Molecules around Late-type stars seen in the infrared at high spectral resolution using EXES on SOFIA

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Wednesday, 24th of April 2024 , 14:00 - 14:30 Uhr,

University of Stuttgart, Raumfahrtzentrum Baden-Württemberg
814. WE-Heraeus Seminar: Heritage of SOFIA – Scientific Highlights and Future Perspectives

Content

I. Late-type stars – the birthplace of molecules and chemistry

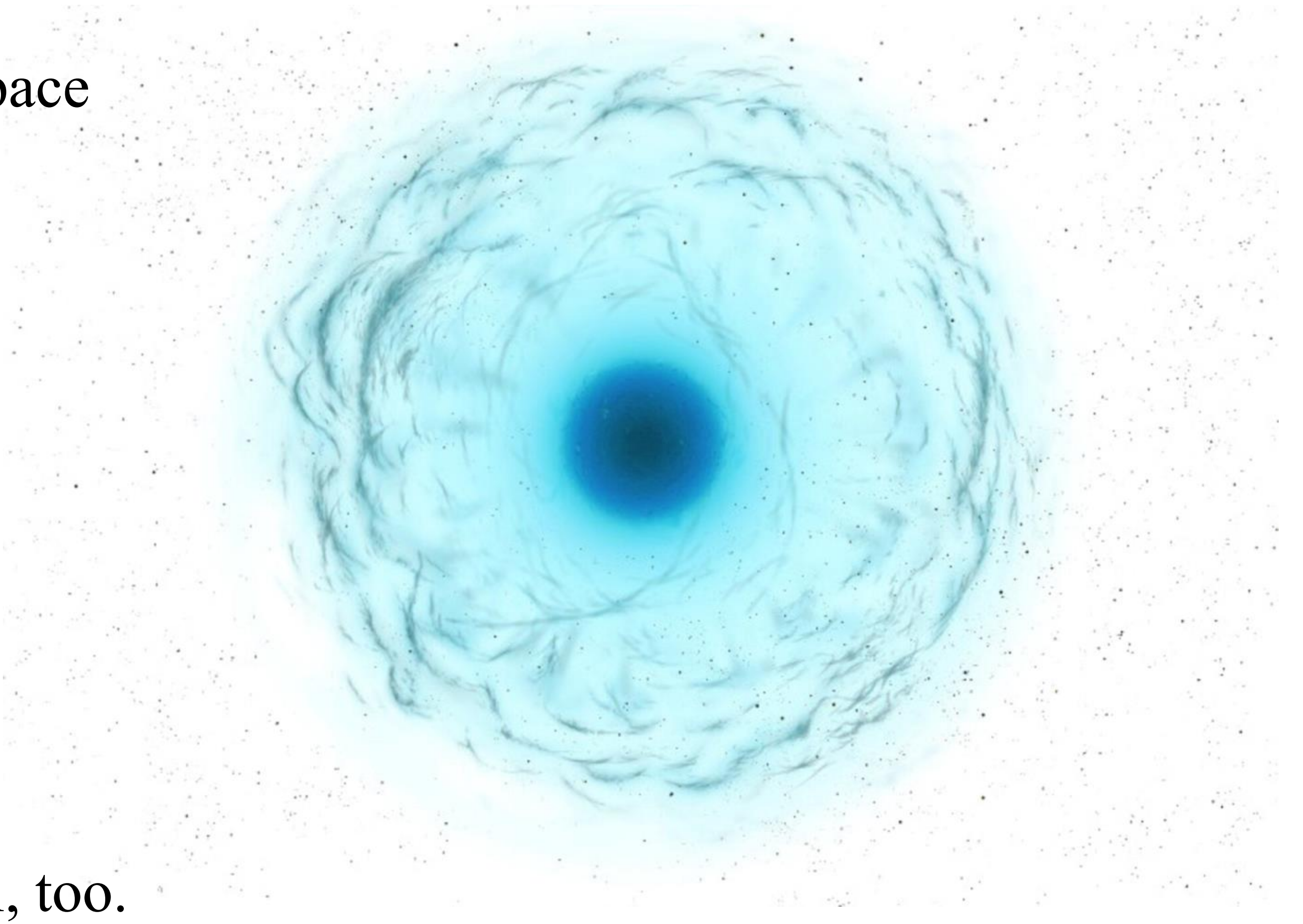
- Stars at late stages eject matter into space
  atoms → molecules (chemistry)

Questions:

1. Which molecules are formed first?
   Can we detect them?

2. What do these molecules tell us
   about the stellar environment?

Radio strong tool, but IR is a strong tool, too.



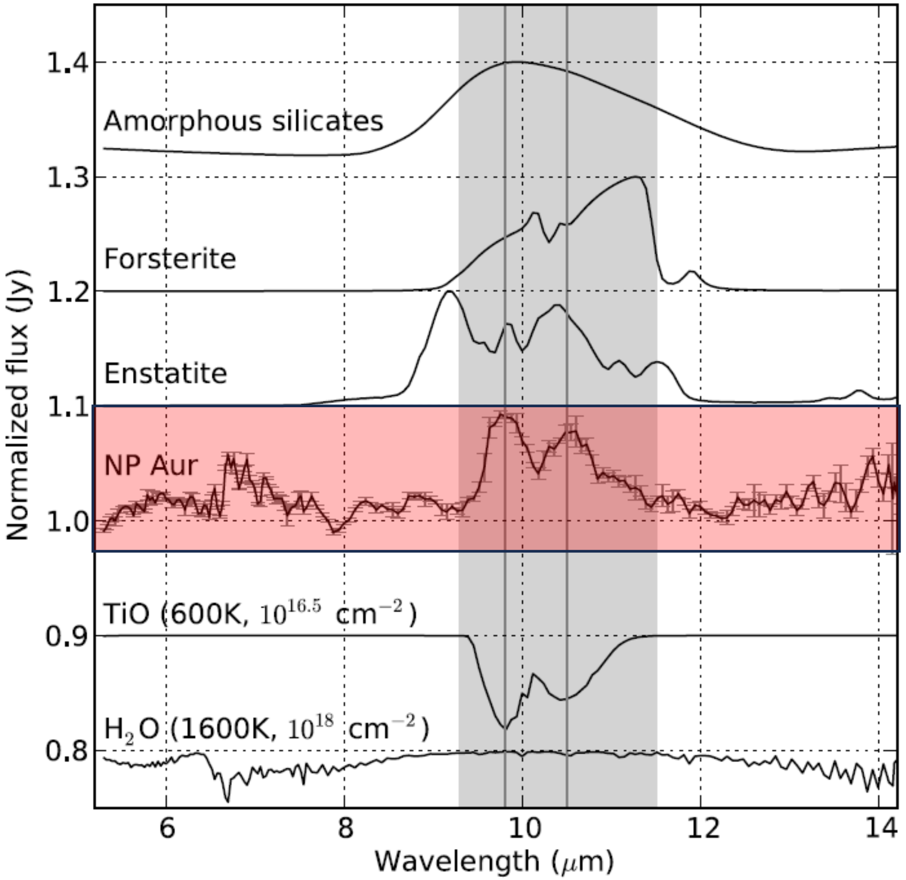
Using high-resolution IR spectroscopy

Advantage 1:
unique molecule identification

- Low resolution good for dust and solids

- Disadvantage: No or only ambiguous identification of the molecules possible

- Example: Spitzer spectrum of S star NP Aur [1]
  TiO? Yes or no?



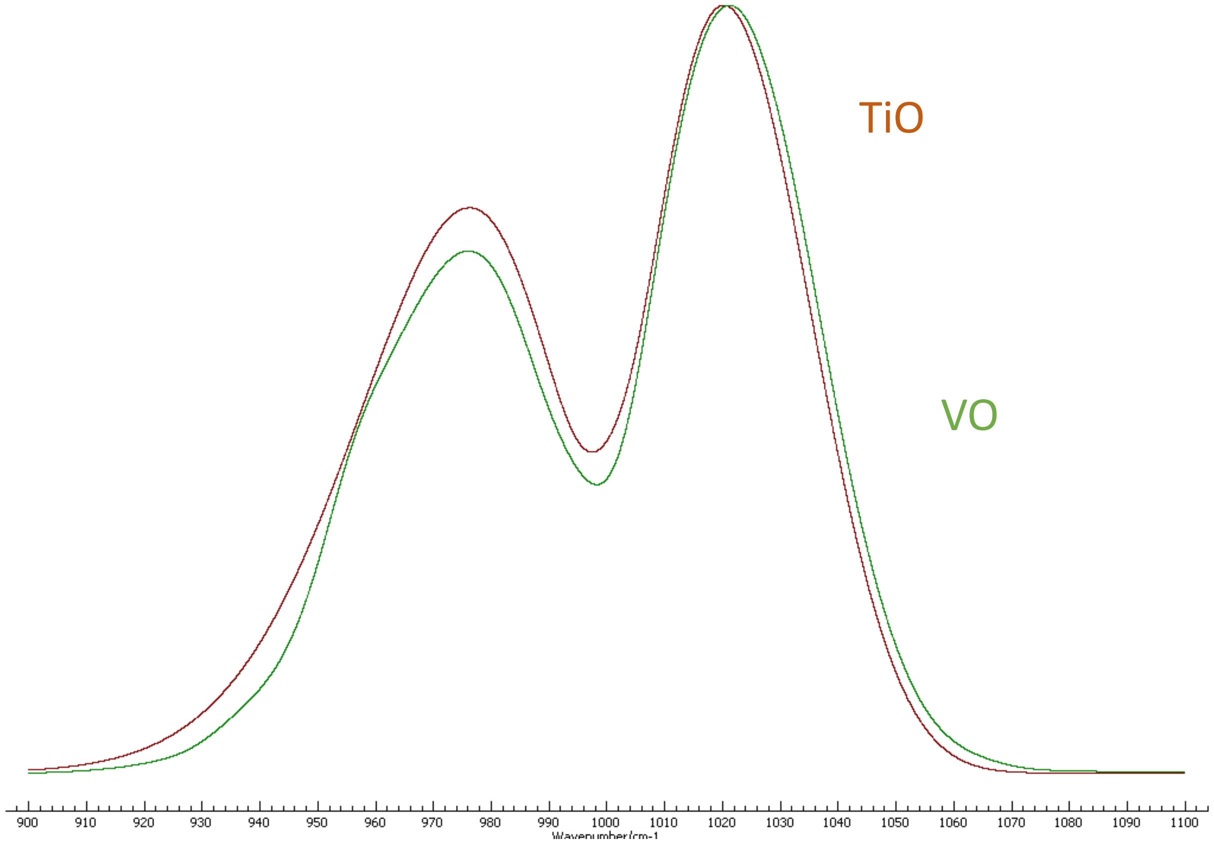
"Normalized Spitzer spectrum of [S star] NP Aur, the opacities of candidate dust species and the normalized absorption of TiO […]" [1]

[1] Smolder et al. (2012), A&A, 543, L2

Using high-resolution IR spectroscopy

Advantage 1:
unique molecule identification

Could it be **VO** instead ?

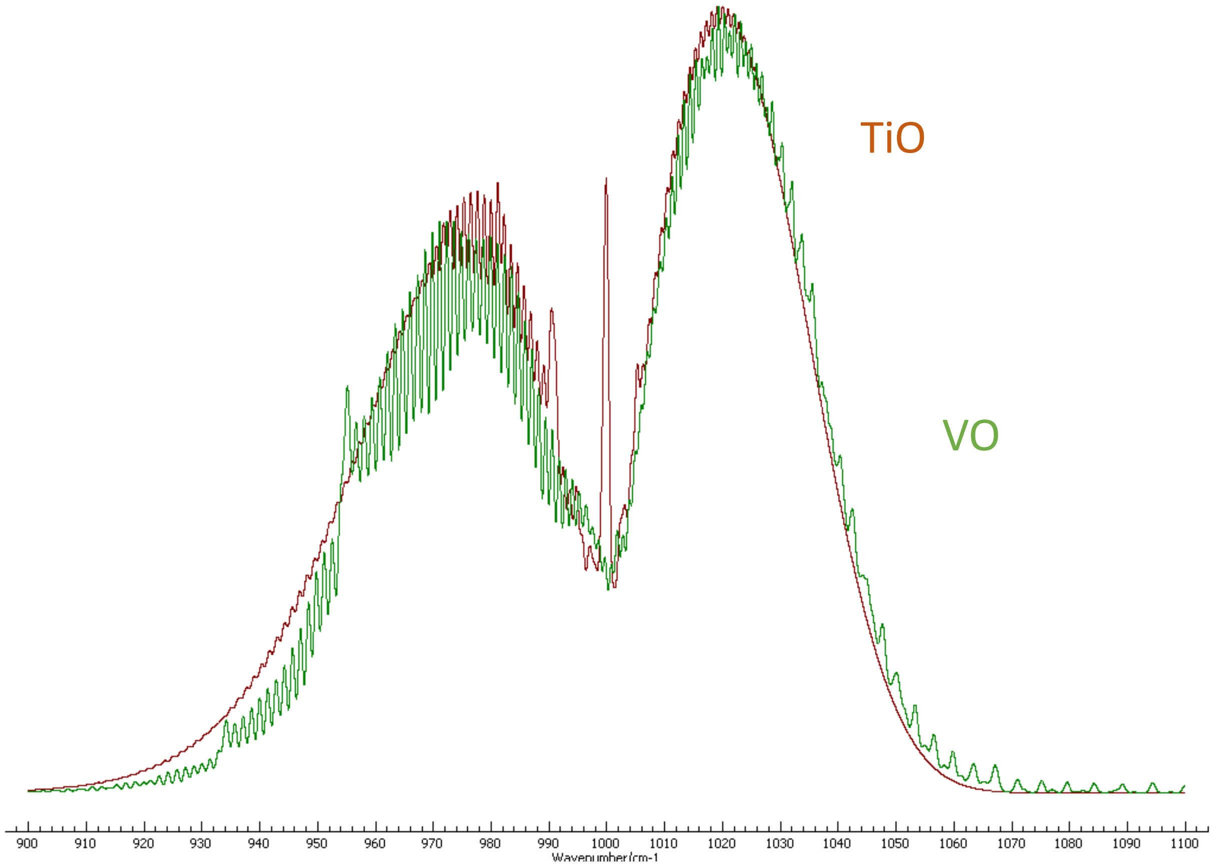


(pgopher) simulated spectrum of TiO and VO at 600K with R=100

Using high-resolution IR spectroscopy

Advantage 1:
unique molecule identification

Could it be **VO** instead ?

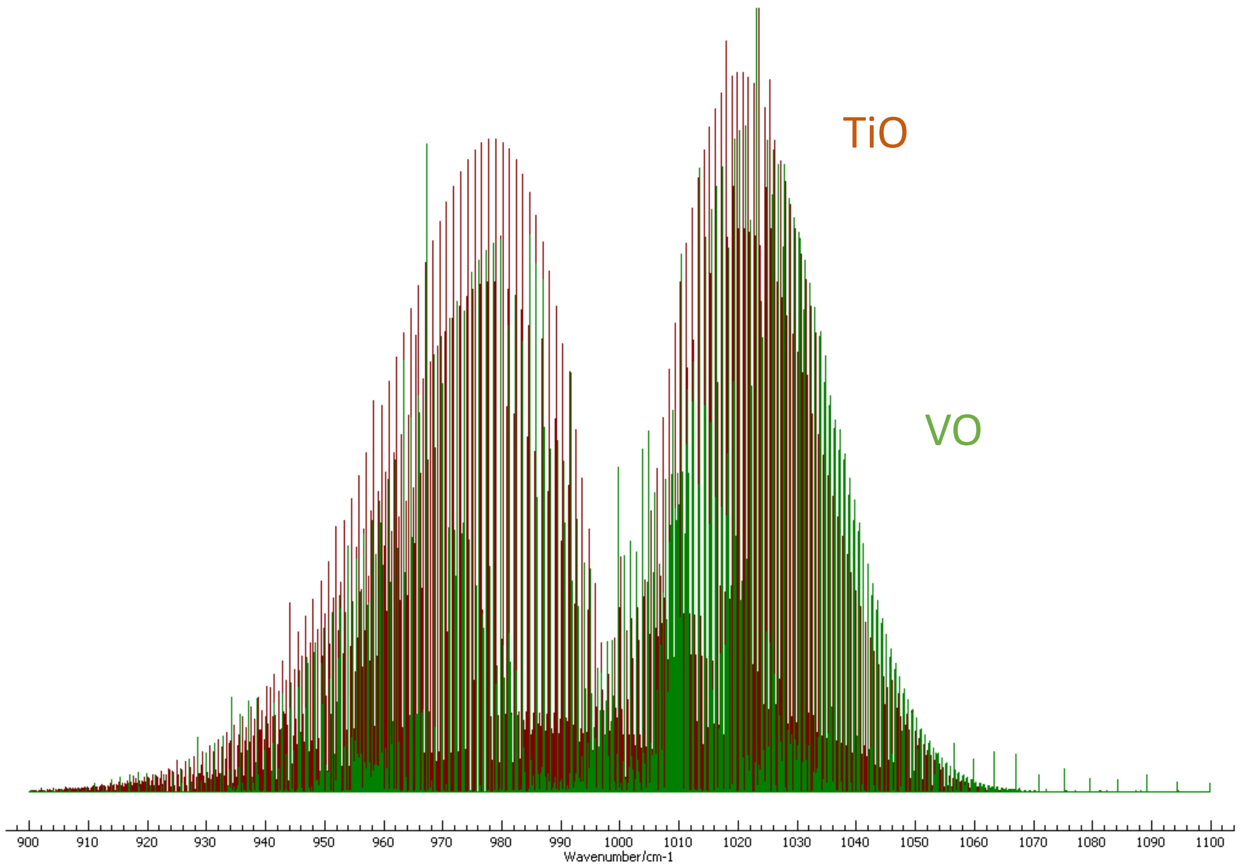


(pgopher) simulated spectrum of TiO and VO at 600K with R=1000

Using high-resolution IR spectroscopy

Advantage 1:
unique molecule identification

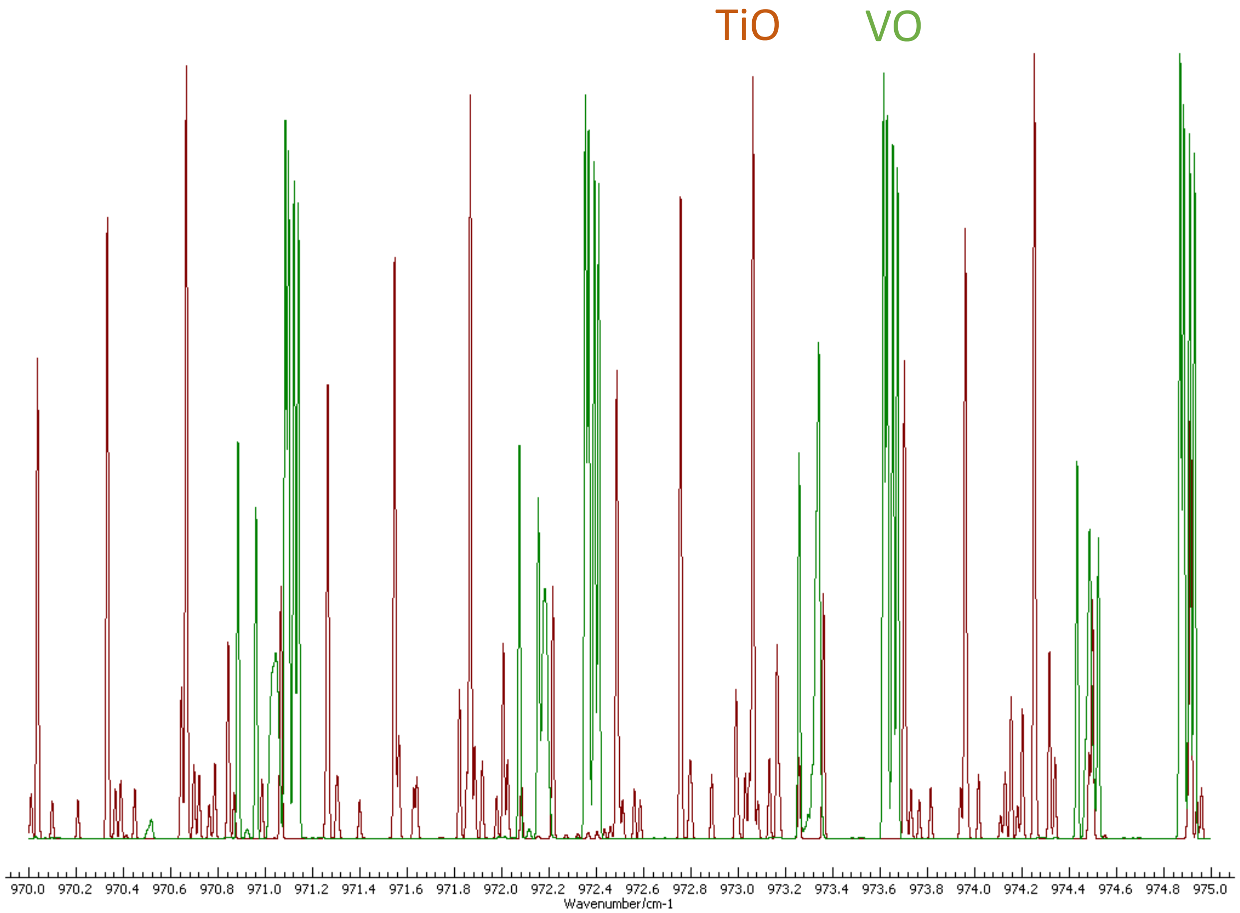
Could it be **VO** instead ?



