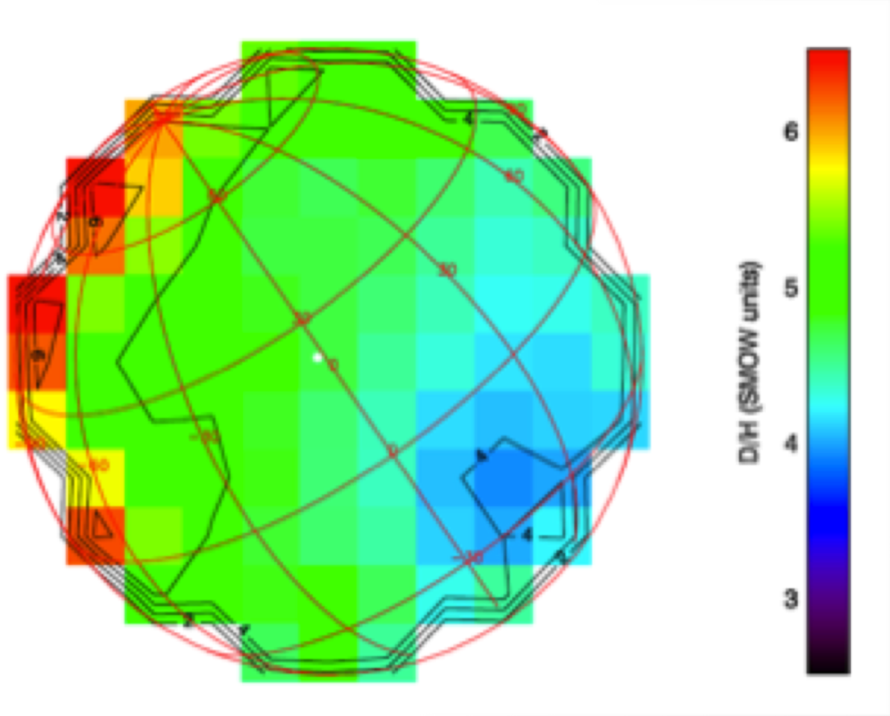
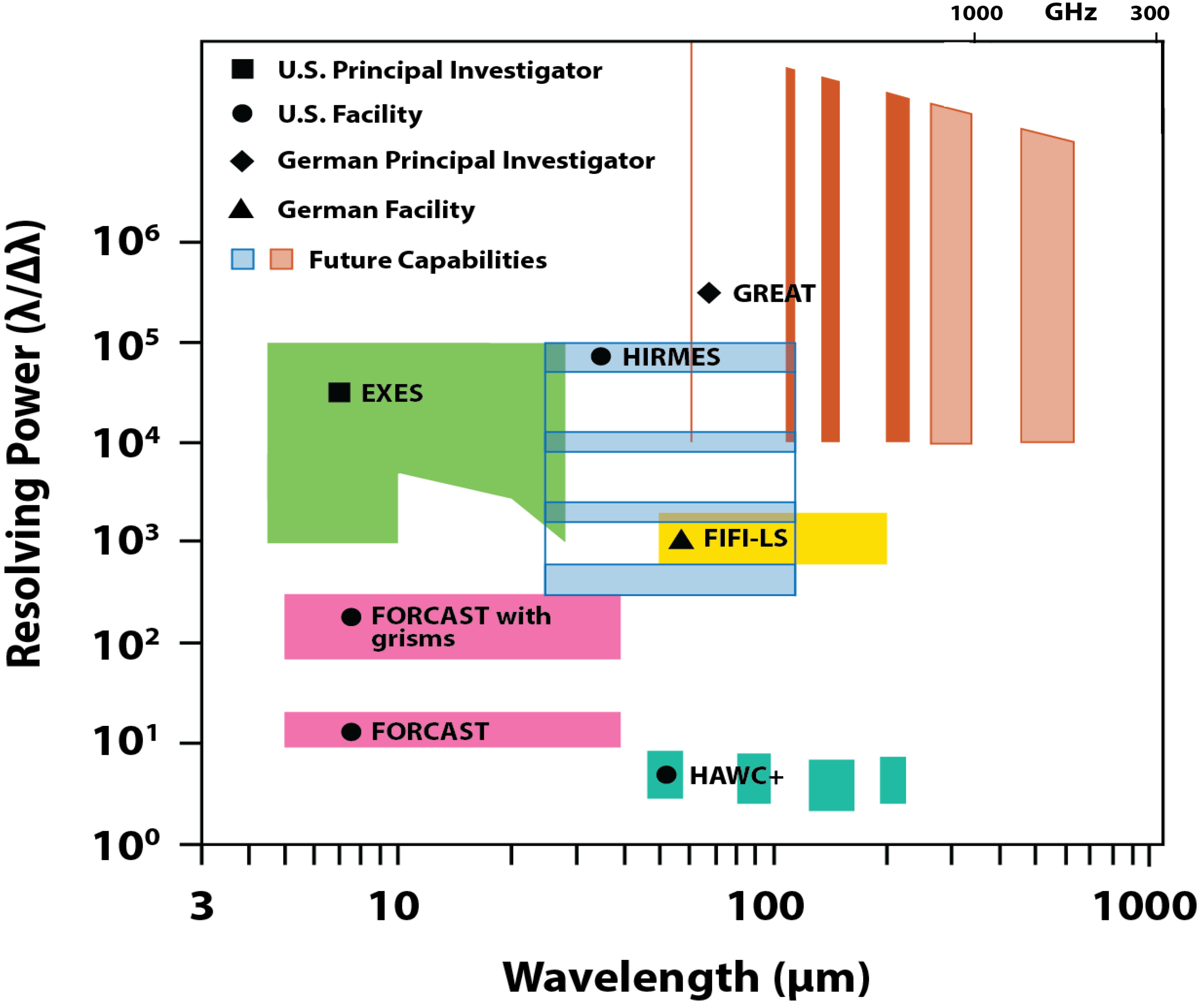
EXES: High-Resolution Mid-IR Spectroscopy with SOFIA



Tracing ancient water on Mars via a D/H map
Encrenaz et al. (2016)

The SOFIA Instrument Suite



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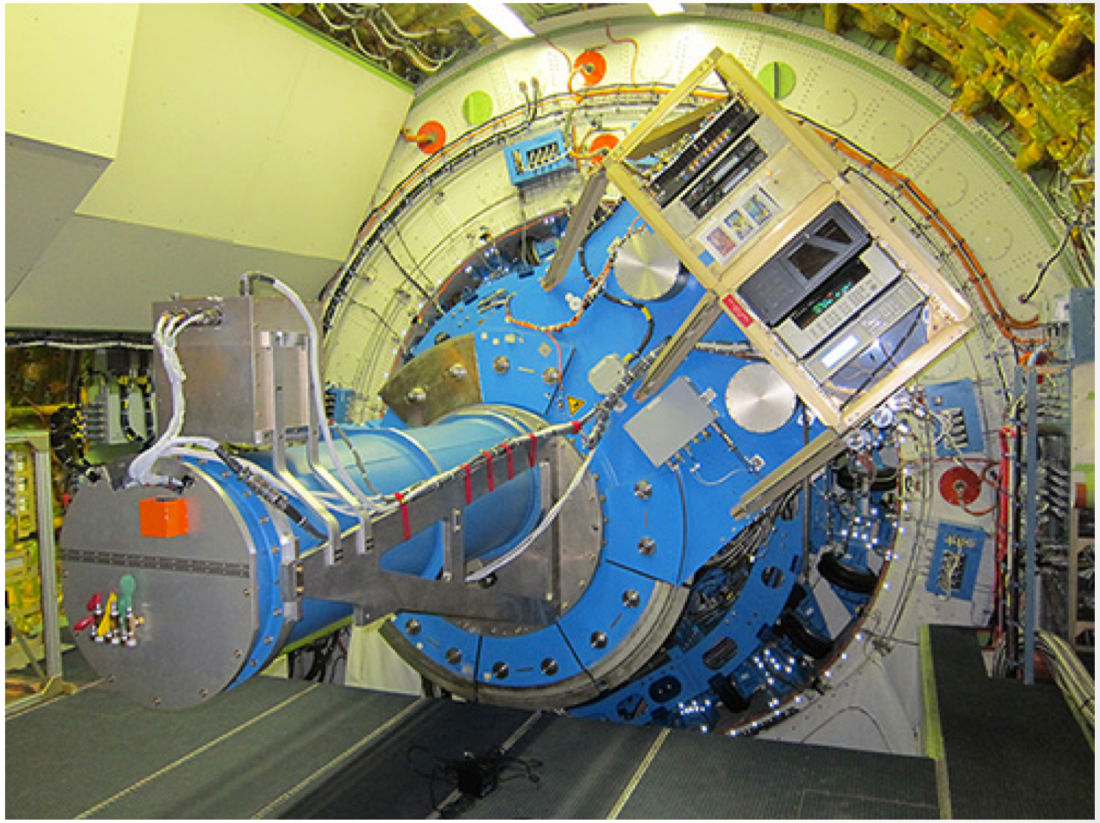
EXES: Echelon Cross Echelle Spectrograph

