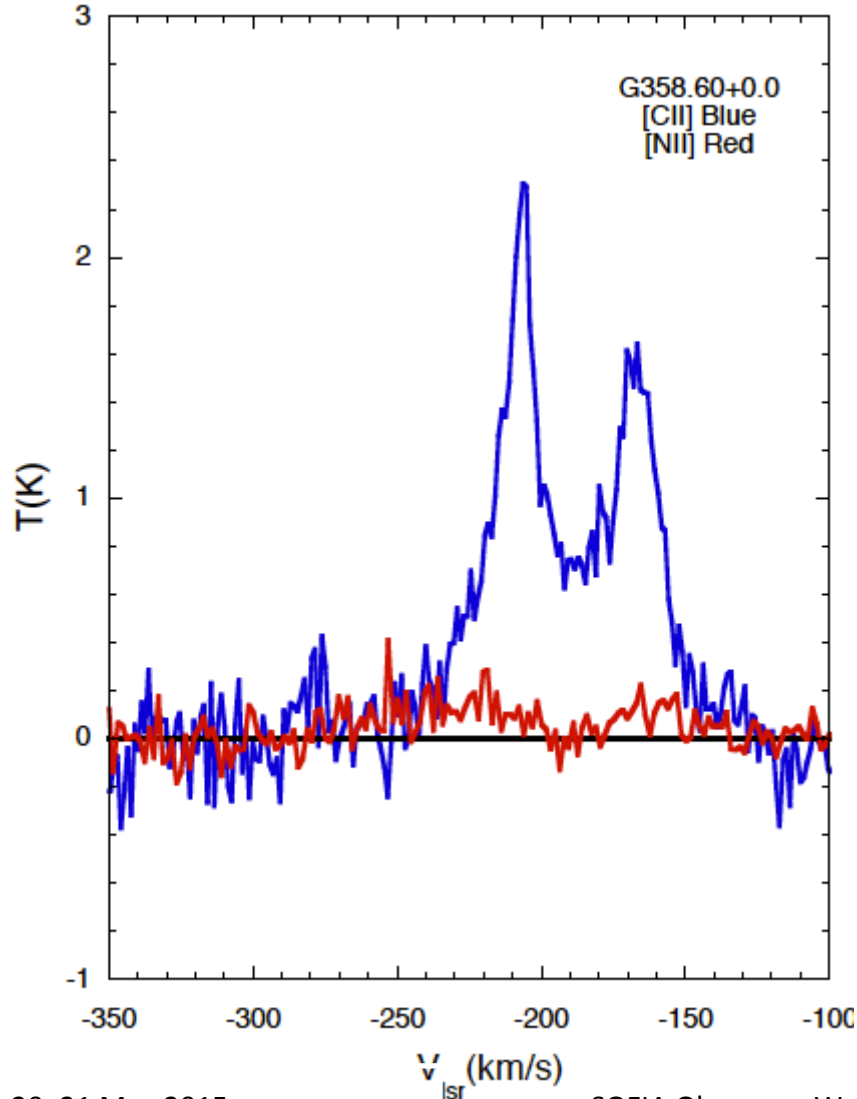


For observations in wavelength regions possible from the ground, EXES sister instrument TEXES may be used. It is offered alternately at Gemini-North and IRTF. Differences with EXES:

- TEXES has smaller array (256^2 versus 1024^2), hurting spectral survey speed
- Ground-based telescopes have much better PSF, and TEXES is more sensitive than EXES/SOFIA, atmosphere permitting.



3. Preparing GREAT Single Point Observation



GREAT position switch (“total power”) observation C⁺ and N⁺ toward the edges of the Central Molecular Zone around the Galactic Center (Langer et al. [2015A&A...576A...1L](https://doi.org/10.1051/0004-6361/201525764))