(pgopher) simulated spectrum of TiO and VO at 600K with R=10^5

Using high-resolution IR spectroscopy

Advantage 1:
unique molecule identification



High-res allows unique
molecule identification

(pgopher) simulated spectrum of TiO and VO at 600K with R=10^5

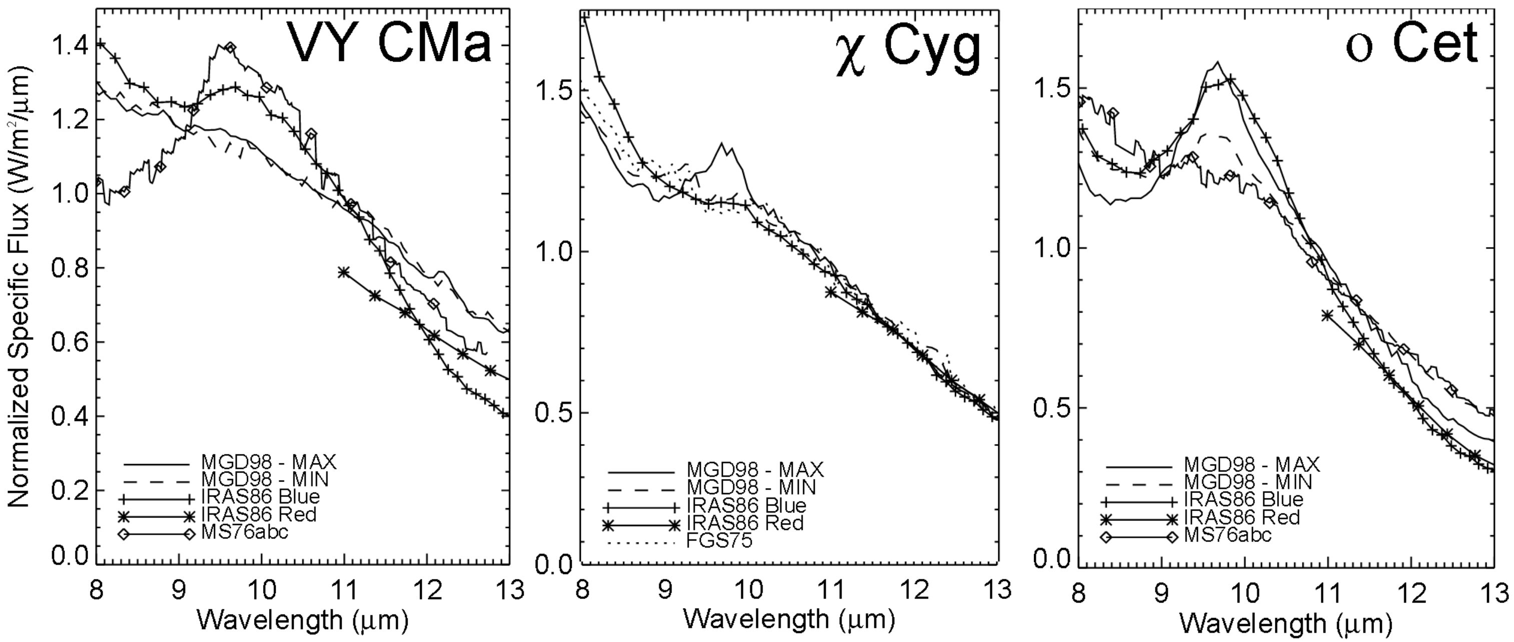
Using high-resolution IR spectroscopy

Advantage 2:
Probing dynamics

- temporal changes of stellar dust envelopes visible at low res
  → epochs [1]

- What are the dynamical processes?

- Are molecules involved?



Three epochs: (I) late 1960s/early 1970s, (II) IRAS-LRS Atlas (1983) (epoch II), and (III) UKIRT data (mid-1990s) [1]

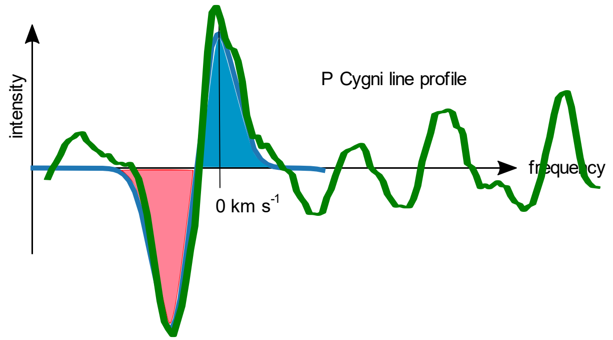
[1] Monnier et al. (1999), ApJ, 521, 261

Using high-resolution IR spectroscopy

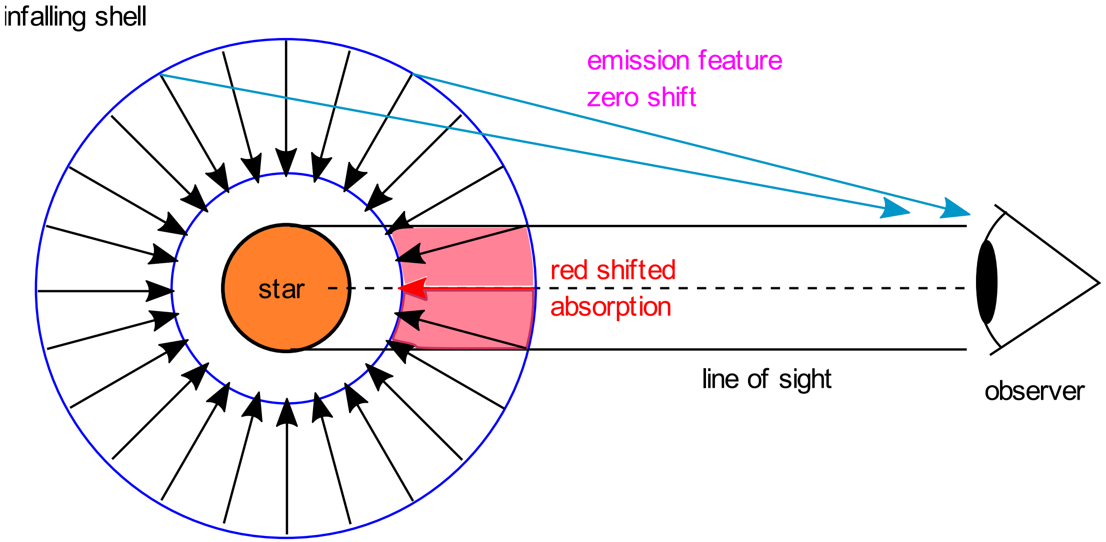
Advantage 2:
Probing dynamics

For molecules:

High-res Line profile / shifts

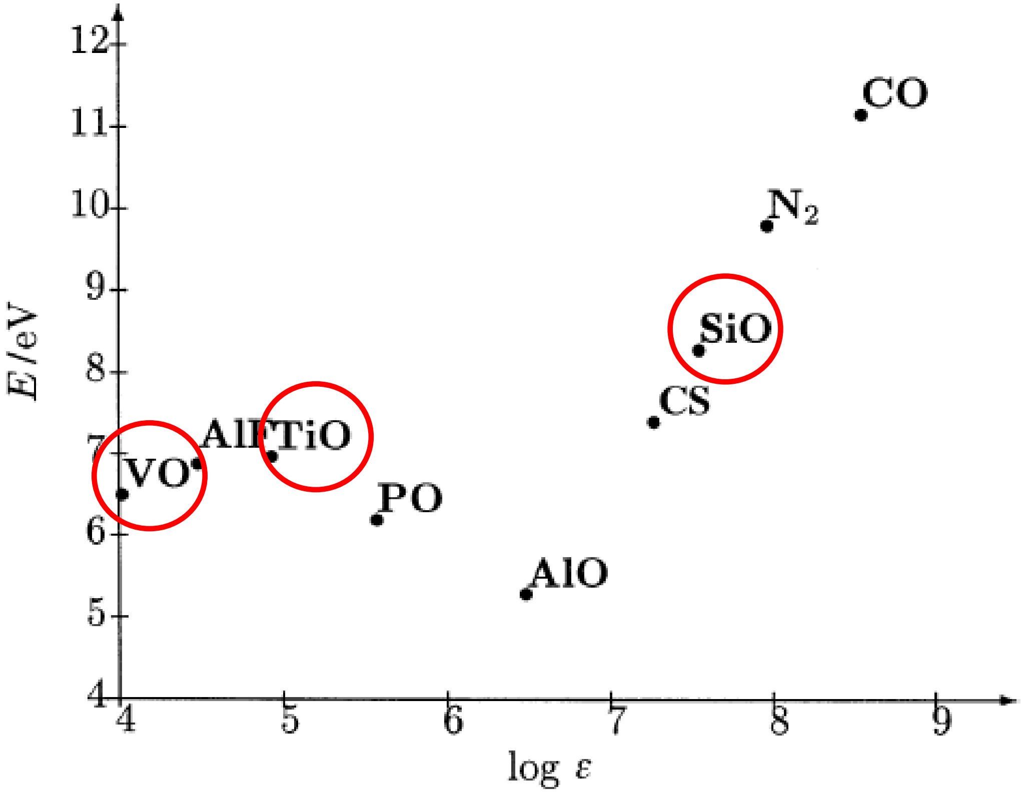


χ Cyg SiO line
at $\phi = 0.26$

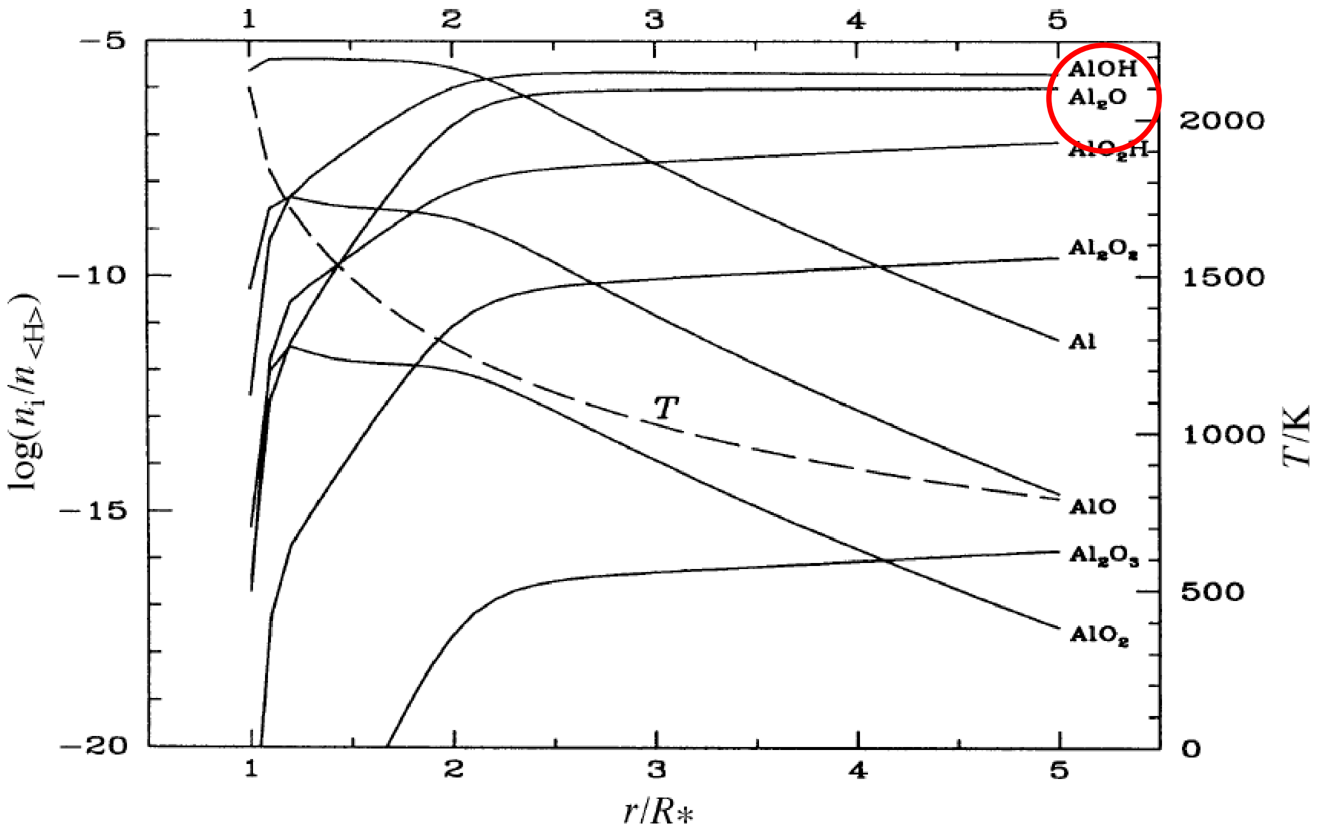


[1] Monnier et al. (1999), ApJ, 521, 261

Which molecules are to be expected?



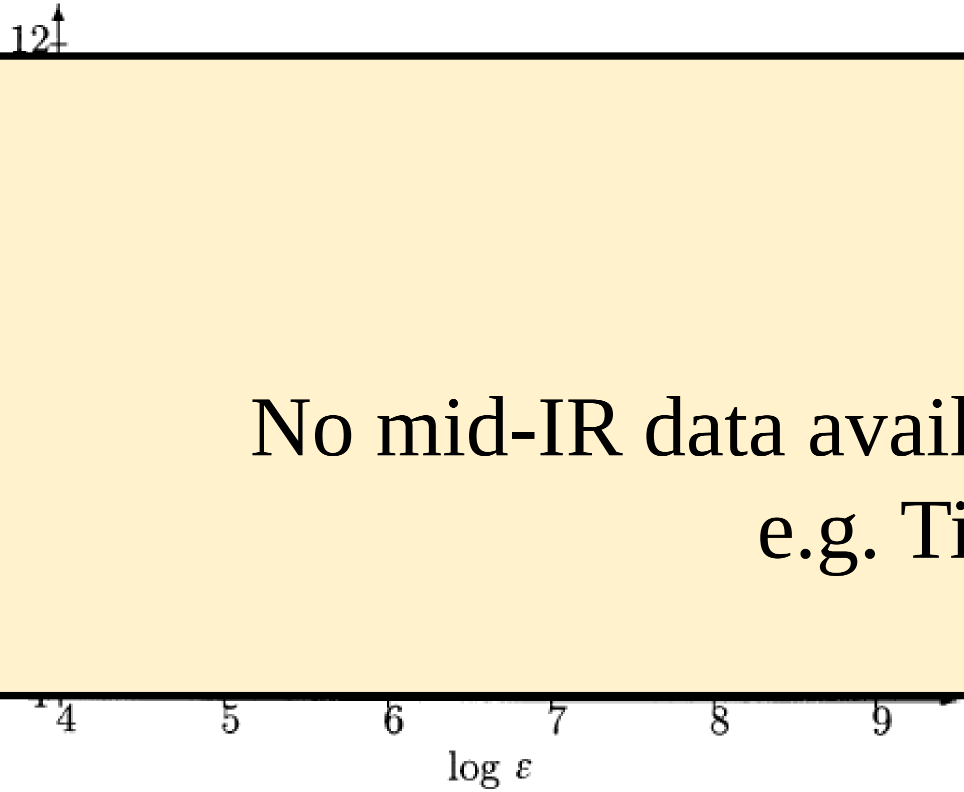
Bond energies of strongly bound diatomic molecules relevant for dust formation, plotted against the abundance of the less abundant of its constituents. [1]



Chemical equilibrium abundances of some gaseous Al/O species in a typical stationary outflow with solar element abundances [1].

[1] Gail & Sedlmayr (1998), Far. Disc. **109**, 303

Which molecules are to be expected?



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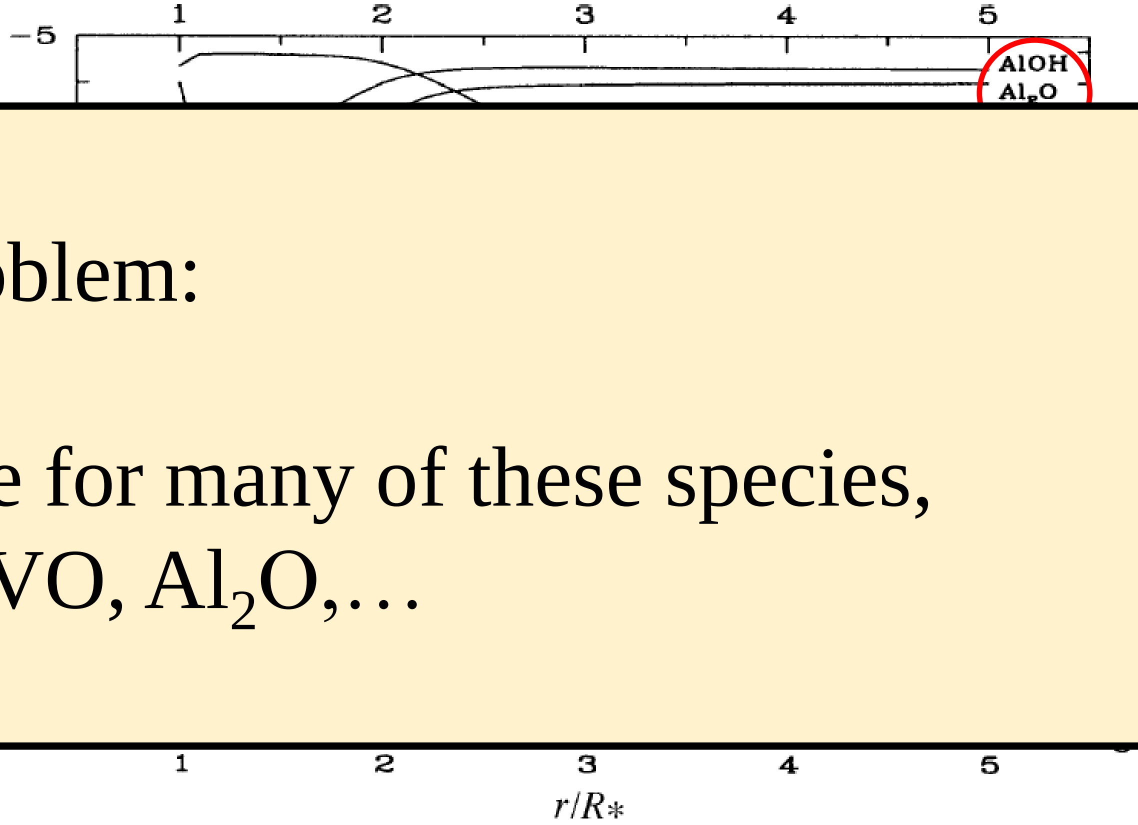


Chemical equilibrium abundances of some gaseous Al/O species in a typical stationary outflow with solar element abundances [1].