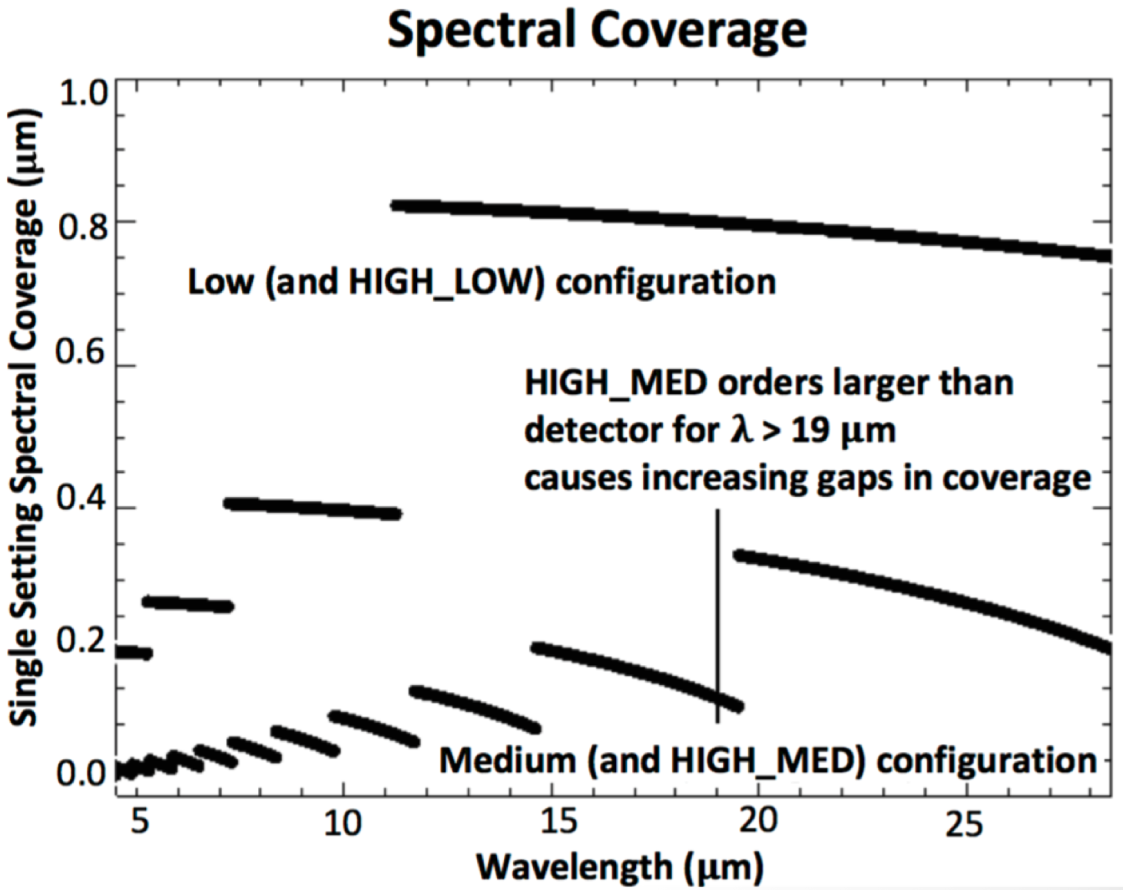
- Mid-IR High-Resolution Spectrometer: 4.5-28.3 μm
- Optimized for High-resolution: R=50000-100000
- Spatial resolution, ~3.5-4.5”
- Array size 1024x1024 Si:As BIB (same as JWST/MIRI)
- Designed and built at UT by J. Lacy and team.
- PI : Matthew Richter, UC Davis



Specifications

Configuration	Slit Length	Spectral Resolution
Low	25"– 180"	1,000 – 3,000
Medium		5,000 – 20,000
HIGH_MED	1.5" – 45"	50,000 – 100,000
HIGH_LOW	1" – 12"	

In the Medium and Low configurations the slit lengths vary from 25" to 180" depending on the number of rows to be read.



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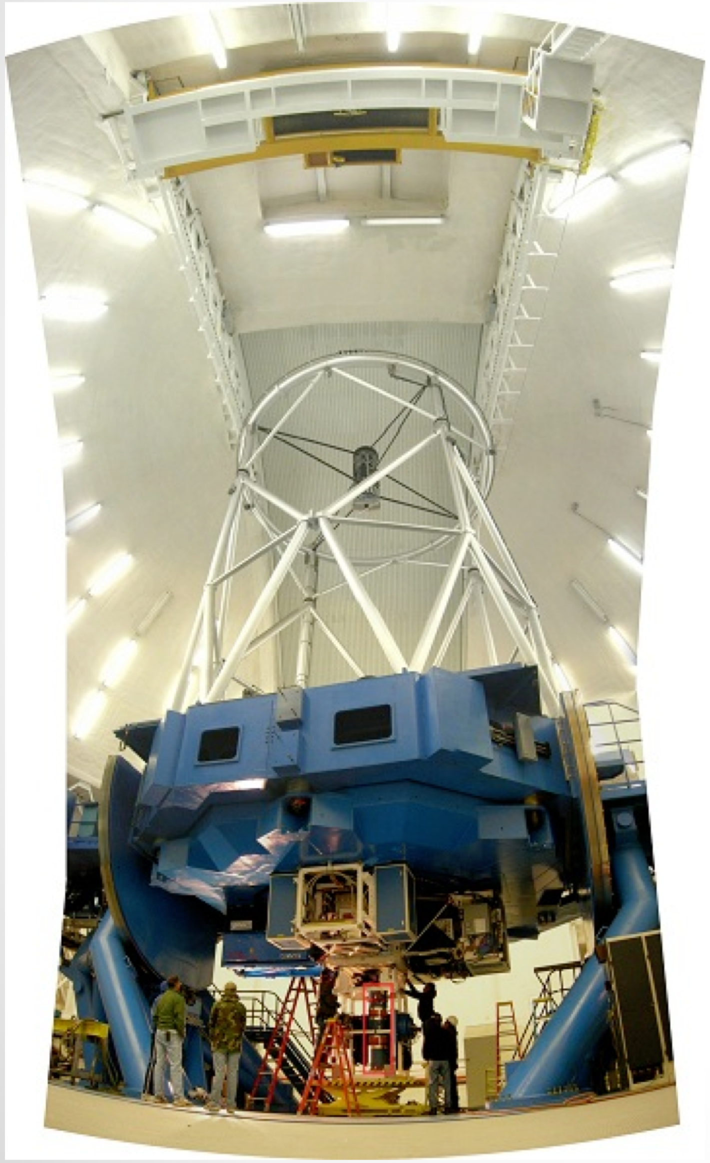
TEXES & EXES



TEXES STANDARD OBSERVING CONFIGUATIONS RESOLVING POWERS, WAVELENGTH COVERAGES, SLIT LENGTHS		
Gemini OT Name	**4.5-14μm 0.52 arcsec wide slit**	**17-20μm, 22-25μm 0.75 arcsec wide slit**
Echelon + 32 l/mm echelle	R~85,000 (high) Δλ ~ 0.006 λ slit length: 4 arcsec	R~60,000 (high) Δλ ~ 0.006 λ slit length: 8 arcsec
Echelon + 75 l/mm grating	R~85,000 (high) Δλ ~ 0.25μm slit length: 1.7 arcsec	-
32 l/mm echelle	R~15,000 (medium) Δλ ~ 0.006 λ slit length: 20 arcsec	R~11,000 (medium) Δλ ~ 0.006 λ slit length: 20 arcsec
75 l/mm grating	R~4,000 (low) Δλ ~ 0.25μm slit length: 20 arcsec (7.5-14μm only)	-

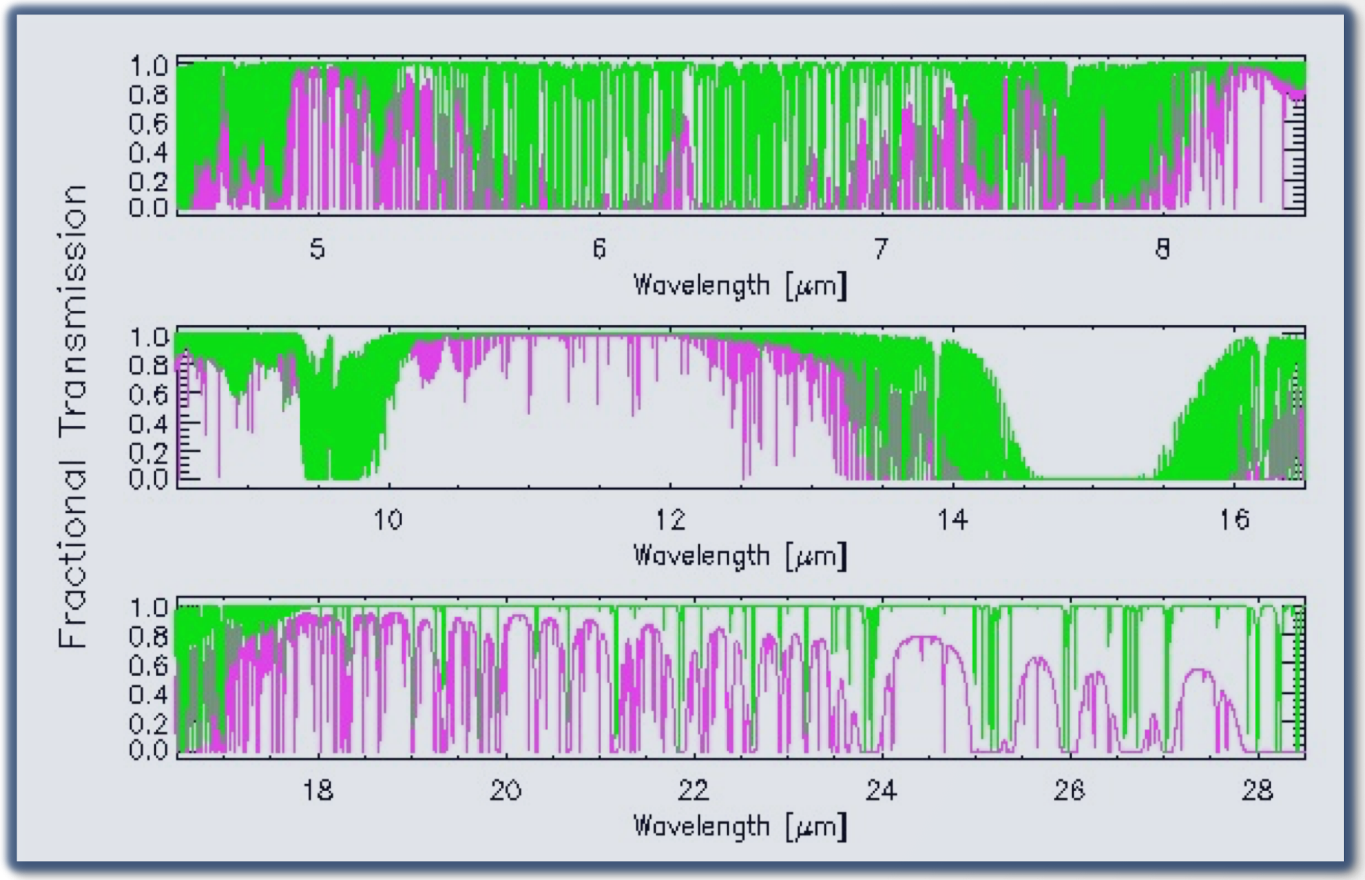
EXES has a companion instrument (TEXES) which is a proprietary instrument which can be mounted at the IRTF and at the GEMINI North telescope in Mauna Kea.
Lines which can be observed with TEXES should not be proposed with EXES. The two instruments are seen as complementary.