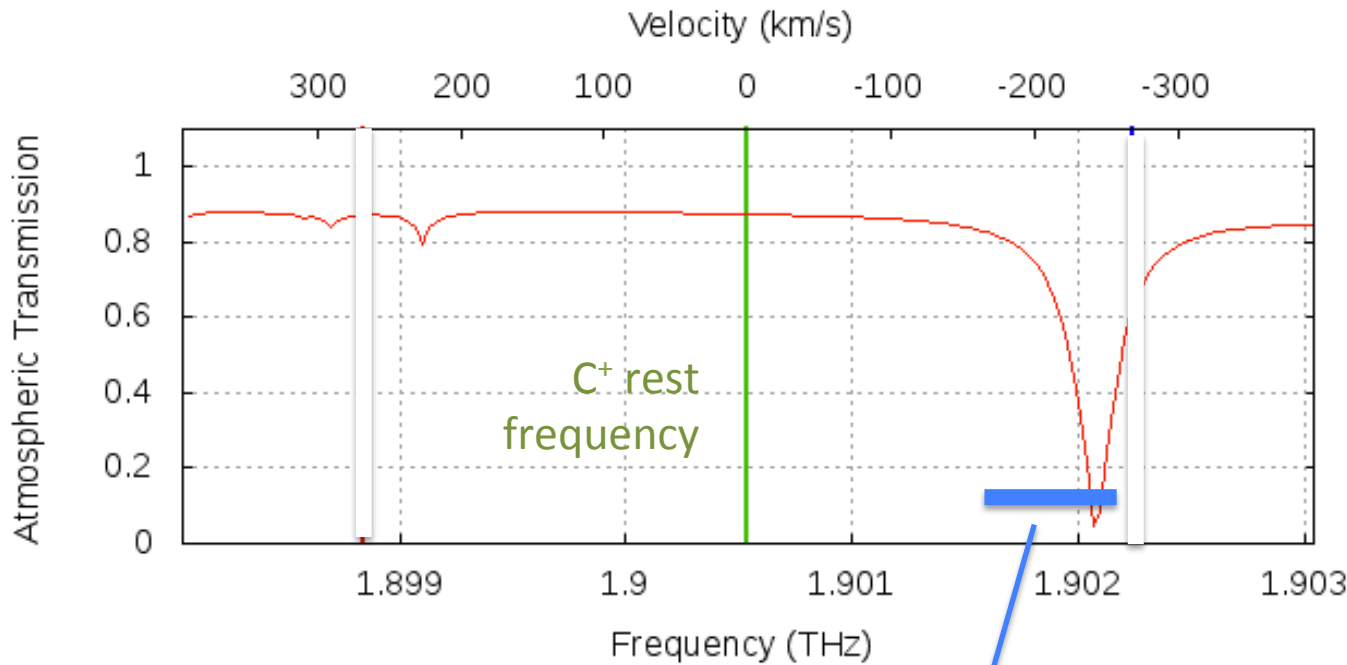
3. Preparing GREAT Single Point Observation: Atmosphere



Use GREAT time estimator tool to determine the atmospheric transmission:

<https://great.sofia.usra.edu/cgi-bin/great/great.cgi>

Atmosphere around C+ line good, but not for strongly blue shifted lines of CMZ targets:



$$V_{LSR} = -150 - 150 \text{ km/s}$$

$$V_{HELIO} = -159 - 259 \text{ km/s}$$

$V_{DOP} = V_{HELIO} \pm 17 \text{ km/s}$
(extremes in october +17 and march -16 km/s).
October a bit better.

Difficult project, but not impossible (see section 2.1 in Langer et al.)

Expected C+ lines CMZ

(for calculation details, see EXES slides)



