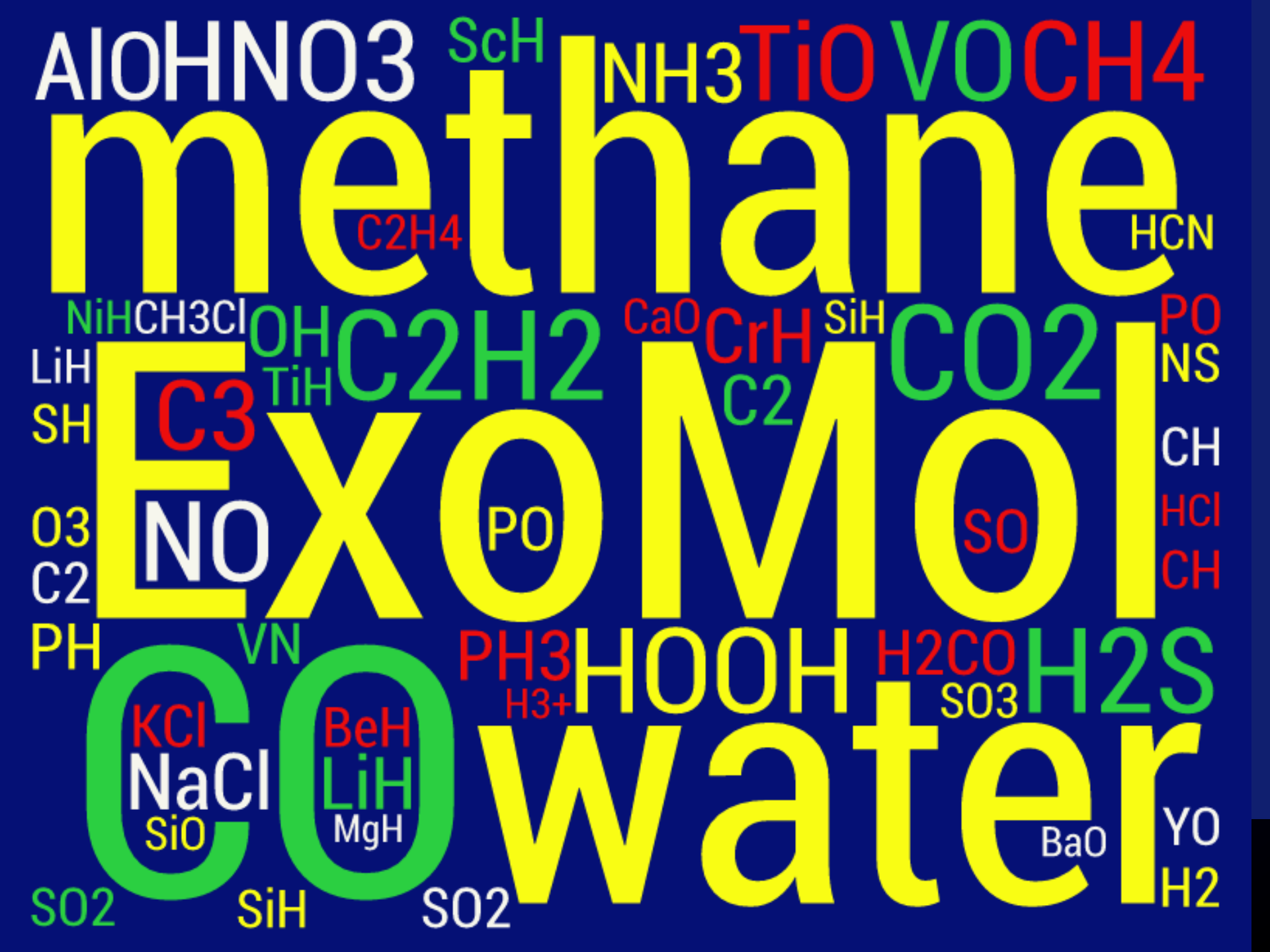
Opacities for modelling atmospheres of exoplanets

S. N. Yurchenko

J. Tennyson and ExoMol team

Physics and Astronomy


AlOHNO3
ScH
NH3
TiO
VO
CH4
methane
C2H4
HCN
NiH
CH3Cl
OH
C2H2
CaO
CrH
SiH
CO2
PO
LiH
TiH
C2
NS
SH
C3
ExoMol
CH
O3
NO
PO
SO
HCl
C2
CH
PH
VN
PH3
HOOH
H2CO
H2S
H3+
SO3
CO
KCl
NaCl
SiO
BeH
LiH
MgH
water
BaO
YO
H2
SO2
SiH
SO2


Dan Underwood
Renia Diamantopoulou
Andrey Yachmenev
SergeyYurchenko
Phillip Coles
Alec Owens
Maire Gorman
Ahmed Al-Refaie
Sarah Rugheimer
Emma Barton
Jonathan Tennyson
UCL
Christian Hill
Katy Chubb
Emil Zak
Oleg Polyansky
Andrei Patrascu
erc
Laura McKemmish
Lorenzo Lodi
Clara Sousa Silva

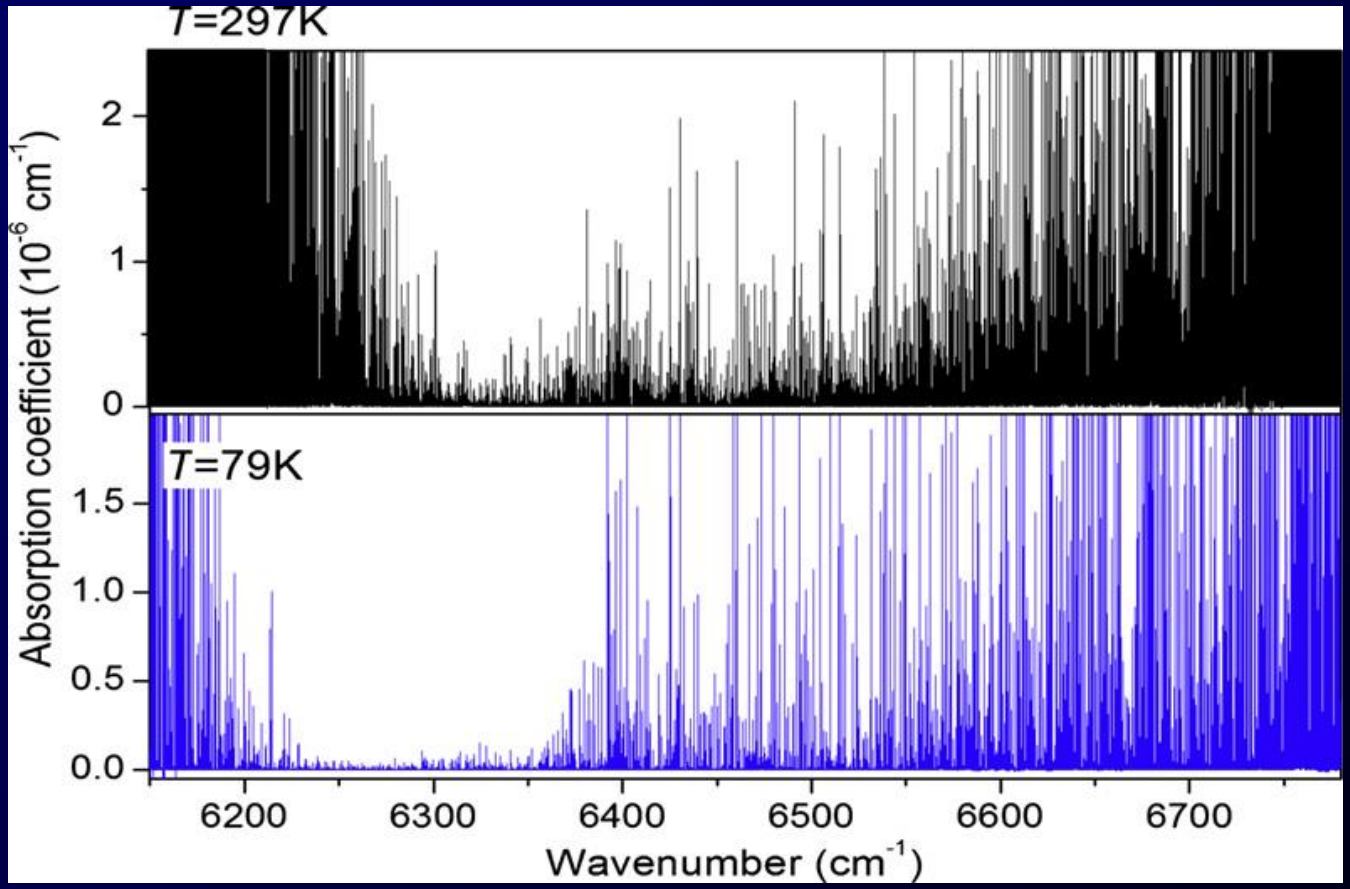
ExoMol produces opacities for *all* molecules likely to be important for exoplanetary atmospheres

Opacities

Intensities

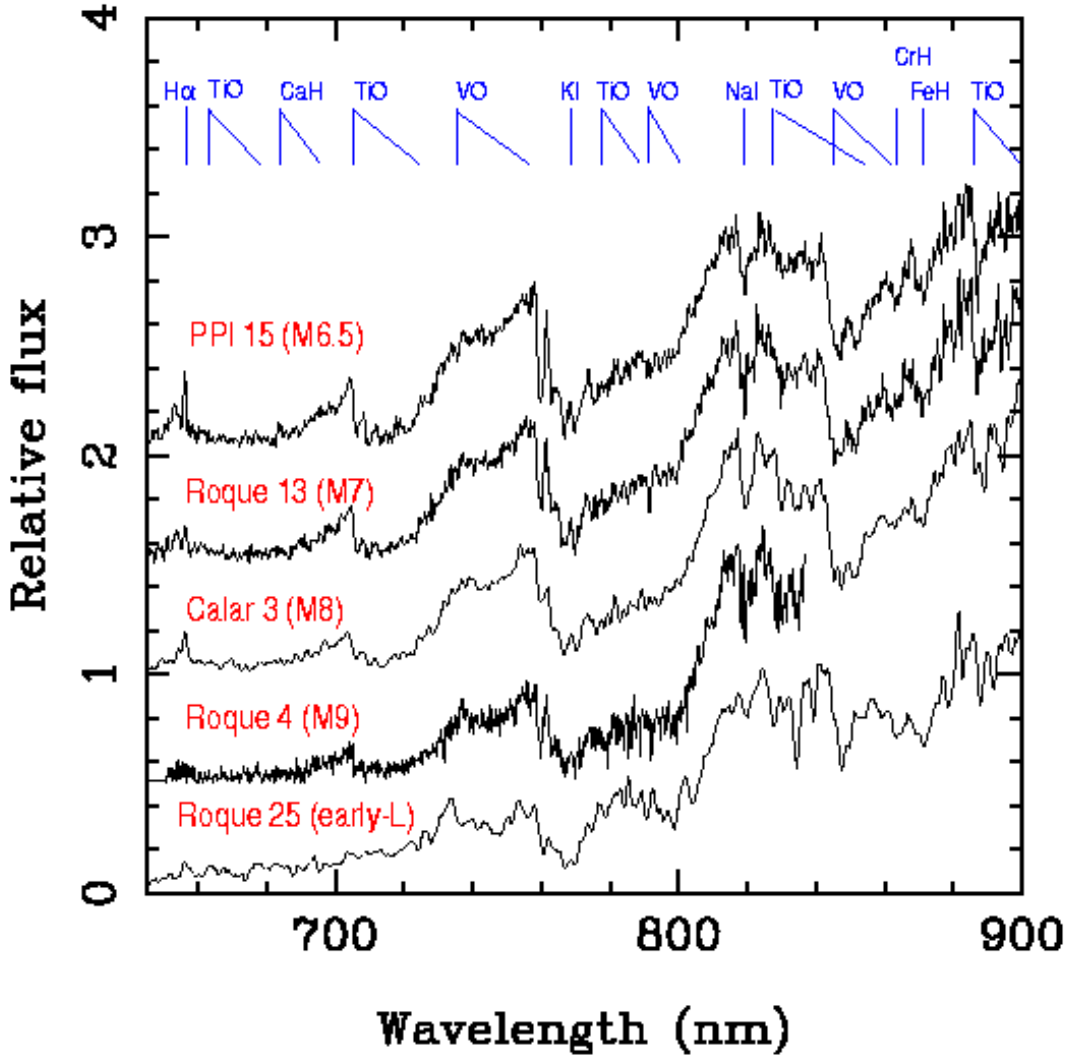
Spectrum

Methane high resolution spectrum



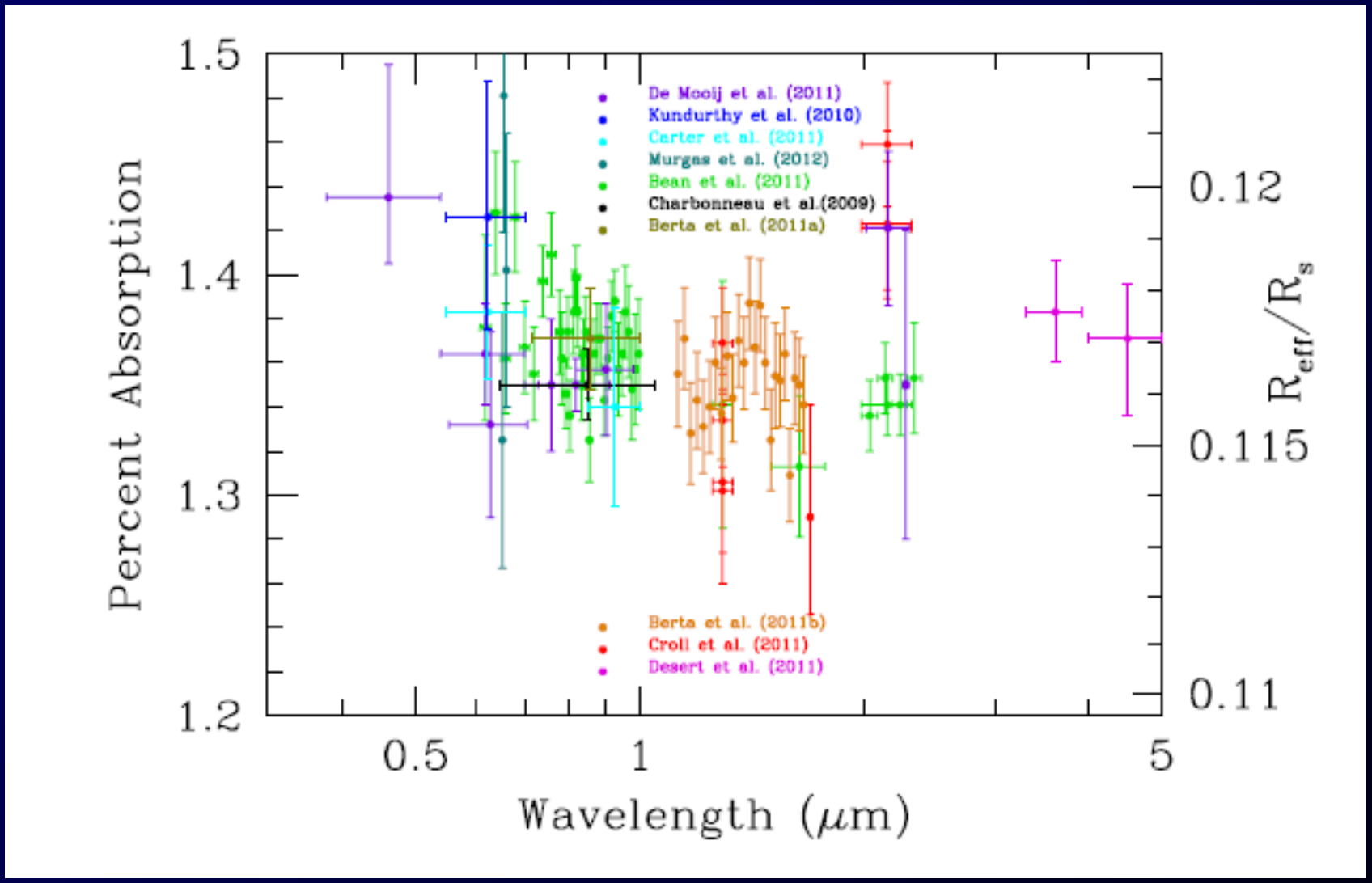
Transmitance

Flux


Hα
TiO
CaH
TiO
VO
KI
TiO
VO
NaI
TiO
VO
CrH
FeH
TiO
PPl 15 (M6.5)
Roque 13 (M7)
Calar 3 (M8)
Roque 4 (M9)
Roque 25 (early-L)
Relative flux
0
1
2
3
4
700
800
900
Wavelength (nm)

For exoplanetary transit:

Opacity = R(planet)/R(star)

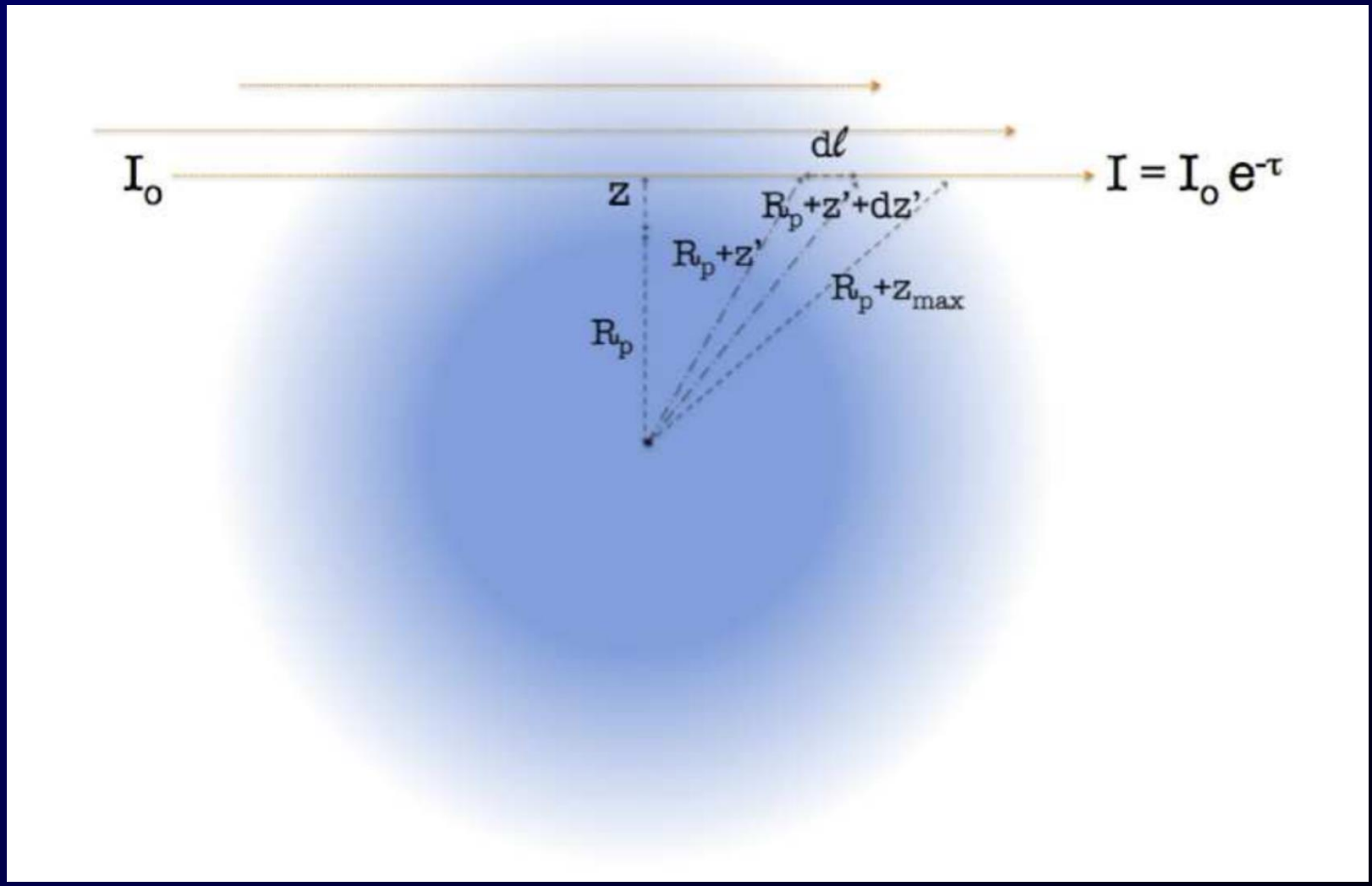


NASA's Hubble

Howe and Burrows, 2012 *ApJ* **756** 176

Our Opacity = cross-sections

Opacity is  -Lambert Law


I_o
$d\ell$
$I = I_o e^{-\tau}$
z
$R_p+z'+dz'$
R_p+z'
R_p+z_{max}
R_p

$$I_\lambda(z) = I_\lambda(0) e_\lambda^{-\tau_\lambda(z)}$$

Optical depth

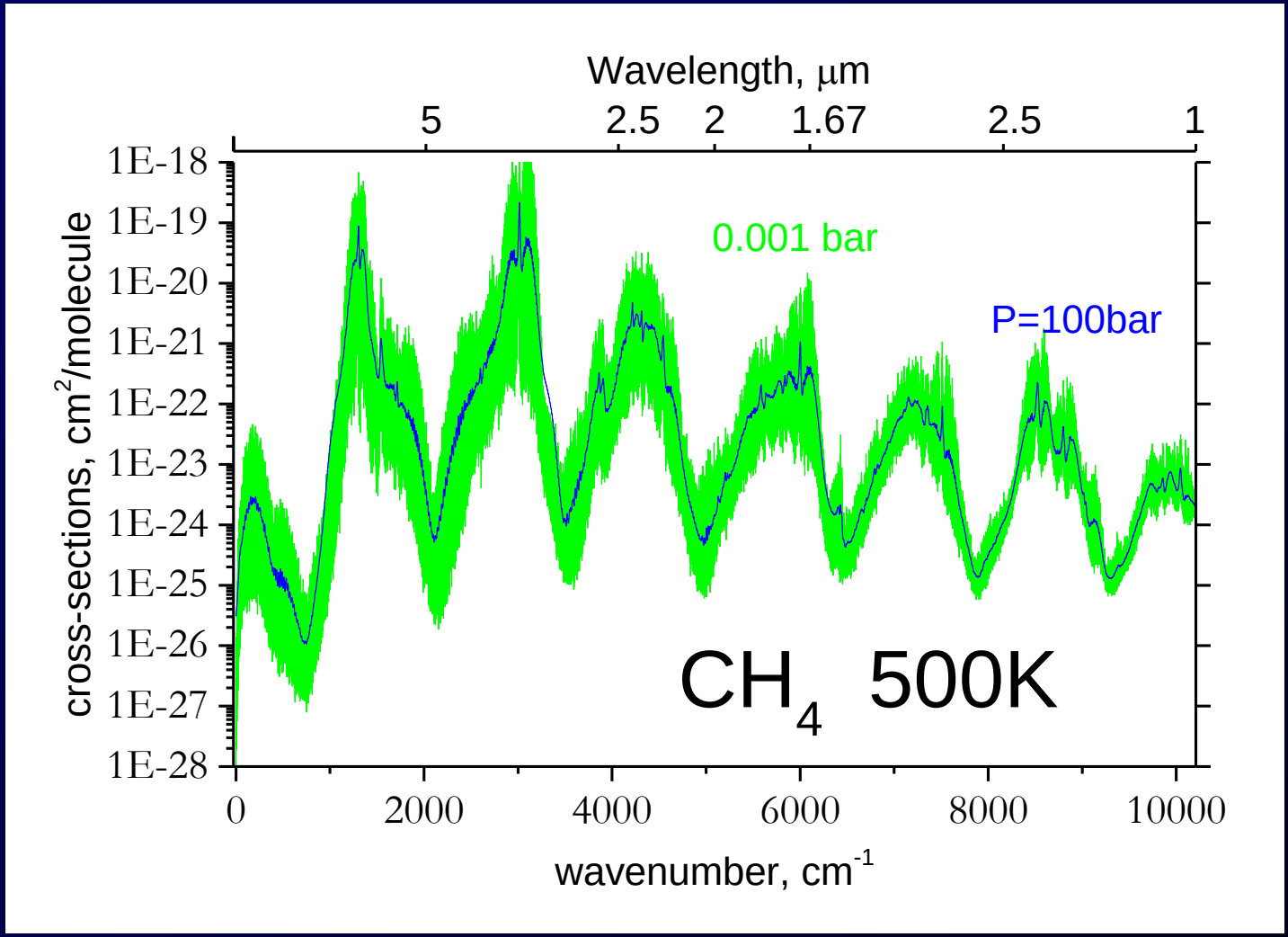
$$\tau_\lambda^n(z) = \int_0^{l(z)} \sigma_n(\lambda)\chi_n(z')\rho_N(z')dl$$