Atmospheric transmission

Range: 4.5μm – 28.3μm

Spitzer/IRS and ISO/SWS were limited R=100-1000.

Even though SOFIA flies about 99.9% of water vapor, you still have to work around the remaining 0.1%.



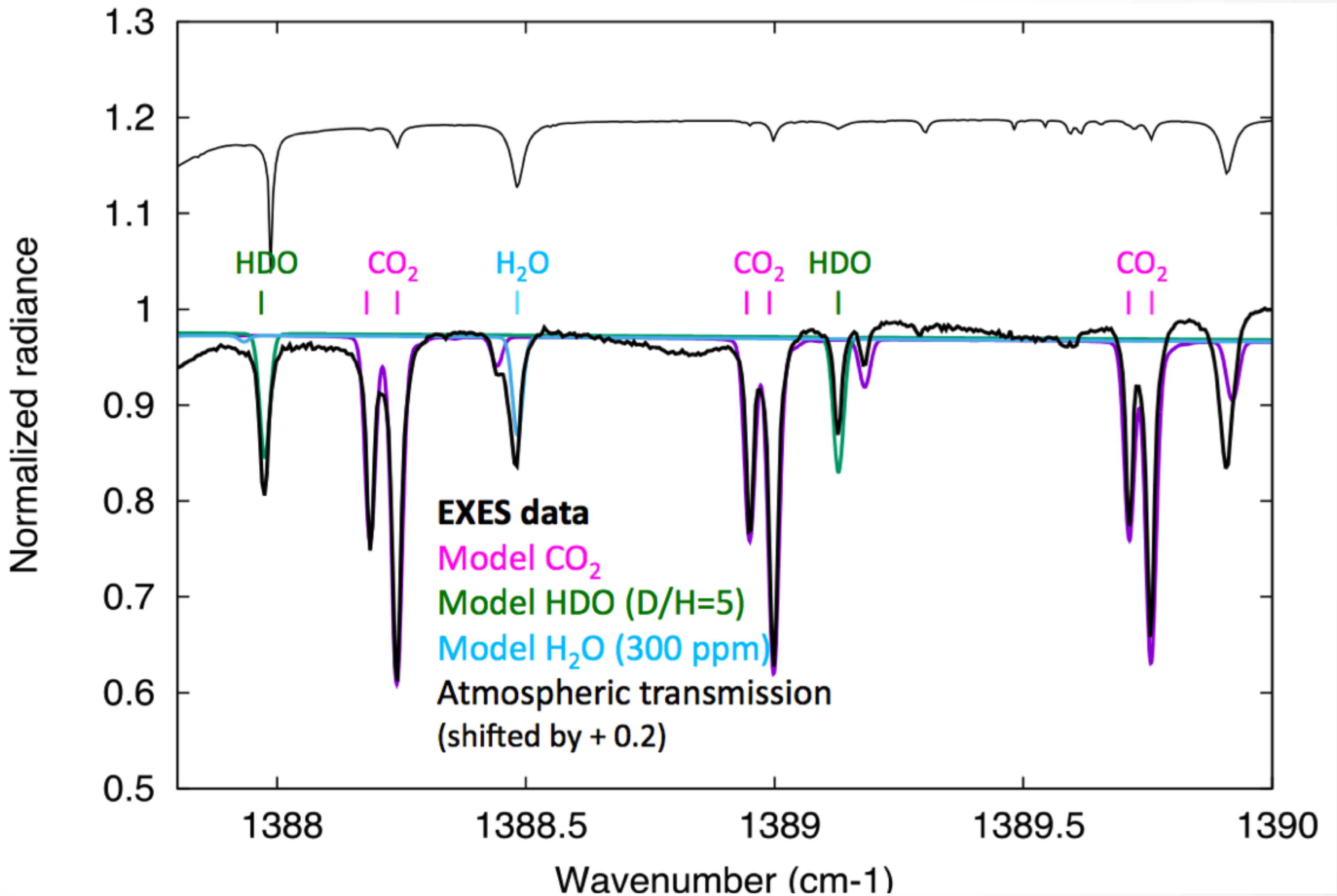
Atm. Transmission for SOFIA (green) and Mauna Kea (magenta)

High Resolution Spectroscopy Science

- Many molecular and ionic lines of interest in the 4.5-28.3μm
- Resolved line profiles yield kinematic origin of line emission/absorption, e.g.:
  - Infall
  - Outflow
  - Rotation
- Separation of spectroscopically crowded line regions
  - P-Cygni profiles, multiple components
  - Closely spaced (roto-)vibrational transitions
- Higher contrast peak emission/absorption line increases detectability
- Separation of telluric and astronomical line improves sky correction

Separation of telluric and astronomical lines

At resolving powers worse than 10^4, telluric and astronomical features are hopelessly blended



Mars, Encrenaz (2016)

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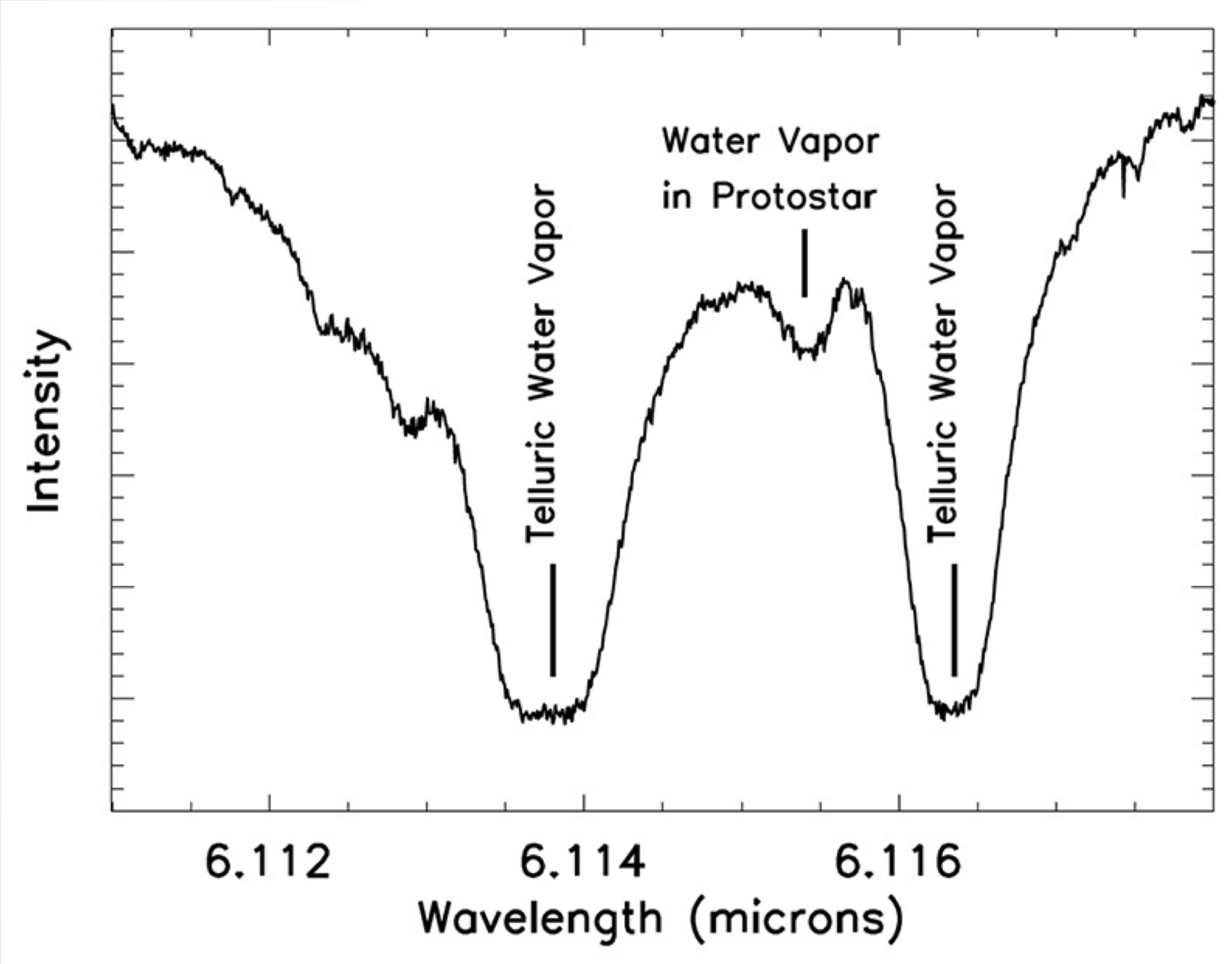
EXES Highlights: Doppler shift