20+21 May 2015

SOFIA Observers Workshop





3. Preparing GREAT Single Point Observation: Atmosphere

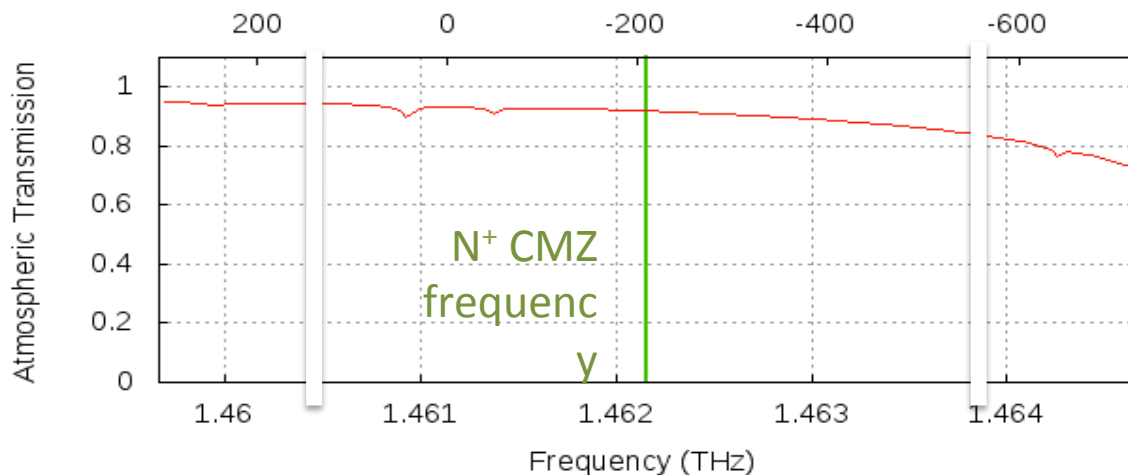
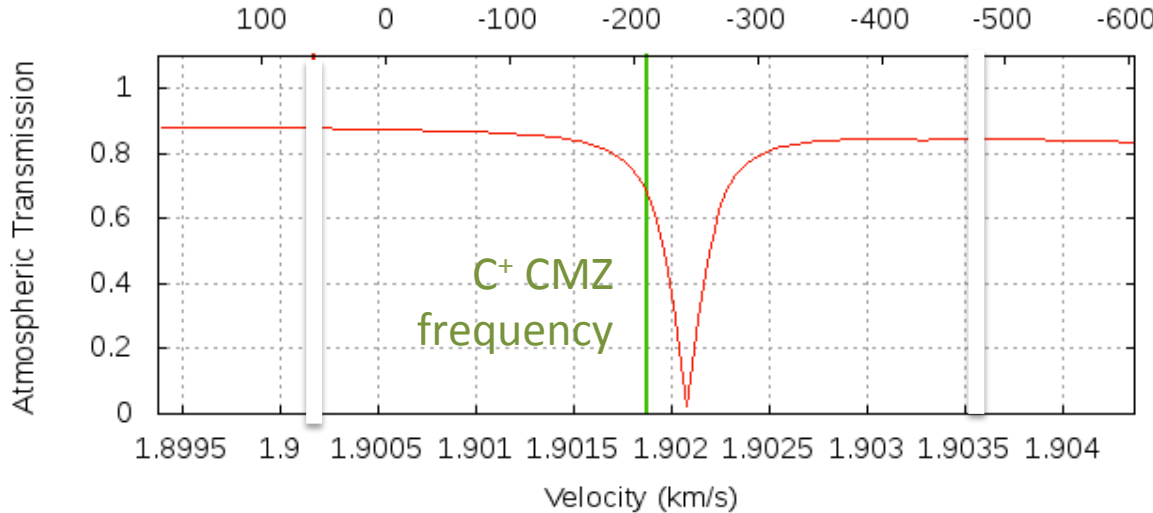


Use GREAT time estimator tool to determine the atmospheric transmission:

<https://great.sofia.usra.edu/cgi-bin/great/great.cgi>

C⁺ difficult at CMZ velocity shift

N⁺ much easier





3. GREAT Instrument Status and Configurations Offered for Cycle 4



GREAT mixer bands:

- **L1 1.25 – 1.52 THz**: not all frequencies available! Contact team or helpdesk.
 - E.g.: CO 12-11, OD, SH, H₂D⁺, CO 13-12, [NII]
- **L2 1.81 – 1.91 THz**: not all freq available! Contact team or helpdesk.
 - E.g., CO 16-15, [CII], NH₃ 3-2, OH 2Π_{1/2}
- **H 4.74 THz**: -25 to +90 km/s or -30 to -140 km/s
 - [OI]
- **M channel**: not offered in cycle 4
 - HD 1-0, 18OH 2Π_{3/2}

Simultaneous observation L1+L2 (e.g., N+ and C+) or L2+H (e.g., C+ and O), depends on results of call.

Instantaneous usable band width ~1.8-2 GHz, but 0.9 GHz for H channel.

upGREAT: 7 pixel map around C+ line, if commissioning succesfull, combined with L1. Order of magnitude improved mapping speed compared to single beam! See presentation by Randolf Klein.

3. GREAT Frequency Tuning

GREAT is a Dual Sideband (DSB) receiver. The local oscillator signal is mixed with the sky signal. The difference $|v_{LO} - v_{SKY}|$ (IF, Intermediate Frequency) is detected:

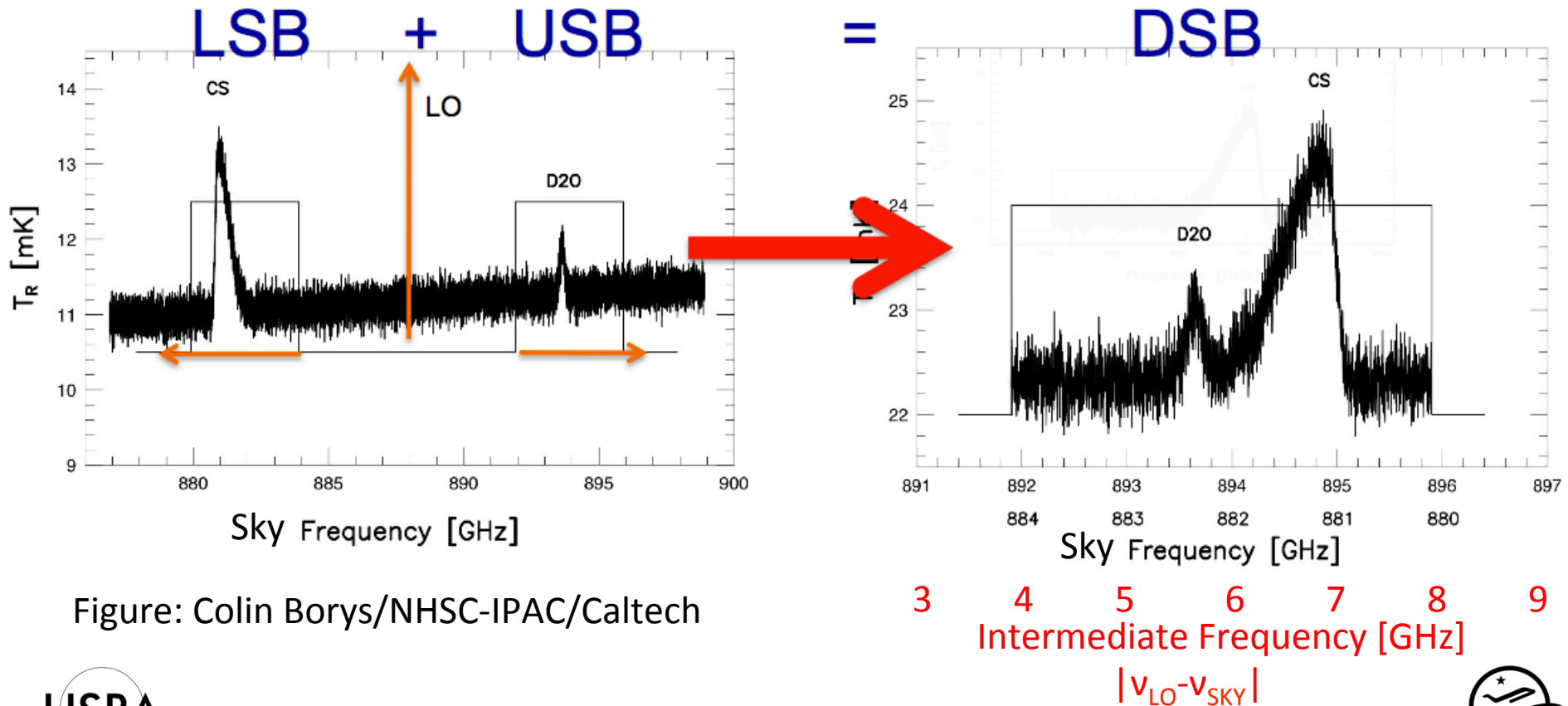


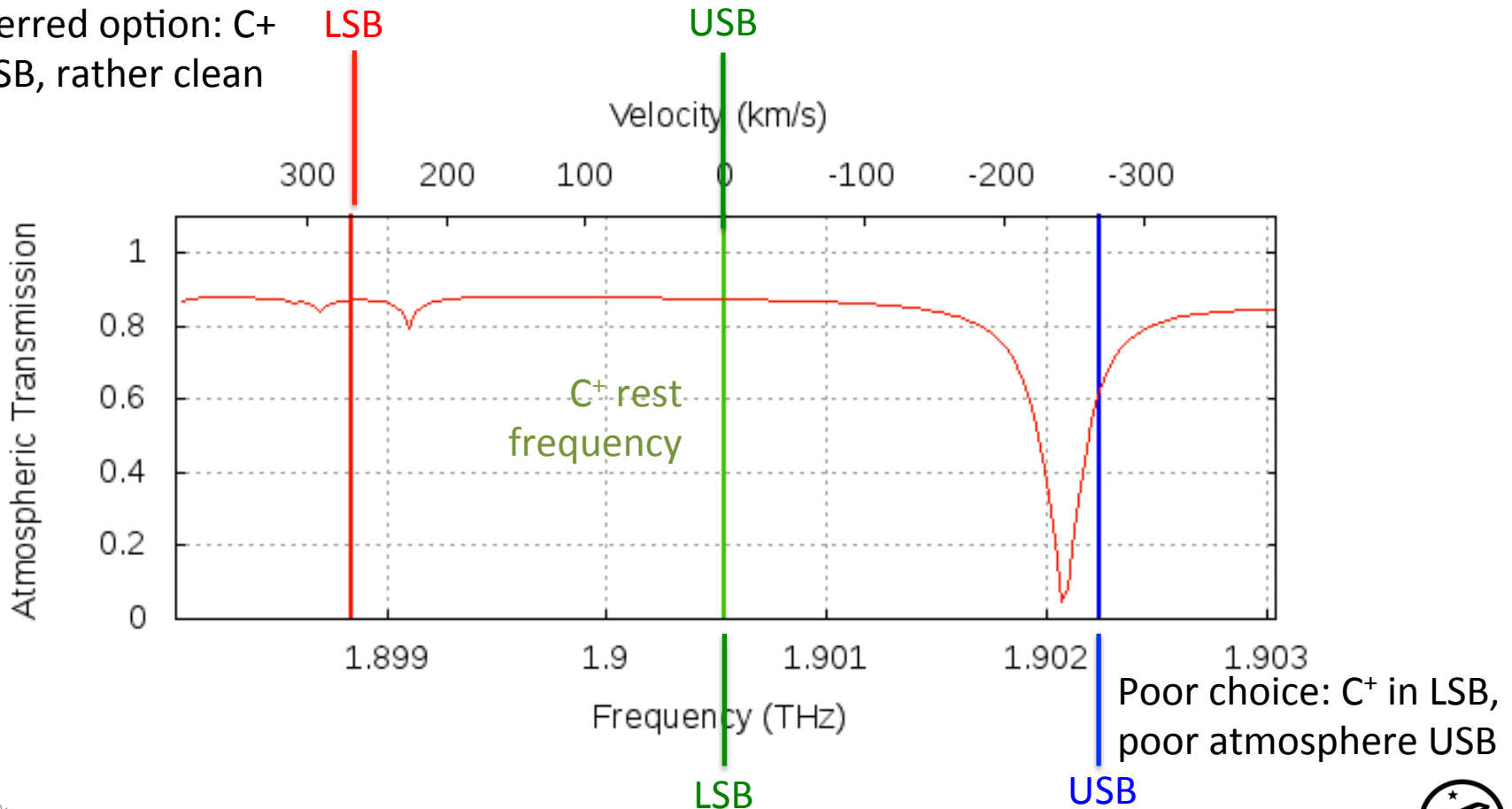
Figure: Colin Borys/NHSC-IPAC/Caltech



3. GREAT Frequency Tuning

At low Doppler shifts, the C+ line is best observed in the upper sideband (USB)