Mixing ratio

density

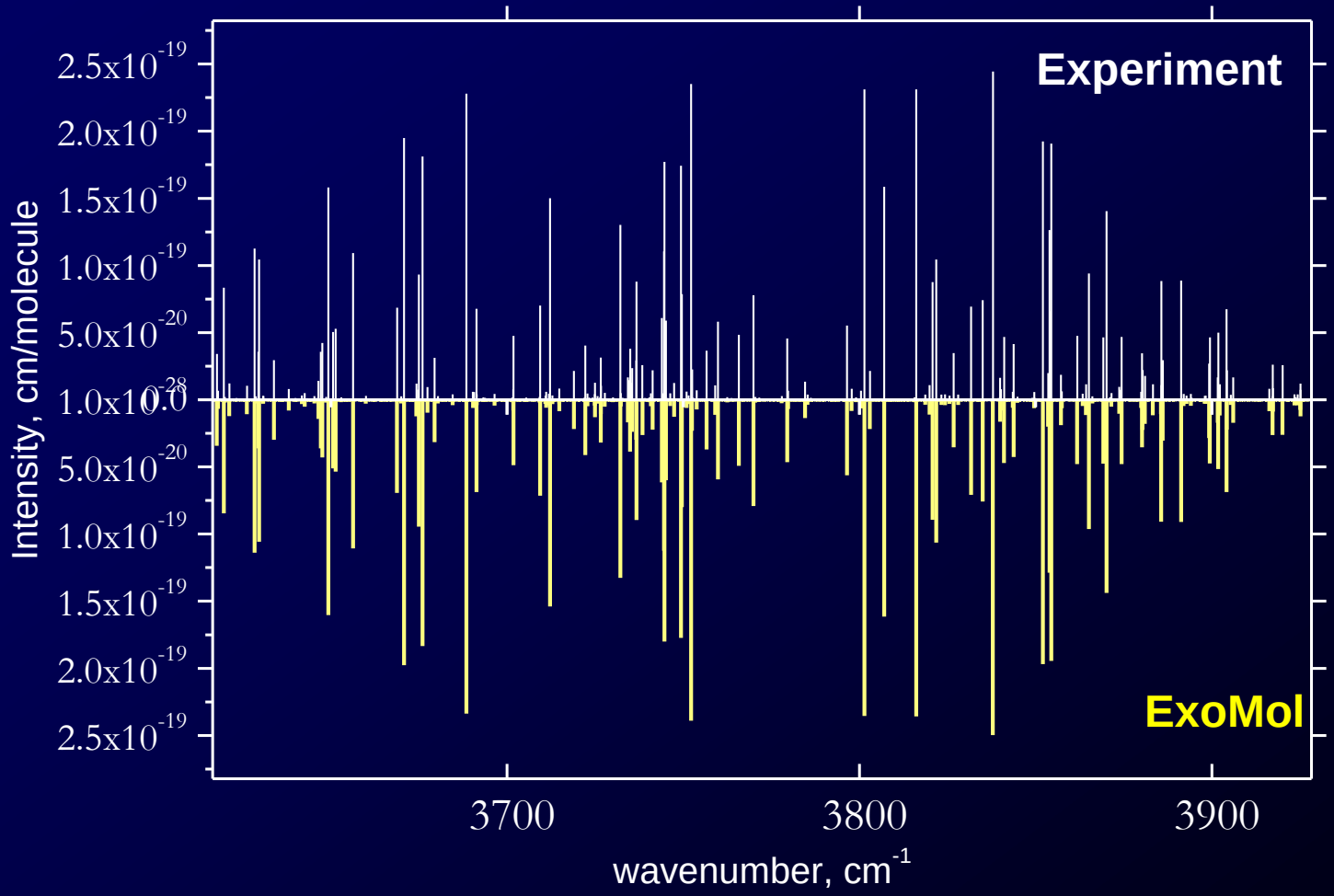
Cross-sections

Here is Methane absorption using different profiles



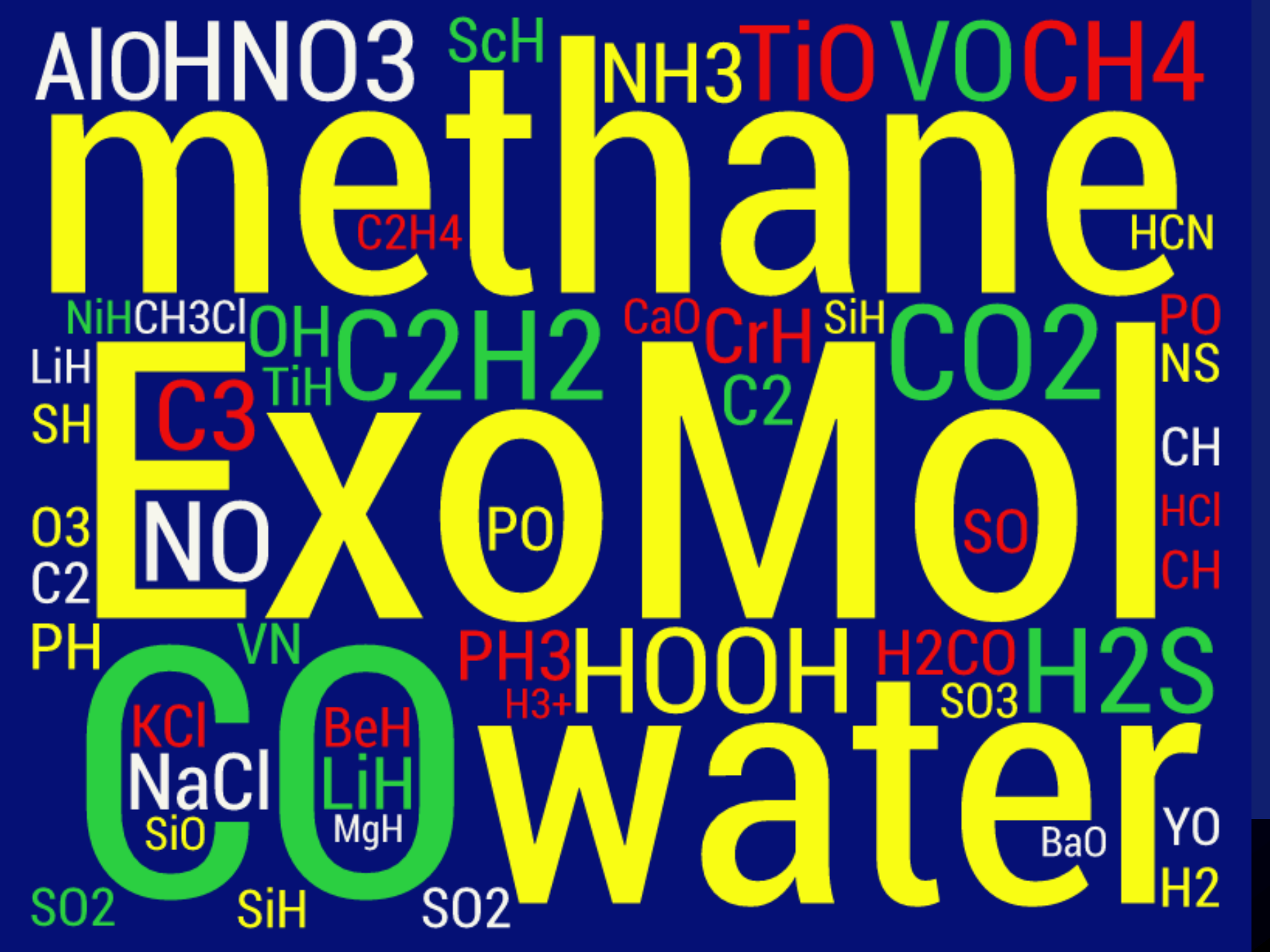
Our Opacity = line list

This is our 2016-line list for water compared to experiment, each line represented by a stick



ExoMol = line lists

Astrophysics with ExoMol


AlOHNO3
ScH
NH3
TiO
VO
CH4
methane
C2H4
HCN
NiH
CH3Cl
OH
C2H2
CaO
CrH
SiH
CO2
PO
LiH
TiH
C2
NS
SH
C3
ExoMol
CH
O3
NO
PO
SO
HCl
C2
CH
PH
VN
PH3
HOOH
H2CO
H2S
H3+
SO3
CO
KCl
NaCl
SiO
BeH
LiH
MgH
water
BaO
YO
H2
SO2
SiH
SO2

I will show examples of ExoMol line land of their (possible or actual) applications

I will go through molecules not necessarily in any special order

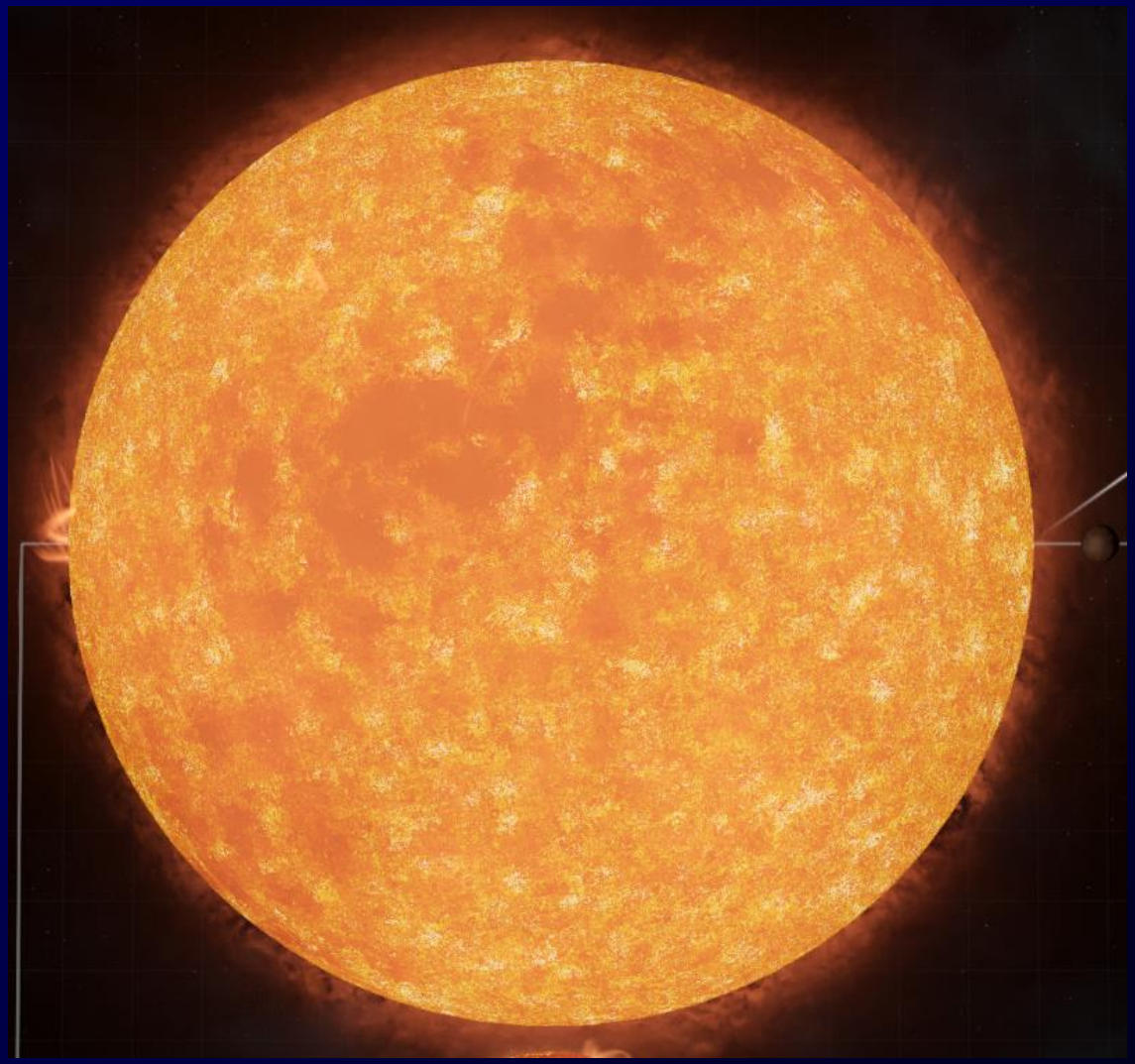
I will start from C_2

C_2

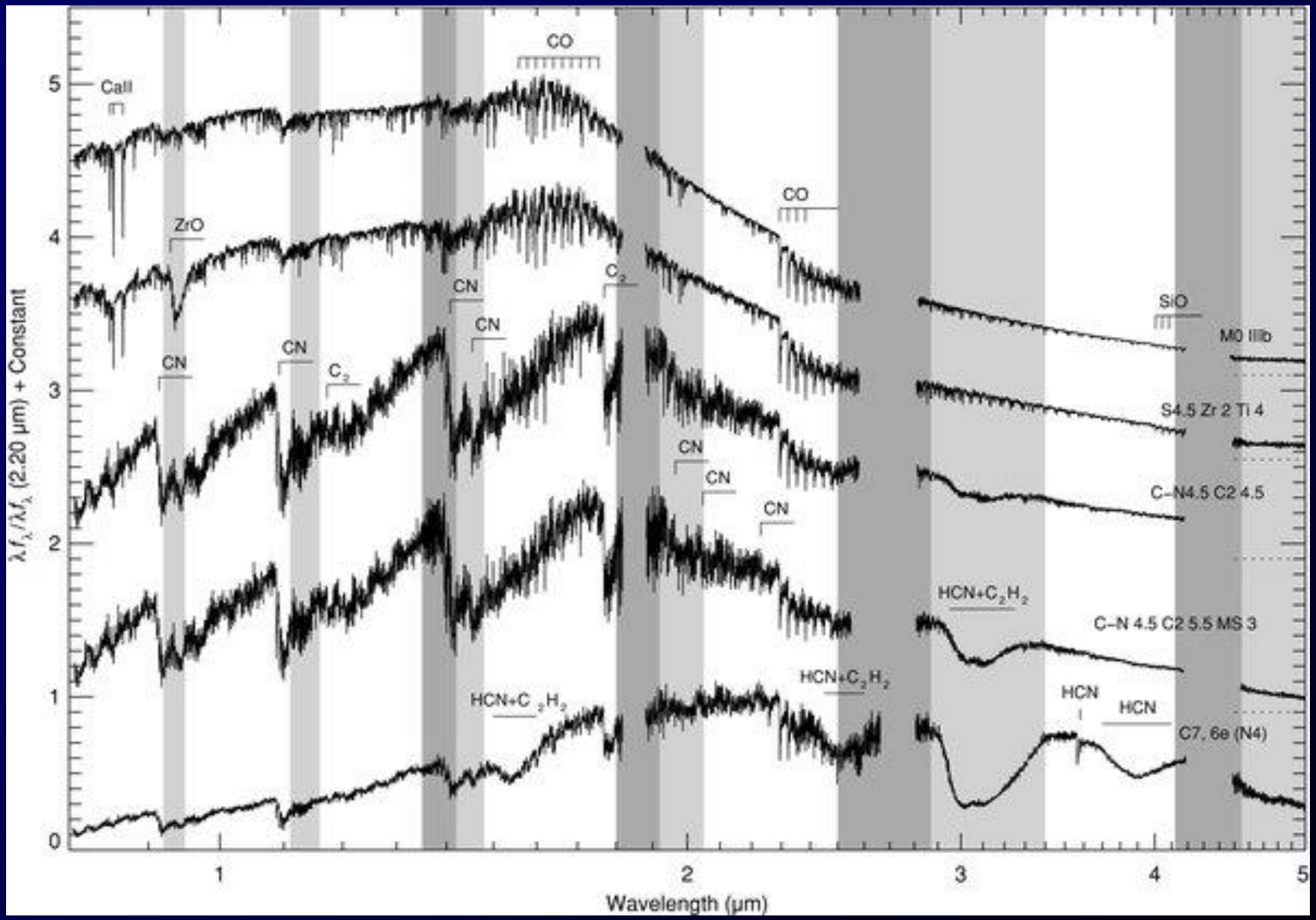
is seen in many places

for example Carbon stars

(obviously)



Here is an example of High-Res Spectra of Carbon stars



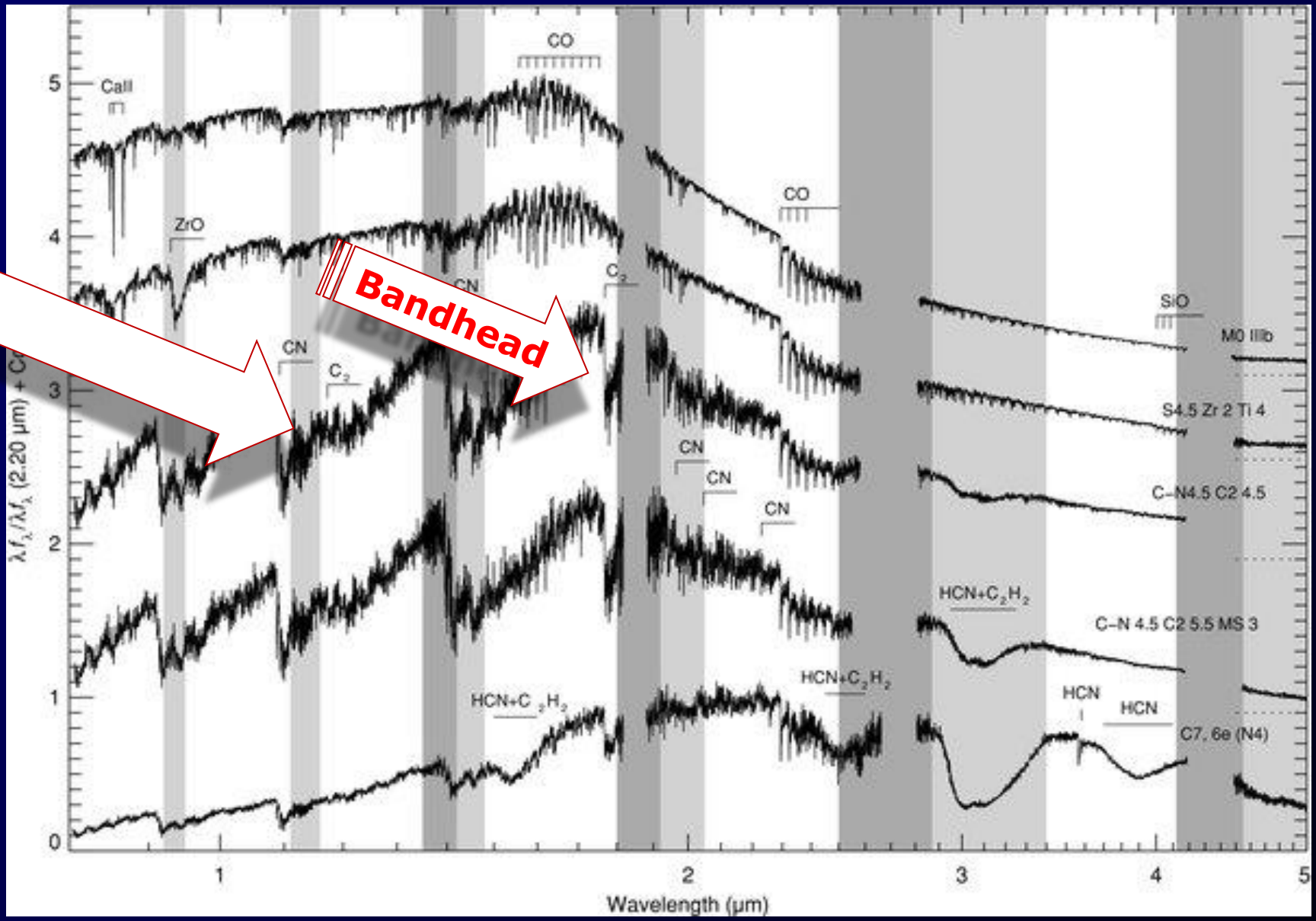
The Astrophysical Journal Supplement Series, 185:289–432, 2009 December doi:10.1088/0067-0049/185/2/289