Problem:

No mid-IR data available for many of these species, e.g. TiO, VO, Al_2O,…

[1] Gail & Sedlmayr (1998), Far. Disc. **109**, 303

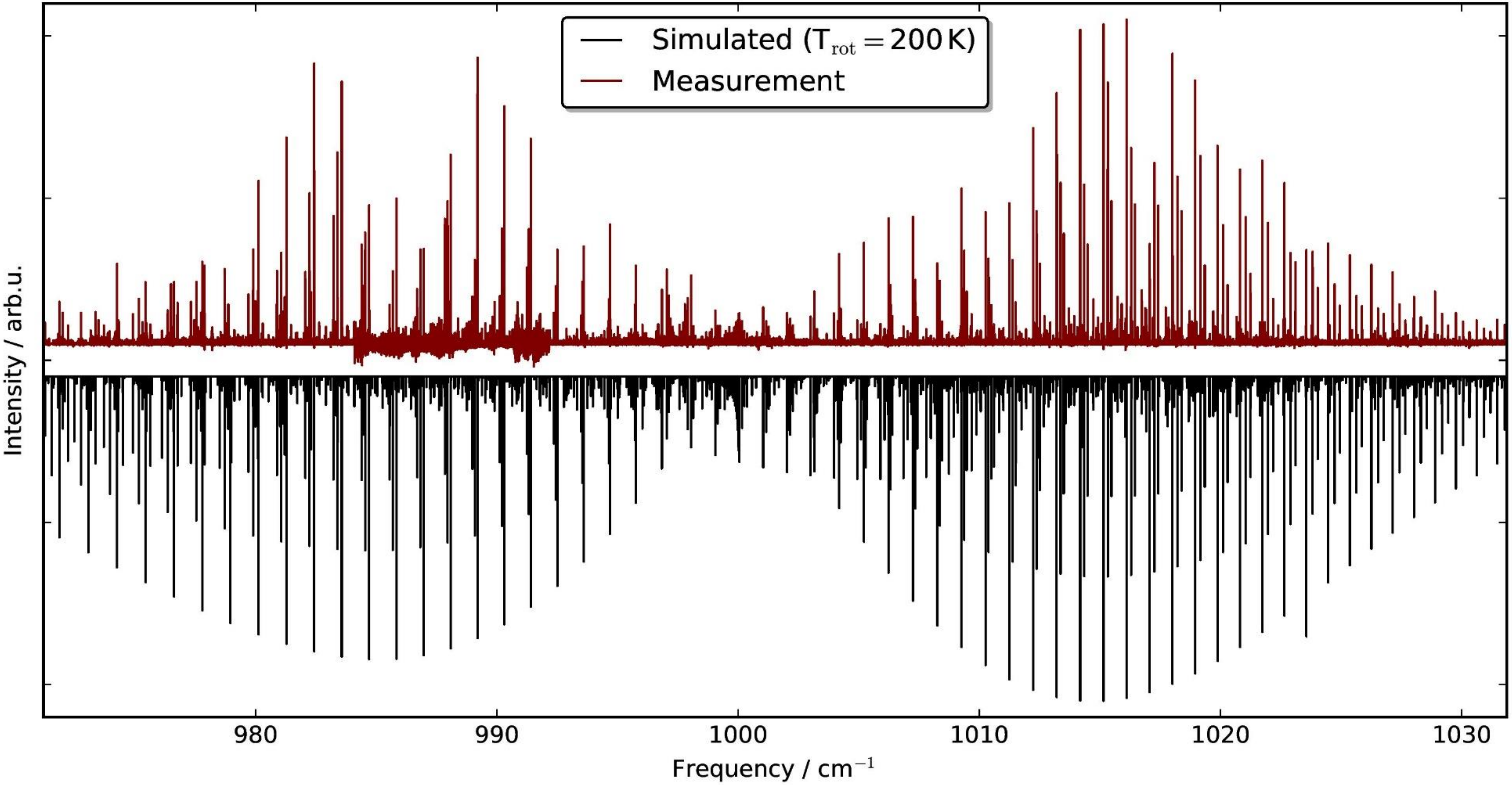
Our aim

Obtaining high-res ($R=10^4$ - 10^5) IR data of late-type stars environments

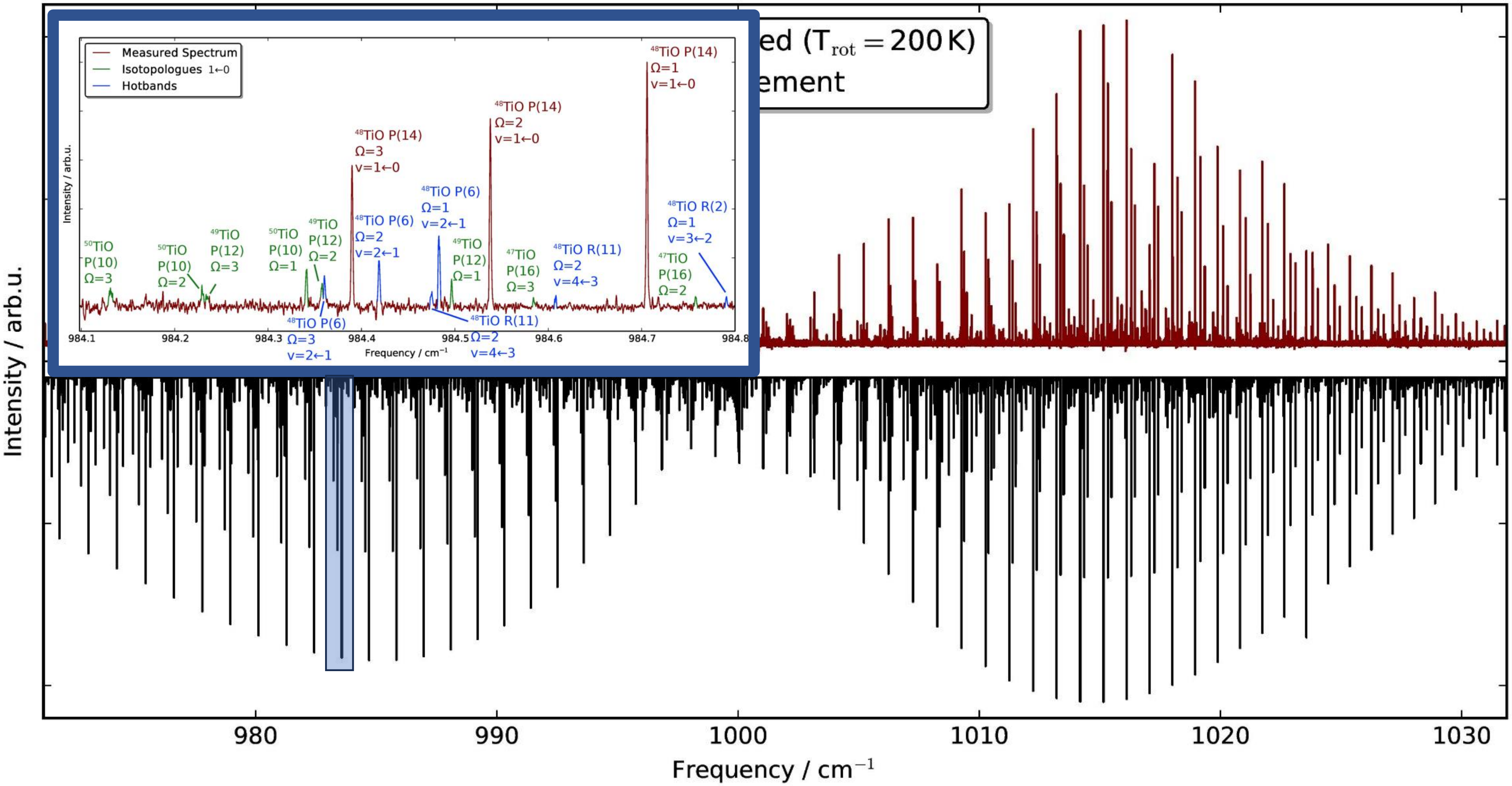
- Enabling IR observations via laboratory experiments
- Looking for new species in the IR
- Line survey of VY CMa and similar stars (e.g., NML Cyg)
- Probing the dynamics of molecular layers of variable stars
  (o Cet, χ Cyg, IK Tau, R Cas)

II. Laboratory infrared experiments on molecules

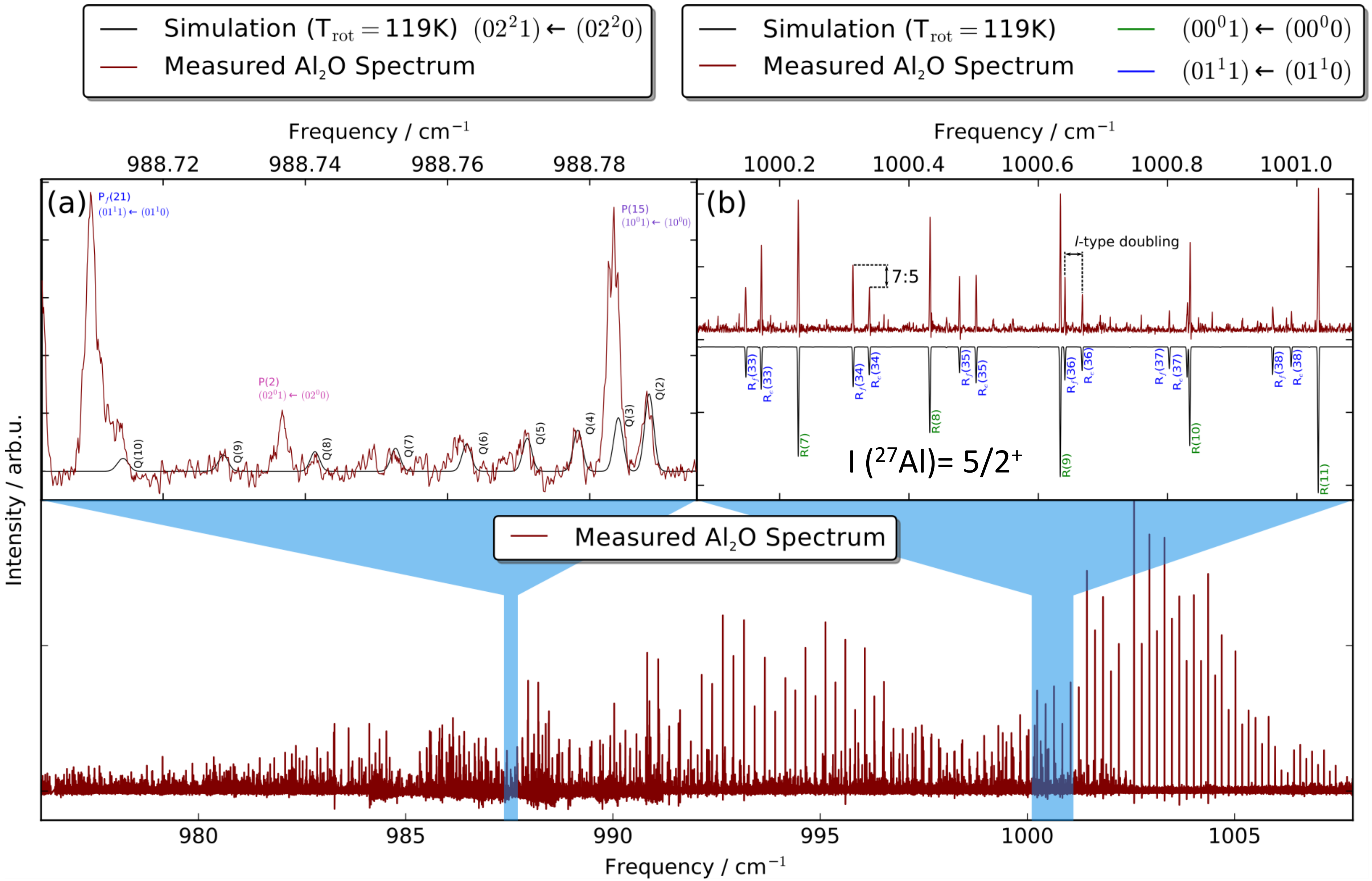
First Mid-Infrared Gas Phase Spectrum of Titanium oxid (TiO, $X\ ^3\Delta_r\ , C_{\infty v}$) incl. isotopologues (^{47}Ti, **^{48}Ti**, ^{49}Ti, ^{50}Ti) around 1000 cm^{-1}

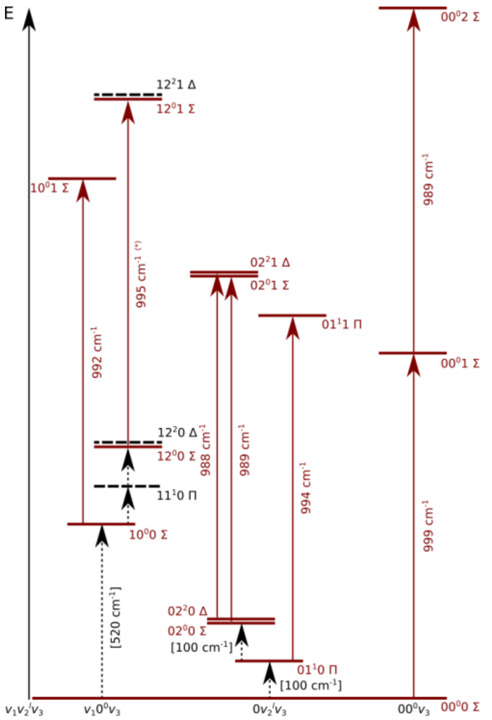


First Mid-Infrared Gas Phase Spectrum of Titanium oxid (TiO, $X\ {}^{3}\Delta_{r}$, $C_{\infty v}$) incl. isotopologues (^{47}Ti, **^{48}Ti**, ^{49}Ti, ^{50}Ti) around 1000 cm^{-1}



Dialuminium oxid, Al_2O ($X\ ^1\Sigma_g^+$), $D_{\infty v}$

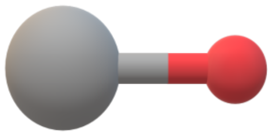




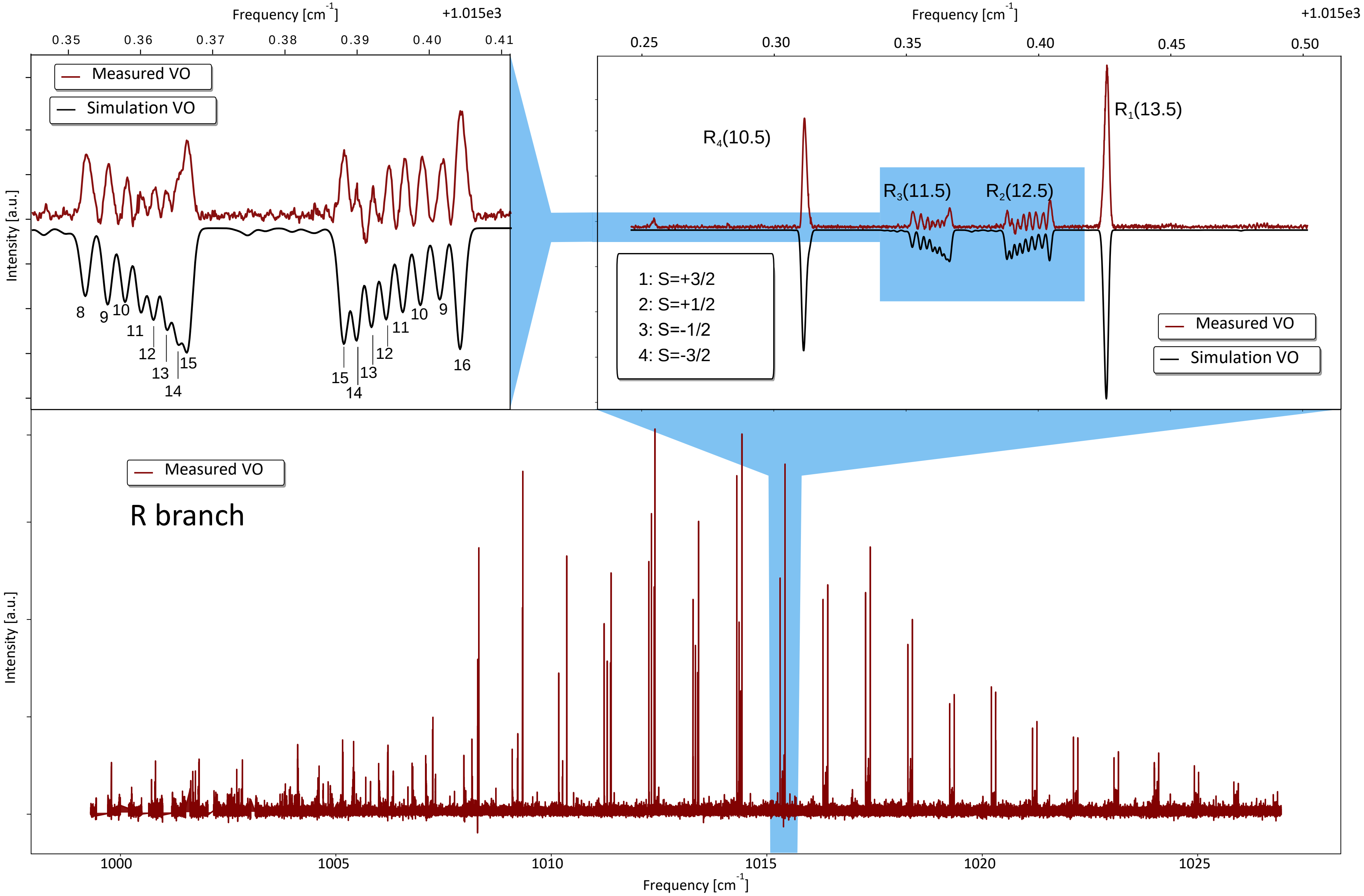
● Measured transitions and obtained states
● Theoretical work [1]

[1] KOPUT & GERTYCH, *J. Chem. Phys.*, **121**, 130-135, 2004.

Vanadium oxid, VO ($X\ ^4\Sigma^-$), $C_{\infty v}$



To be published soon.