Preferred option: C+ in USB, rather clean LSB



Poor choice: C+ in LSB, poor atmosphere USB

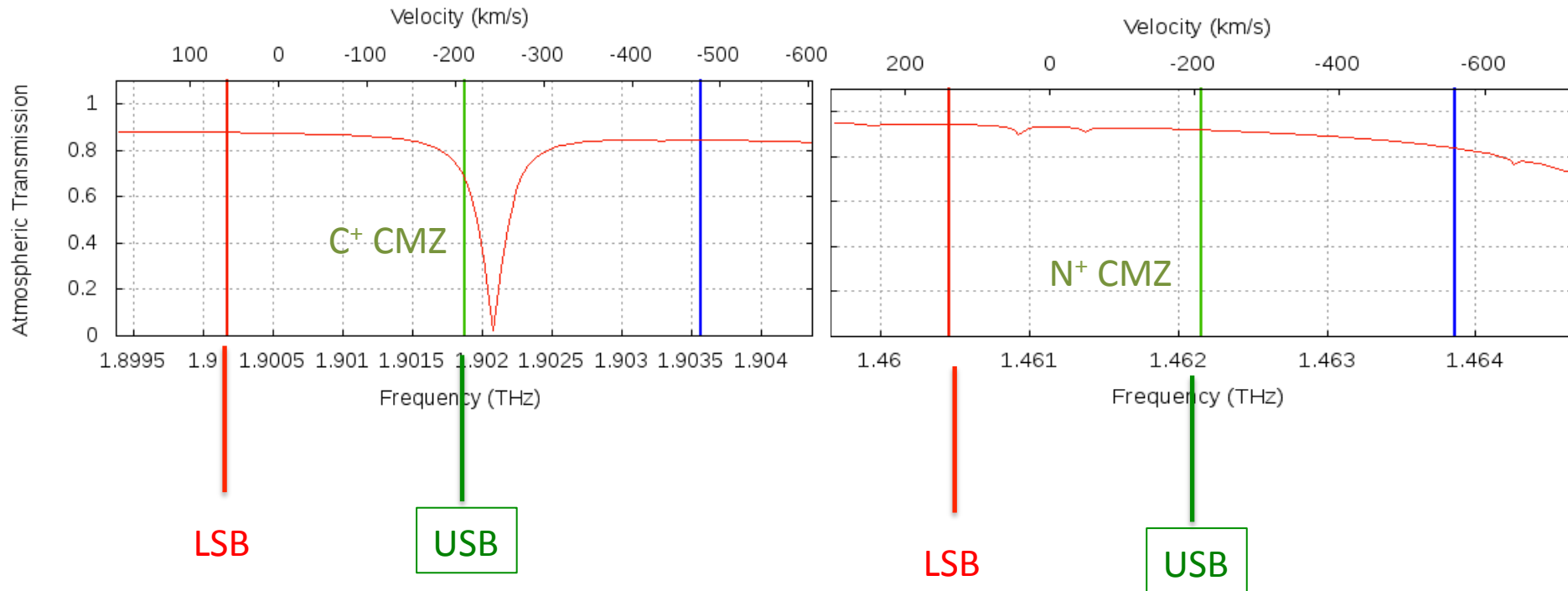




3. GREAT Frequency Tuning



At large, negative Doppler shifts, the sideband choice for C+ is less relevant, though USB slightly preferred, similar to N+ (better transmission in image sideband)





3. GREAT Observing Modes



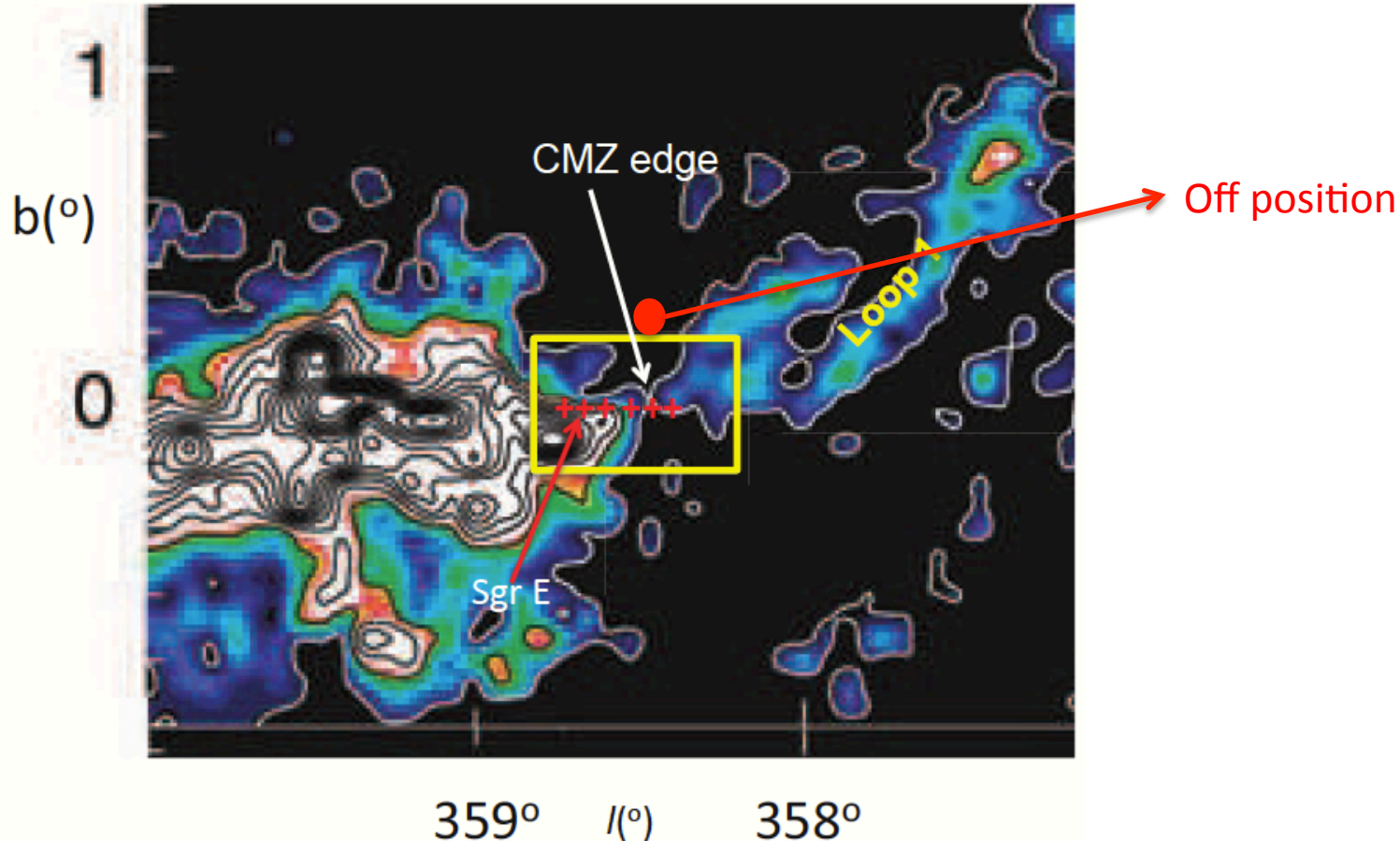
- Single pointing:
 - dual beam switching (DBS) chopping with the secondary
 - position switching (“Total Power”)
- On-the-fly mapping (see presentation by Randolph Klein):
 - position switch (“Total Power”)
 - single beam switch (SBS)
- Raster mapping:
 - dual beam switching (DBS)
 - position switching (“Total Power”)