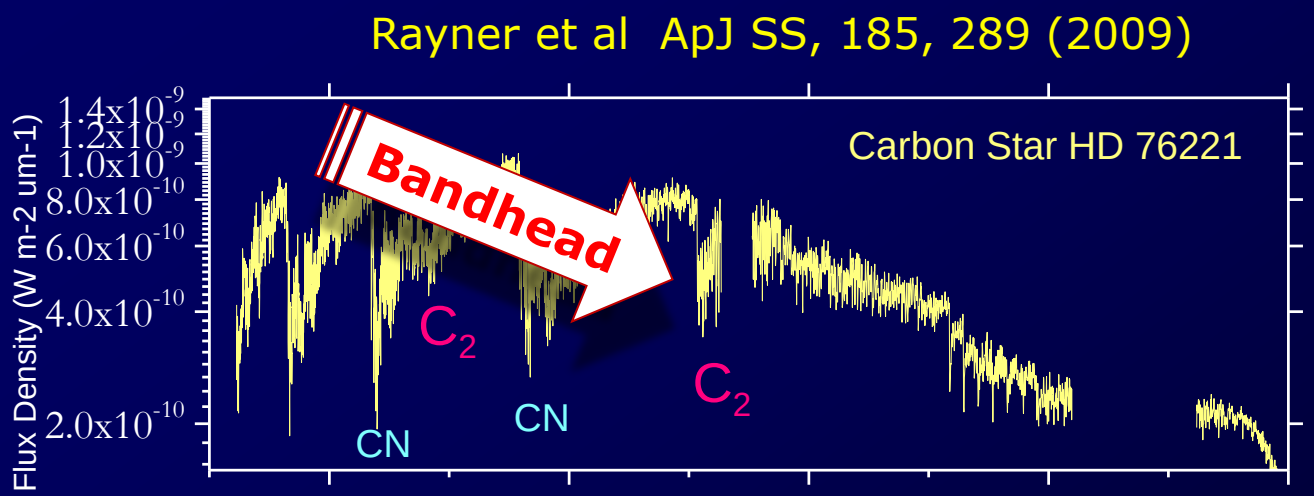
THE INFRARED TELESCOPE FACILITY (IRTF) SPECTRAL LIBRARY: COOL STARS

John T. Rayner[1], Michael C. Cushing[1,3], and William D. Vacca[2]
[1] Institute for Astronomy, University of Hawaií, 2680 Woodlawn Drive, Honolulu, HI 96822, USA; rayner@ifa.hawaii.edu, michael.cushing@gmail.com
[2] SOFIA-USRA, NASA Ames Research Center MS N211-3, Moffett Field, CA 94035, USA; wvacca@sofia.usra.edu
Received 2009 March 5; accepted 2009 September 3; published 2009 November 17

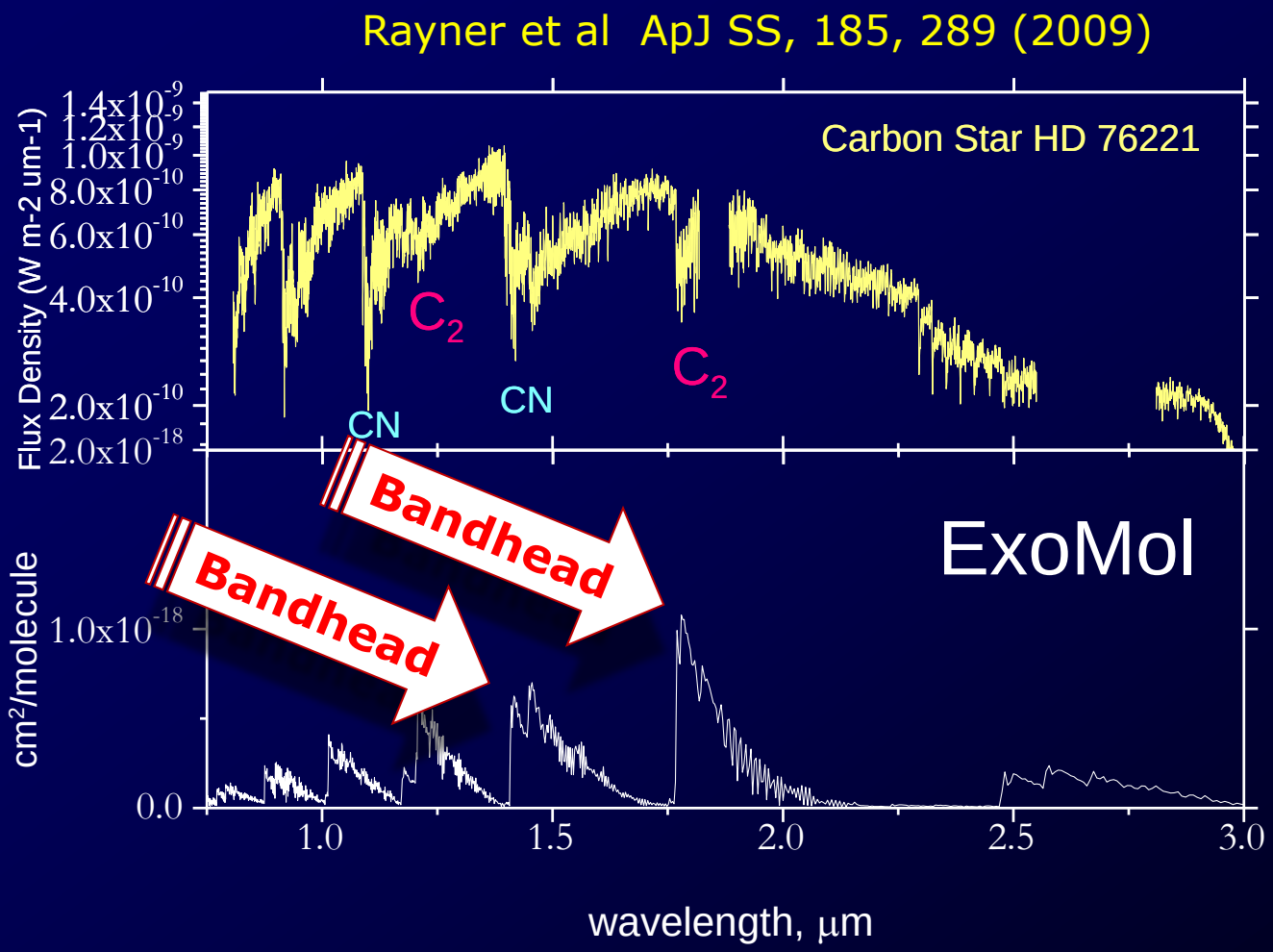
ABSTRACT

We present a 0.8–5 μm spectral library of 210 cool stars observed at a resolving power of $R \equiv \lambda/\Delta\lambda \sim 2000$ with the medium-resolution infrared spectrograph, SpeX, at the 3.0 m NASA Infrared Telescope Facility (IRTF) on Mauna Kea, Hawaii. The stars have well-established MK spectral classifications and are mostly restricted to near-solar metallicities. The sample not only contains the F, G, K, and M spectral types with luminosity classes between I and V, but also includes some AGB, carbon, and S stars. In contrast to some other spectral libraries, the continuum shape of the spectra is measured and preserved in the data reduction process. The spectra are


Bandhead
CaII
CO
ZrO
CN
C2
SiO
M0 IIIb
S4.5 Zr 2 Ti 4
C–N4.5 C2 4.5
HCN+C2H2
C–N 4.5 C2 5.5 MS 3
HCN
C7, 6e (N4)
Wavelength (μm)



Here is a particular example of HD 76221 with nice C_2 band-heads

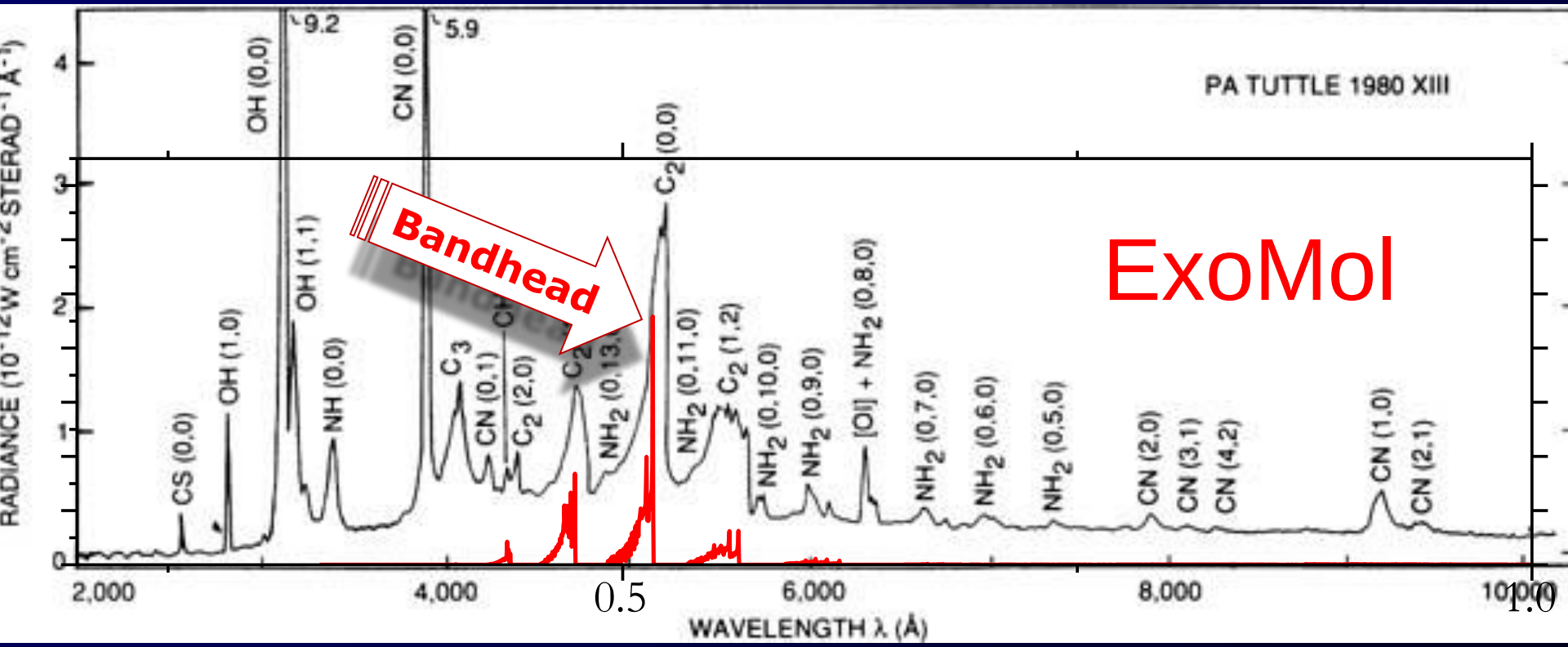


ExoMol's C_2 is shown on the lower display and compares very well

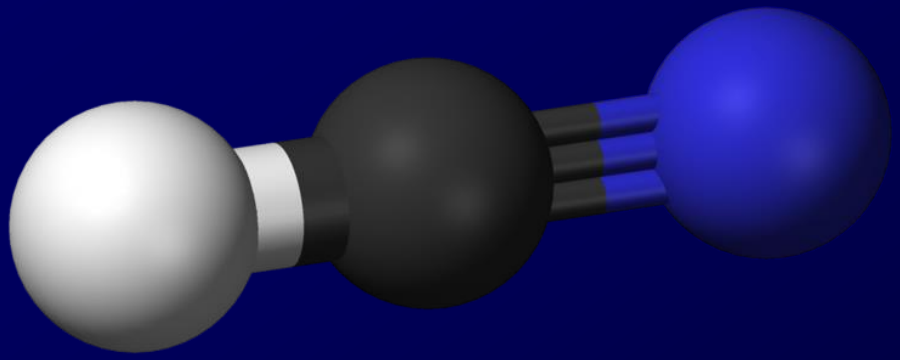
C_2 can be also cold

In comets

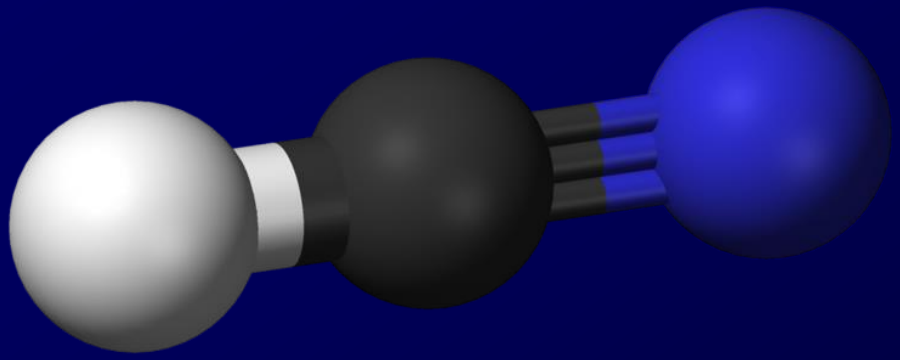
Here is the spectrum of Coma of Comet Tuttle



(Ignore the CN for now, which is also available at ExoMol)

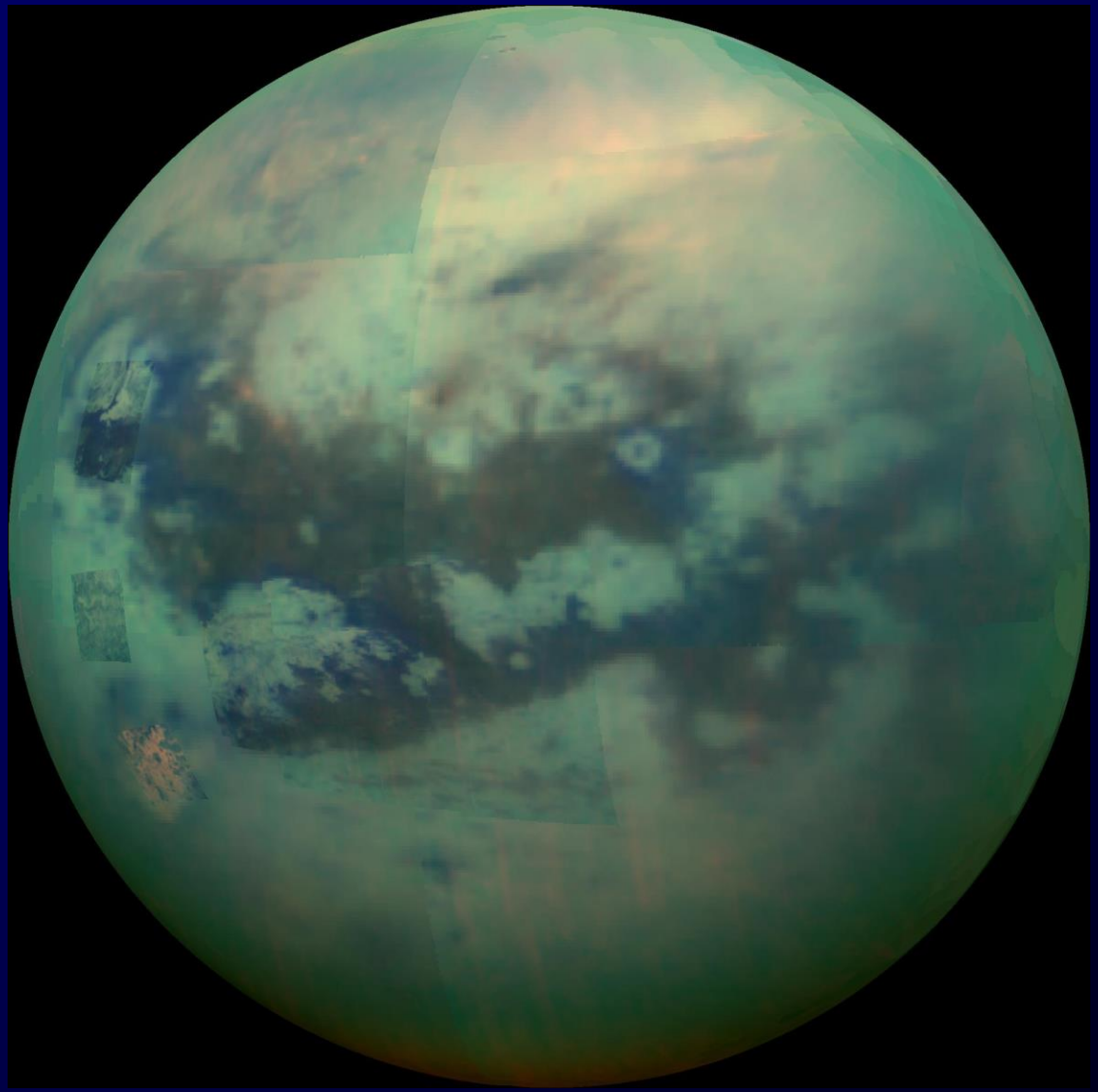


Hydrogen cyanide

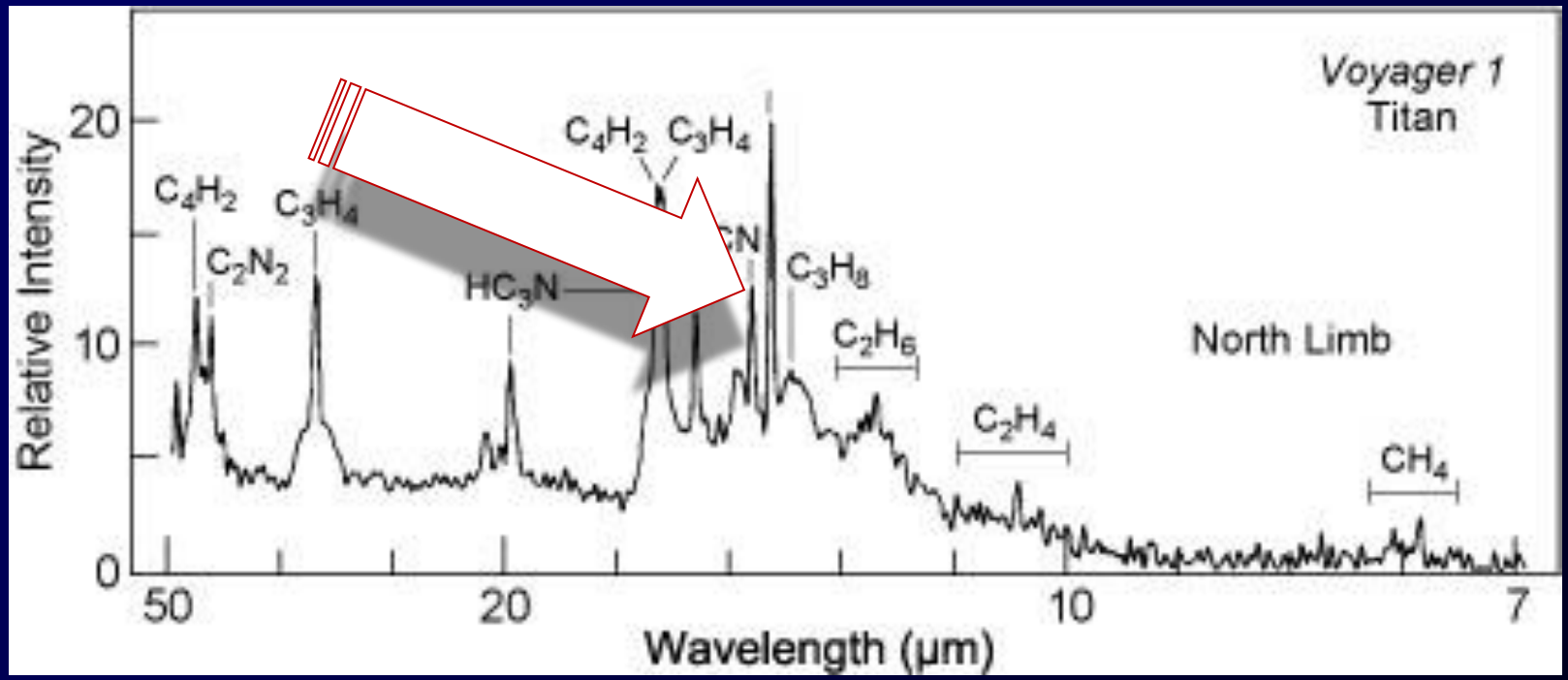


HCN

has been seen in our Solar system

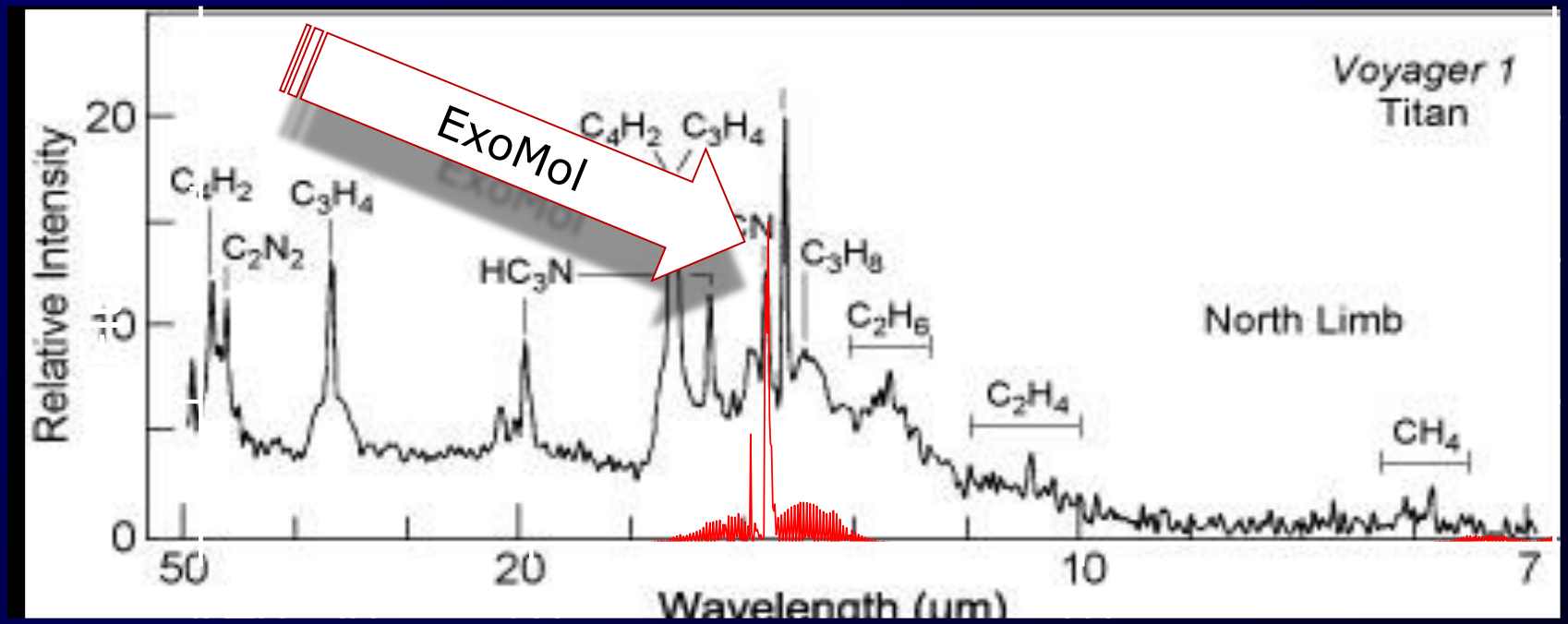


HCN on Titan



ExoMol's has produced HCN
(by Emma Barton)