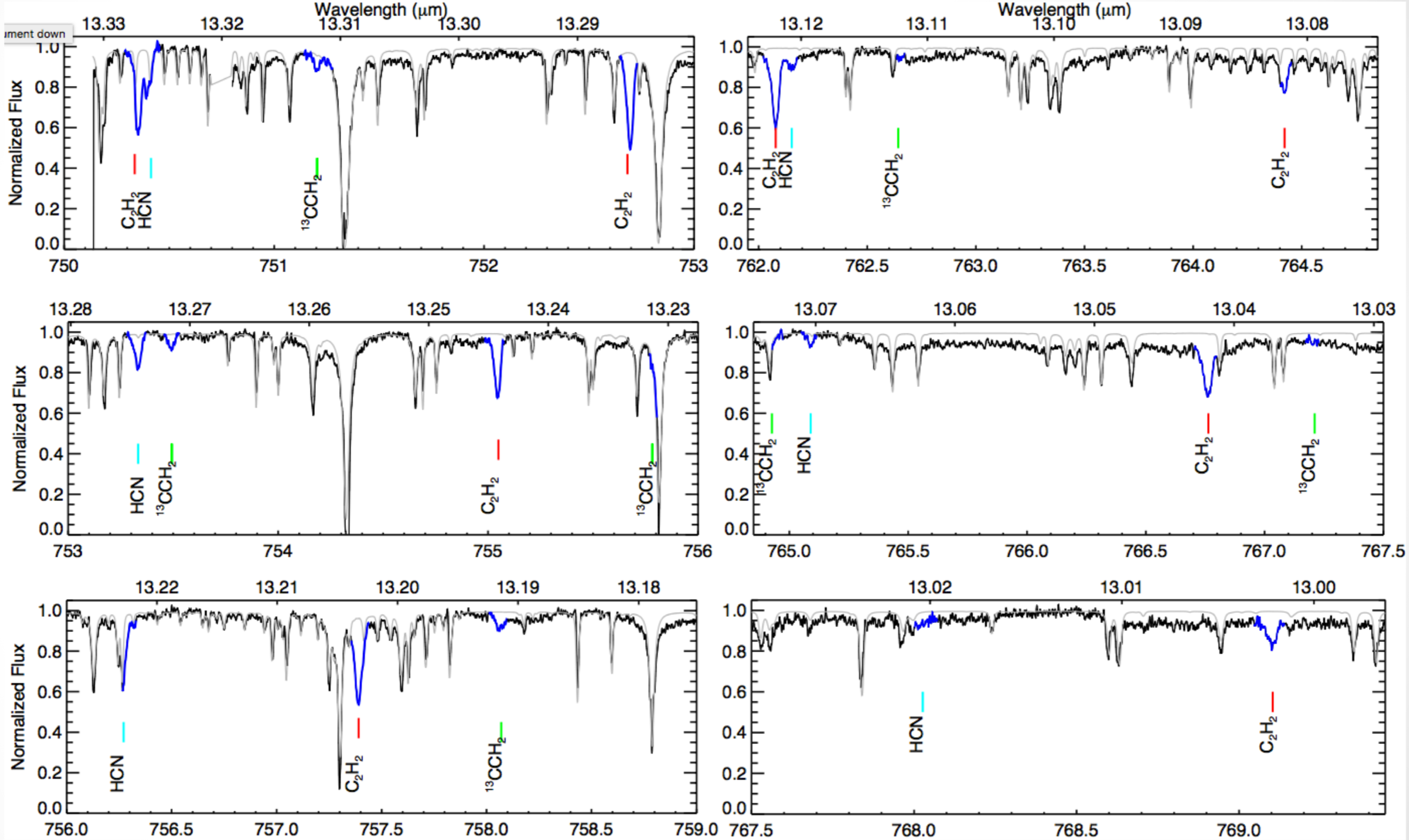
Idriolo et al (2015) used the Doppler shift of AFGL 2591 relative to the Earth to separate its H_2O from the nearby zero-transmission telluric features.

A shift of 34.7 km/s was sufficient.

R=86,000 High - Medium EXES spectrum of massive YSO AFGL 2591
Indriolo et al. [2015ApJ...802L..14I]

Line survey

Spectral survey Orion hot core



Rangwala (ApJ 2018)

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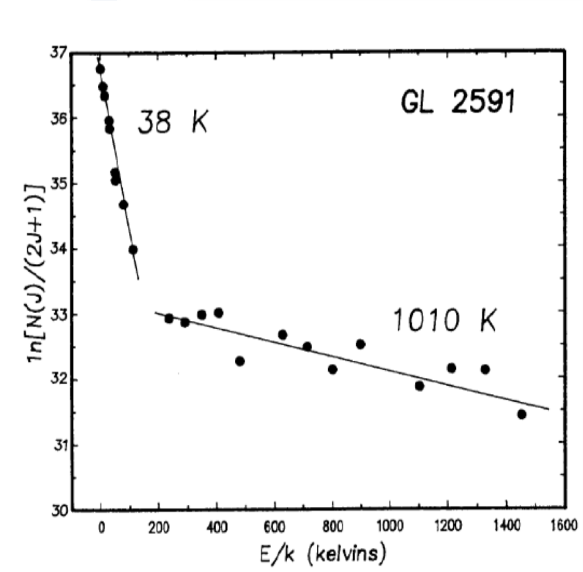
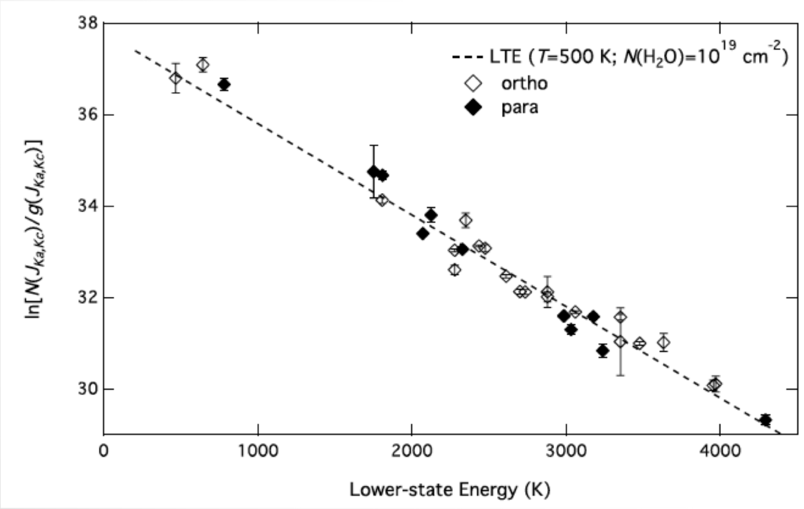
Molecules in massive YSO envelopes

Excitation diagrams to derive the amount of water.

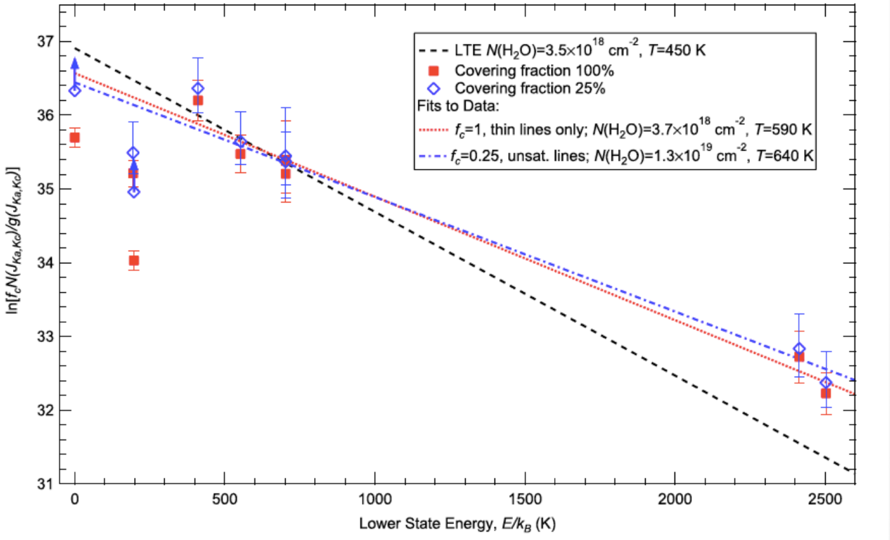
- No ground based access to excitations with
- EXES on SOFIA can detect the ground state para-water and other transitions

Mitchell et al. 1990, ApJ





CRIRES/VLT, lowest level energy, 500 K



SOFIA/EXES, down to 200 K and ground state 0 K

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Organic inventory of massive YSOs 5.4 - 8.0μm

GI: Alexander Tielens

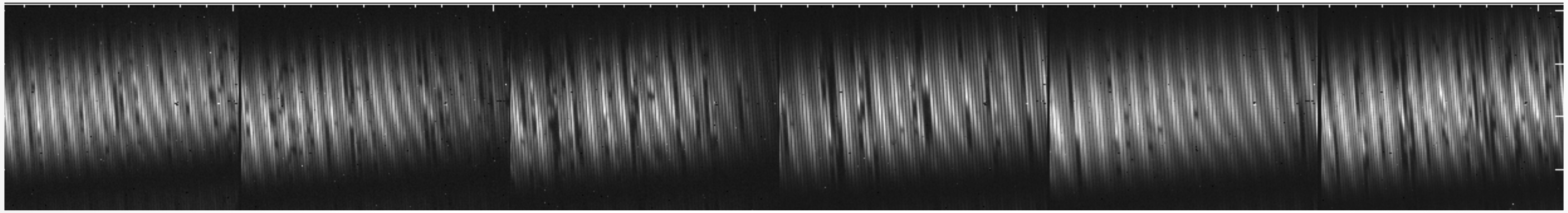
AFGL 2591, AFGL 2316-- using EXES in High-low mode

-- CS, CH_4,NH_3, HCOOH, CH_3CH_2OH, CH_3OCH_3, CH_3CHO, CH_3COCH_3,$HCONH_2$, CH_3CN

27 hr award (1 source completed, 7 hrs remaining)

TEXES/IRTF 2017b: (PI: A. Boogert)

-- Extends the coverage to 8-13 μm and adds 2 YSOs



Hi-lo mode for spectral surveys in action: The O-rich AGB star VY CMa, 5.6-7μm with EXES in 2015. (E. Montiel & P. Fonfria, in prep.)