CMZ: expected lines are weak (esp. N+), and the emission is expected to be very extended: Use single point, position switch mode.

Which position to switch to?

3. GREAT: Off Position

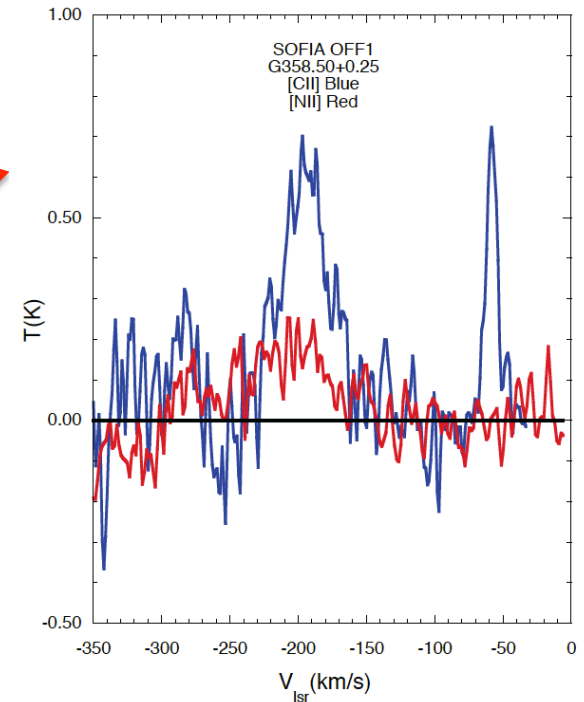
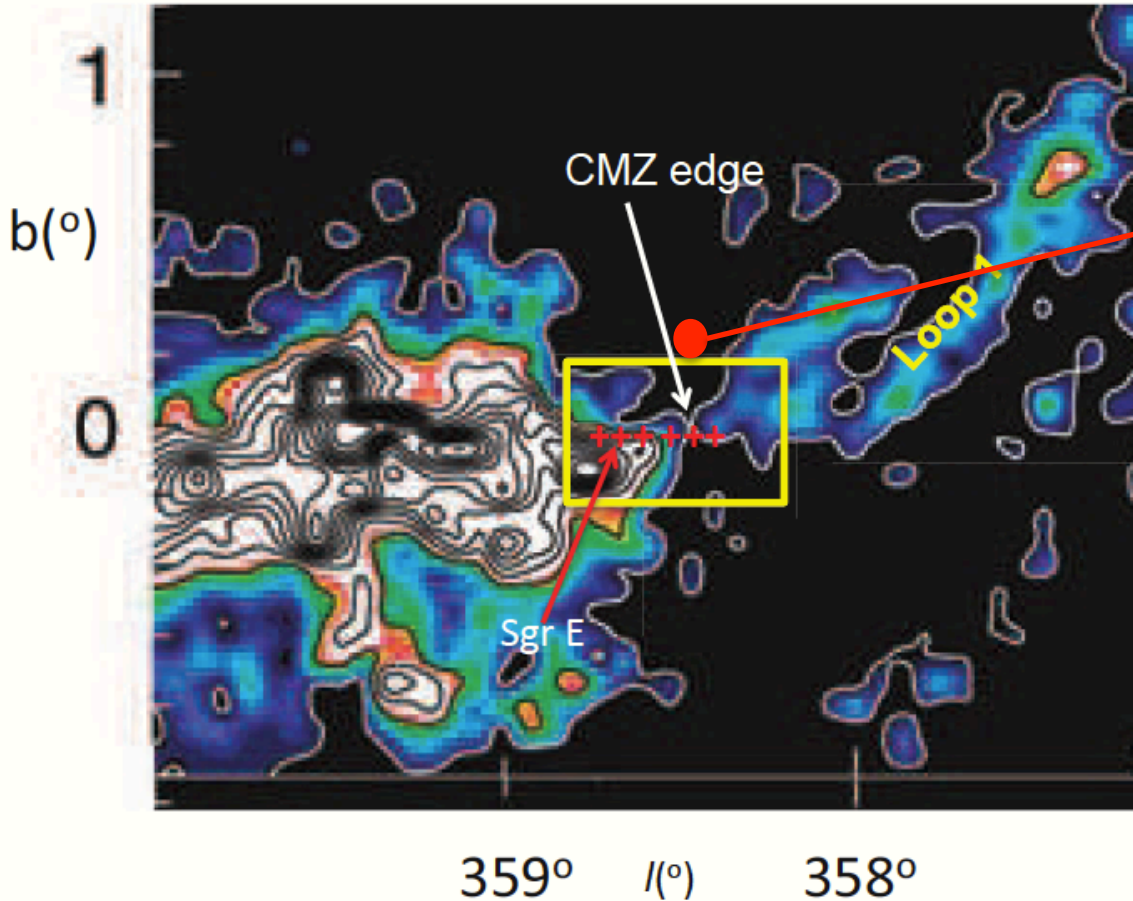
It is important to find a sky 'off' position that is clean (or as clean as possible).
Requires literature search (and sometimes trial and error at the telescope):