Here is our HCN compared to Voyager 1's spectrum



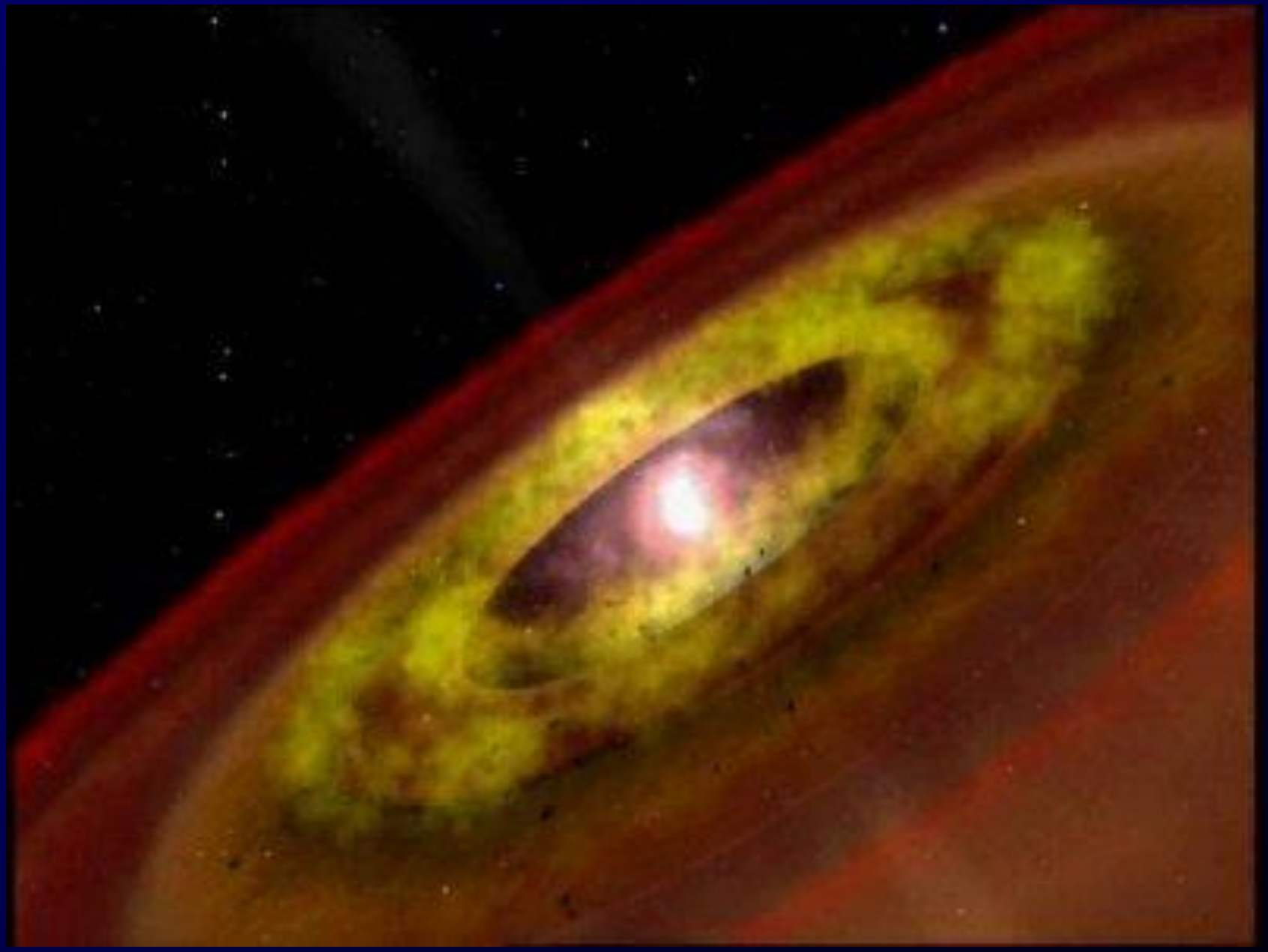
Which contains half a billion lines

and represents it rather well

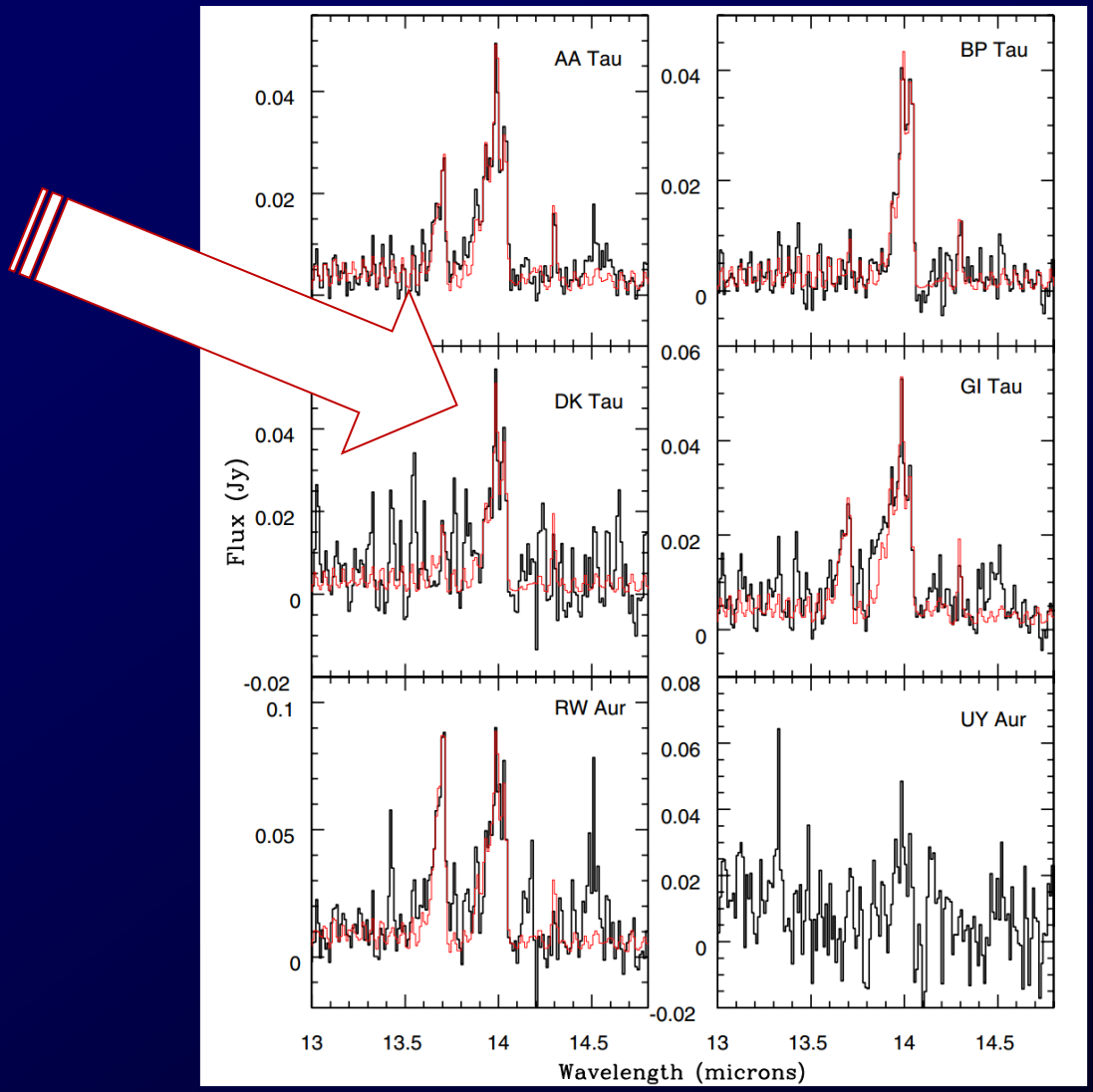
HCN

has been seen on stars

for example T Tauri



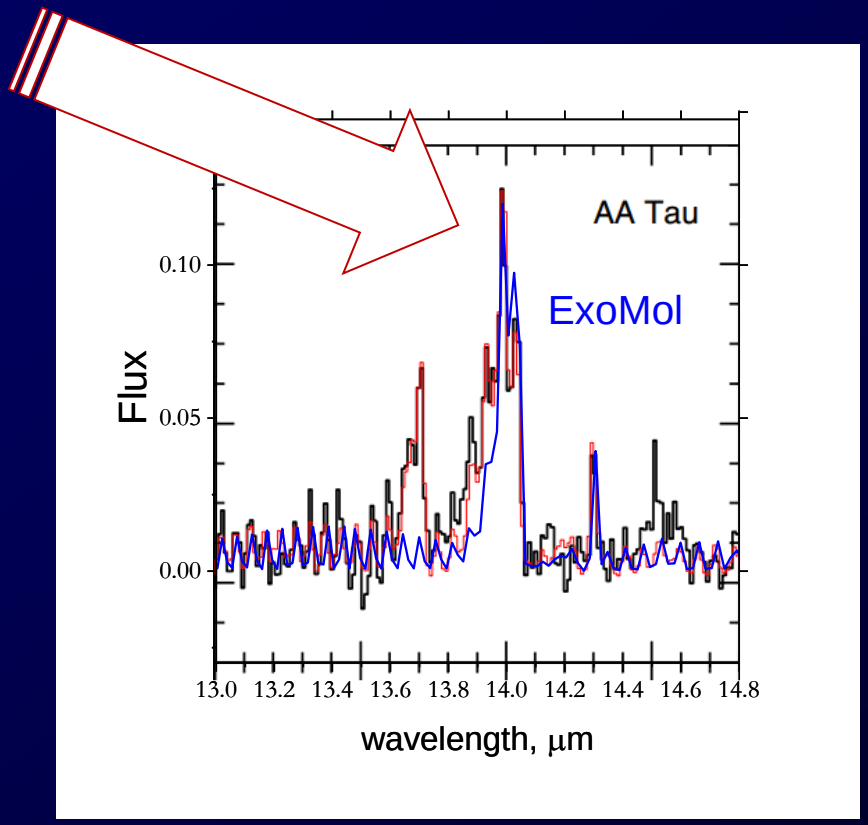
Organic molecules: Inner Disks of T Tauri Stars



Carr & Najita, ApJ, 733, 102 (2011)

ExoMol’s HCN

Here is a zoom-in with ExoMol's HCN

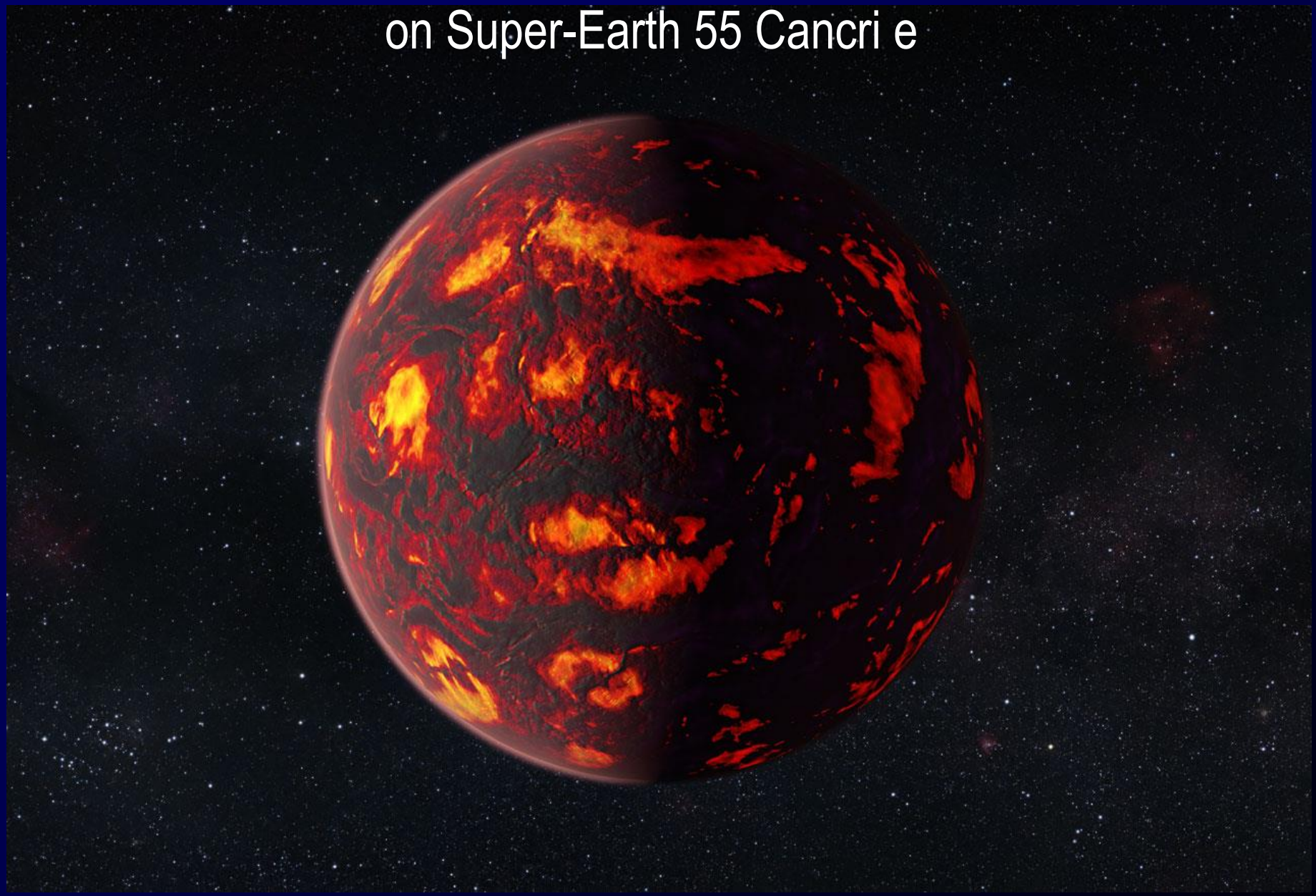


HCN: Inner Disks of T Tauri Stars

Carr & Najita, ApJ, 733, 102 (2011)

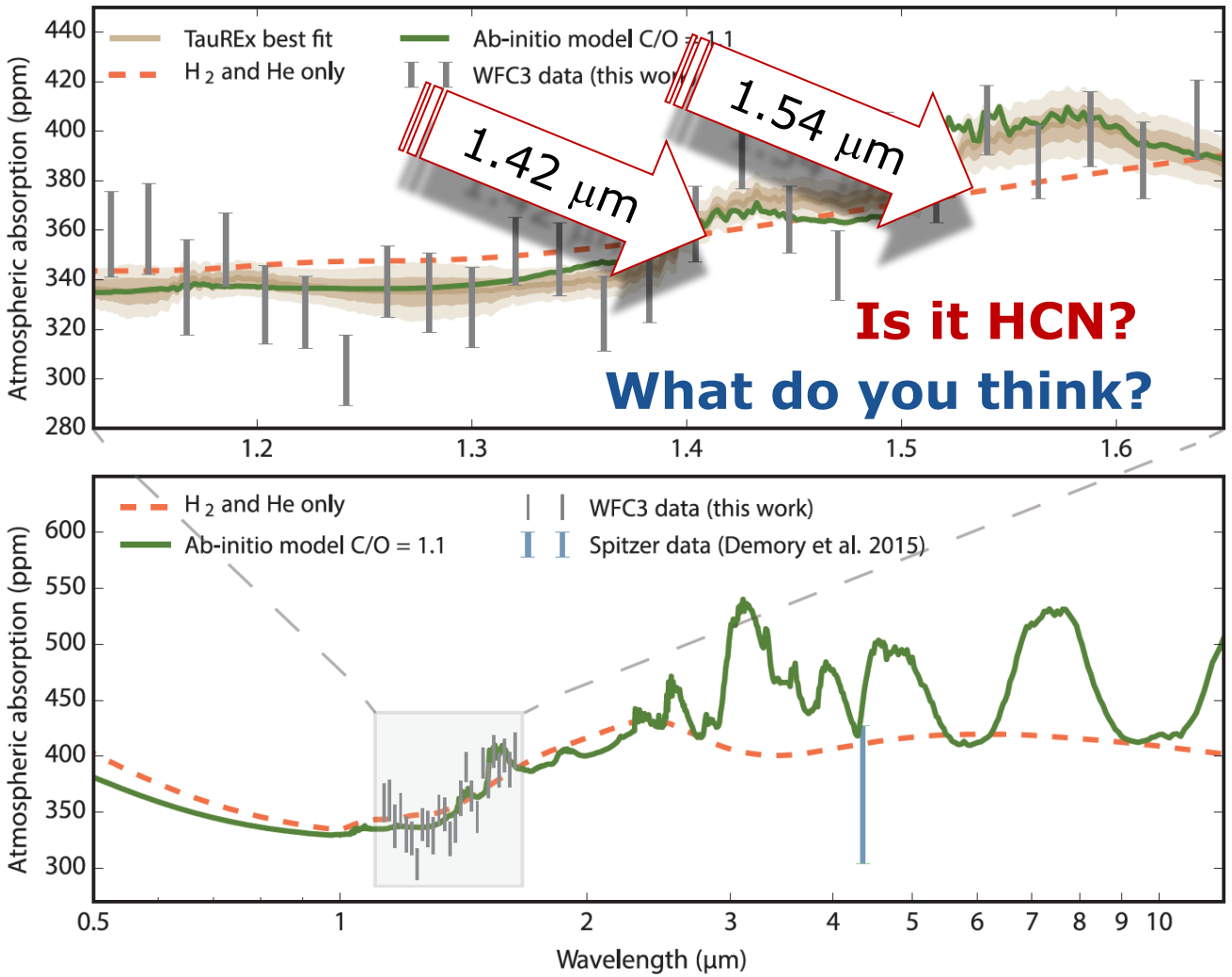
HCN on Exoplanets?

Maybe


on Super-Earth 55 Cancri e

Lets look at the transit of
the Super-Earth 55 Cancri e
with Hubble’s WFC3

Look at these two “features”



A. Tsiaras ApJ (2016)

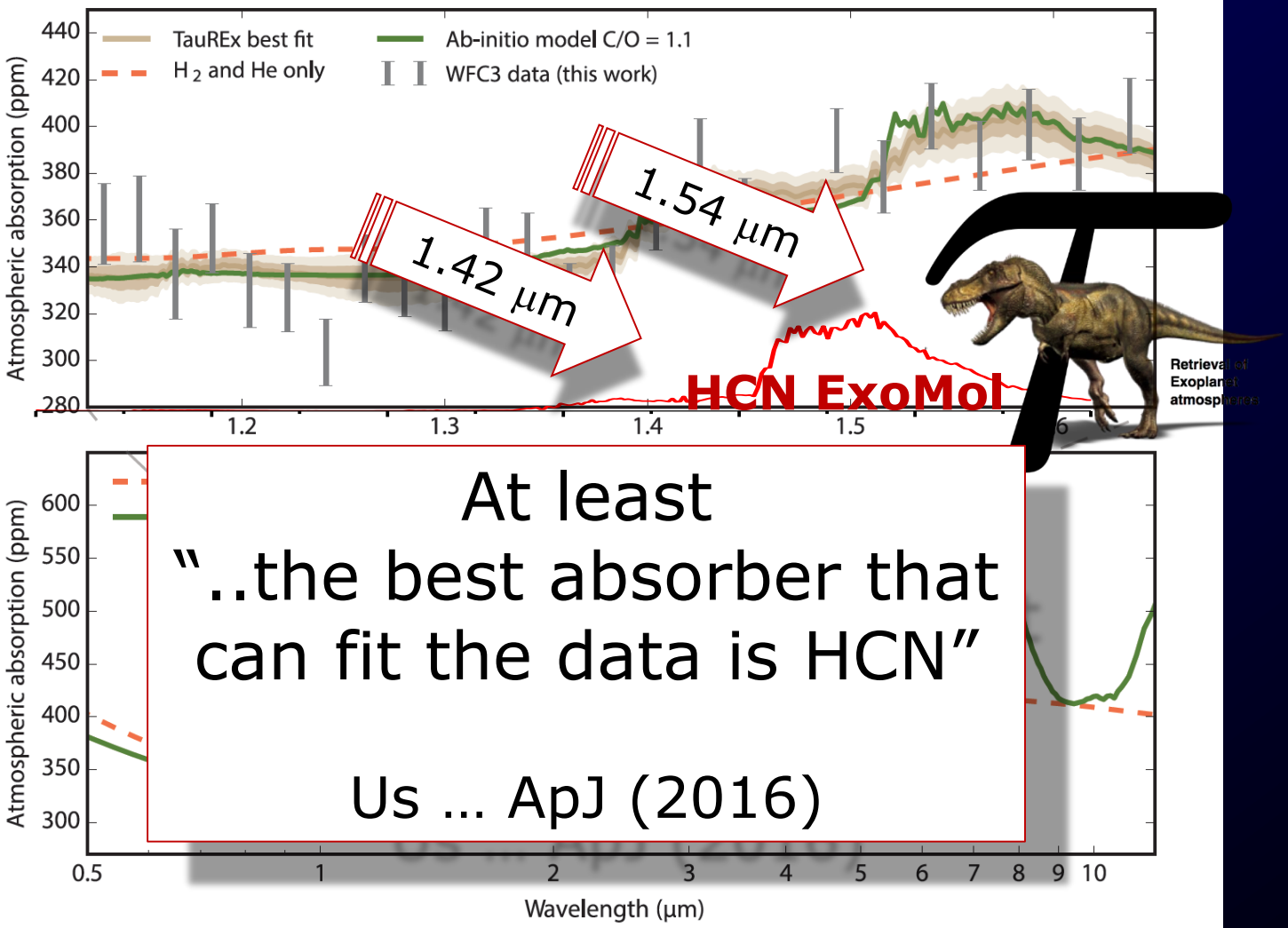
This is what we think (modelling with tau-Rex)

55 Cancri e

WFC3 HST

A. Tsiaras ApJ (2016)

HCN: Why not? (modelling with tau-Rex)