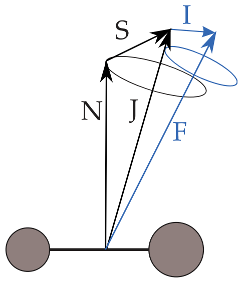


Hyperfine structure

nuclear spin

I (^{51}V)= 7/2$^-$

4 spin (Ω, with Λ=0) components



Hund's coupling case (b)

Beside own data…

We use databases like

- HITRAN (NH_3, CO_2, H_2O,…) [1]
- EXOMOL (NH_3) [2]

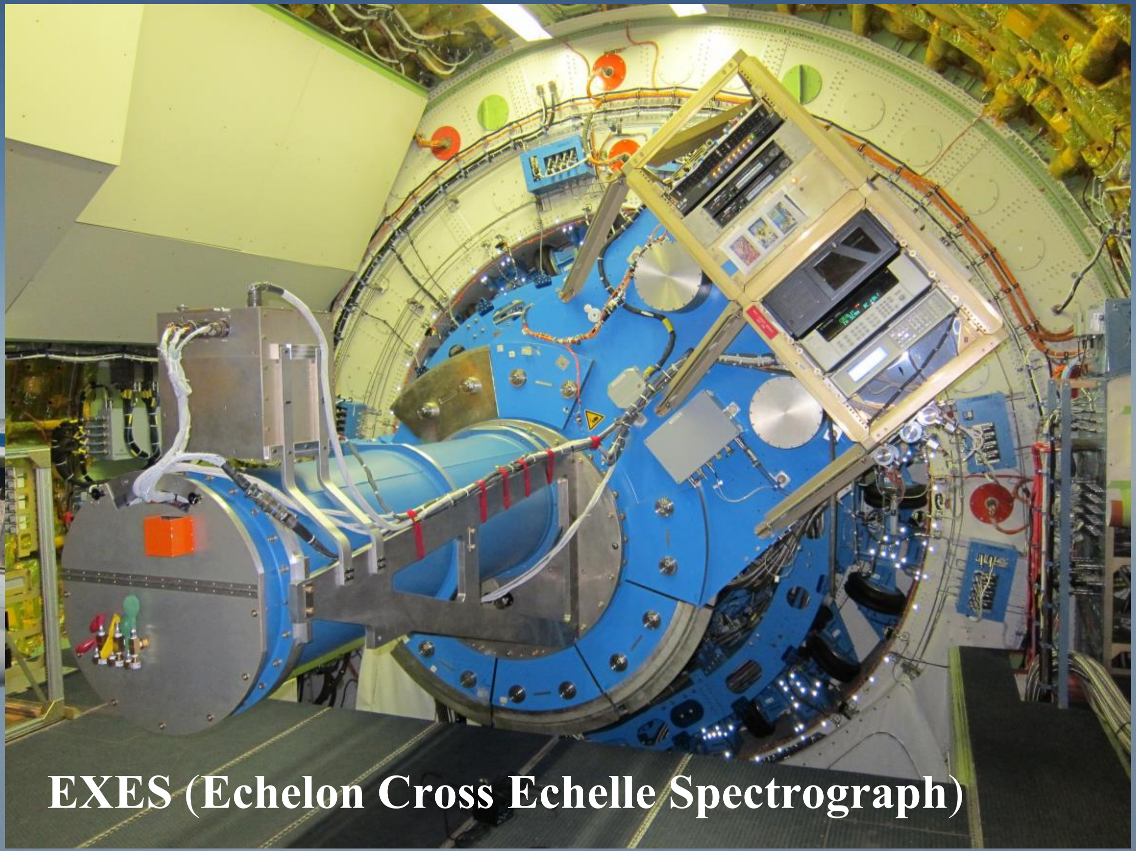
for line assignments

[1] URL: https://hitran.org/ , Down et al. (2013), J. Quant. Spectros. Radiat. Trans., 130, 260
[2] URL https://www.exomol.com/

III. IR astrophysical observations

SOFIA

Stratospheric Observatory
For Infrared Astronomy


EXES (Echelon Cross Echelle Spectrograph)

4.5 – 28.3 μm wavelength region,
R ≈ 50,000 – 100,000
1024 x 1024 Si:As detector array
Cross-dispersed spectrum: Echelon (coarsely-ruled, steeply-blazed aluminum reflection grating) + echelle grating

TEXES / IRTF (Mauna Kea)

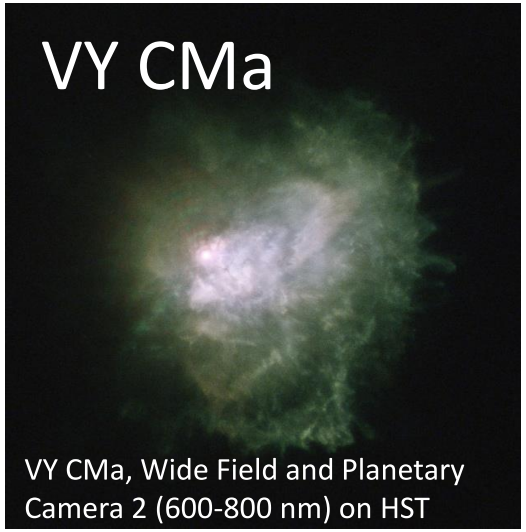
3m NASA Infrared Telescope Facililty (IRTF)

TEXES (**Texas Echelon Cross Echelle Spectrograph**)
4.5 – 25 μm wavelength region
R ≈ 50,000 – 100,000

III. IR astrophysical observations

i. Hypergiants:
(17-40 $M_\odot$)

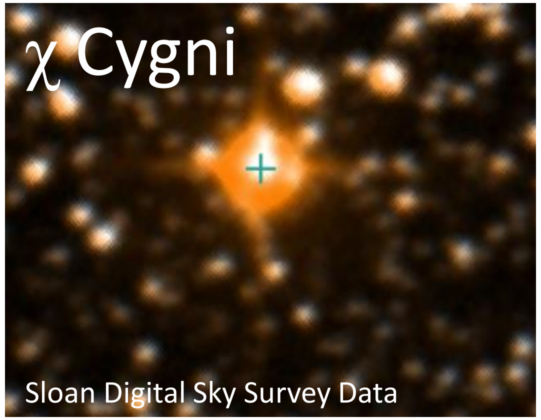
1. **VY CMa**
2. NML Cyg
3. IRC+10216



VY CMa, Wide Field and Planetary Camera 2 (600-800 nm) on HST

ii. Variable stars:
red giants & AGBs
(1 to 2 $M_\odot$)

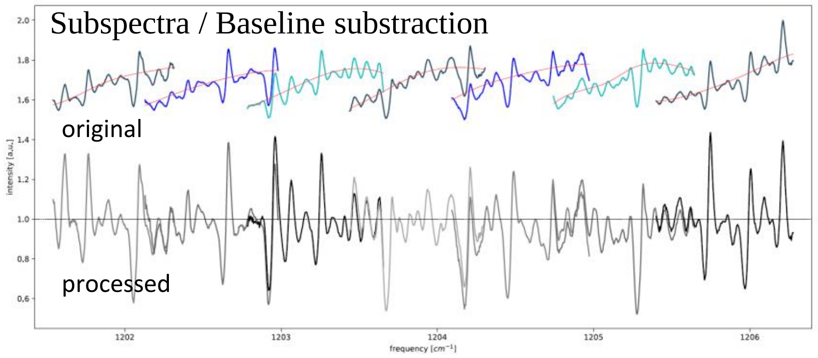
1. **χ Cyg**
2. O Cet (Mira)
3. IK Tau
4. R Cas

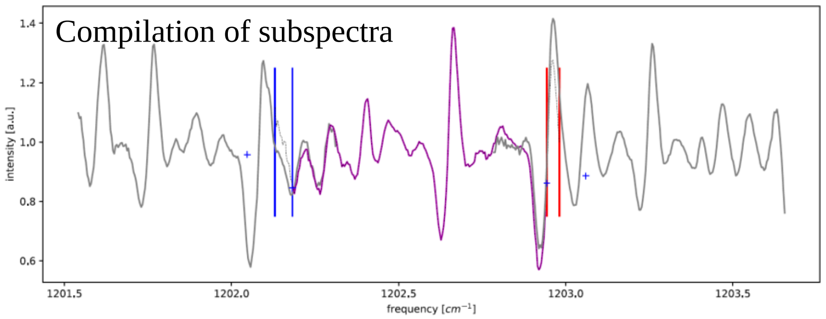


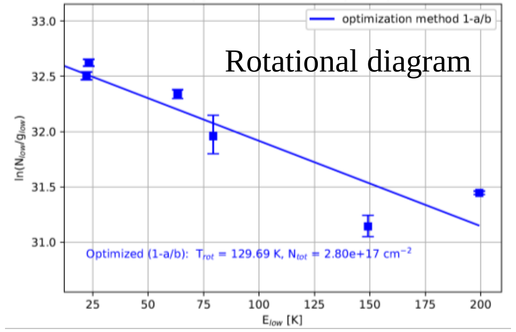
Sloan Digital Sky Survey Data

Home made data analysis software

- Problems with standard software to deal with complicated baseline of TEXES/EXES observations
- Homemade software package SpExes (A – D), python code
- Features:
  - Baseline substraction (including instrument signature, and terrestric atmosphere)
  - Compilation of subspectra
  - Simulation of target molecular species
  - Line profile analysis
  - Excitation diagram analysis (new method!)



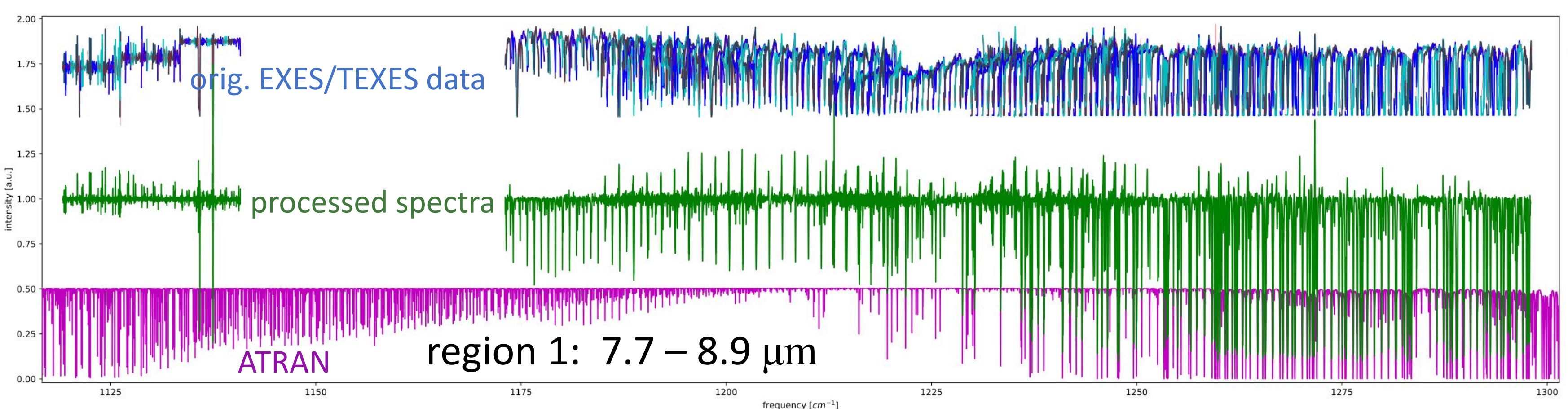




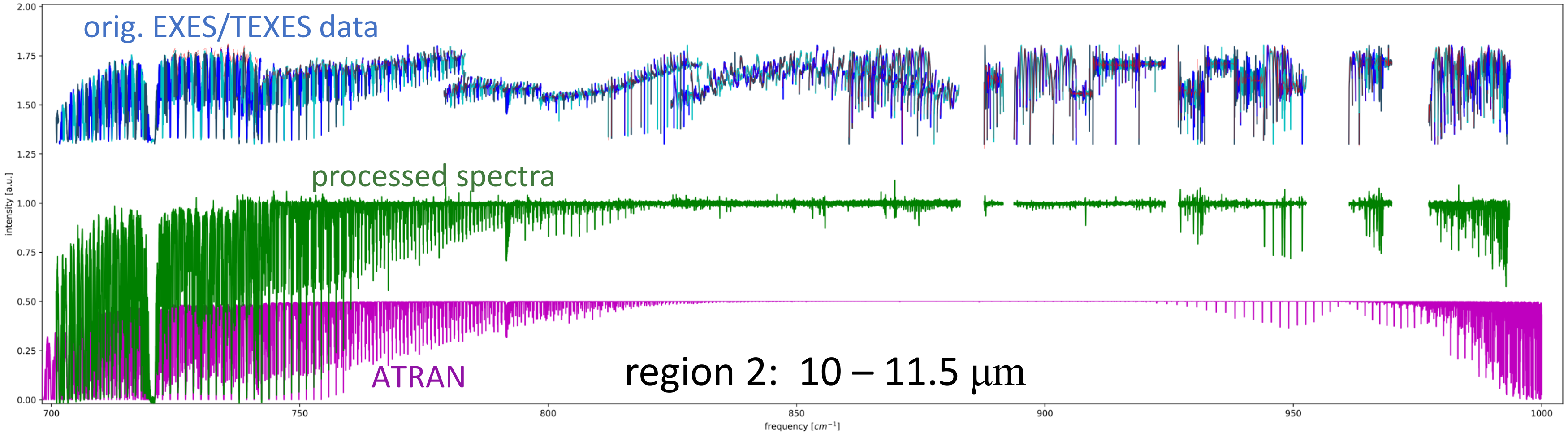
Optimized (1-a/b): T_{rot} = 129.69 K, N_{tot} = 2.80e+17 cm^{-2}

i) The mid-IR high-resolution line survey of VY CMa

part I



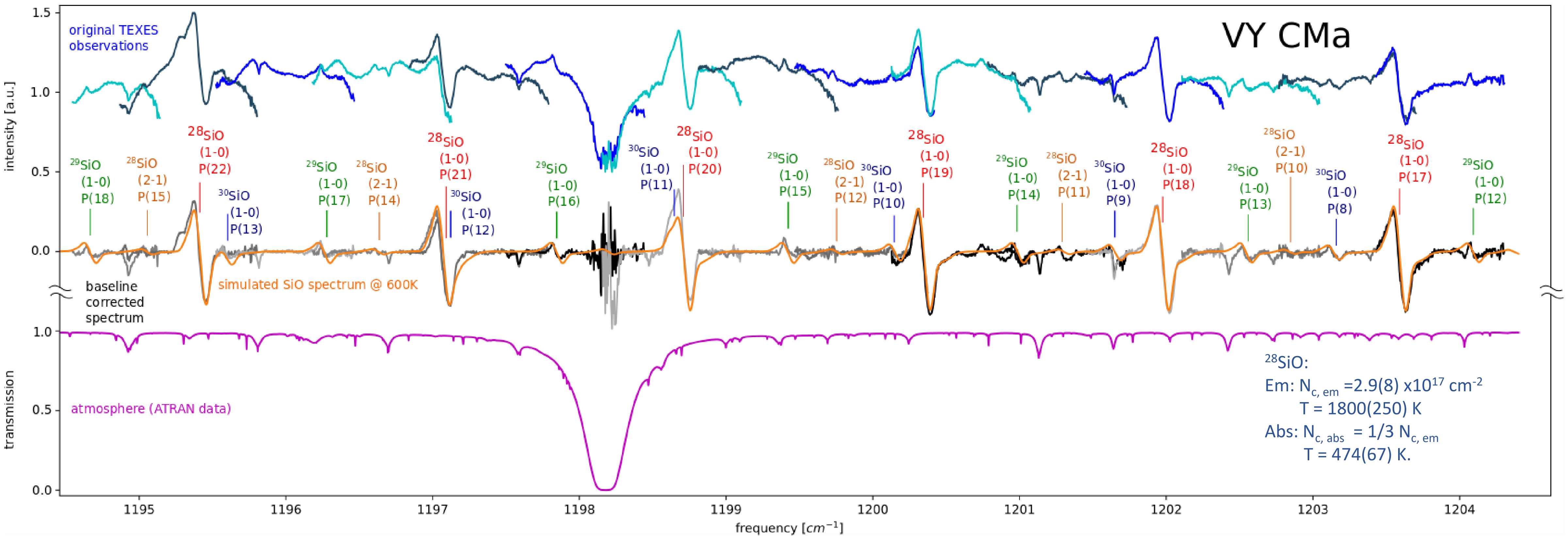
part II



part III

region 3: 6.6 - 7.4 μm (not shown in this talk ⇒ stellar water lines)

i. Hypergiants: SiO isotopologues in the VY CMa envelope TEXES /IRTF



1) Ro-vibration (unique molecule identification)

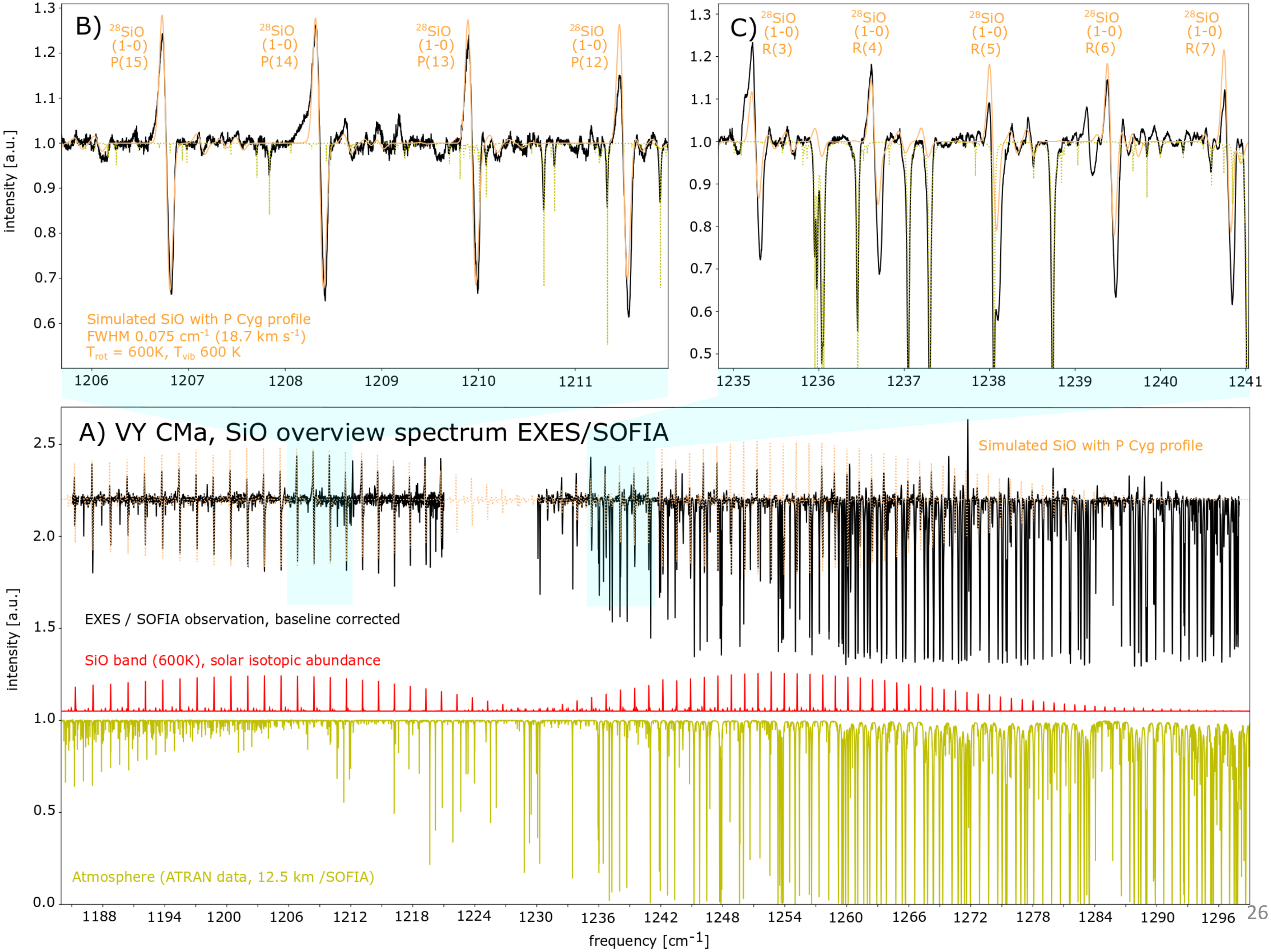
2) Isotope sensitve

3) excitation (temperature)