NANTEN CO(1-0) map (Fukui et al. 2006)

3. GREAT: Off Position

It is important to find a sky 'off' position that is clean (or as clean as possible):



Not so clean after all, but ok, and in fact correctable in data reduction.



3. GREAT Sensitivities, Exposure Time Calculations



GREAT observing time estimator is linked on SOFIA "SITE" page:

<https://dcs.arc.nasa.gov/proposalDevelopment/SITE/index.jsp>

<https://great.sofia.usra.edu/cgi-bin/great/great.cgi>

N⁺ input:

- Rest frequency=1461.1319 GHz
- Velocity correction=-210 km/s
- Expected peak intensity $T_R^* = 0.1$ K ($T_R^* = T_{MB} * \eta_{MB} = 0.15 * 0.67$; Langer et al.)
- Desired S/N in line peak=3
- Resolution after smoothing: 2 km/s (native 88 KHz= 0.015 km/s)

→ 1350 seconds ON+OFF time. Add 100% overhead for nodding and chopping overhead, and add X minutes for tuning, and other setup overhead.

For C⁺ line, observed simultaneously, 1350 sec ON+OFF: S/N=20 in 1 K line peak.

Note: smoothing parameter yields noise on all frequency scales
(channel -channel, baseline fluctuations)





3. SOFIA/GREAT versus Herschel/HIFI



GREAT mixers significantly improved over those at HIFI, in system temperature and baseline quality (standing waves). Despite presence of atmosphere, GREAT (nearly) as sensitive as HIFI:

- C⁺ line at 1900.5369 GHz, at rest velocity, 41,000 ft, smoothed over 2 km/s, 1000 seconds ON+OFF on T_R^* scale, fully extended emission:
 - GREAT: RMS=53 mK, $T_{\text{sys}}=2840$ K (T_{sys} includes atmosphere!)
 - HIFI: RMS=45 mK, $T_{\text{sys}}=2760$ K
- Same after smoothing to 50 km/s (stability for broad lines):
 - GREAT: RMS=11 mK
 - HIFI: RMS=12 mK
- Also, HIFI had no mixers for N⁺ and OI, and Herschel out of Helium
- However, HIFI more sensitive for point source emission (3.5 vs 2.5 meter mirror!).



4. GREAT and EXES: For Further Reading



GREAT:

- Guide to Planning Observations with SOFIA/GREAT
http://www.sofia.usra.edu/Science/proposals/cycle3/Guide_To_GREAT_v7.pdf
- MPIfR sub-millimeter group (GREAT instrument team):
<http://www3.mpifr-bonn.mpg.de/div/submmtech/>

EXES:

- “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/>



5. EXES and GREAT as PSI Instruments



Both EXES and GREAT are Principal Investigator-class Science Instruments (PSI):

It is highly encouraged (not required) to contact the SOFIA helpdesk (sofia_help@sofia.usra.edu) or instrument teams (EXES: Matt Richter, 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 and GREAT teams."

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

GREAT: "The GREAT PI may designate up to 3 coauthors."