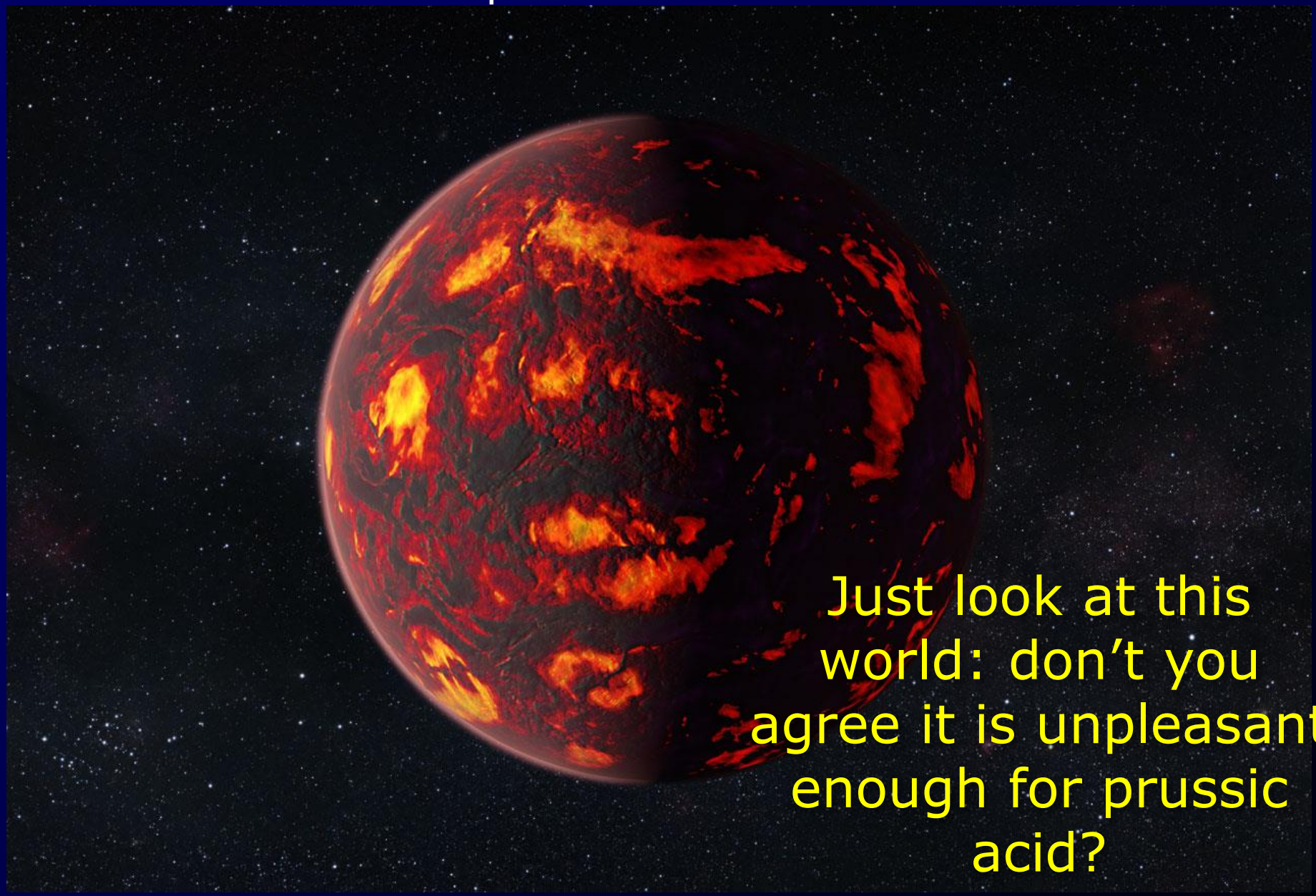


55 Cancri e

WFC3 HST

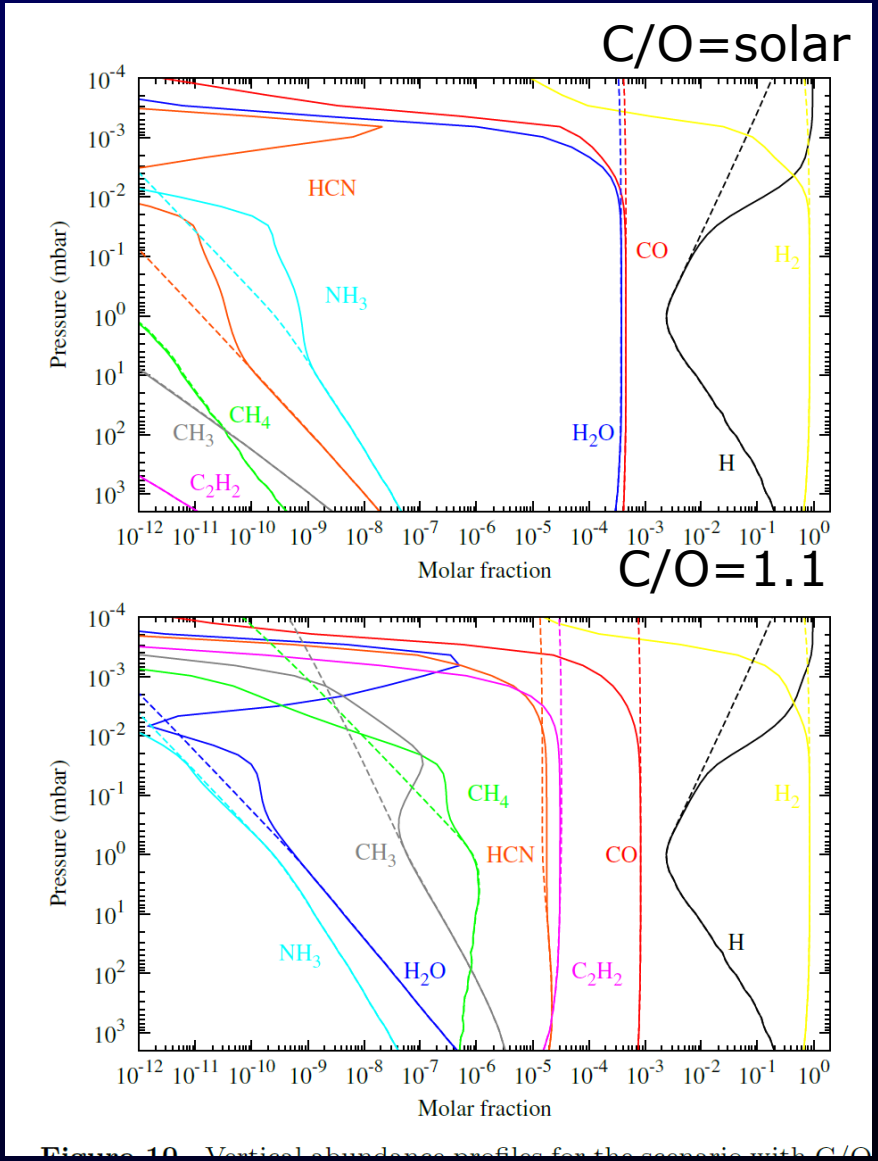
A. Tsiaras ApJ (2016)

Super-Earth 55 Cancri e



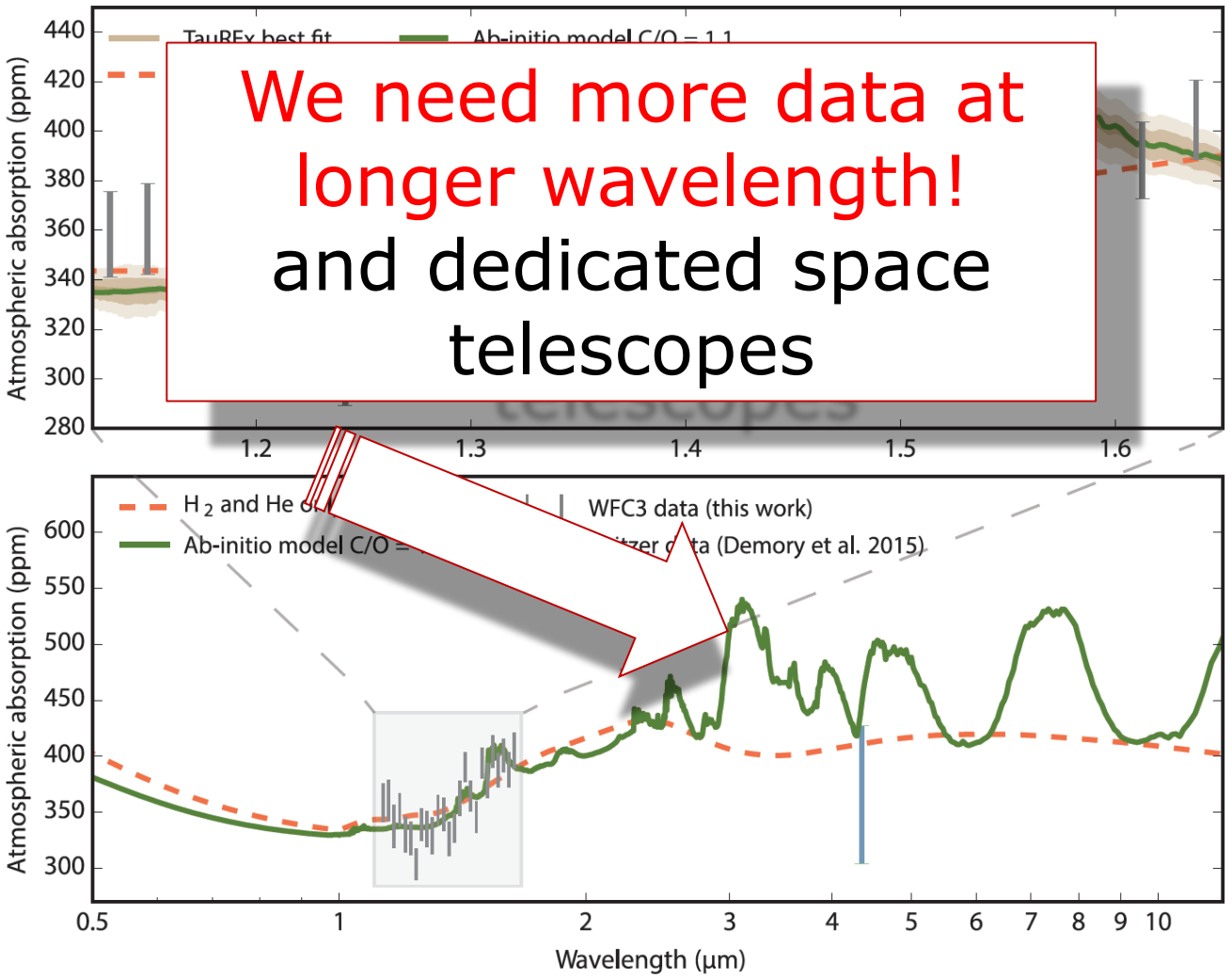
Also support by chemical model by O. Venot

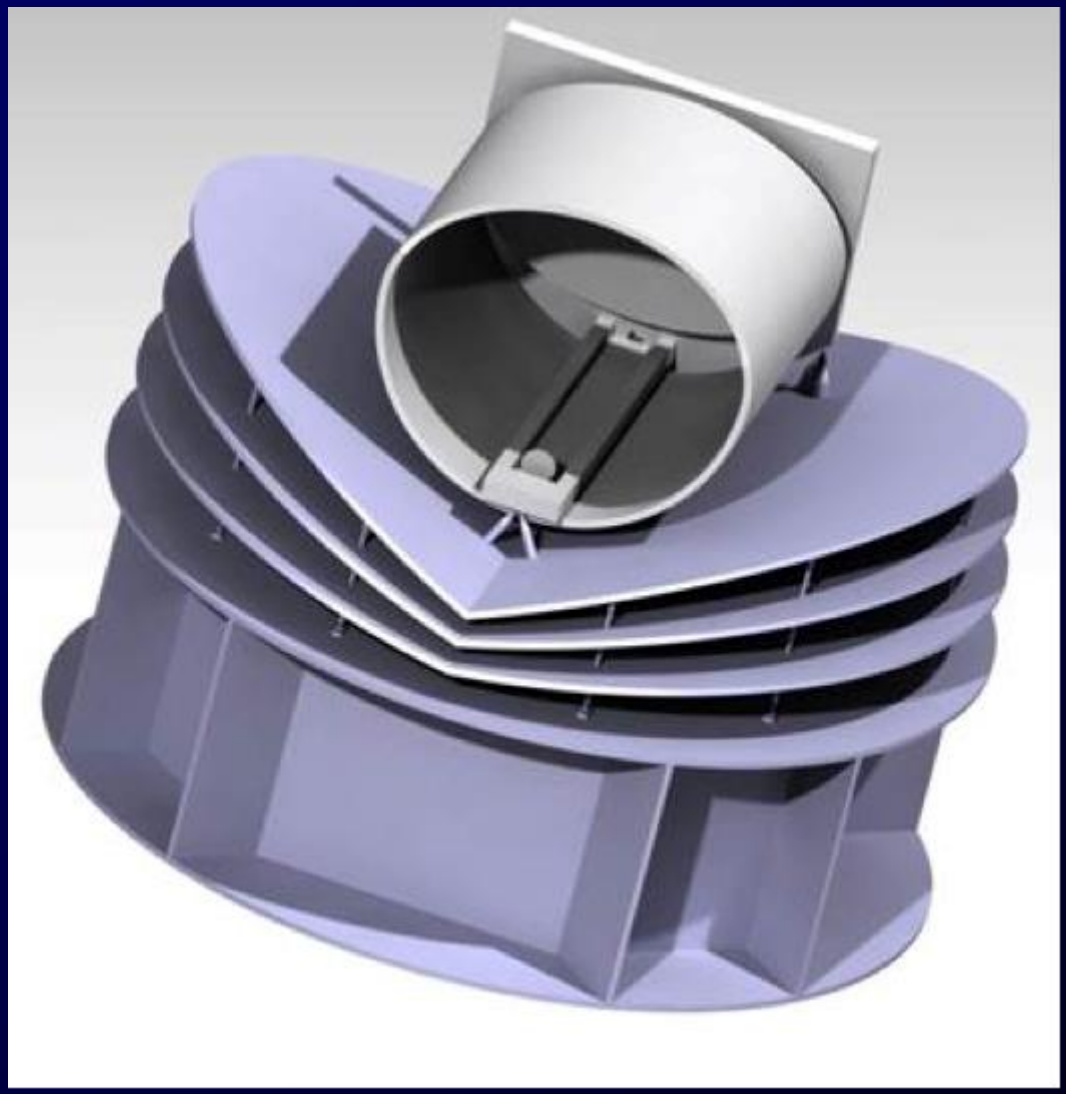
The model included not only HCN: also H_2O, CO, NO, H_2S, CO_2, CH_4, NH_3

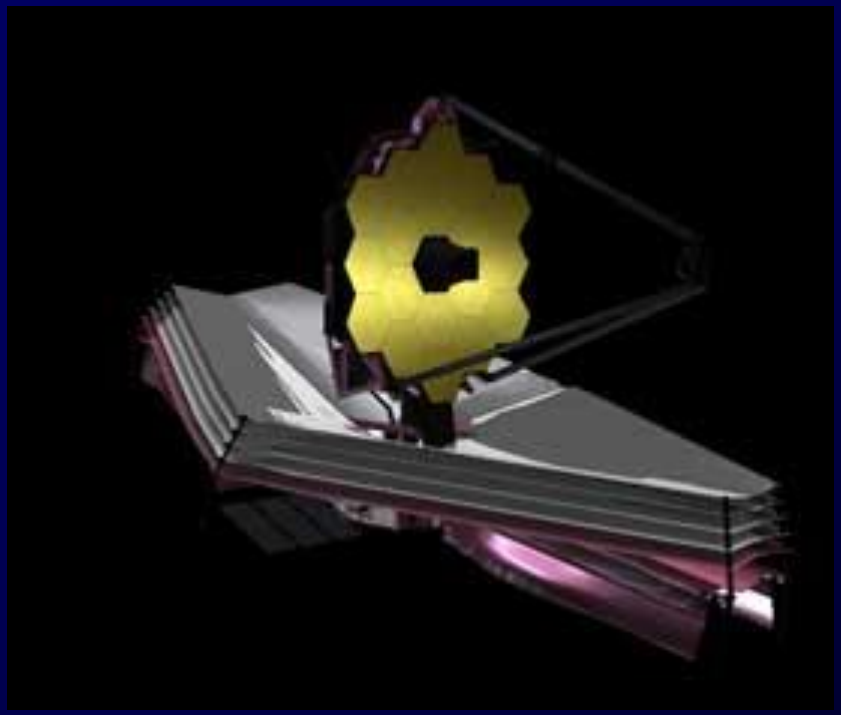


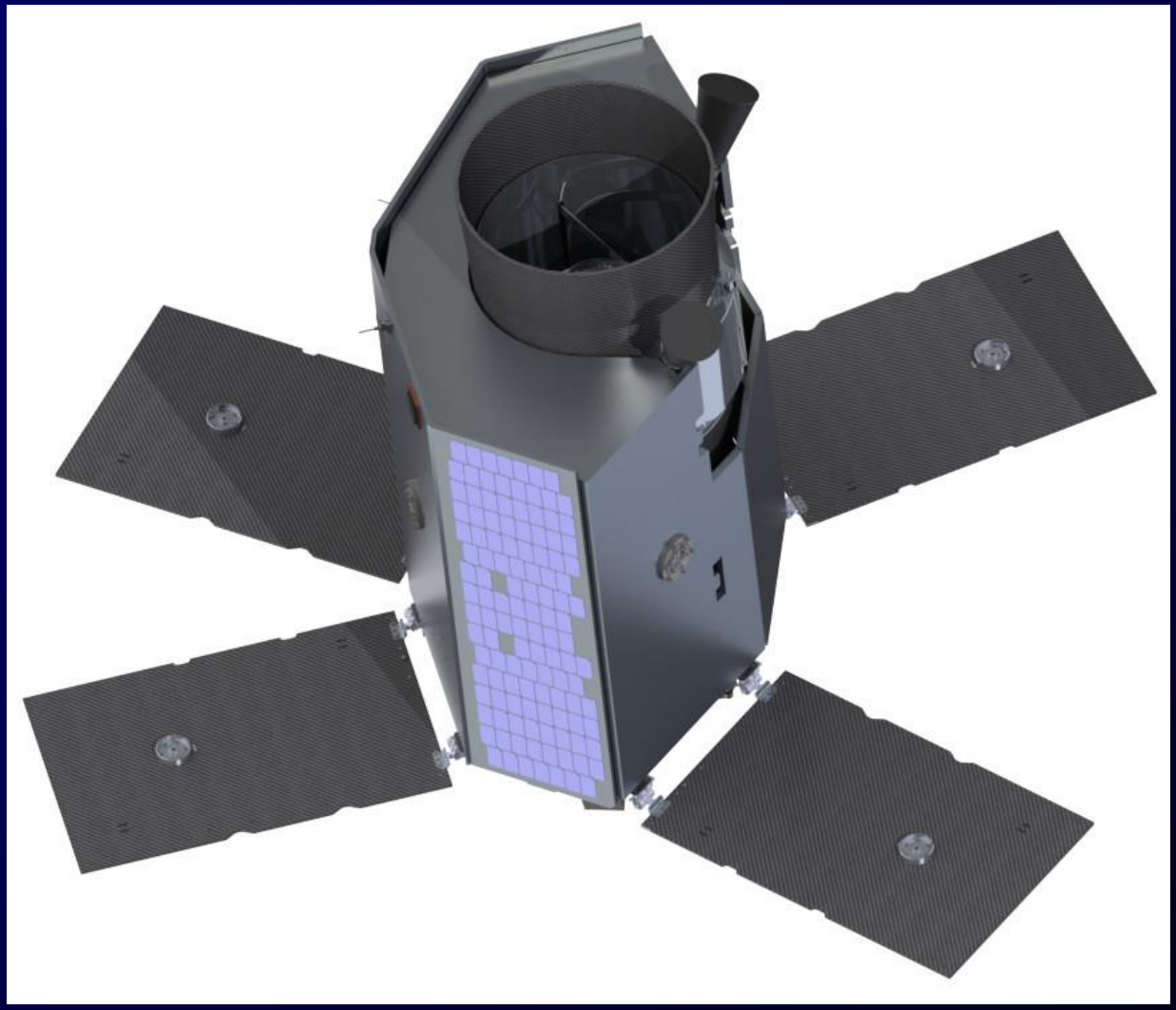
A. Tsiaras ApJ (2016)