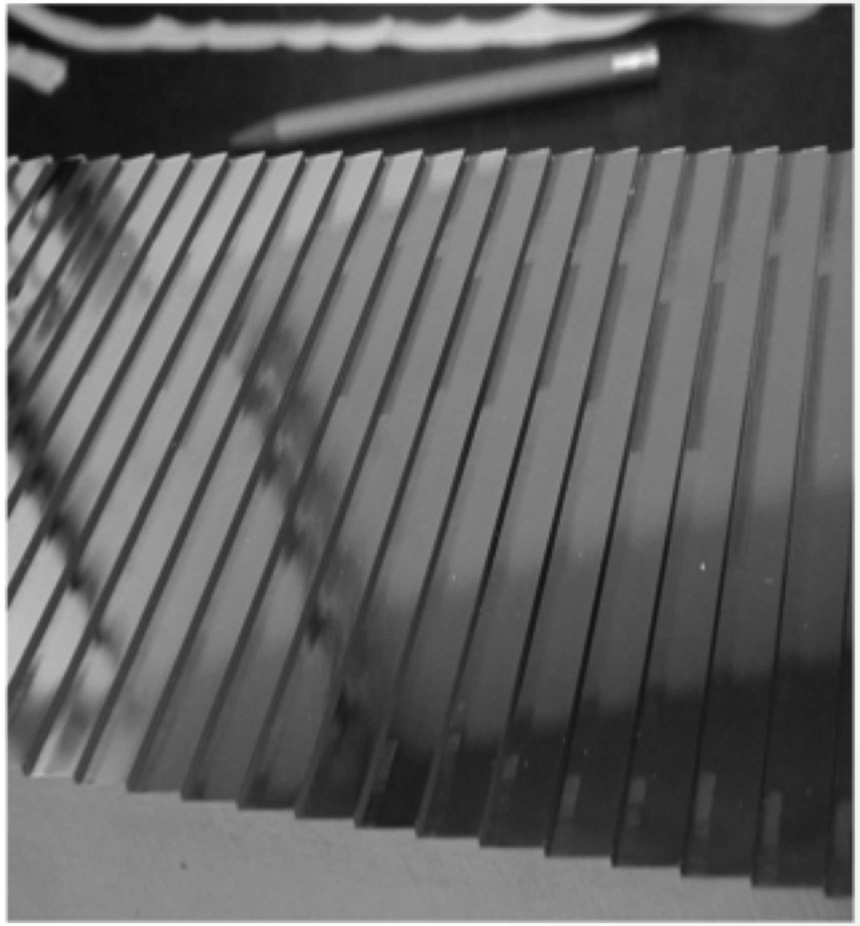
Molecular lines already observed

Molecule	Wavelength	Project
H_2O	6.1	AFGL 2591
H_2O, HDO	7.2	Mars, Venus
H_2	6.9	IC 443
C_2H_2, $^{13}CCH_2$, HCN	13	Orion IRC2
CH_4	7.5	Mars, YSOs

EXES: configurations

Two dispersive elements set the instrument configuration:

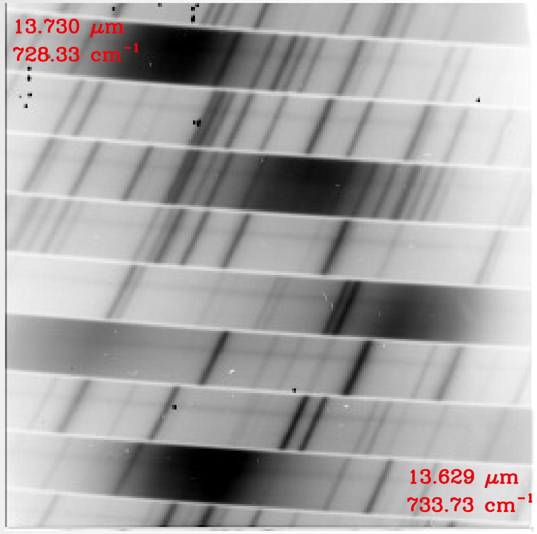
- Echelon: provides high spectral resolution
- Echelle:
  - medium or low resolution cross dispersion of echelon orders
  - medium or low resolution spectroscopy (echelon bypassed)



EXES echelon

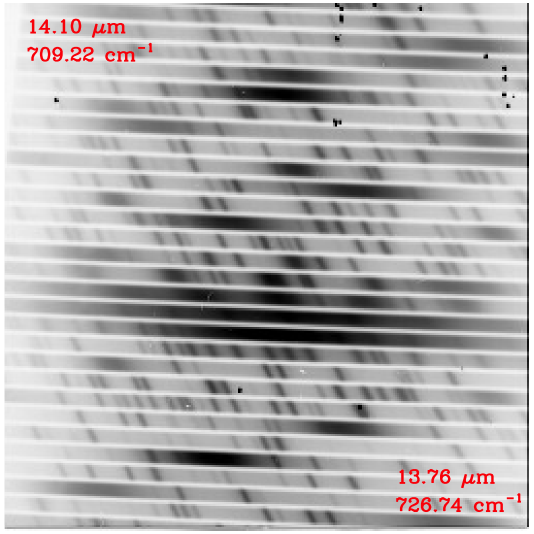
EXES High Resolution Modes

HIGH_MED Configuration

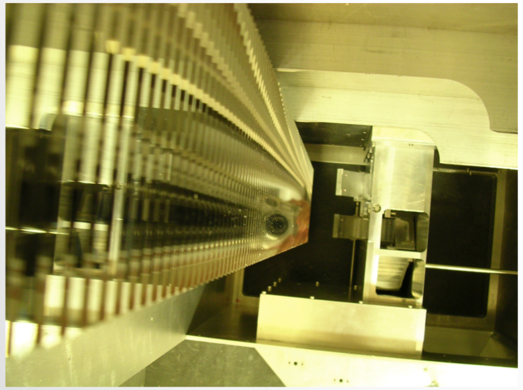


23″ slit length,
6 cm^{-1} coverage

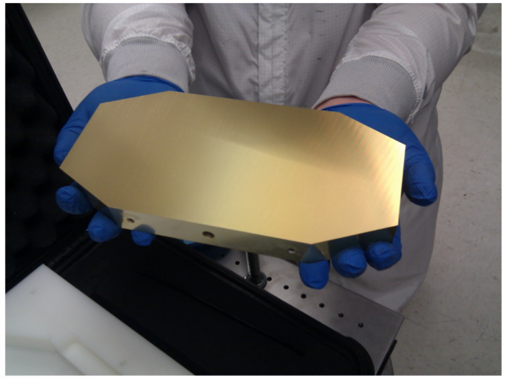
HIGH_LOW Configuration



5″ slit length,
20 cm^{-1} coverage



Echelon



Echelle

HIGH_MEDIUM & HIGH_LOW

- Same high resolution from the echelon grating, R=50,000-100,000, depending on slit width
- Cross disperser angle selects the order – blaze efficiency peaks for both low angles and high-angles
- When slit length is ~3x PSF size, can do on-slit nodding for 2x sensitivity

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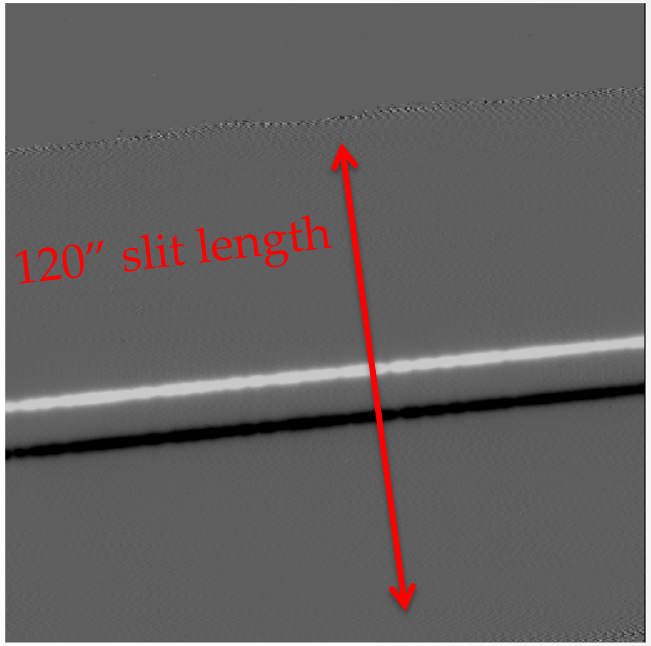
EXES Medium / Low modes

- 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, 6x higher sensitivity, and longer slit.
- Application: e.g., sensitive spatial mapping lines at medium resolution