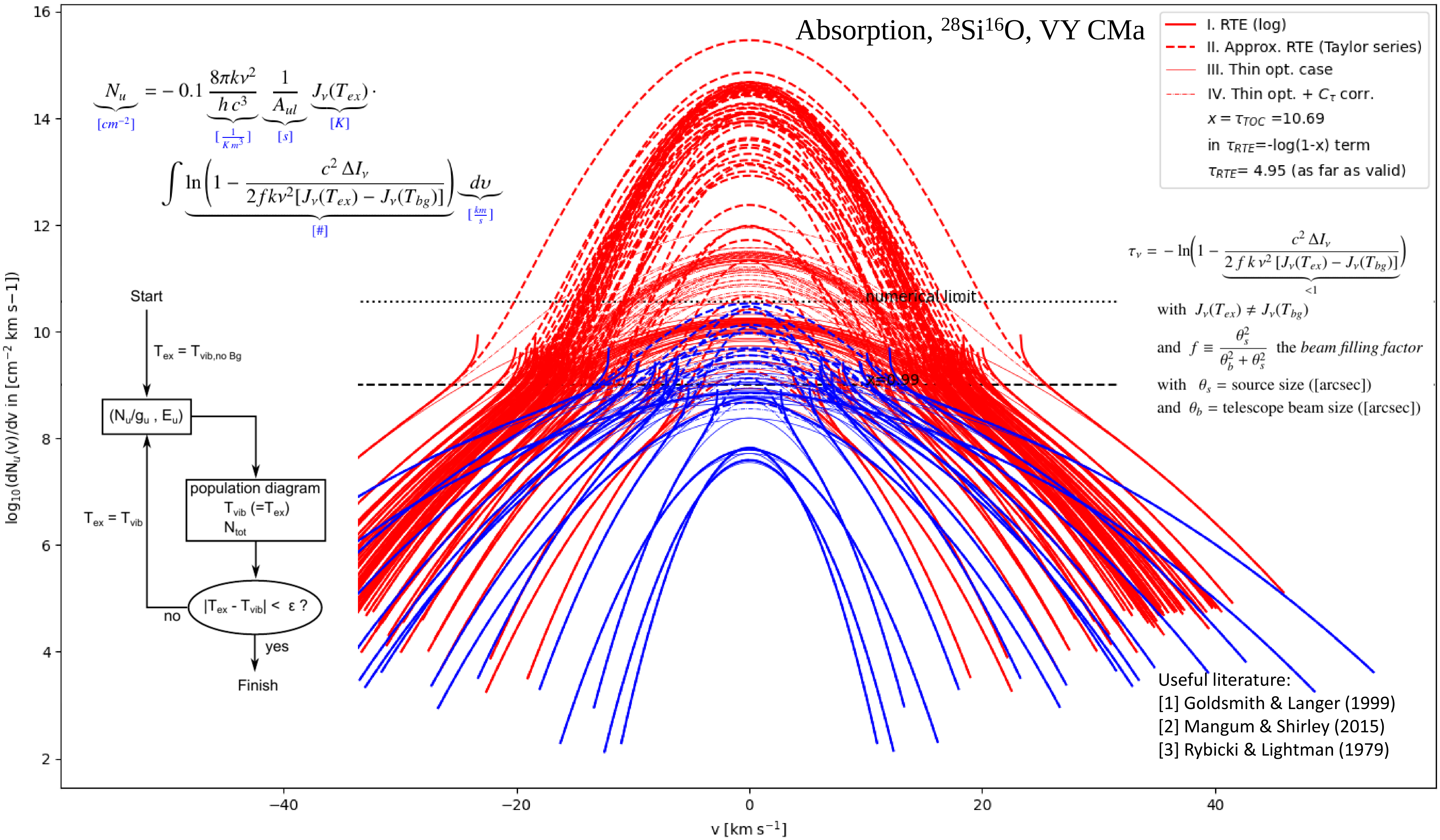
4) Geometrical structure and dynamics (P-Cygni)

SiO in VY CMa Envelope using EXES/SOFIA

- Broader frequency coverage
- Improved line shape analysis (smaller telluroic features)



RTE: Function



$$\underbrace{N_u}_{[cm^{-2}]} = -0.1 \underbrace{\frac{8\pi k \nu^2}{h\, c^3}}_{[\frac{1}{K\, m^3}]} \underbrace{\frac{1}{A_{ul}}}_{[s]} \underbrace{J_\nu(T_{ex})}_{[K]} \cdot$$

$$\int \underbrace{\ln\left(1 - \frac{c^2\, \Delta I_\nu}{2 f k \nu^2 [J_\nu(T_{ex}) - J_\nu(T_{bg})]}\right)}_{[\#]} \underbrace{d\upsilon}_{[\frac{km}{s}]}$$

$$\tau_\nu = -\ln\left(1 - \underbrace{\frac{c^2\, \Delta I_\nu}{2\, f\, k\, \nu^2\, [J_\nu(T_{ex}) - J_\nu(T_{bg})]}}_{<1}\right)$$

with $J_\nu(T_{ex}) \neq J_\nu(T_{bg})$

and $f \equiv \frac{\theta_s^2}{\theta_b^2 + \theta_s^2}$ the *beam filling factor*

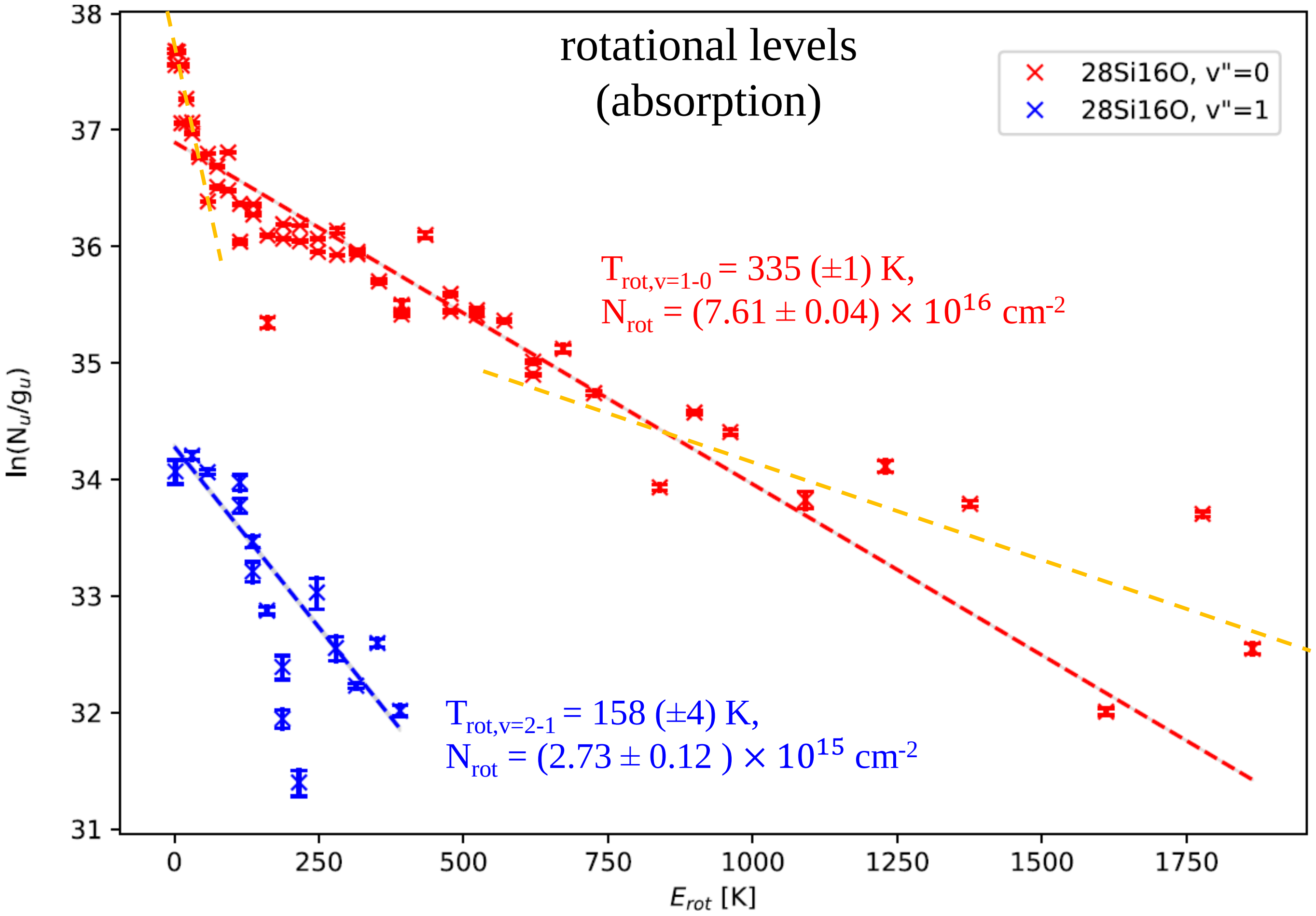
with θ_s = source size ([arcsec])

and θ_b = telescope beam size ([arcsec])

Useful literature:
[1] Goldsmith & Langer (1999)
[2] Mangum & Shirley (2015)
[3] Rybicki & Lightman (1979)

Excitation diagram analysis of SiO, VY CMa

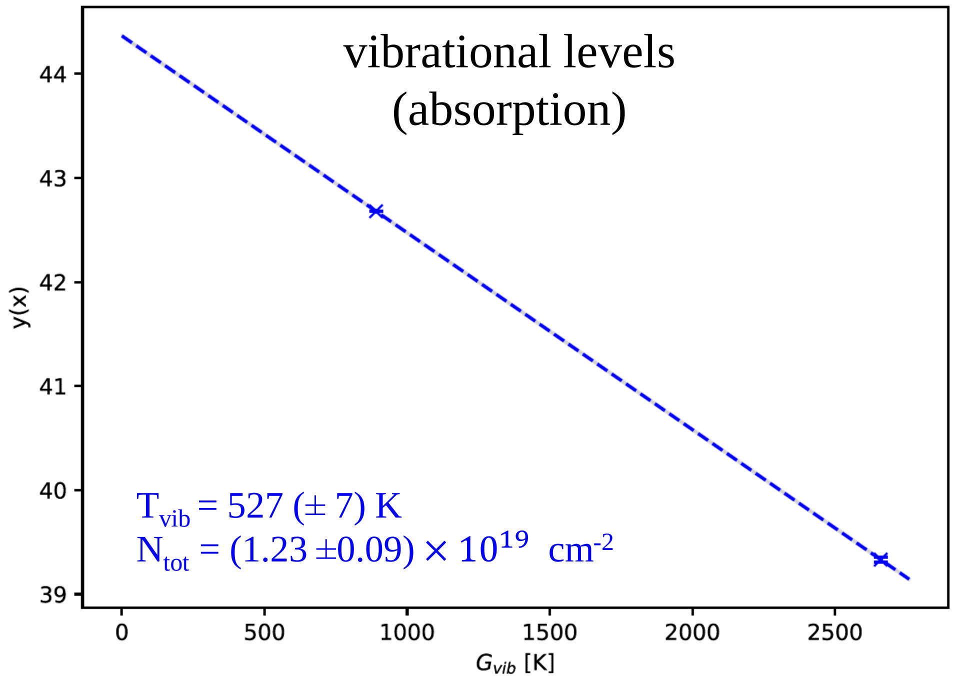
- getting the rotational & vibrational excitation disentangled



$T_{rot,v=1-0}$ = 335 (±1) K,
N_{rot} = $(7.61 \pm 0.04) \times 10^{16}$ cm^{-2}

$T_{rot,v=2-1}$ = 158 (±4) K,
N_{rot} = $(2.73 \pm 0.12) \times 10^{15}$ cm^{-2}

Thin optical case + T_{bg} = 3700 K



T_{vib} = 527 (± 7) K
N_{tot} = $(1.23 \pm 0.09) \times 10^{19}$ cm^{-2}

multi level excitation diagram method

Preliminary results!

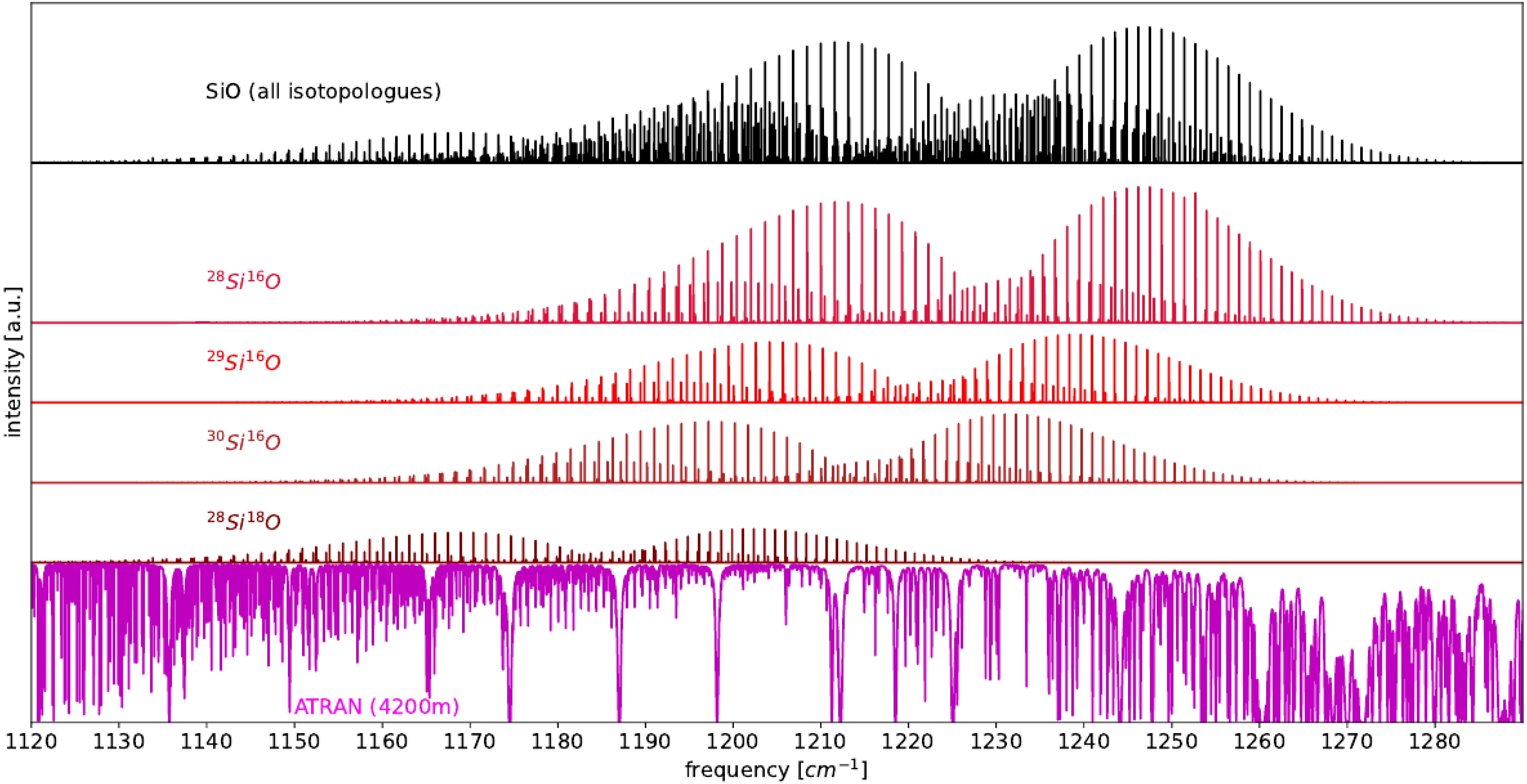
SiO in VY CMa

$^{28}Si^{16}O$	**Geballe et al. (1979) [1] (absorption)**	**Cernicharo et al. (1993) [2] (emission)**	**This work (absorption)***	**(emission)***
T_{rot} (v=1-0)	525±50 K		335 (±1) K	480 (±3) K
T_{rot} (v=2-1)	600±100 K		158 (±4) K	521 (±45) K
T_{vib}	600±100 K		527 (±7) K	542 (±17) K
N_L	**$(7\pm3)\times 10^{17}$ cm^{-1}**	**$> \times 10^{20}$ cm^{-1}**	**$(1.23\pm0.09)\times 10^{19}$**	**$(2.7\pm0.4)\times 10^{20}$**
$N_{L,\ \tau\ corr}$			$(7.1\pm0.7)\times 10^{19}$	$(4\pm2)\times 10^{24}$

*Thin optical case (TOC), T_{bg} = 3700 K

Problem: Lines of $^{28}Si^{16}O$ are optically thick.

[1] Geballe et al. (1979), ApJ, 230, L47; [2] Cernicharo et al. (1993), ApJ, 407, L33


SiO (all isotopologues)
$^{28}Si^{16}O$
$^{29}Si^{16}O$
$^{30}Si^{16}O$
$^{28}Si^{18}O$
ATRAN (4200m)
intensity [a.u.]
1120
1130
1140
1150
1160
1170
1180
1190
1200
1210
1220
1230
1240
1250
1260
1270
1280
frequency [cm^{-1}]

Preliminary results!