However ts is only indication of HCN



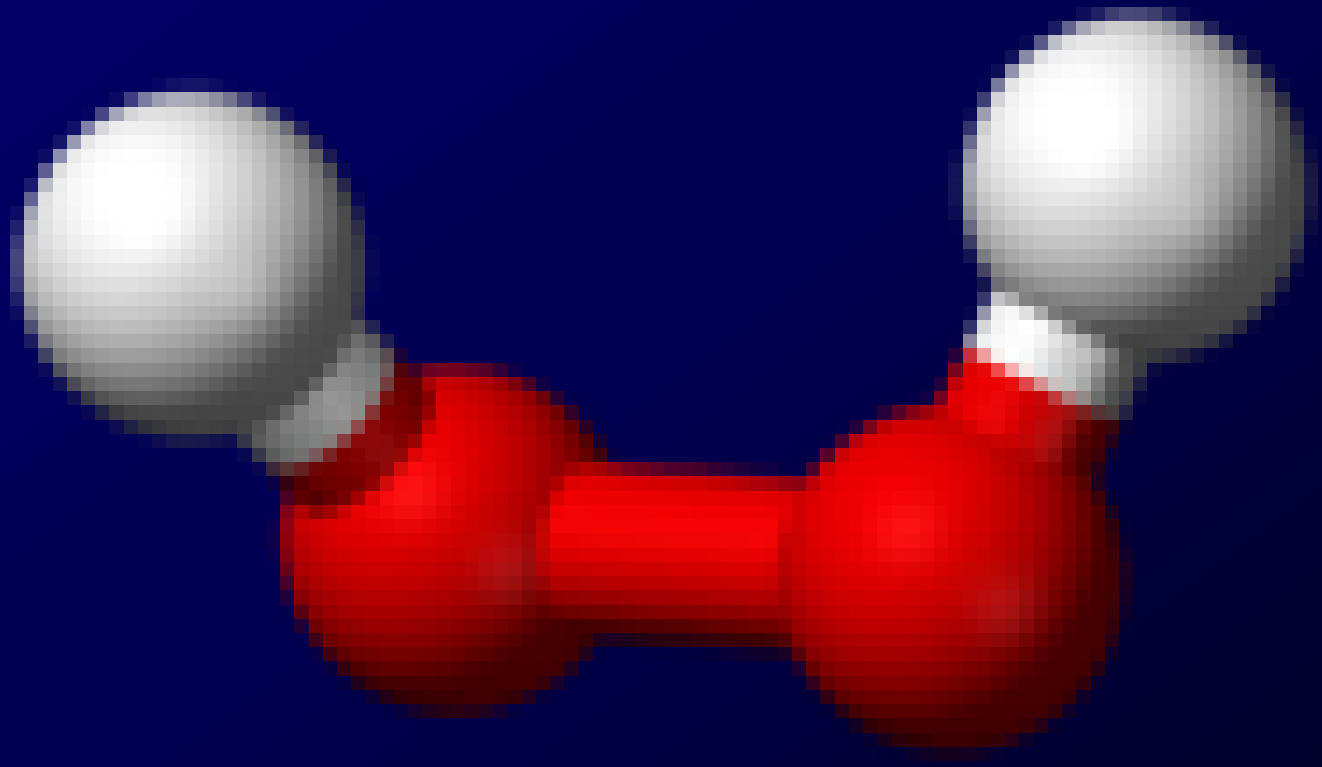






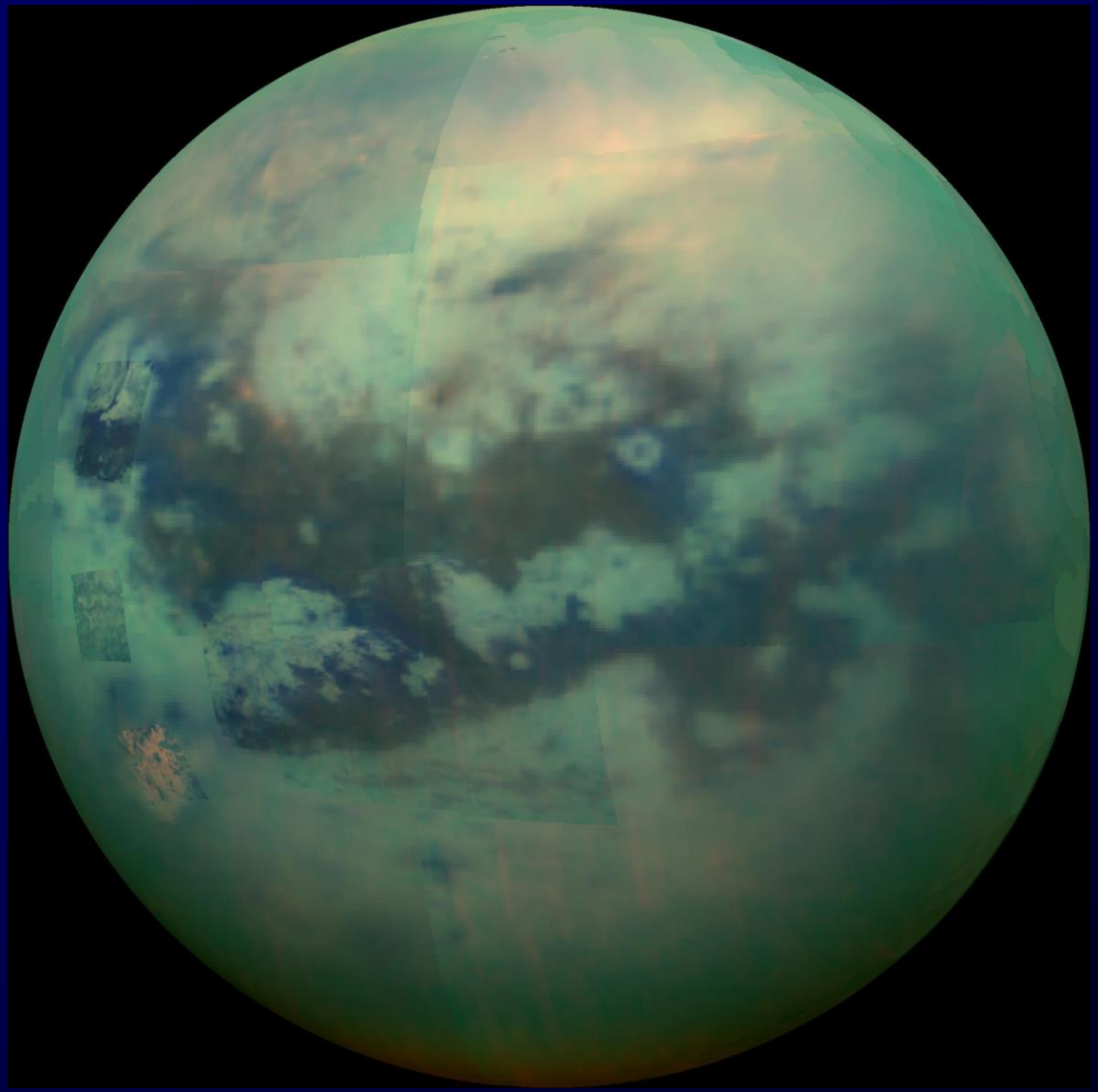
Hydrogen peroxide

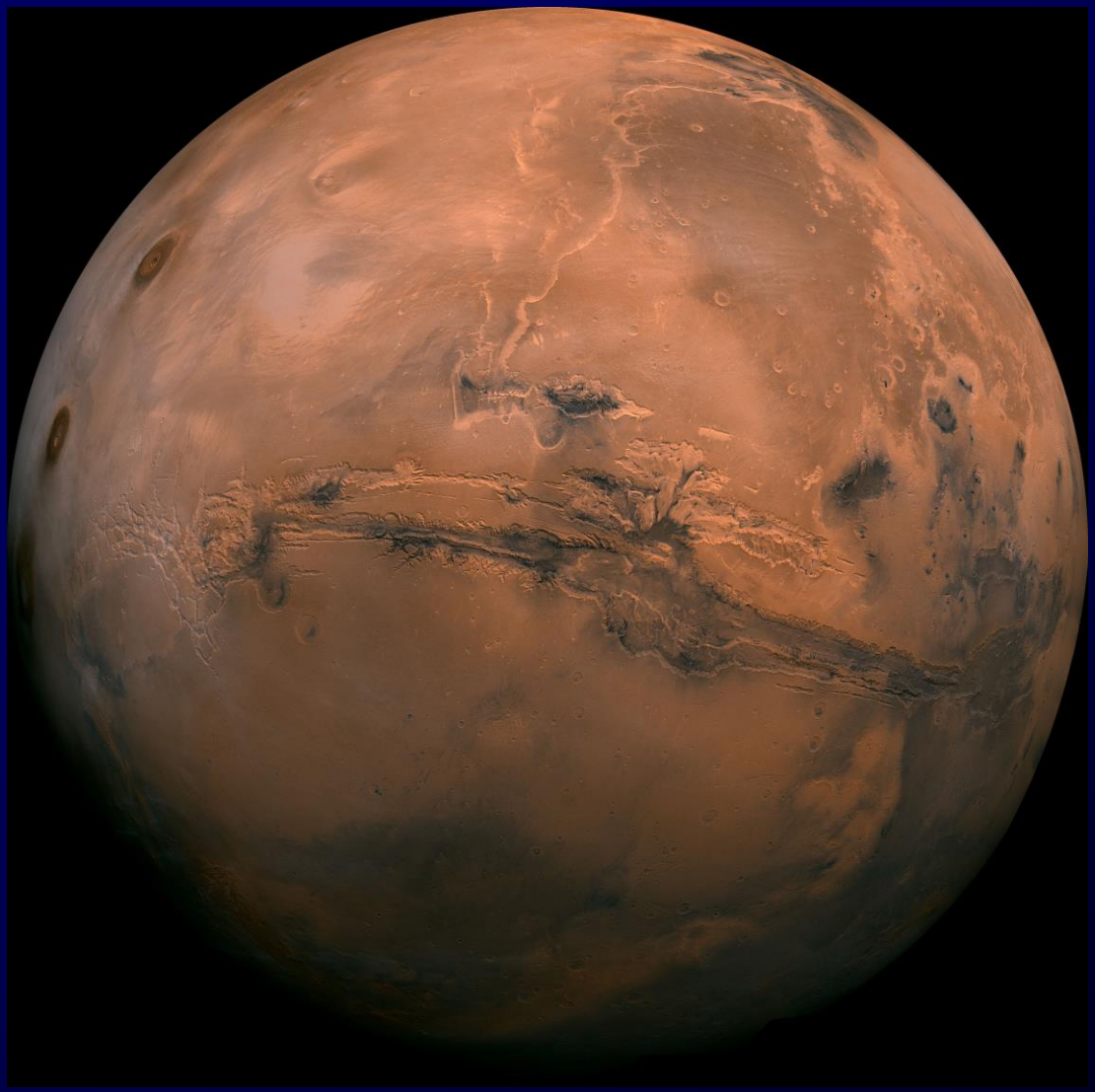
H_2O_2



Hydrogen peroxide
H_2O_2

has been seen in Solar system as well

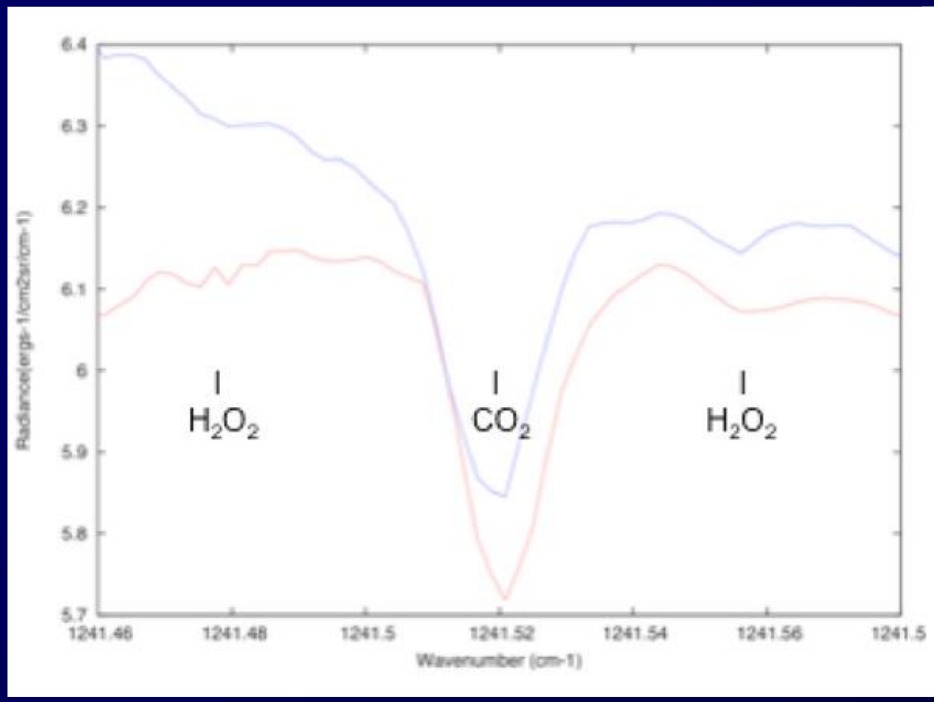


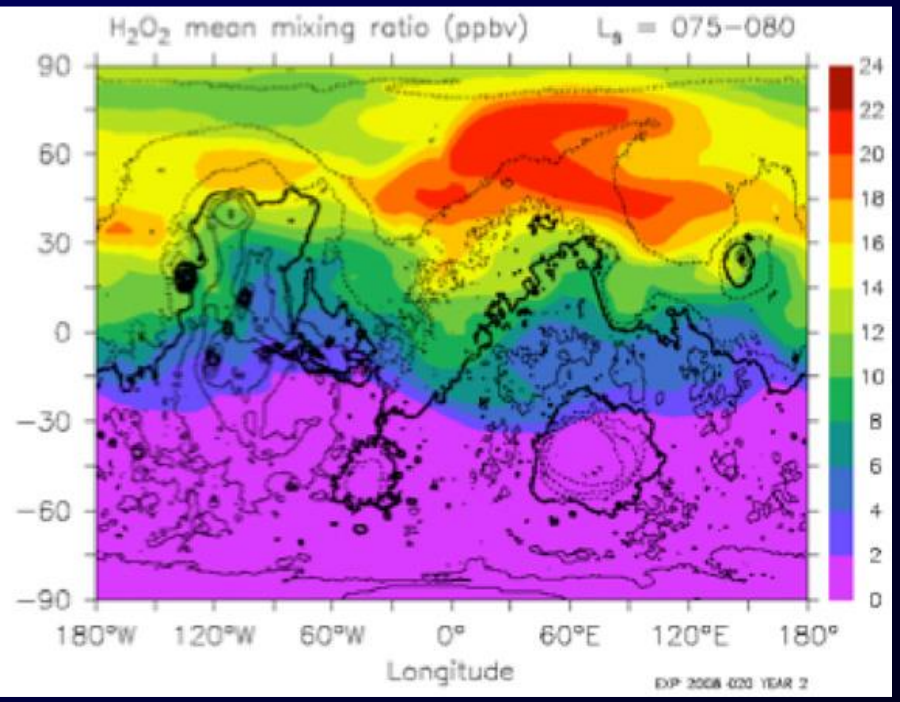


Hydrogen peroxide
H_2O_2

On Mars, where it is used to monitor the seasonal changes of the atmosphere

H_2O_2: Martial seasonal changes





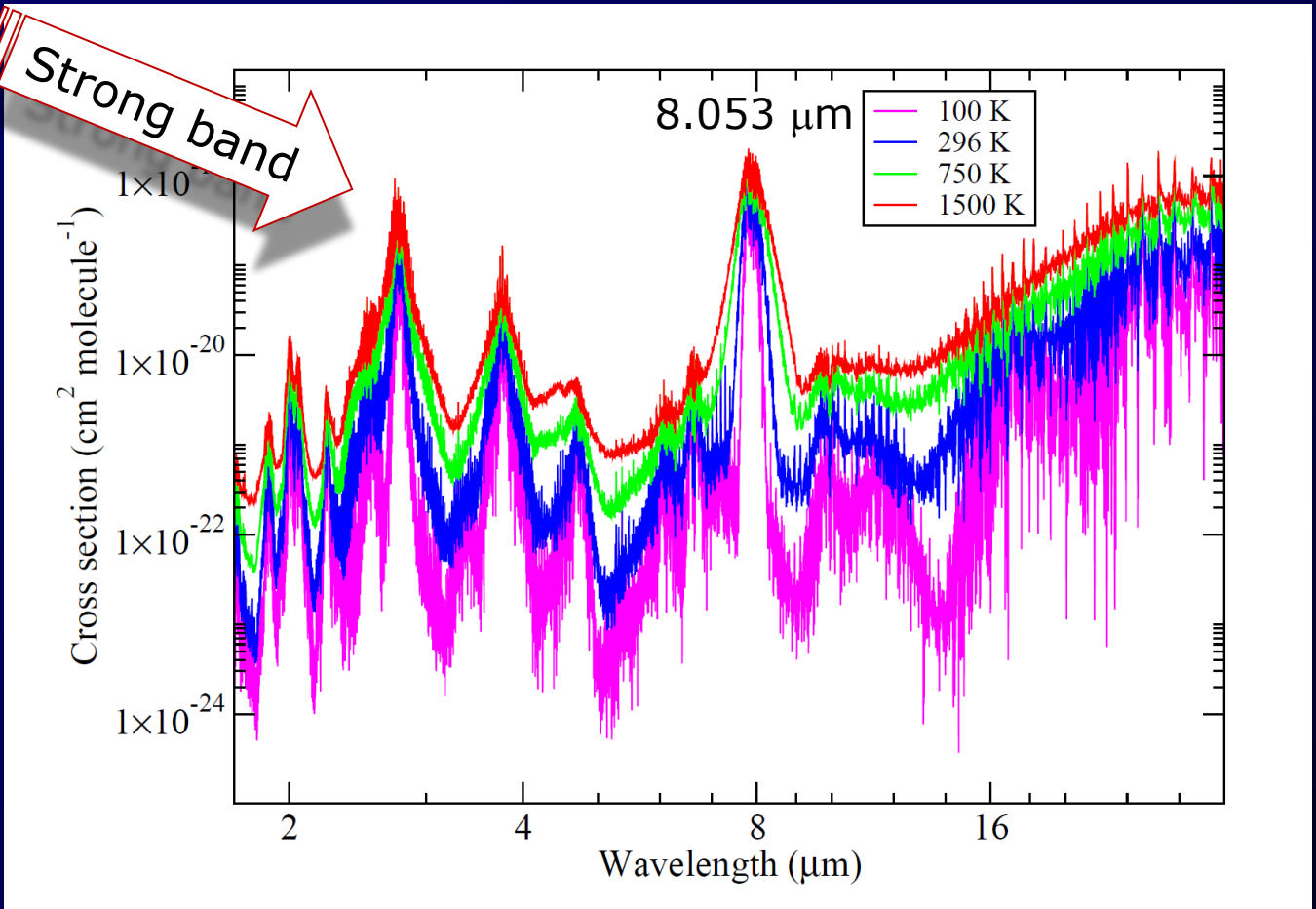
Well, just a few lines of
H_2O_2 at least

Encrenaz Planetary and Space Science 68 (2012) 3–17

ExoMol's H_2O_2 by Ahmed Al-Refeie is hot!

It is new and designed to model hot (800 K) environments

ExoMol: hot H_2O_2, containing these monitoring features at 8 μm



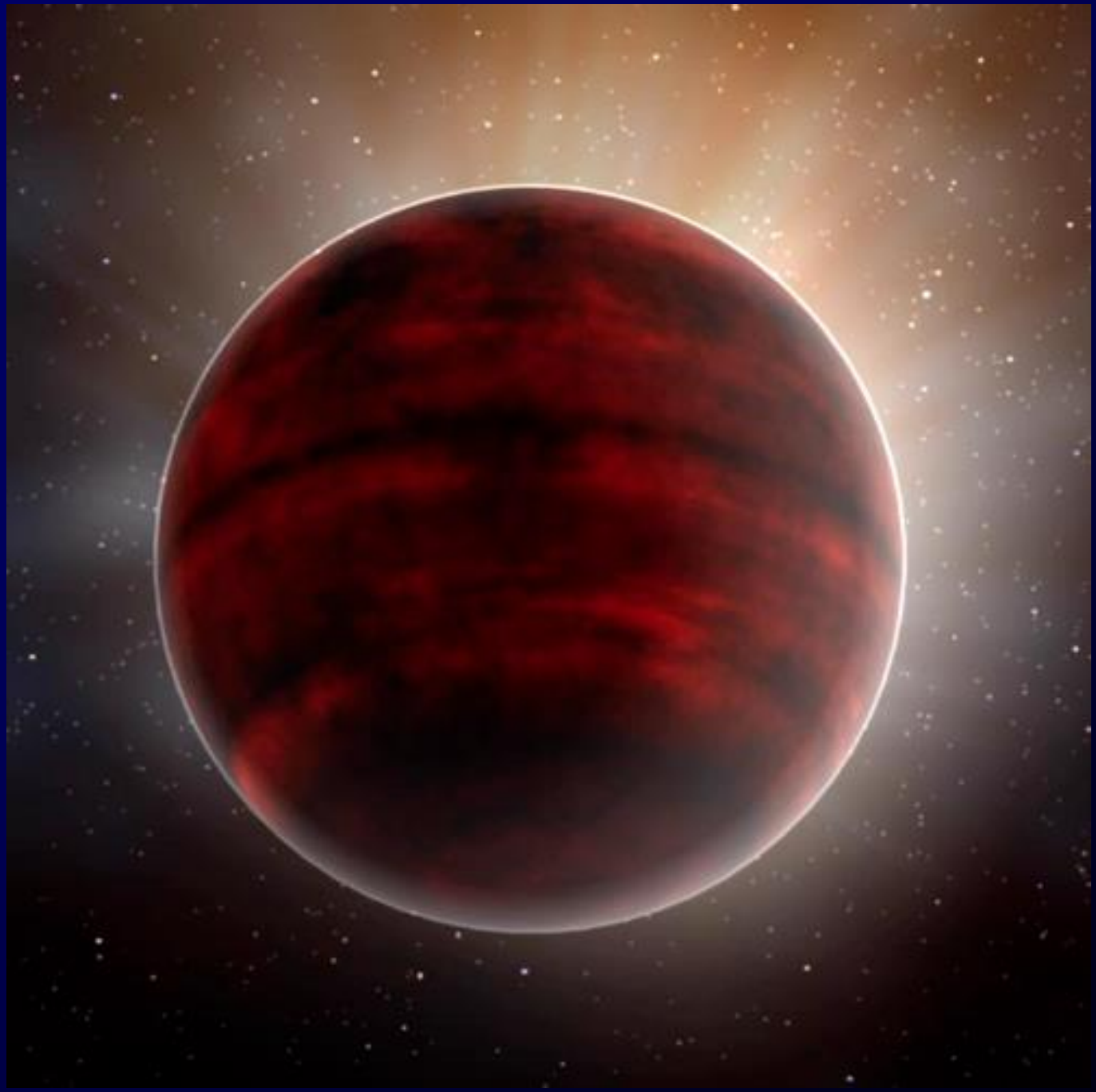
It contains 20 billion lines

Going hotter

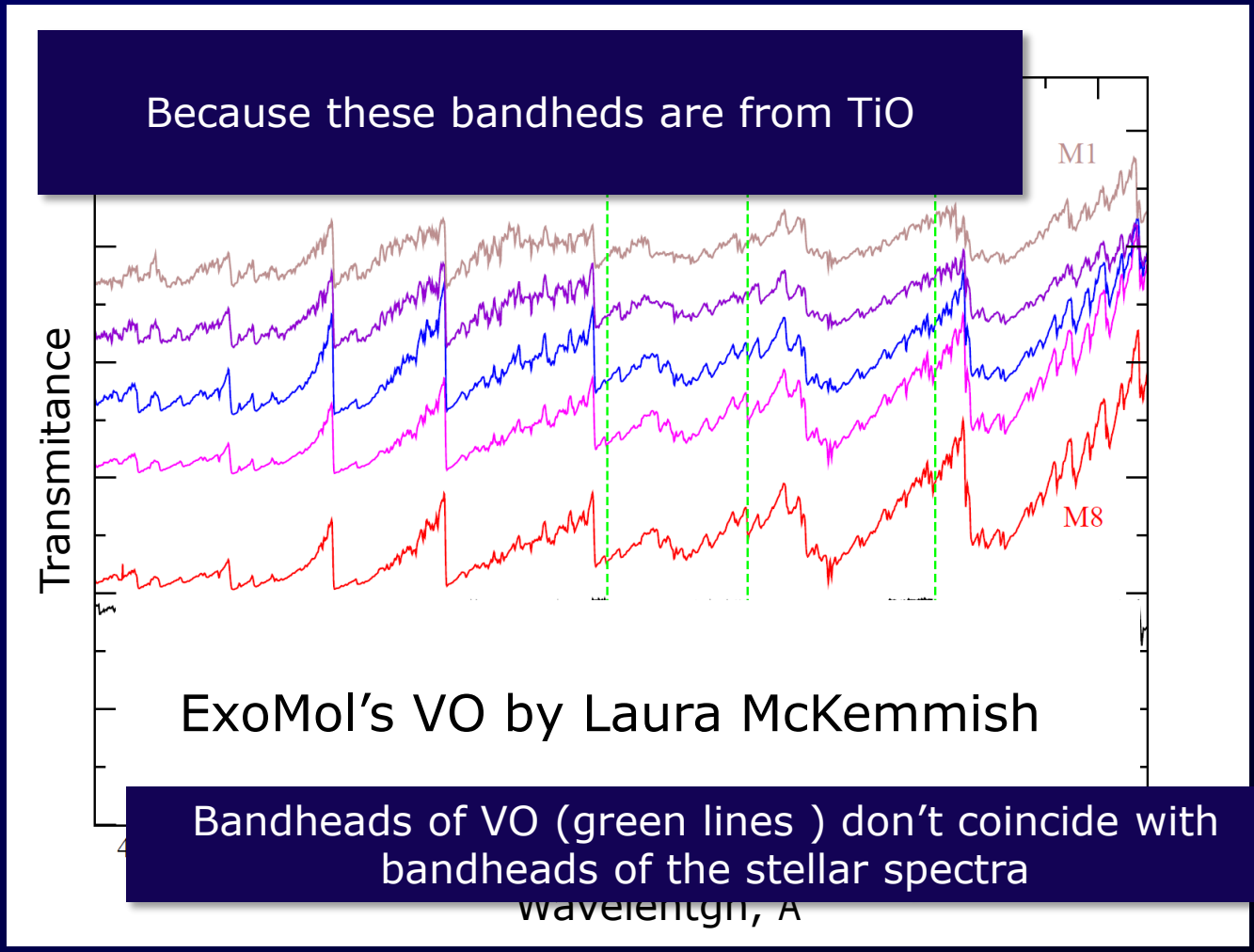
Vanadium oxide (VO)