Nod-subtracted data, showing star in positive and negative beams

Observing modes

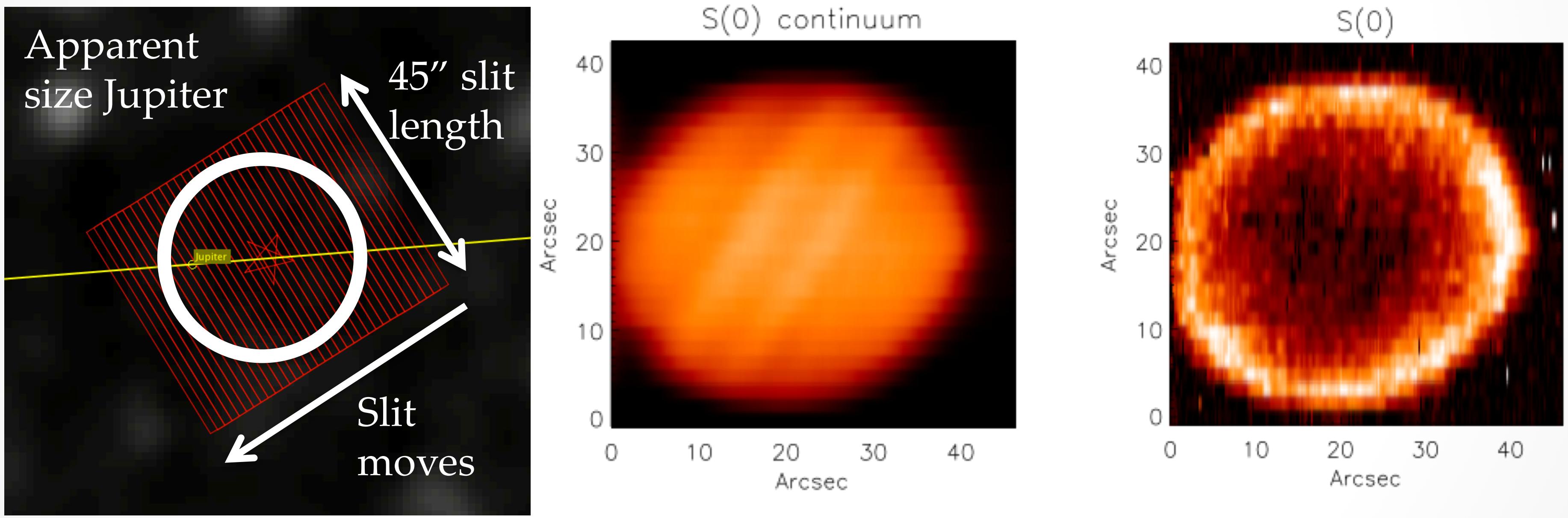
EXES does not use the chopper.

There are three possible observing modes:

- **Nod_on_slit**: compact sources, if the slit is long enough (typical longer than 4 times PSF FWHM). Note that slit length is a strong function of wavelength.
- **Nod_off_slit**: extended sources and if slit is too short.
- **Mapping**: slit scan.

Mapping

EXES is an efficient mapper, although the slit length and thus the instantaneous map size is strongly wavelength dependent.



Map H_2 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”.

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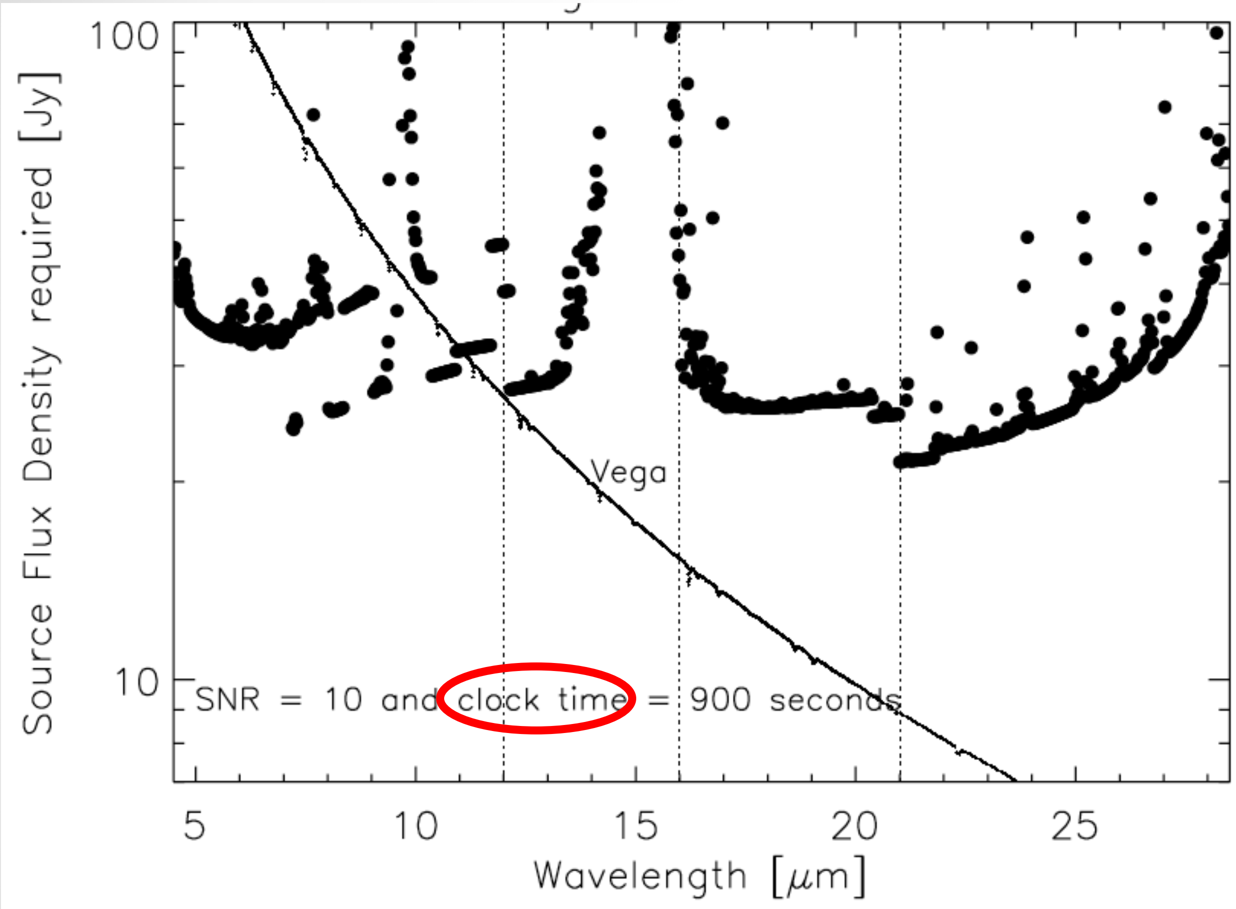
EXES Point Source Sensitivity



Most up-to-date sensitivities in
http://irastro.physics.ucdavis.edu/exes/etc/

High_medium

Sources should be more than 20 Jy to be feasible (varies with wavelength, generally worse with long wavelengths with high background)

High_low

Typically factor of ~2 less sensitive due to among others, shorter slit.

Medium & Low

x10 times more sensitive than High-Med.
~7 Jy T-Tauri source successfully studied in Cycle 5 in medium mode, R = 10000 with about 2 hrs per wavelength setting

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Tips for Preparing an EXES Observation

Key instrument/observation parameters:

1. Feasibility check: check line's wavelength against the atmospheric transmission. How to choose best dates for optimal Doppler velocity.

2. Spectral resolution and instantaneous wavelength coverage needed: instrumental configuration, slit width, echelon order, bypass high-resolution grating ?

3. Background emission subtraction: nodding mode.

4. Compute the clock time needed. Use the ETC tool for EXES.

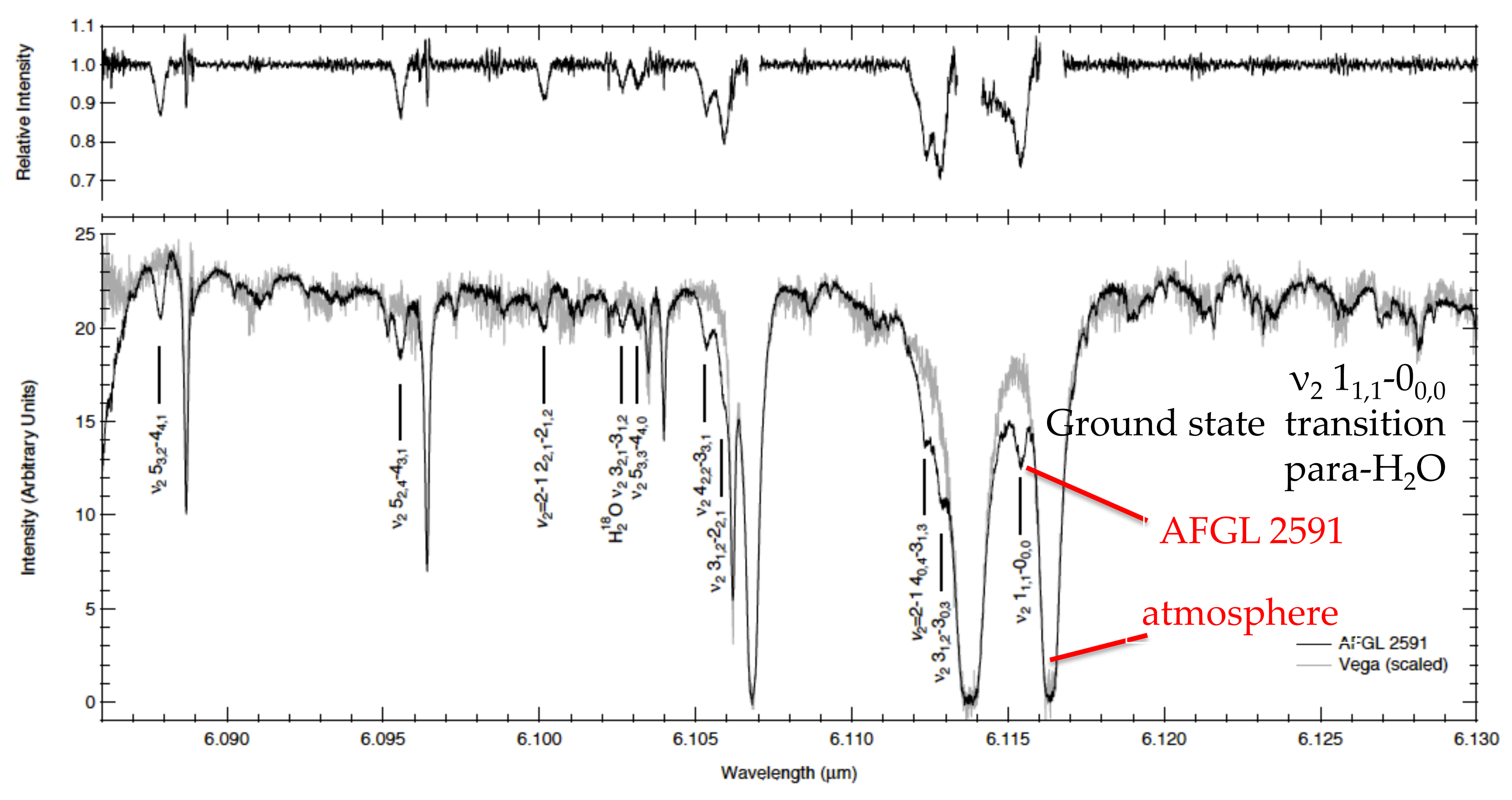
5. Is a telluric calibrator needed for atmospheric line and fringe correction ?