SiO isotopologues in VY CMa

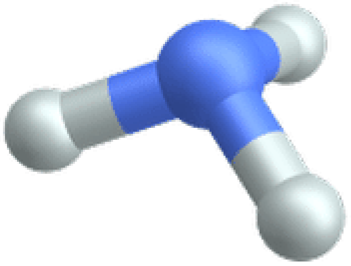
$^{28}Si^{16}O$	**This work (absorption)*** $^{28}Si^{16}O$	$^{29}Si^{16}O$	$^{30}Si^{16}O$	**Geballe et al. (1979)** $^{28}Si^{16}O$ **[1]**
T_{rot} (v=1-0)	335 (±1) K	316 (±8) K	235 (±5) K	525±50 K
T_{rot} (v=2-1)	158 (±4) K	-	-	600±100 K
T_{vib}	527 (±7) K	527 (fixed) K	527 (fixed) K	600±100 K
N_L	$(1.23 \pm 0.09) \times 10^{19}$	1.1×10^{18}	1.2×10^{18}	$(7 \pm 3) \times 10^{17}$ cm^{-1}

*Thin optical case (TOC), T_{bg} = 3700 K

Ratios:	**This work**	**Geballe et al. (1979) [1]**
$^{28}Si/^{29}Si$	11^{+20}_{-1} **	20(±5)
$^{29}Si/^{30}Si$	0.93 (±0.1)	1.0(±0.3)

**Using τ correction for upper limit

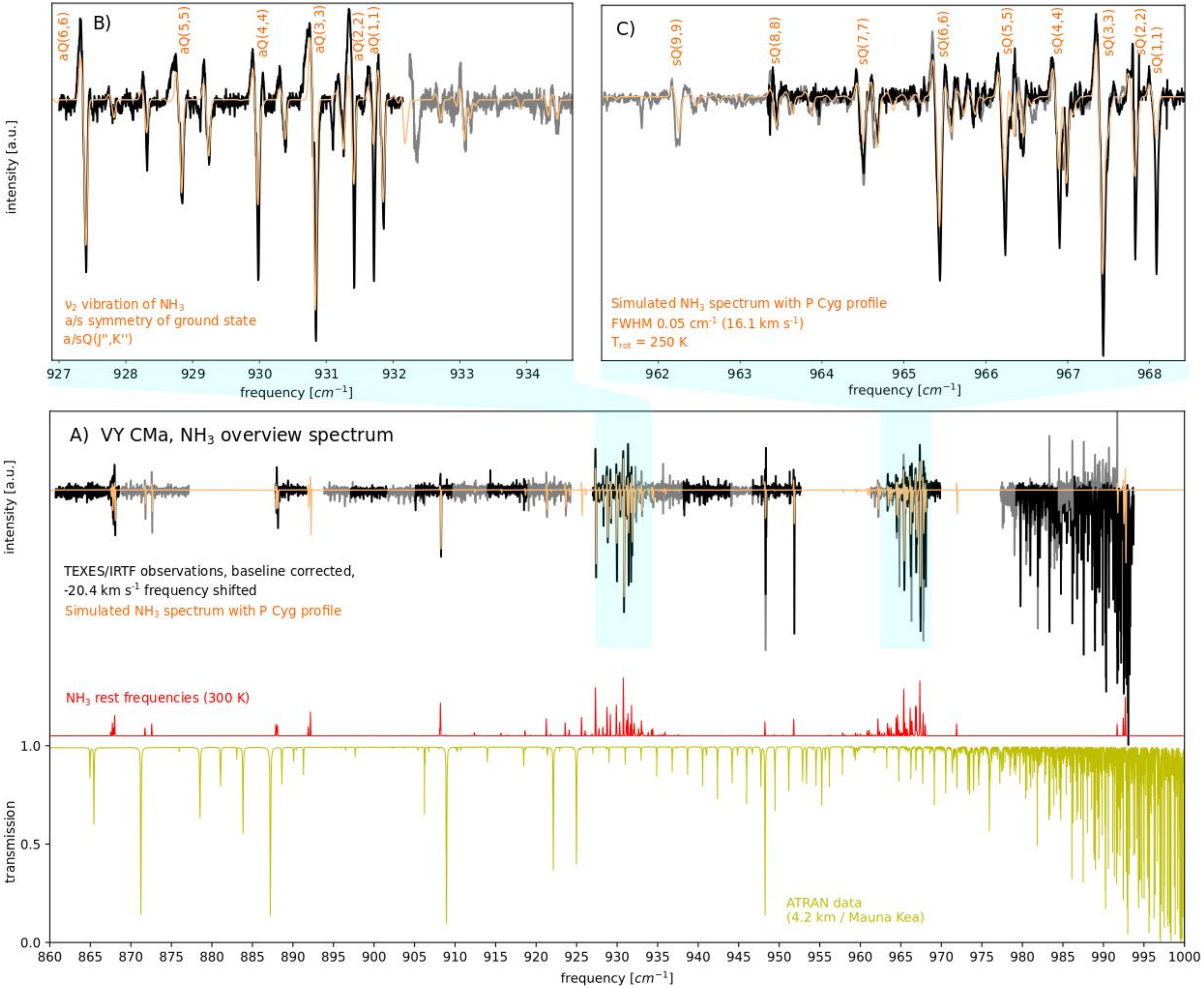
Ammonia in the envelope of VY CMa @ 10 – 11.5 µm (EXES+TEXES)



- Broader frequency coverage than in [1]

- Consistent NH_3 simulation in LTE

ν_2 N-H umbrella mode



[1] Wong et al. (2018), A&A, 580, A36

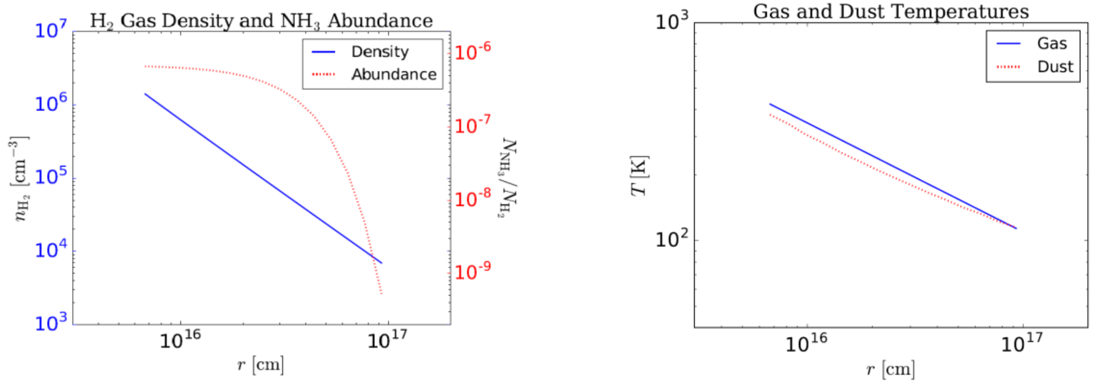
Preliminary results!

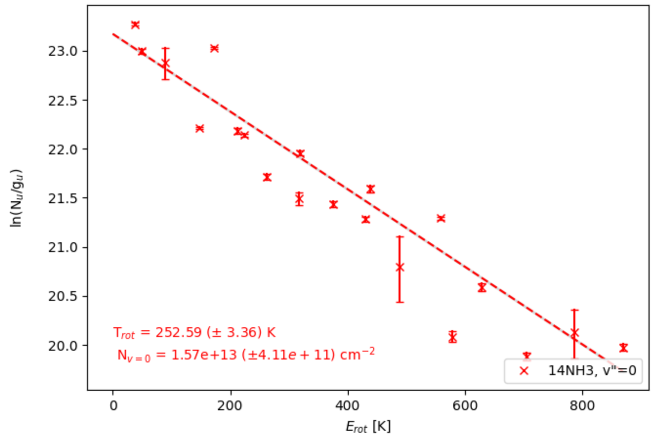
Excitation diagram analysis NH_3 in VY CMa

$^{28}Si^{16}O$	**Wong et al. (2018) [1] (radio + IR)**	**This work (absorption)***	**ortho**	**para**
T_{rot} (v_2=1-0)		253 (±3) K	~328 (±6) K	~223 (±3) K
T_{vib}	100 – 400 K	300 (fixed) K	300 (fixed) K	300 (fixed) K
$\tau_{max, RTE}$		0.01	0.01	0.01
N_L	~2 × 10^{15} cm^{-1} (@ 10^{16} cm)	(1.5 – 3.5)× 10^{15}	(0.8 – 1.1)× 10^{15}	(1.4 – 6.6)× 10^{15}

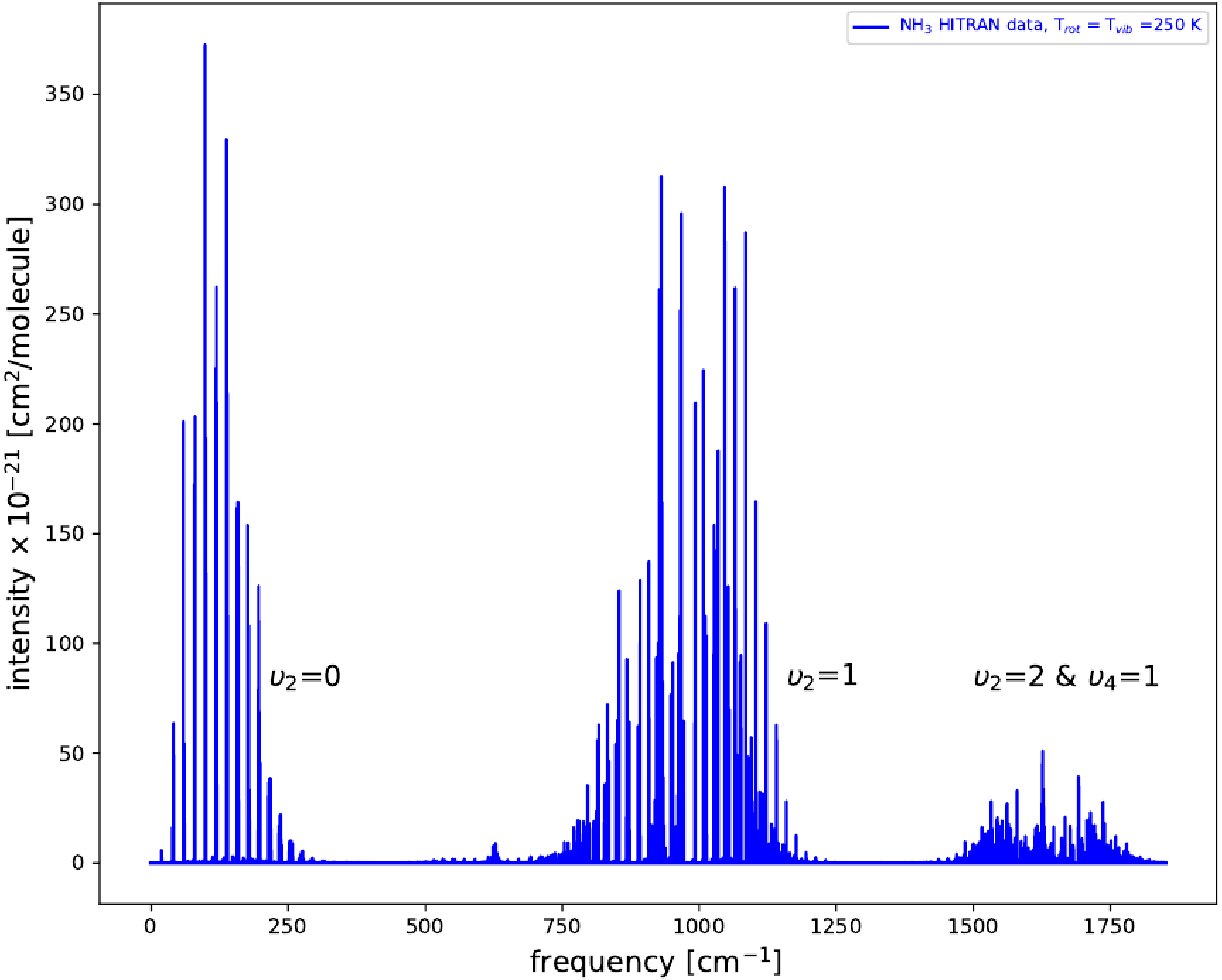
*Full RTE , T_{ex} = T_{vib} = 300 K, T_{bg} = 2400 K

Fig 16 [1]:

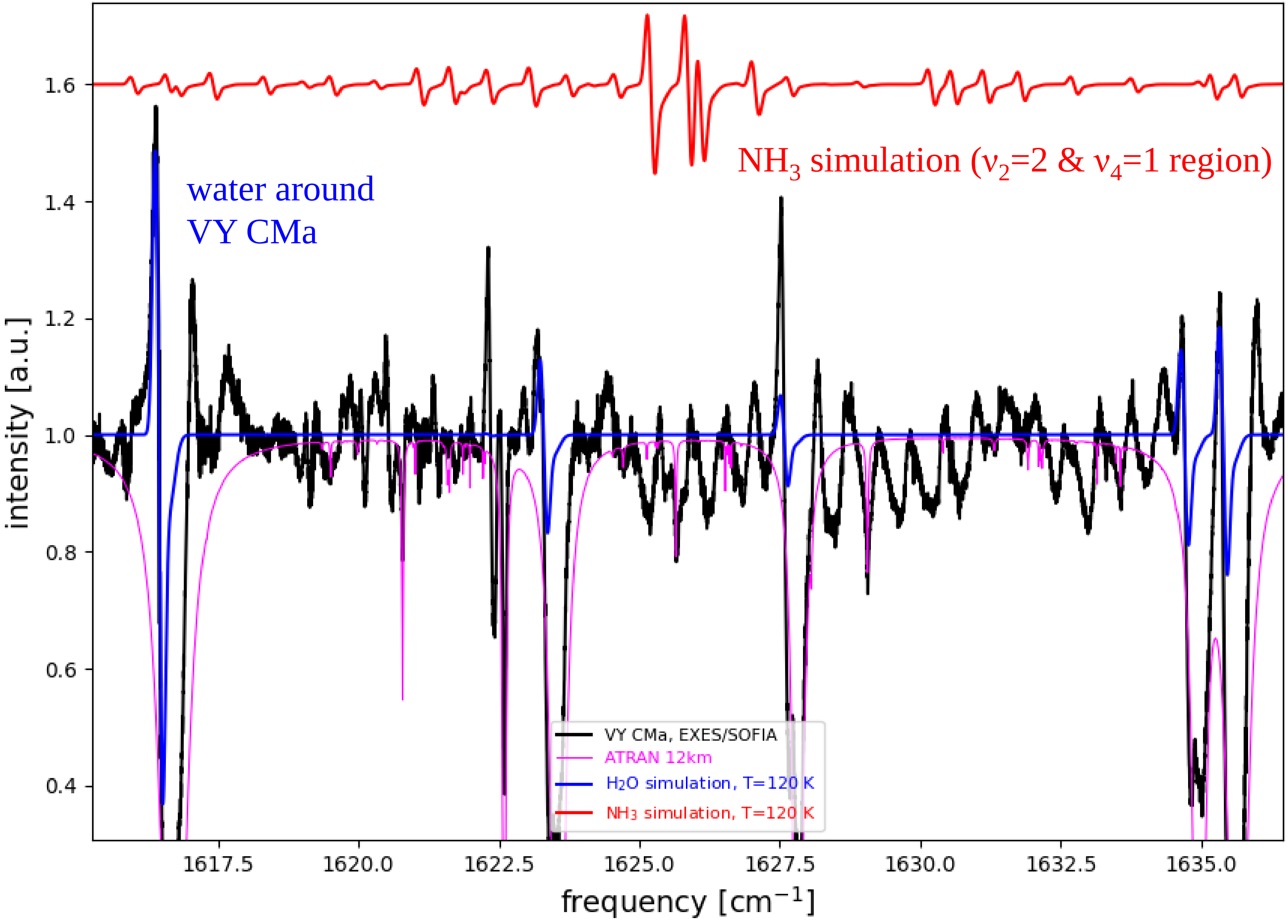




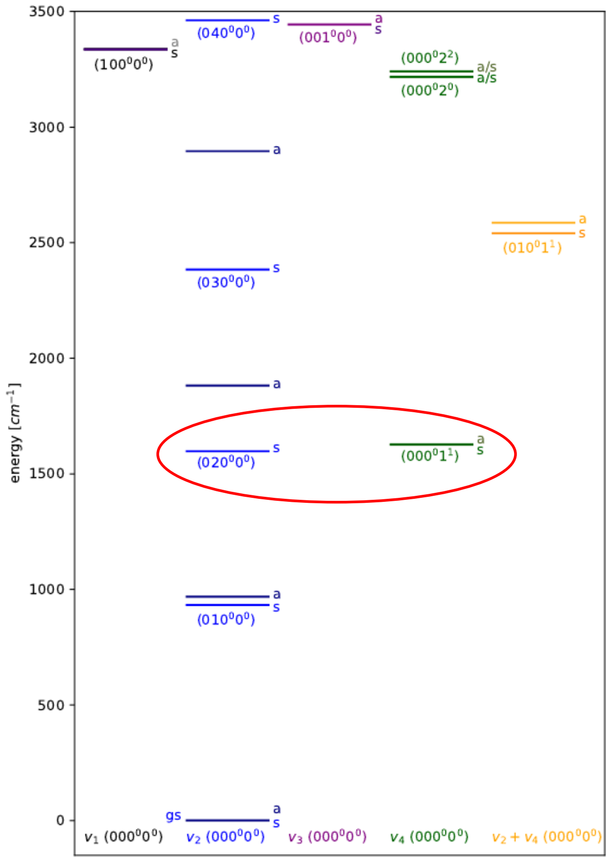
[1] Wong et al. (2018), A&A 612, A48


NH$_3$ HITRAN data, T$_{rot}$ = T$_{vib}$ =250 K
intensity × 10^{-21} [cm^2/molecule]
0
50
100
150
200
250
300
350
frequency [cm^{-1}]
0
250
500
750
1000
1250
1500
1750
υ_2=0
υ_2=1
υ_2=2 & υ_4=1

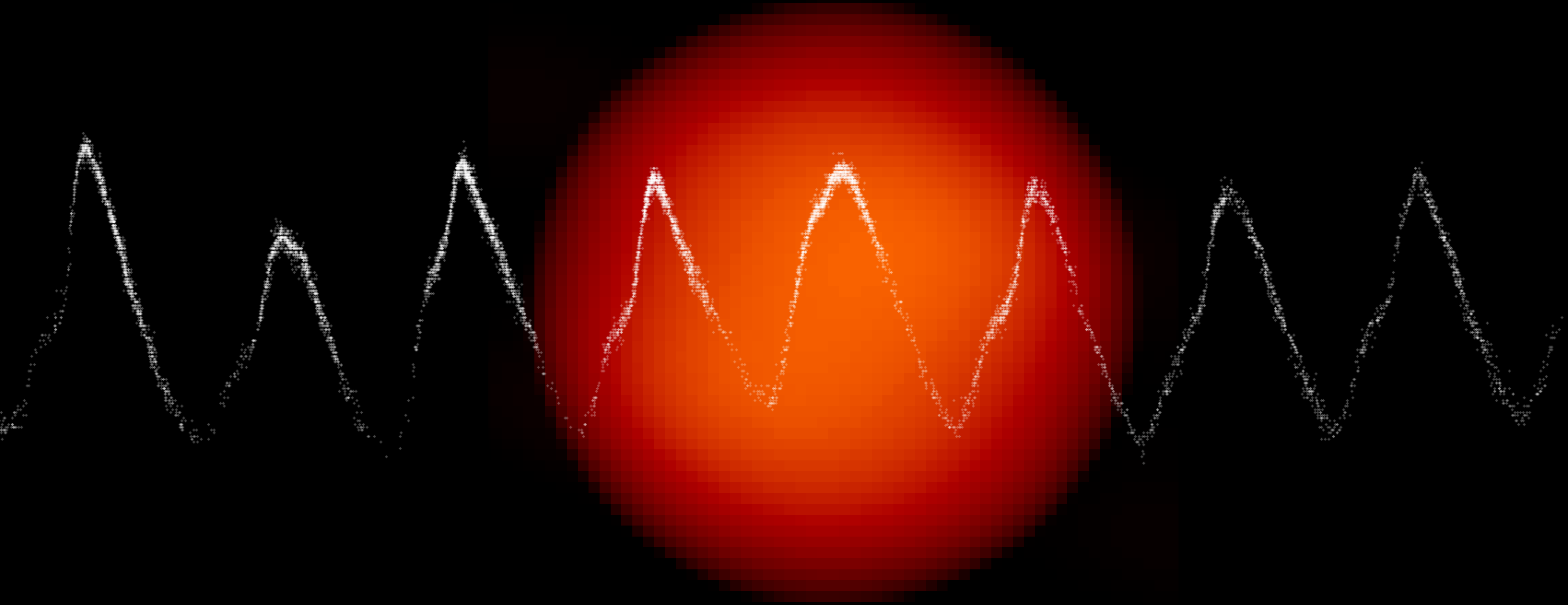
EXES/SOFIA, VY CMa



No evidence for ν_2=2 or ν_4=1 excitation.



ii) Variable stars



The case of χ Cyg

- Mira-type (regular) variable
  408 days periode,
  Magnitude from +4.5 to +12.8
- Intermediate mass star ≈ 2 $M_\odot$
  Lifetime: 500 Mio – 10^9 years
- Distance: 169 pc (553 ly)[1]
- Radius: 348 – 480 $R_\odot$ [1]
- Luminosity: 6,000 – 9,000 $L_\odot$ [1]
- Temperature: 2,441 – 2,742 K [1]