and TiO

VO/TiO
are found a lot in
M-type stars spectra



Here is an example of M dwarfs high resolution spectra



HD199799, M1

HD163990, M6Svar

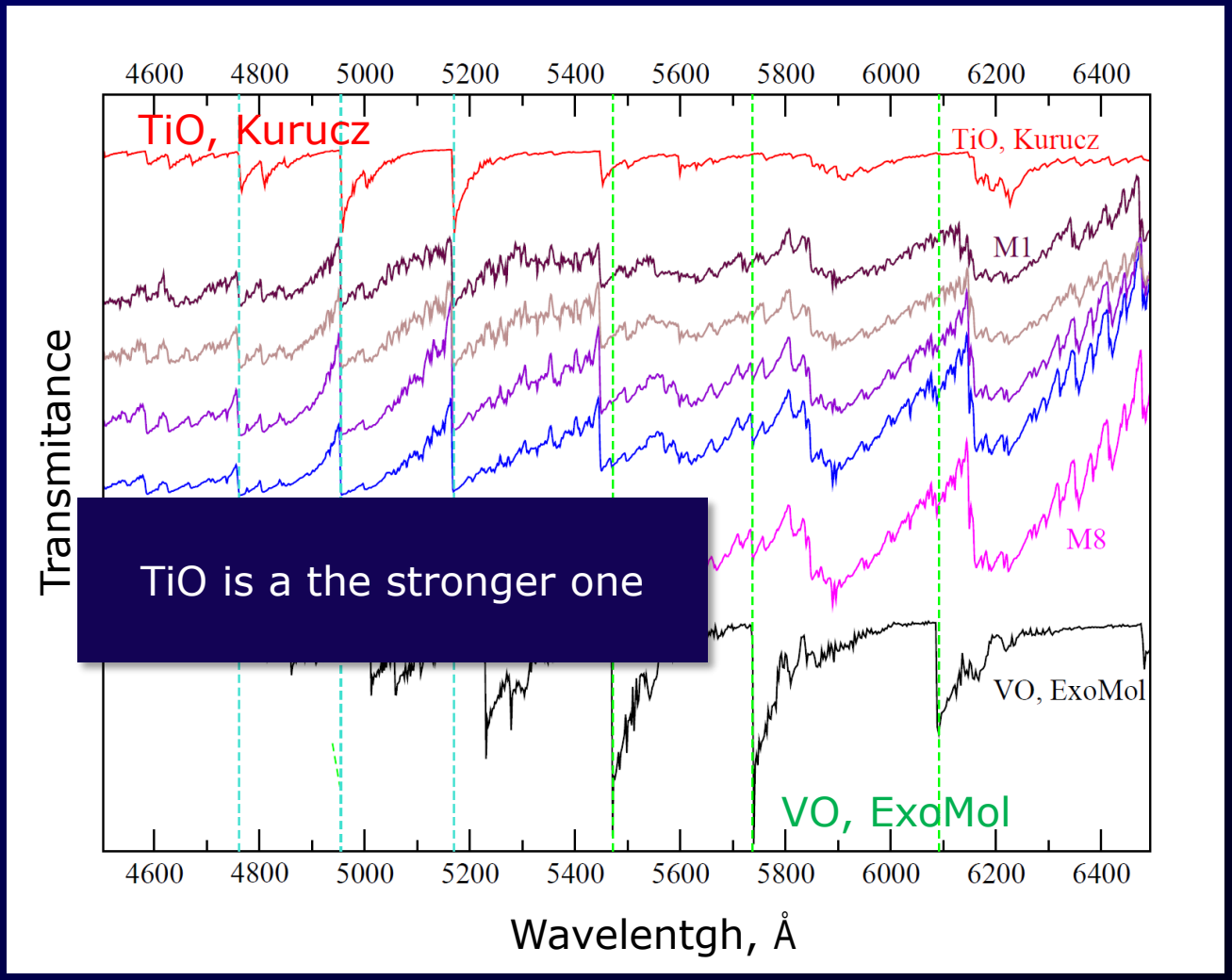
HD207076, M7 III

HD126327, M7.5 I

HD113285, M8 III

Falcón-Barroso et al. (2011)

Here it is overlaid with synthetic TiO spectrum



TiO is a the stronger one

HD199799, M1

HD163990, M6Svar

HD207076, M7 III

HD126327, M7.5 I

HD113285, M8 III

VO/TiO
Can be detected on Exoplanets?

Apparently yes, learning from this conference

WASP-121b?

Aluminum Oxide

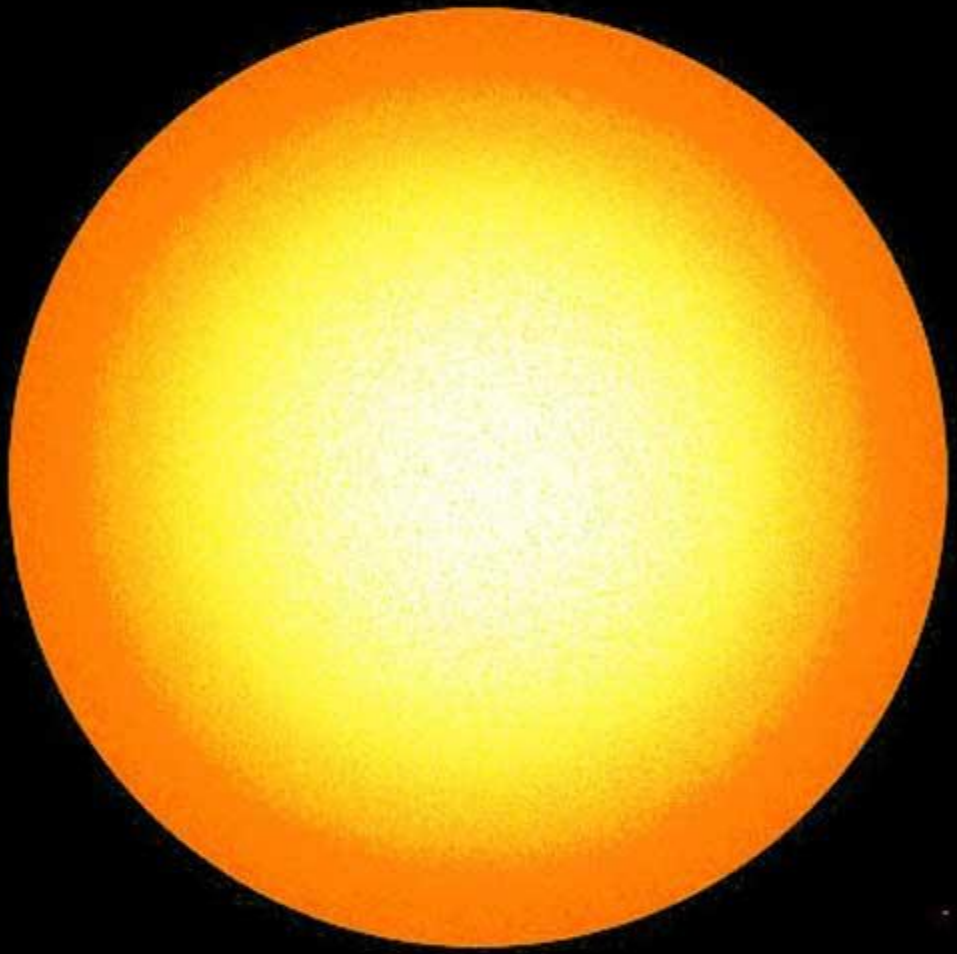
Not very often featured by the exoplanetary models

Is it because of T?

Aluminum Oxide

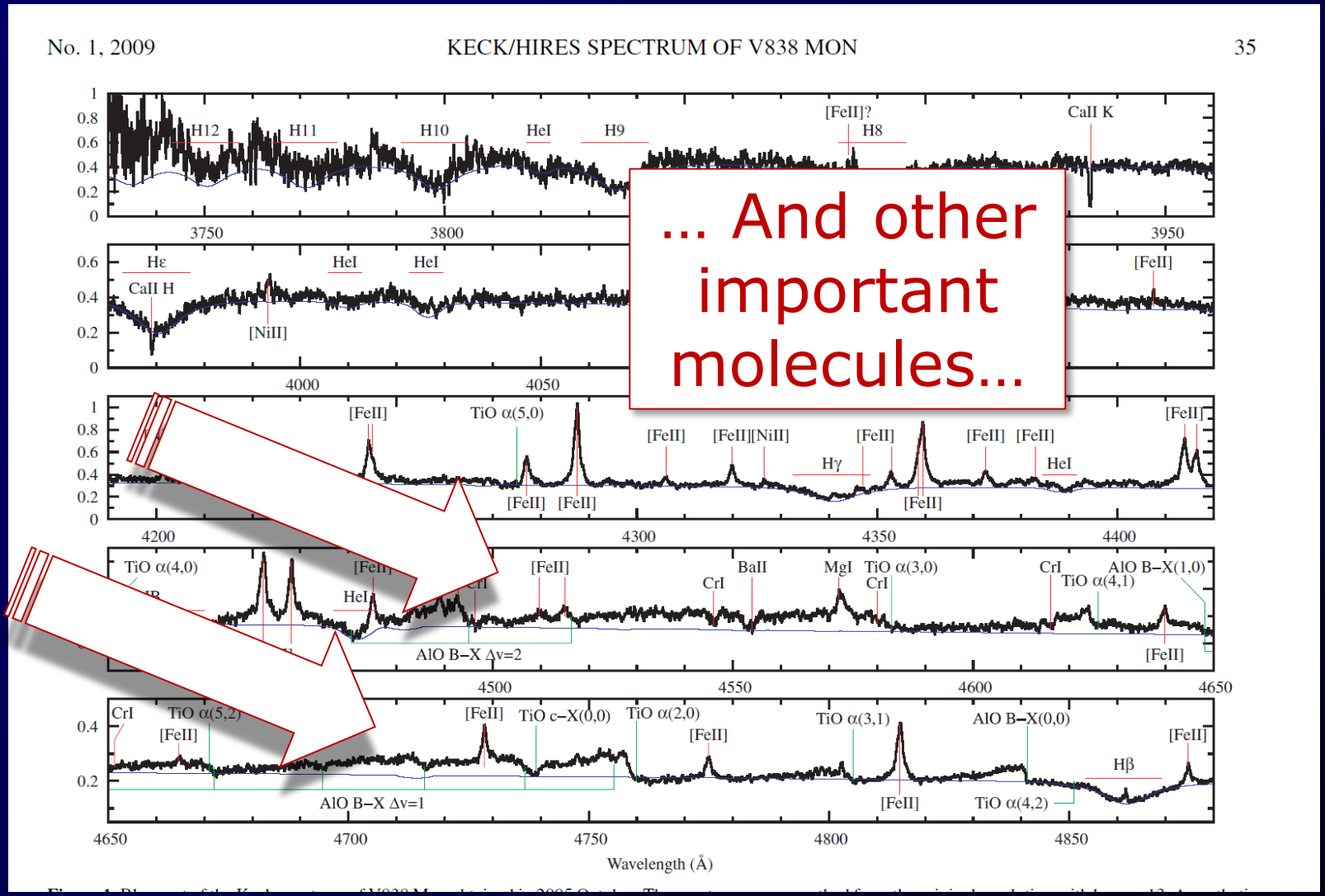
in red supergiant

VY Canis Majoris



Sun

Here is an example of AlO in red supergiant VY Canis Majoris



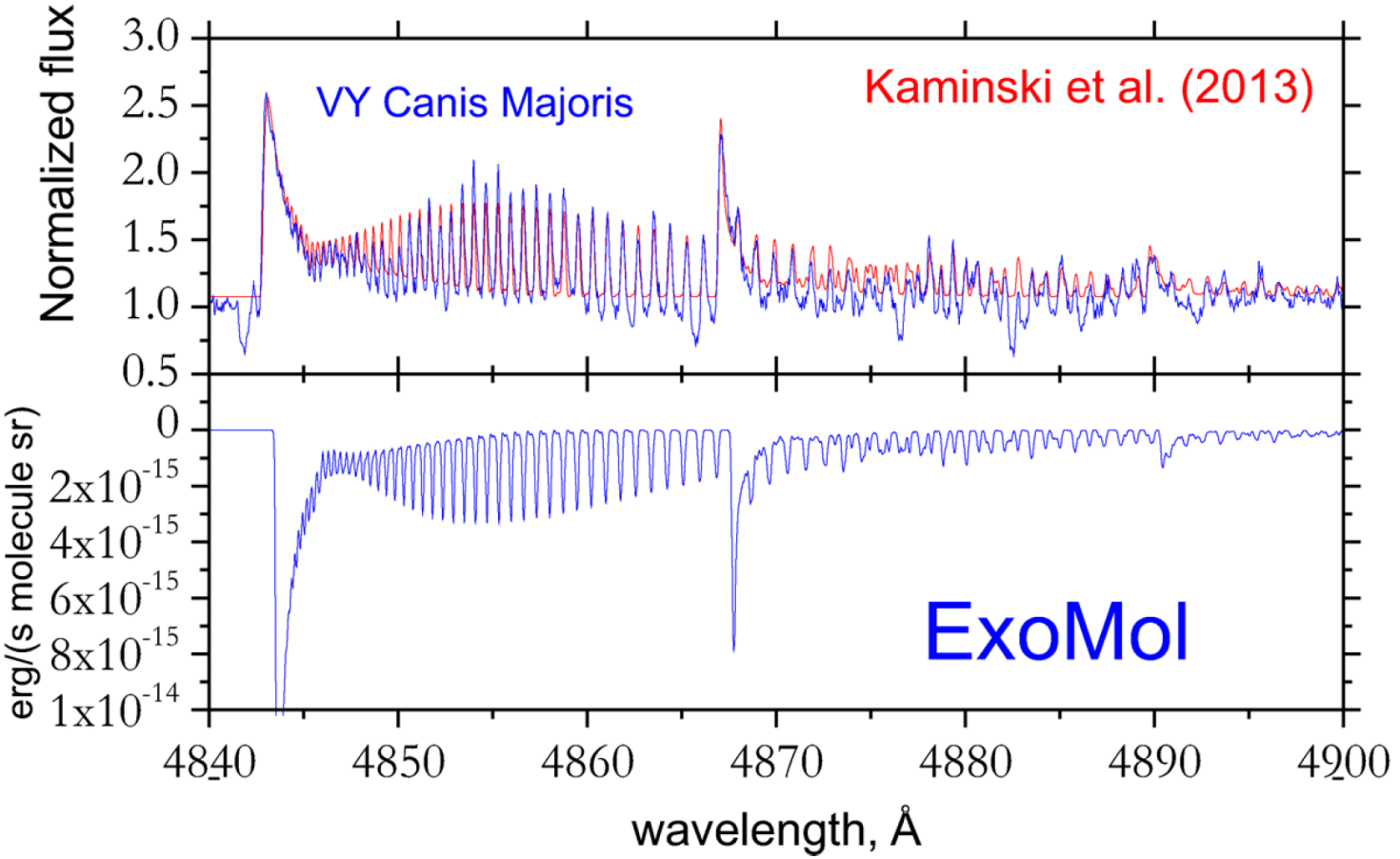
… And other important molecules…

Kaminski, Schmidt & Menten (2013)

AlO

ExoMol’s line list (Andrei Patrascu) is pretty good even for high Temperatures

AlO was seen in red supergiant VY Canis Majoris

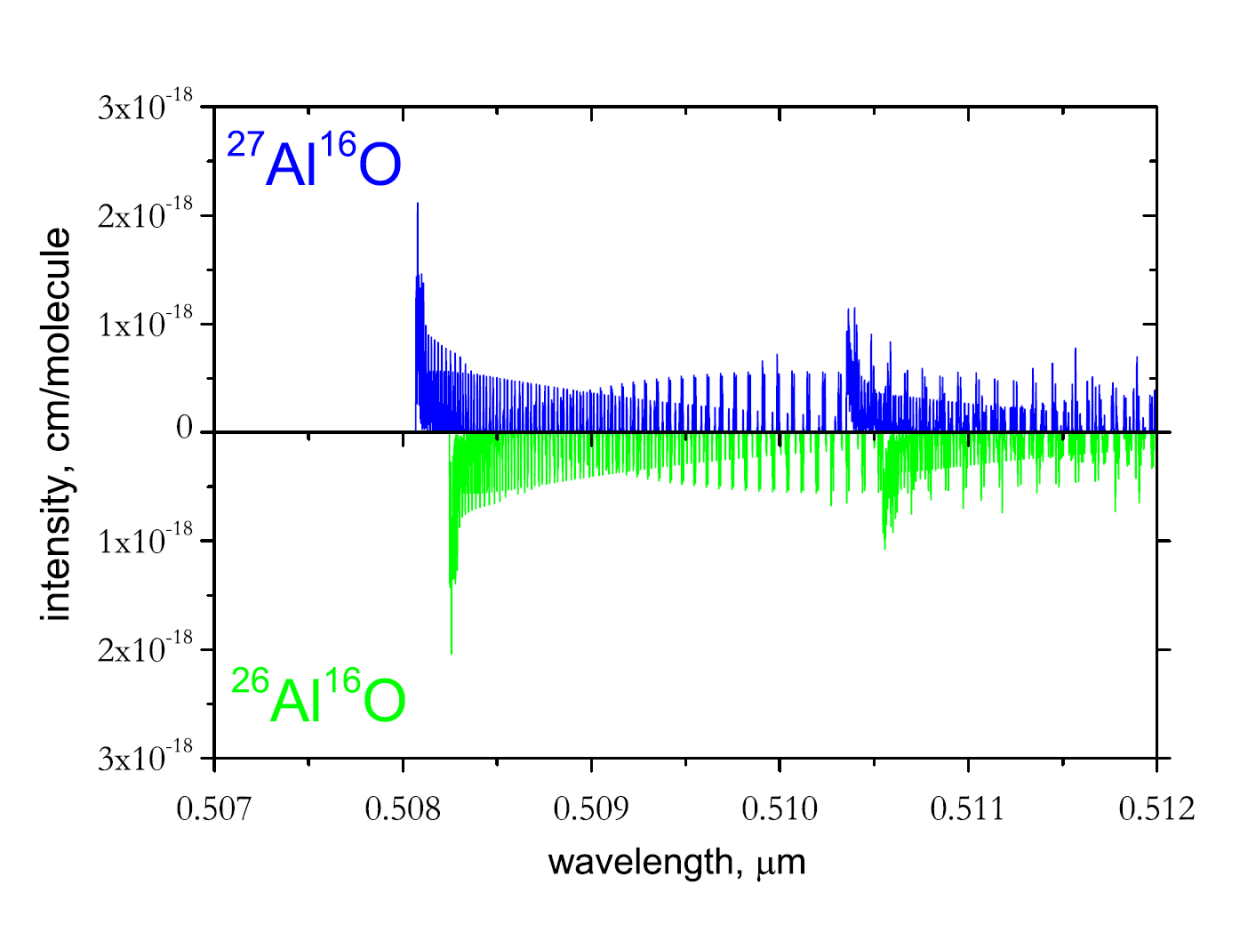


Kaminski, Schmidt & Menten (2013)

AlO

It has very nice bandheads, easy to detect at around 0.5 μm sensitive to isotopic variation

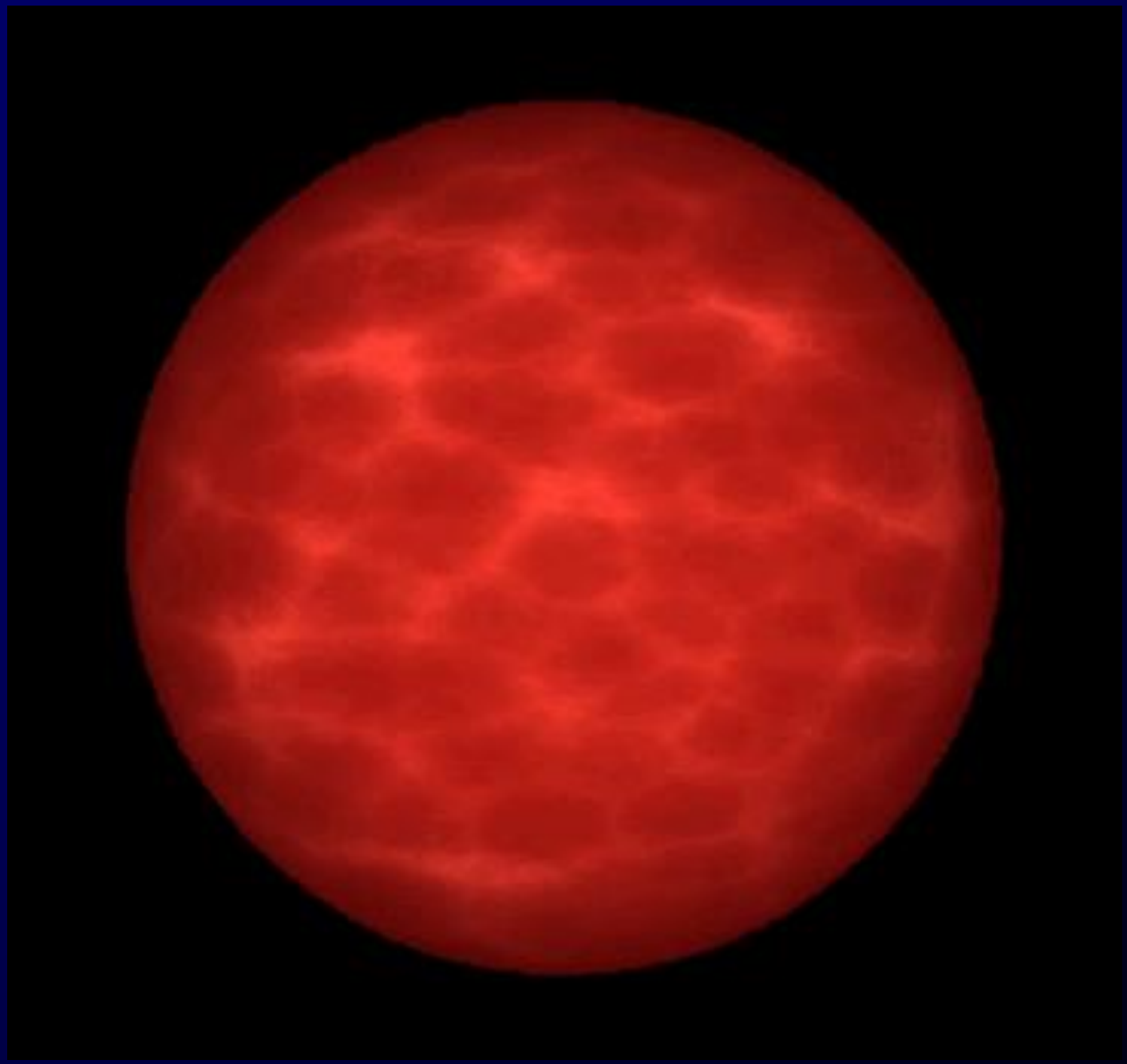
Isotope substitution: 27 to 28



ExoMol: Patrascu et al MNRAS 449, 3613 (2015)