Example EXES observation

We will work out the following example:

- Massive protostar AFGL 2591, ~500 Jy at 6 µm
- obtain S/N=100, R=80,000-100,000
- Resolve line profiles of water vapor to reveal its location and perhaps chemical origin. Previously detected at R=1000 with ISO/SWS spectrum.
- Detect ν_2 $1_{1,1}$-$0_{0,0}$ ground state transition para-H_2O at 6.116 micron (never detected before), for total 'cool' gas column.

Preparing EXES Observation

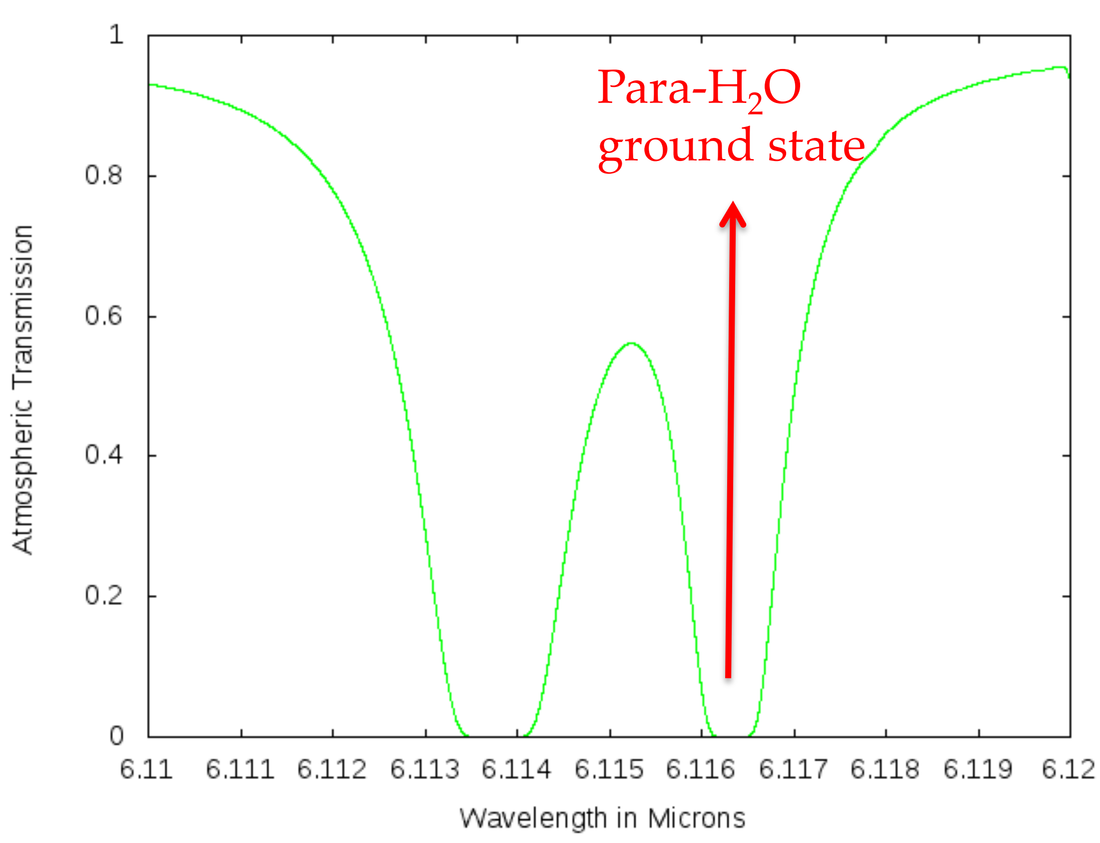


R=86,000 High_Medium EXES spectrum massive YSO AFGL 2591
Indriolo et al. 2015ApJ...802L..14I

Doppler Shifts

ν_2 $1_{1,1}$-$0_{0,0}$ ground state transition para-H_2O at 6.116 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.sofia.usra.edu/cgi-bin/atran/atran.cgi



Seems hopeless?

Need Doppler shift!

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Doppler Shifts

Velocity of line absorption on a 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 orbits around sun at ~ 30 km/s.

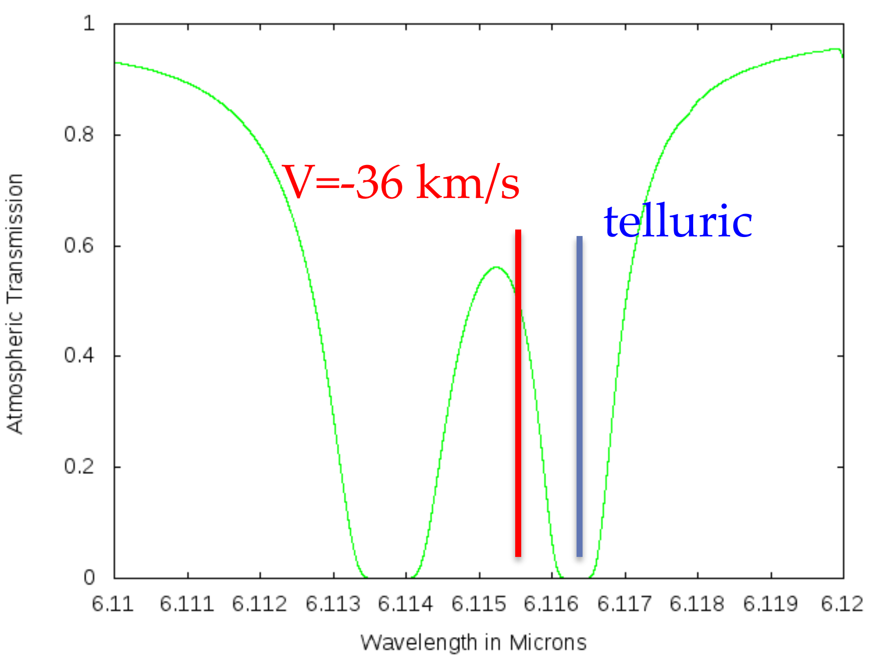
AFGL 2591: V_{LSR}=-5.5 km/s (submm CO lines) →
V_{HEL}=-23.5Km/s

V_{DOP}=-36 km/s on April 10, 2014

=- 6 km/s in Dec

Derive acceptable Doppler shift and set time constraints on 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!



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Preparing EXES Observation: Doppler Shifts

These are the steps to compute the Doppler shift with IDL. Similar codes exist in Python (astropy).

- Convert normal date into Julian date:;
  jdcnv, year, month, day, hour, jd

- Compute the heliocentric velocity of the Earth for given date in km/s
  baryvel, jd, epoch, vh, vb

- Project earth velocity toward target. RA and Dec are the target position in radians
  V_{EARTH}=vh[0]*cos(Dec)*cos(RA) + vh[1]*cos(Dec)*sin(RA)+vh[2]*sin(Dec)

- Add radial heliocentric velocity of target to radial heliocentric velocity of the Earth at given date. The sign of V_{EARTH} is negative!
  $V_{DOP}=V_{HELIO}-V_{EARTH}$

- Note: to convert V_{LSR} to V_{HEL} use helio2lsr.pro
  (Erik Rosolowsky; https://people.ok.ubc.ca/erosolo/idl/lib/helio2lsr.pro)