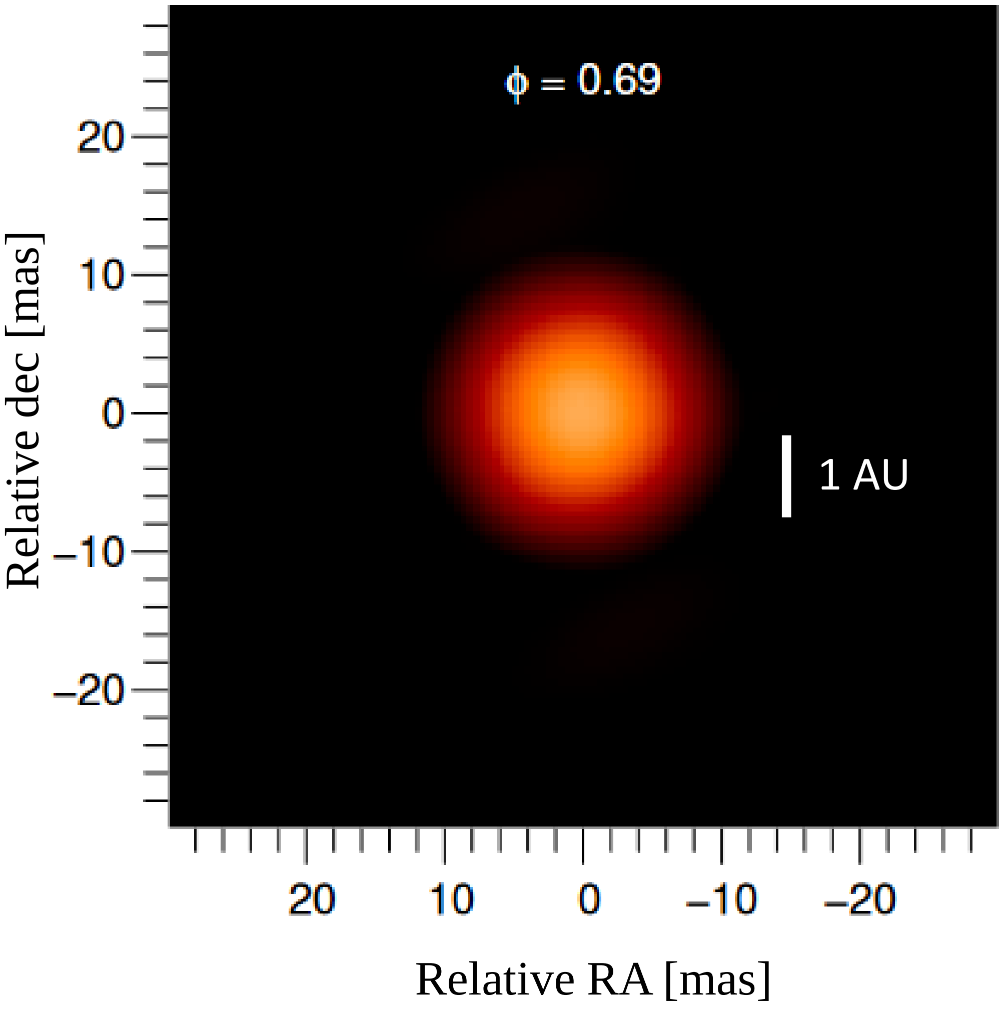


Figure 4 from [1], IOTA interferometer, 1.6 μm, Mt. Hopkins in southern Arizona

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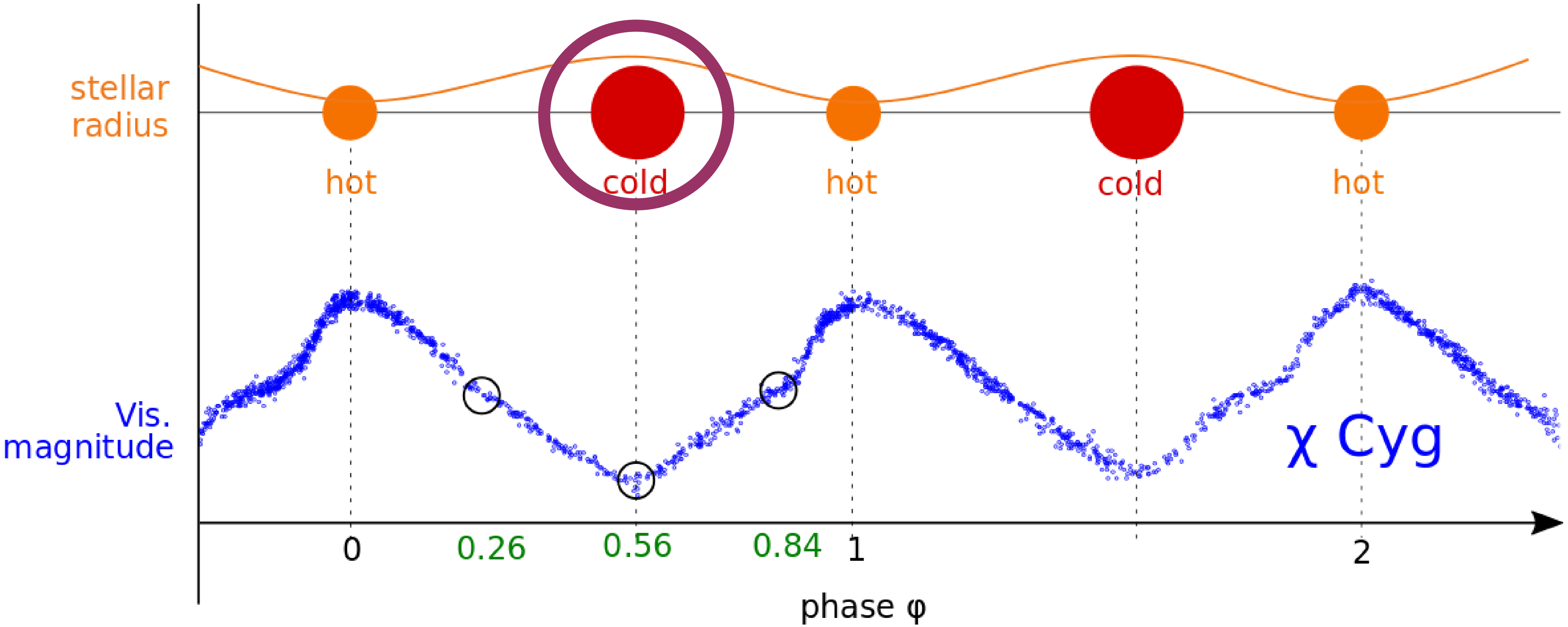
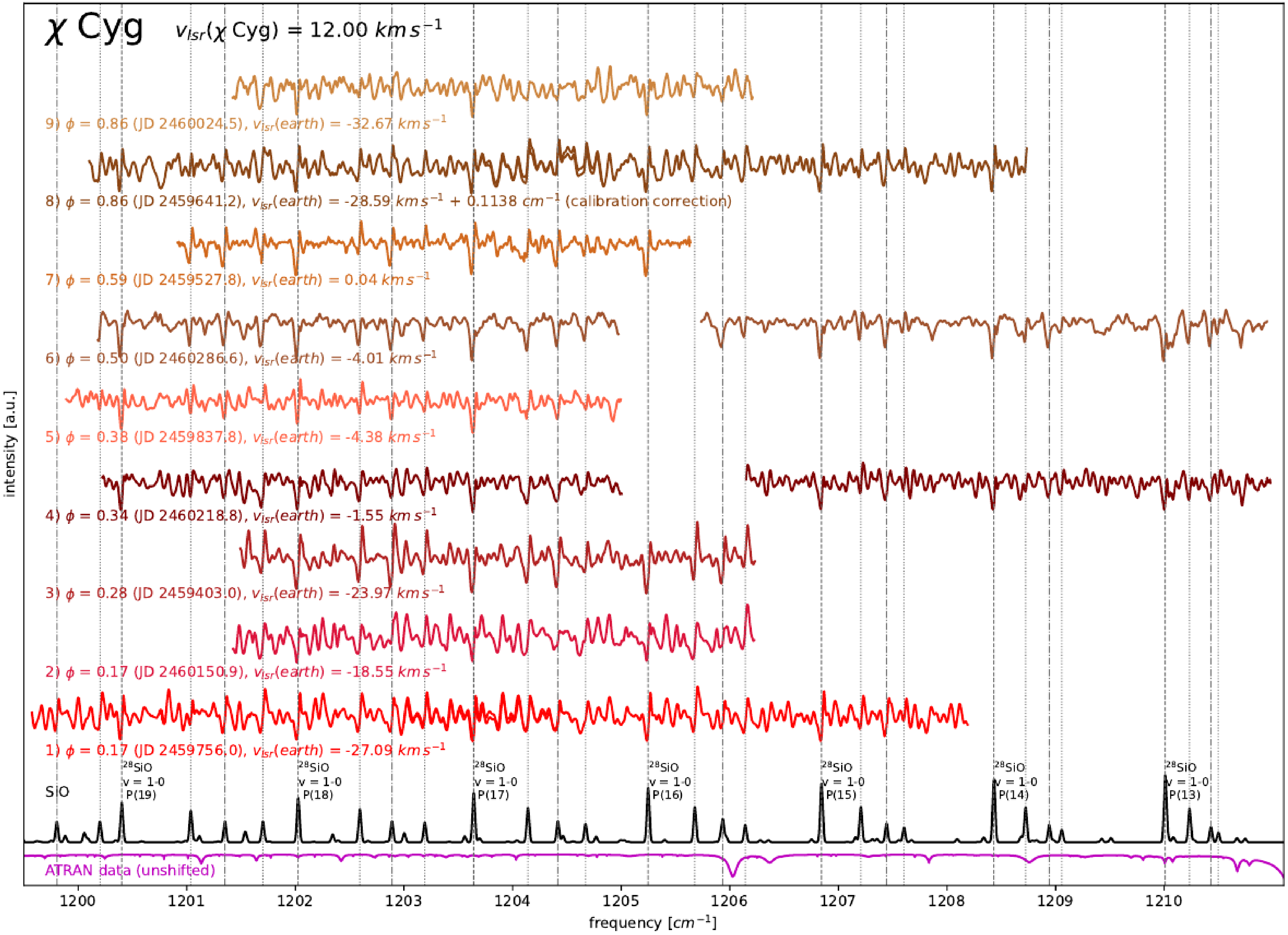
[1] Lacour et al. (2009), ApJ, 707, 632


stellar radius
hot
cold
hot
cold
hot
Vis. magnitude
χ Cyg
0
0.26
0.56
0.84
1
2
phase φ

SiO around
χ Cyg
at various
stellar phases
(TEXES/IRTF)

→ line profile
analysis

→ infall motion
of SiO

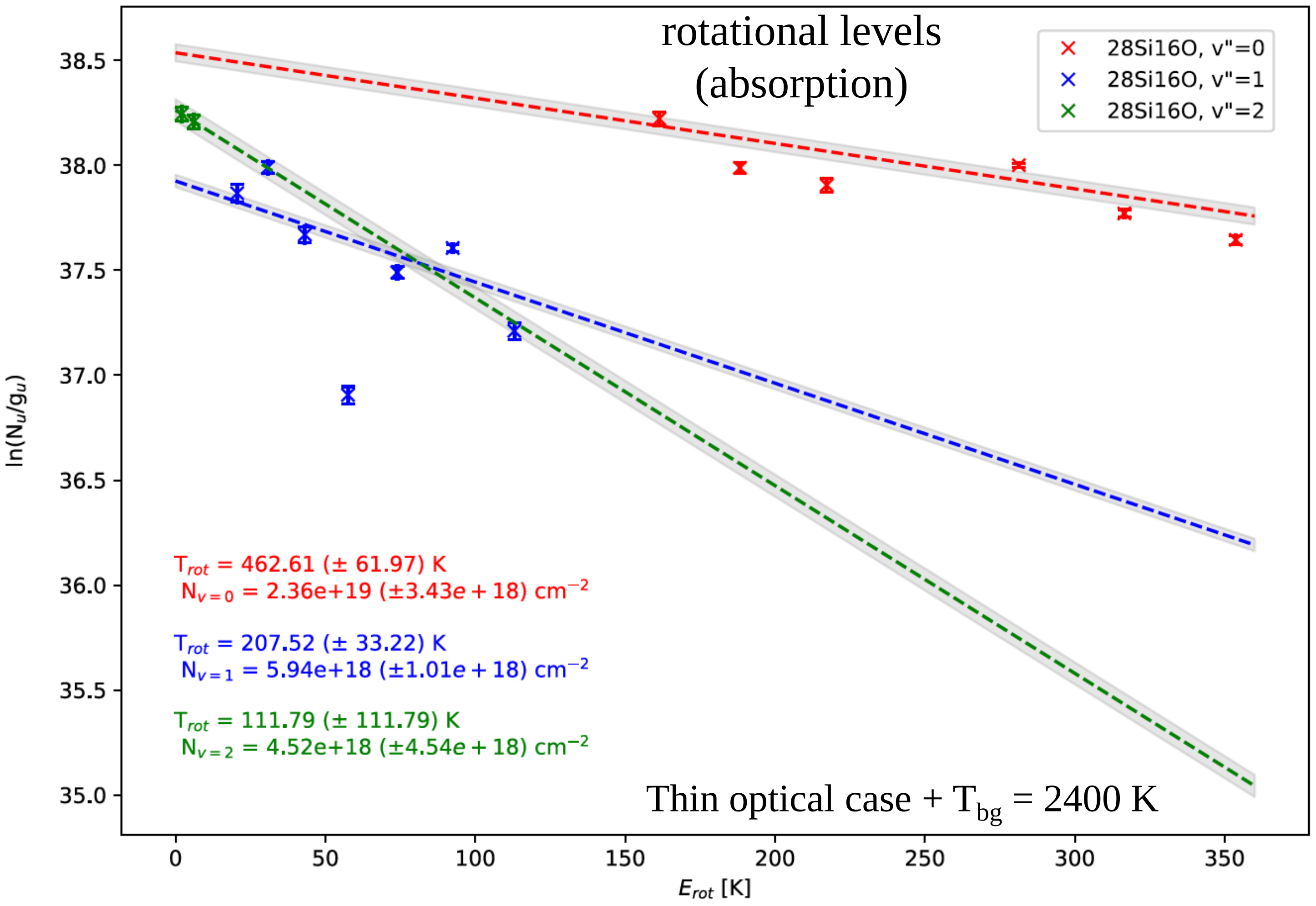


Ongoing work

Excitation diagram analysis of $^{28}Si^{16}O$, χ Cyg

(separate rotational & vibrational excitation diagram method)

TEXES /IRTF, Dec 8, 2023 (φ~0.5)

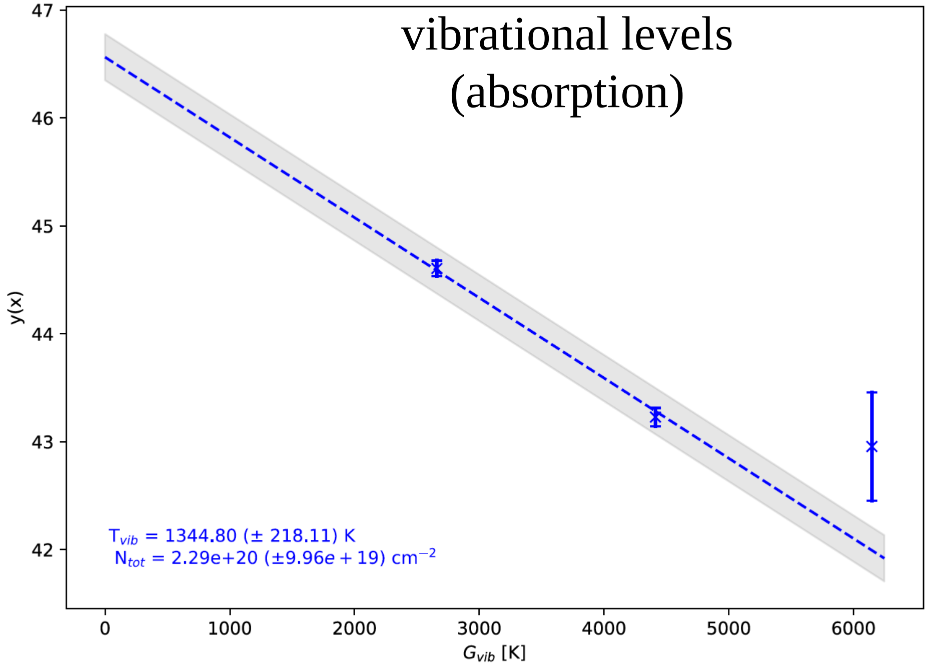

rotational levels (absorption)

T_{rot} = 462.61 (± 61.97) K
$N_{v=0} = 2.36e+19\ (\pm 3.43e+18)\ \mathrm{cm}^{-2}$

T_{rot} = 207.52 (± 33.22) K
$N_{v=1} = 5.94e+18\ (\pm 1.01e+18)\ \mathrm{cm}^{-2}$

T_{rot} = 111.79 (± 111.79) K
$N_{v=2} = 4.52e+18\ (\pm 4.54e+18)\ \mathrm{cm}^{-2}$

Thin optical case + T_{bg} = 2400 K


vibrational levels (absorption)

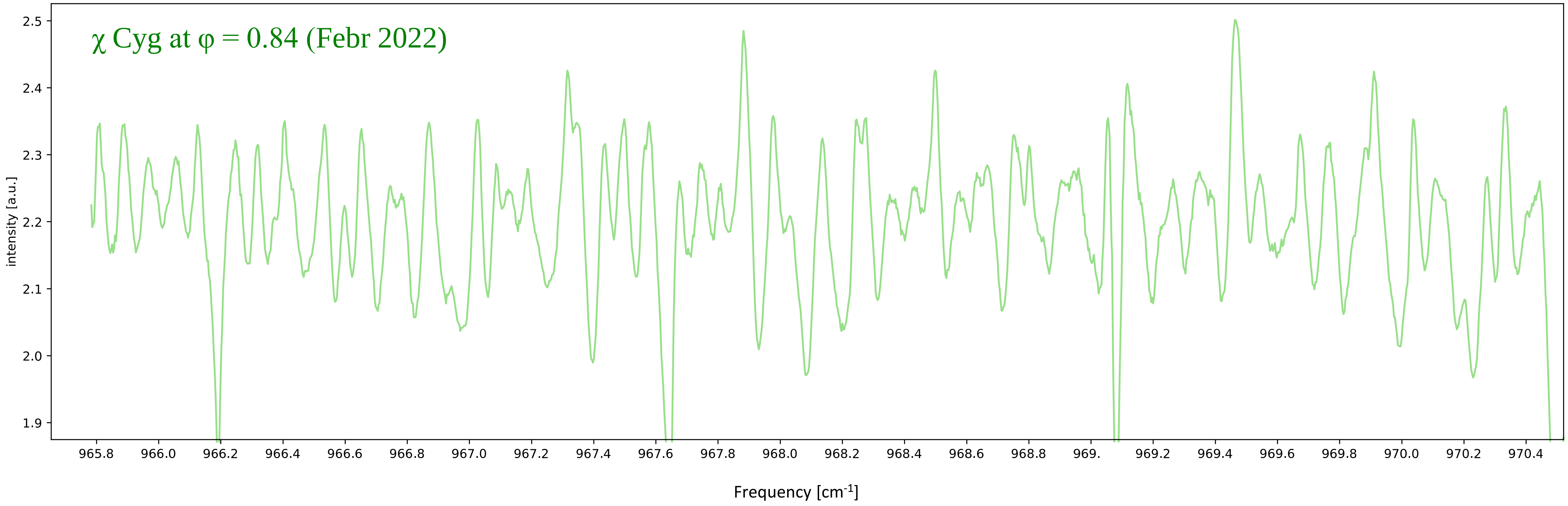
T_{vib} = 1344.80 (± 218.11) K
$N_{tot} = 2.29e+20\ (\pm 9.96e+19)\ \mathrm{cm}^{-2}$

What about something new?