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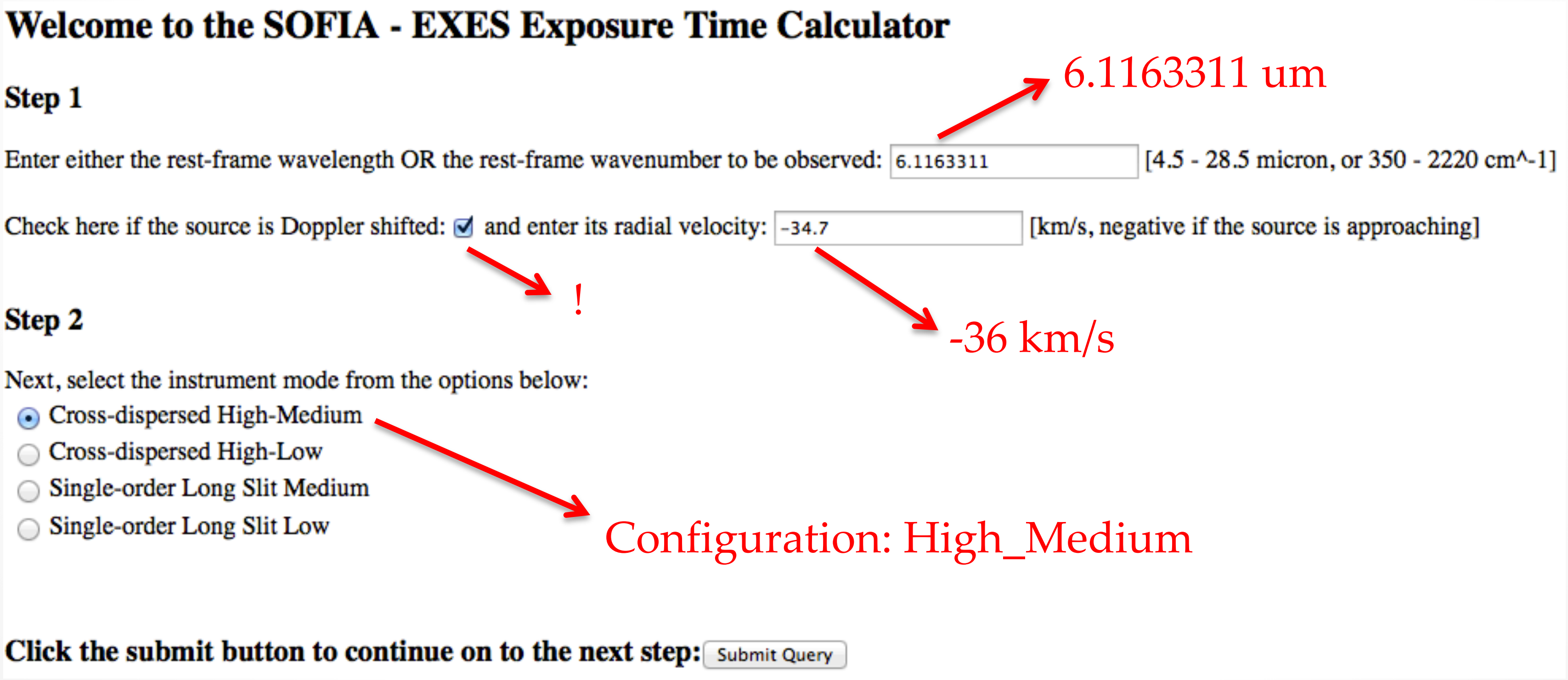
Exposure Time Calculator

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/



Exposure Time Calculator: grating order

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 determines 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
○	6	32.854	112000	6.06134	6.17088	1620.51	1649.8	3.75	Must be off-slit.
○	7	39.63	112000	6.07295	6.15889	1623.67	1646.65	5.06	Must be off-slit.
○	8	47.192	112000	6.08283	6.14877	1626.34	1643.97	6.9	Must be off-slit.
◉	9	56.118	112000	6.09202	6.1394	1628.82	1641.49	10.01	Must be off-slit

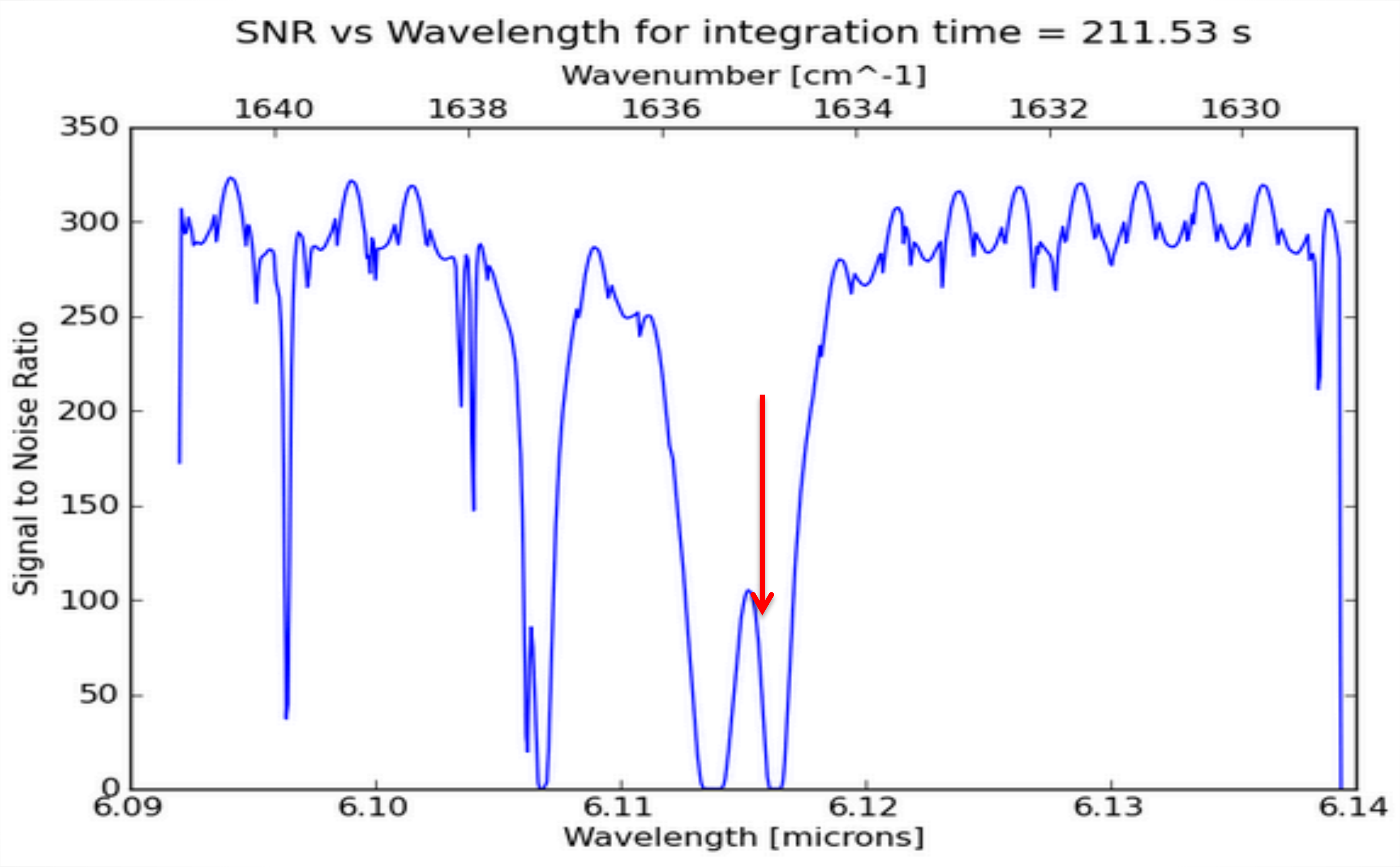
Exposure Time Calculator: slit width

Slit width sets the resolution. Narrower slits block more star light: SOFIA PSF is 3.5". There is a trade off between resolving power and S/N. Consider if the highest resolution is really necessary.

Step 4 - Select a slit width

	Slit Width (arcsec)	Ext. Source Aperture (Slit Width x IQ, arcsec^2)	R 6th order	R 7th order	R 8th order	R 9th order
○	1.44	4.77	112000	112000	112000	112000
◉	1.89	6.24	85590	85590	85590	85590
○	2.43	8.01	66667	66667	66667	66667
○	3.23	10.68	50000	50000	50000	50000

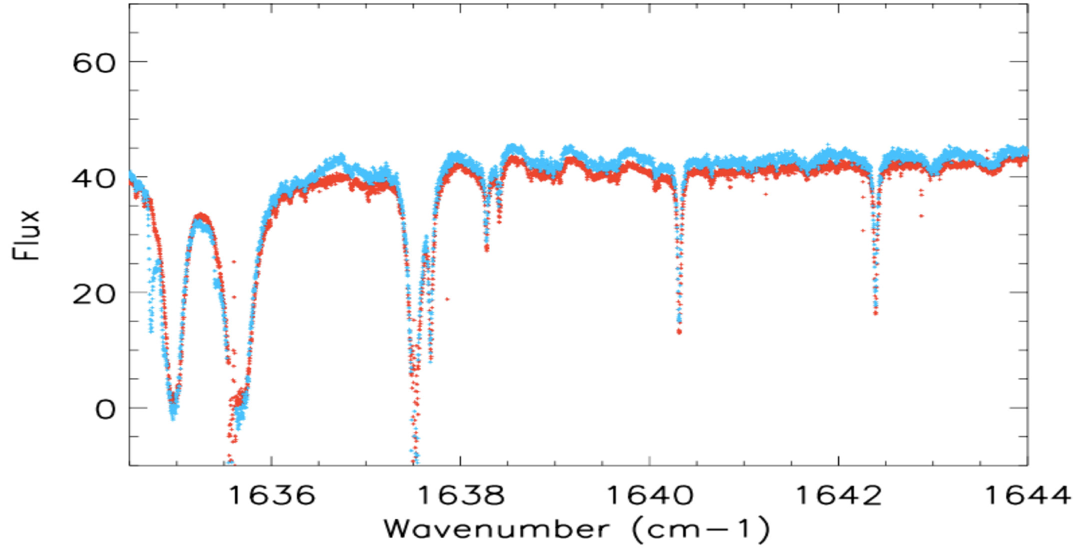
2. Preparing EXES Observation: Clock Time and S/N



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

Telluric Calibration

- Sparse Options in the sky!
  - $\lambda < 9$ μm: only 2 early-type stars have flux densities > 100 Jy: Sirius and Vega
  - $\lambda > 12$ μm: Jovian moons and asteroids are also available.
- Telluric standards also help flatten fringes that make it through the flat fielding step. If features are > 50 km/s, you should consider requesting a telluric calibrator.
- To request a calibrator, include a generic target request, and ask instrument team to suggest an exposure time



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More Information

Contacting instrument team is *ENCOURAGED*

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SOFIA Help Desk

sofia_help@sofia.usra.edu

SOFIA Information for Researchers Website, including SOFIA *Observers Manual*

http://www.sofia.usra.edu/