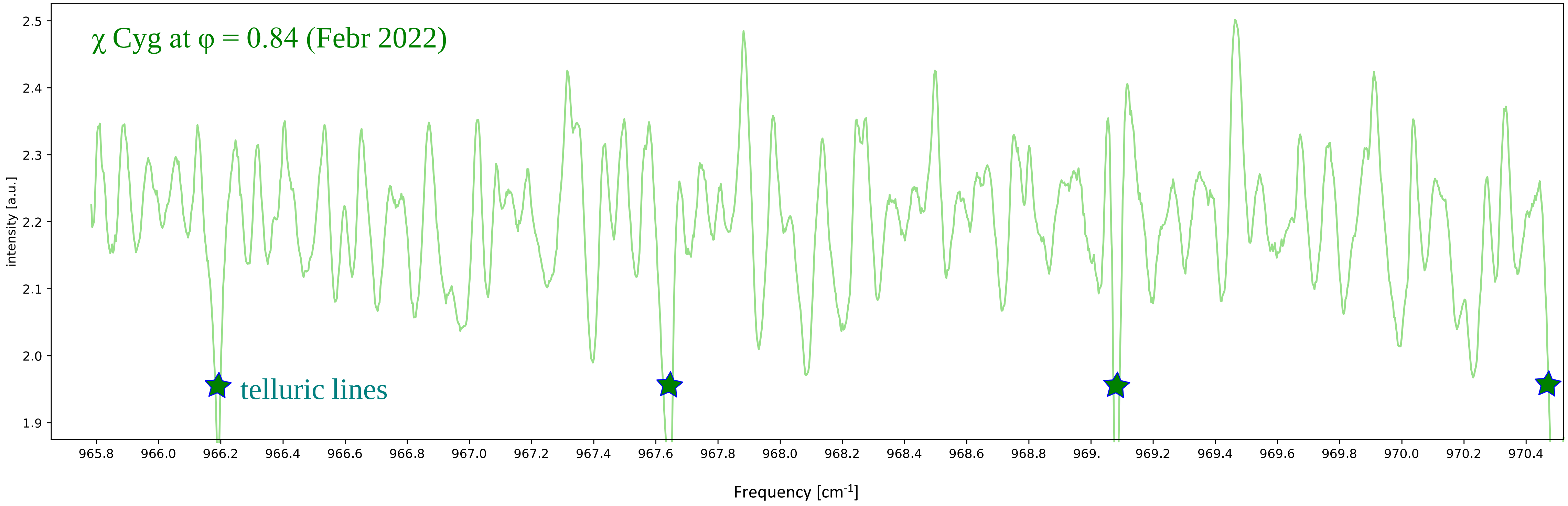
Something that has not been seen in the IR before?

What about TiO?

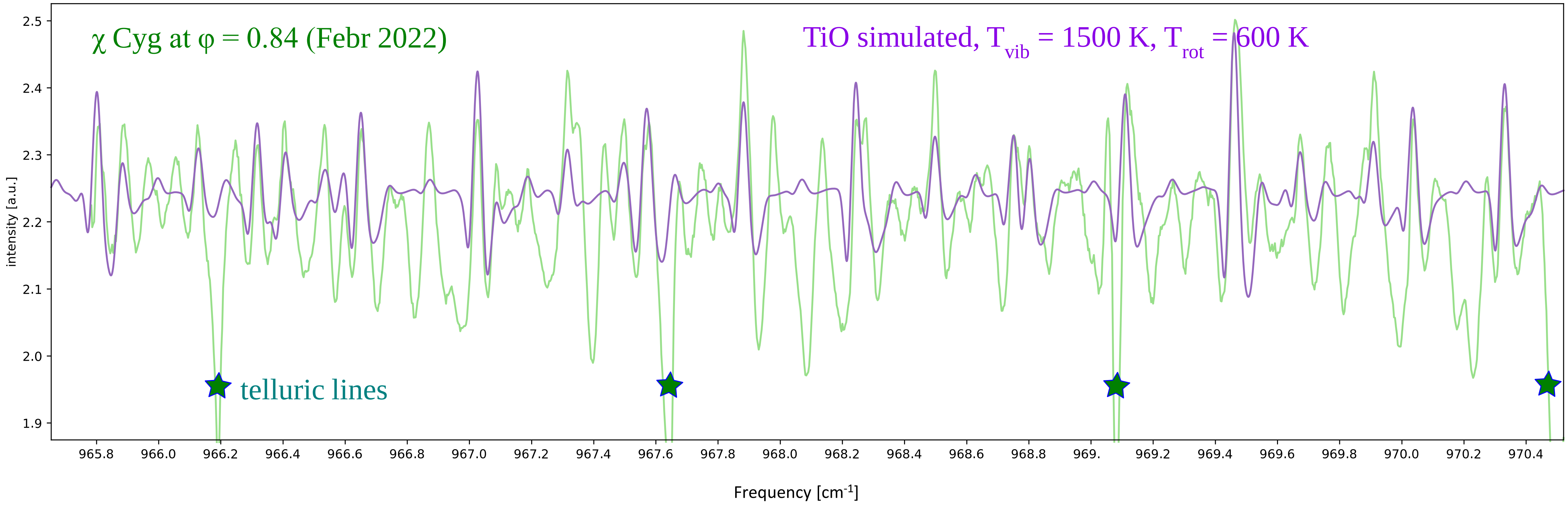
Is TiO around χ Cyg @ mid-IR ?



Is TiO around χ Cyg @ mid-IR ?

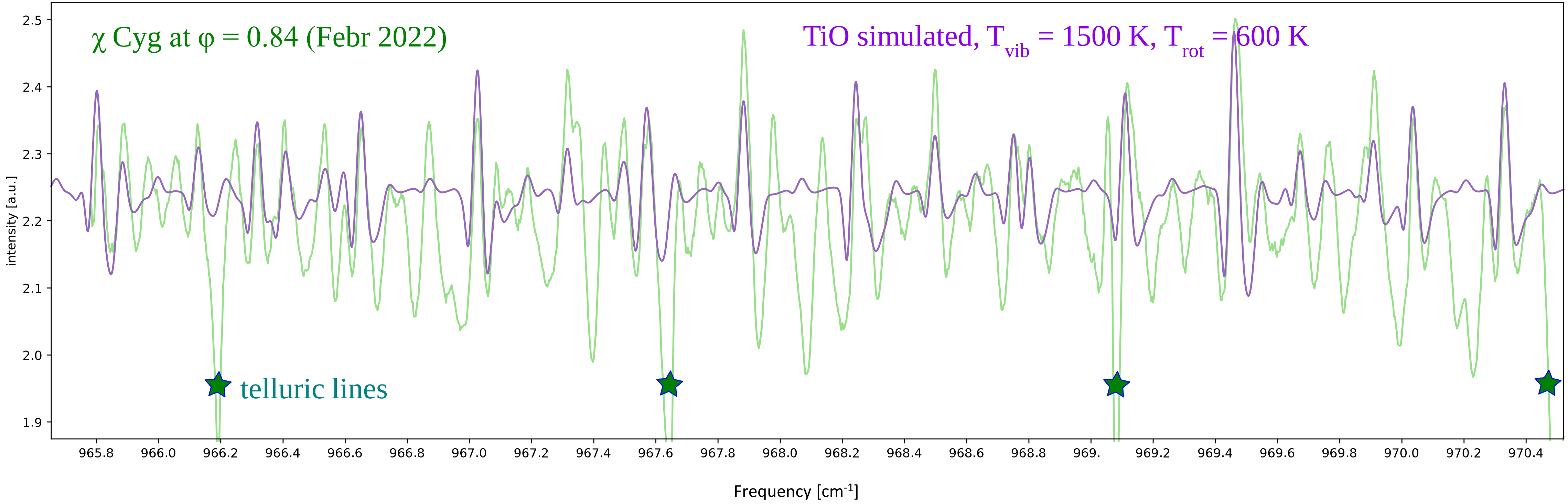


Is TiO around χ Cyg @ mid-IR ?

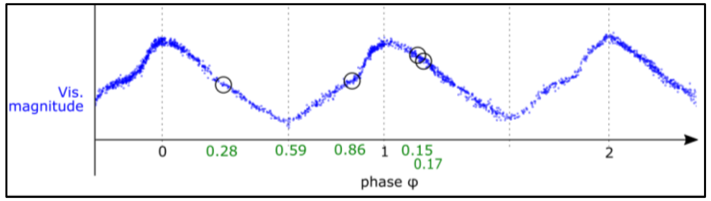


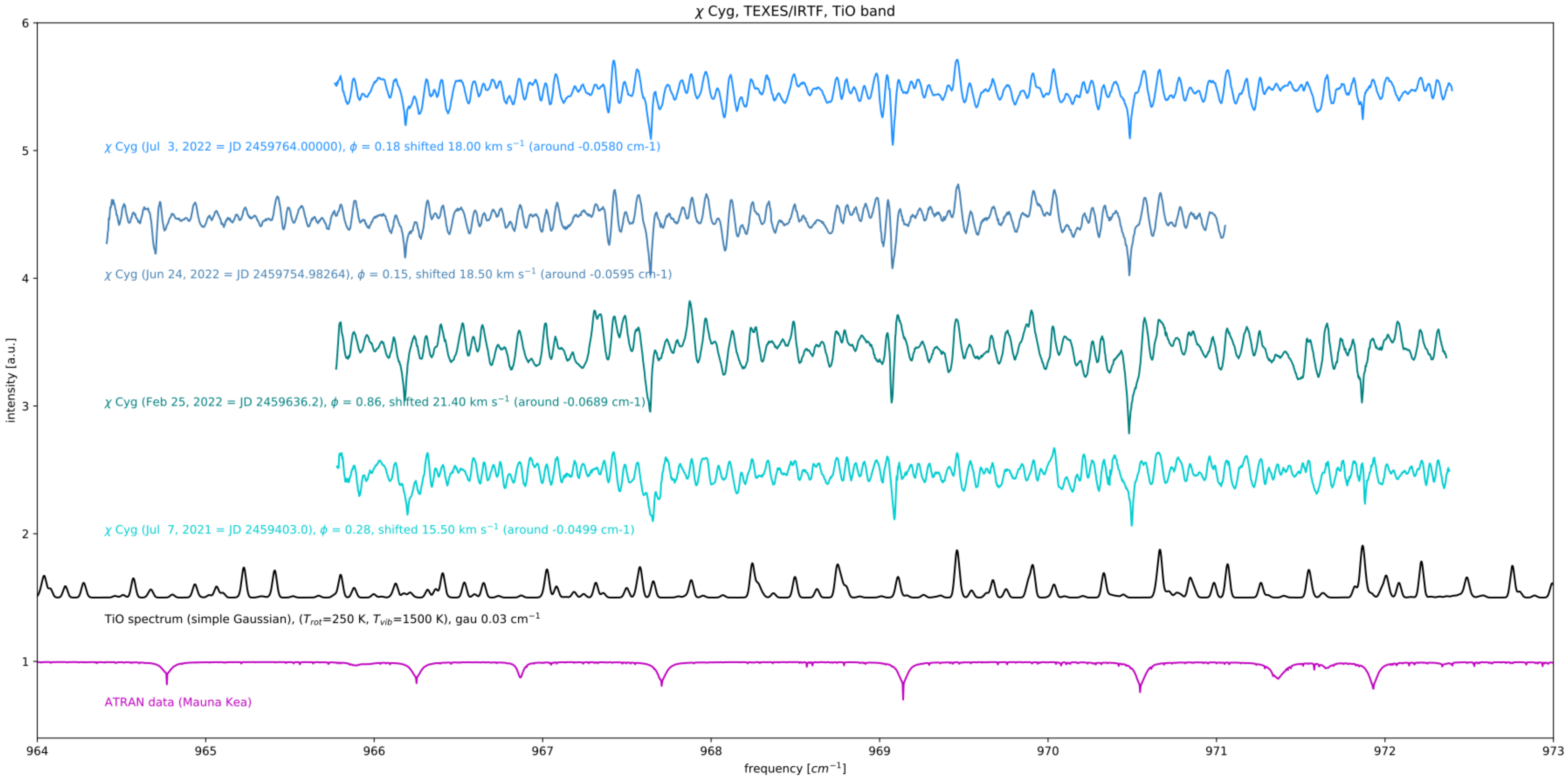
Is TiO around χ Cyg @ mid-IR ?

First time TiO detection in the mid-IR region!
Temp., line profile & shifts indicative of origin within inner molecular layer



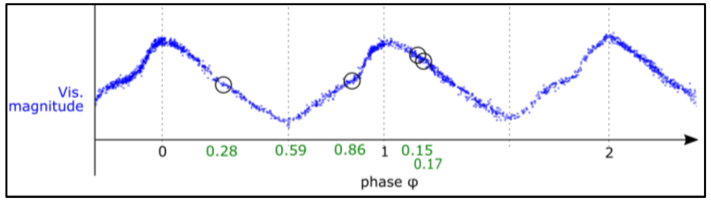
TiO in χ Cyg @ different phases

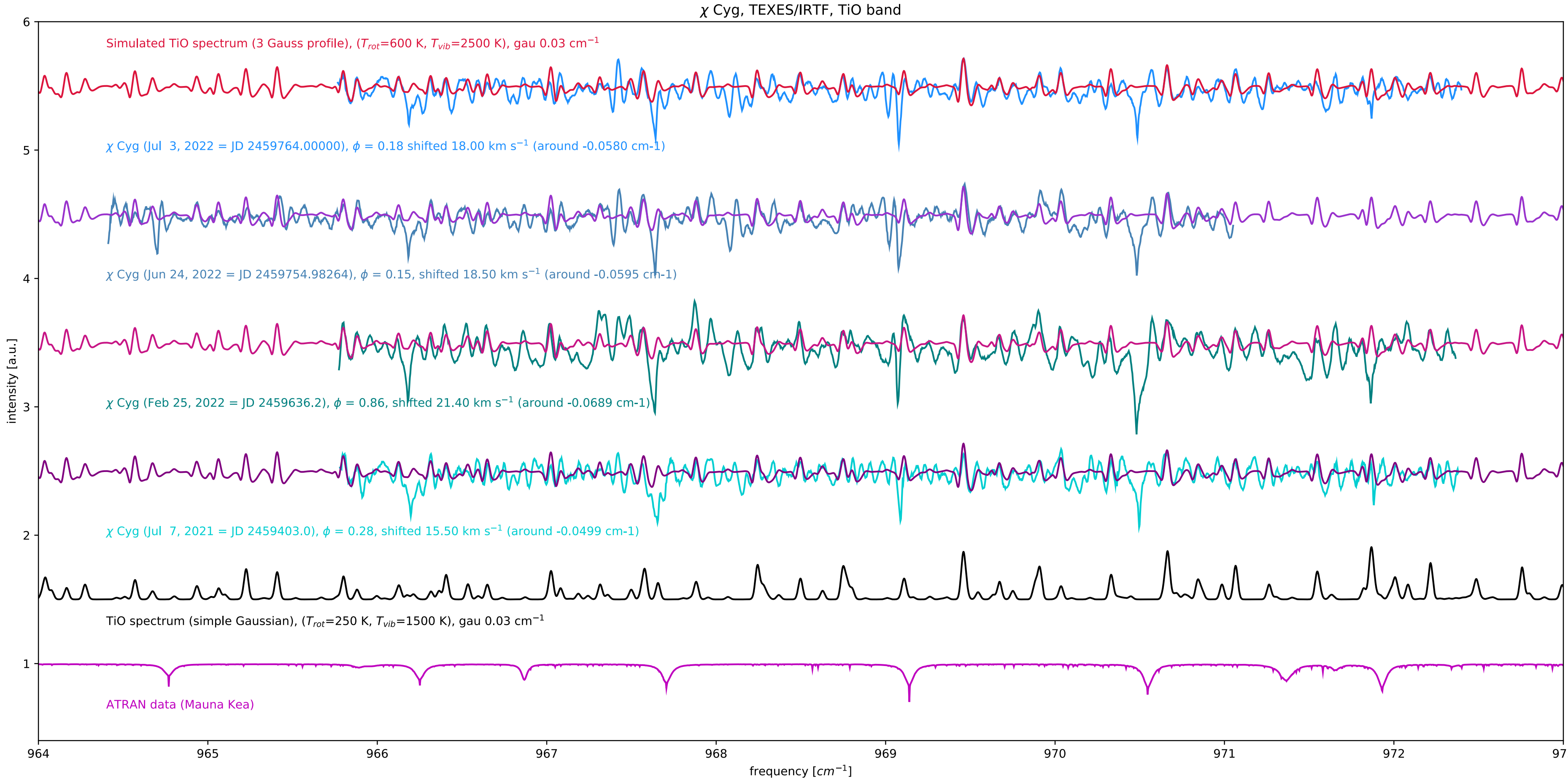




TiO simulations work fine for all phases

TiO in χ Cyg @ different phases





TiO simulations work fine for all phases

IV. Summary

- Mid-IR high-resolution spectroscopy useful tool
    - molecule identification in CSE
    - as analytic tool of dynamical processes (e.g. SiO observations of VY CMa & χ Cyg)

- Laboratory investigations indispensable basis for astrophysical studies (e.g., TiO, VO, Al_2O)

- We found TiO in the molecular layer of χ Cyg!

IV. Outlook

- Further laboratory measurements on astrophysically relevant small molecules

- Finish current projects (variable stars / line survey towards VY CMa and other late-type stars → data mining in EXES/SOFIA archive)

- Use JWST MIRI to investigate suitable molecules (R=1,500 to 3,500)

- What about balloons, airships, or an IR telescope on the moon?

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(2) Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany,(3) AIST, Tsukuba-West, Japan

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SOFIA/EXES: Edward Montiel(4) , Curtis DeWitt(4), Matt Richter(5)
(4)SOFIA/USRA, Universities Space Research Association, (5)Department of Physics, University of California, Davis, CA, USA

IRTF/TEXES: Thomas K. Greathouse(6), Rohini S. Giles(6), John H. Lacy(7)
(6) Southwest Research Institute, San Antonio, Texas, USA, (7) University of Texas at Austin, Department of Astronomy, Austin, Texas, USA

SOFIA
STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY
NASA · USRA DLR · DSI

IRTF

UNIKASSEL VERSITÄT
MATHEMATICS AND NATURAL SCIENCES

DFG Deutsche Forschungsgemeinschaft

DLR Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center

Laborastrophysik
Universität Kassel

Thank you for your attention!

Title: Molecules around Late-type stars seen in the infrared at high spectral resolution using EXES on SOFIA

Speaker: Guido W. Fuchs (University of Kassel, Germany)

Abstract:

Our universe is full of molecules. Most molecules have been discovered with the help of radio or MM telescopes based on their rotational spectra. But molecules can also be detected unambiguously in the infrared (IR) range. Here, even those can be detected that do not have a permanent electric dipole moment. If available IR high-resolution laboratory spectra can be used to identify molecules from astrophysical observations. The molecular envelopes around aging stars provide an excellent opportunity to study molecular species and also the dynamics of their environment like the outflows, shock waves, the expansion of molecular shells or the infall of material into a star. For this purpose, observations with the SOFIA aircraft telescope using the EXES spectropgraph were performed as well as observations using the TEXES instrument at the IRTF telescope on Mauna Kea. Hawaii on selected astronomical objects. Example IR spectra from hypergiant stars such as VY CMa and NML Cyg will be presented. With the help of the high-resolution spectra, molecular abundances, ambient temperatures, and dynamical processes can be determined. This will be demonstrated on the molecule silicon monoxide (SiO), ammonia (NH_3) and others.