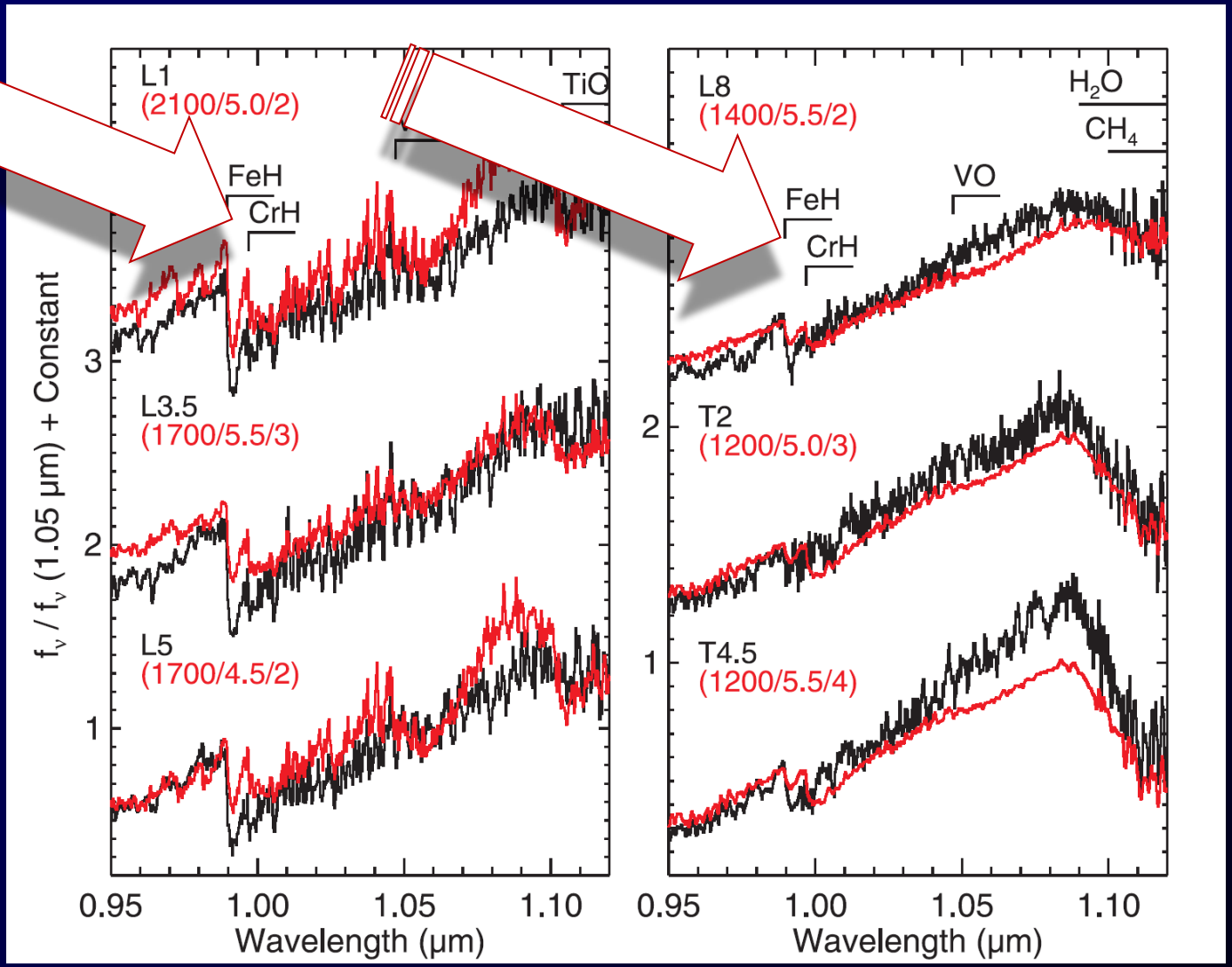
CrH and FeH

CrH and FeH
seen on L-type dwarfs a lot



CrH and FeH
used to classify the L-type dwarfs
by Kirkpatrick et al. (1999)

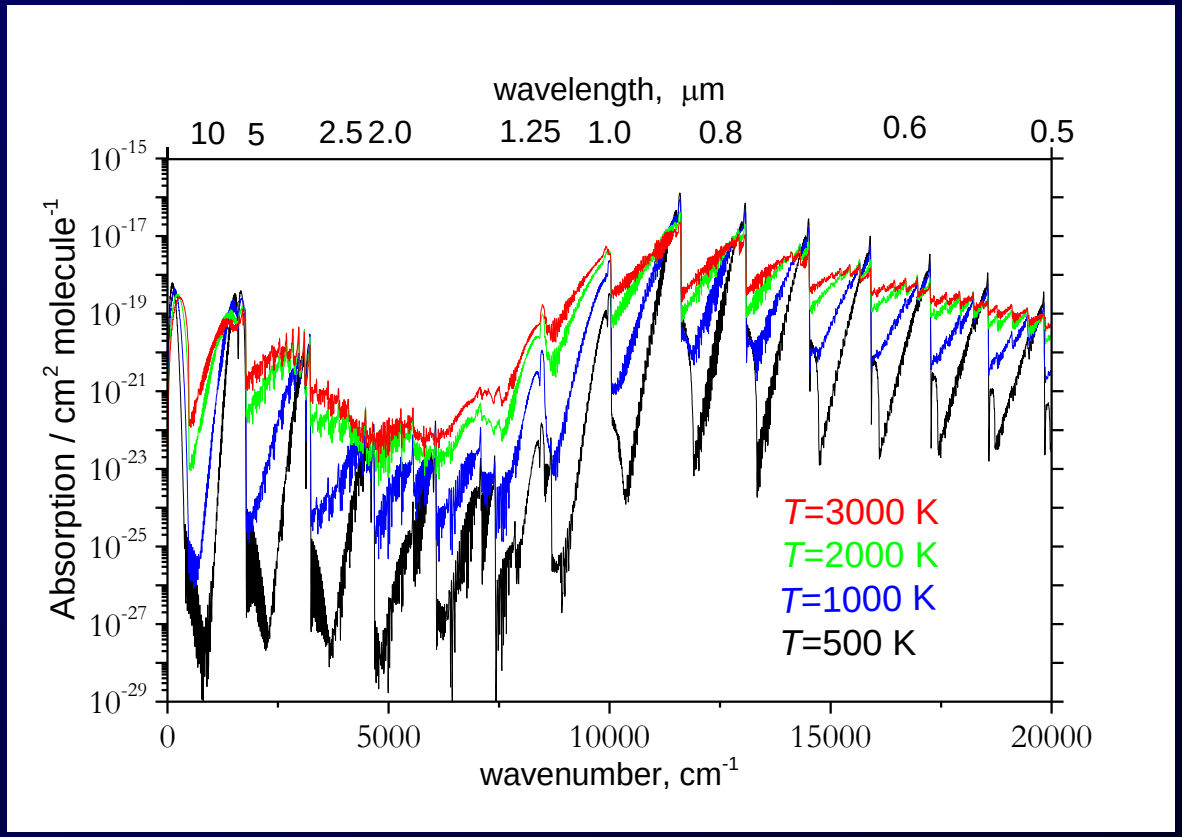
Here is an example of L-type dwarfs spectra with CrH and FeH



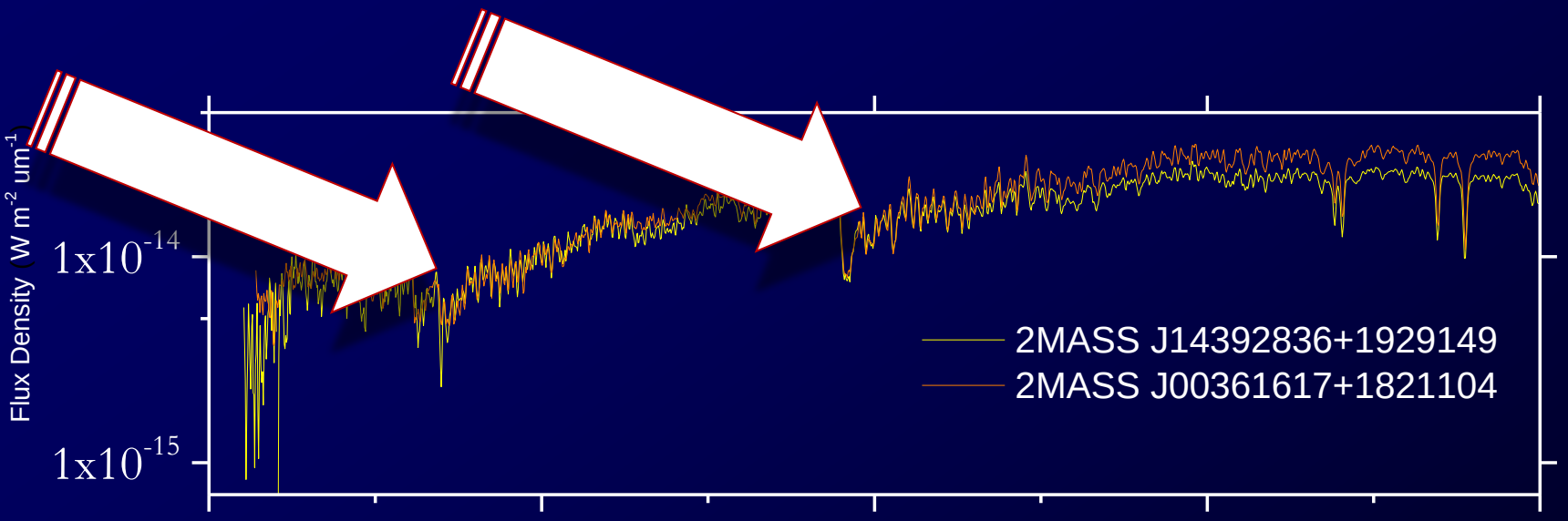
Maire Gorman (ExoMol PhD)

has produced
a new CrH line list

The line list is
to replace Burrow's line list

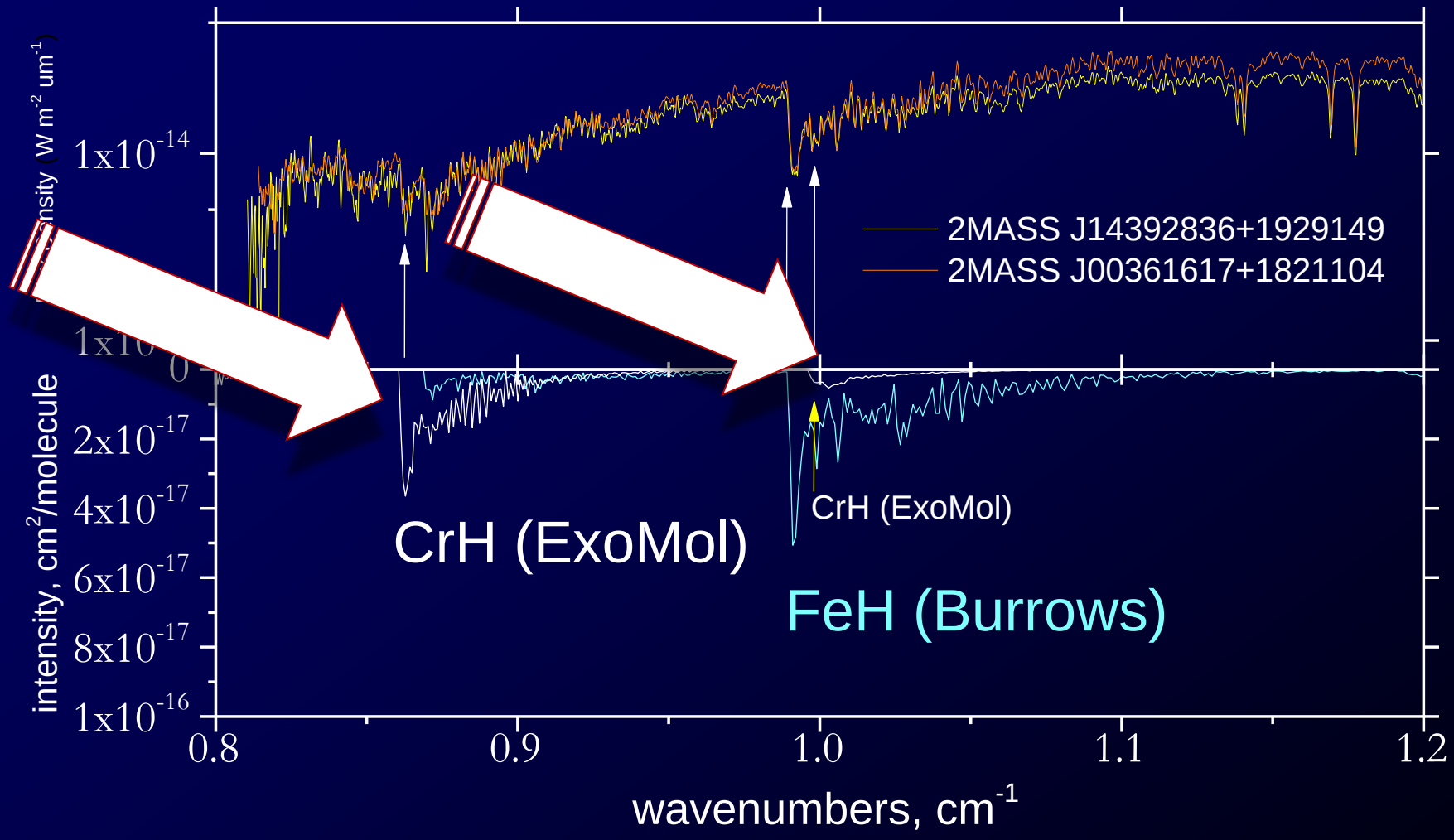

wavelength, μm
10
5
2.5
2.0
1.25
1.0
0.8
0.6
0.5
Absorption / cm2 molecule-1
10-15
10-17
10-19
10-21
10-23
10-25
10-27
10-29
T=3000 K
T=2000 K
T=1000 K
T=500 K
0
5000
10000
15000
20000
wavenumber, cm-1

Here is example of L-dwarf spectra with



Rayner et al ApJ SS, 185, 289 (2009)

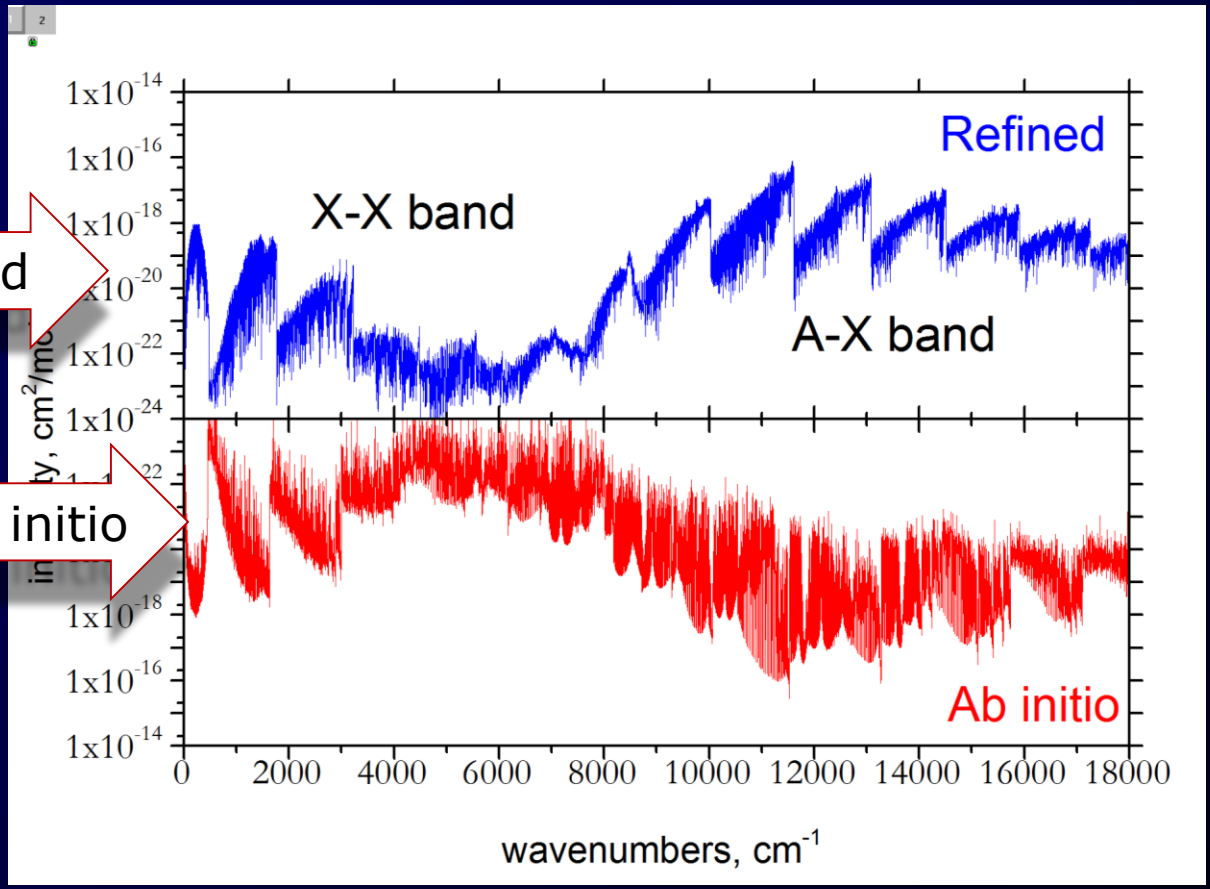
Here is example of L-dwarf spectra with CrH from ExoMol



CrH is transition metal and very difficult to get right

Empirically Refined

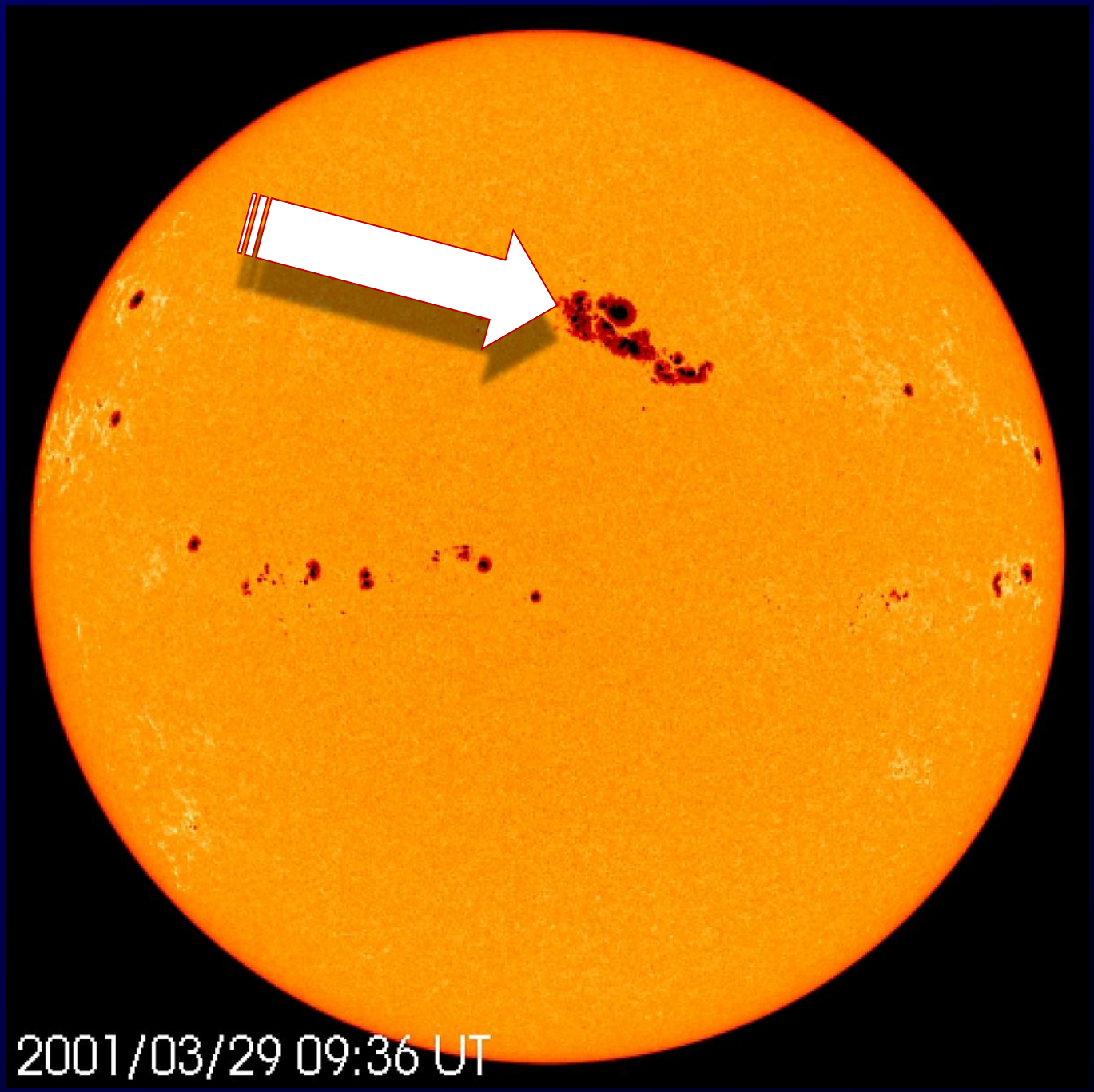
Ab initio



Going hotter:

SiO

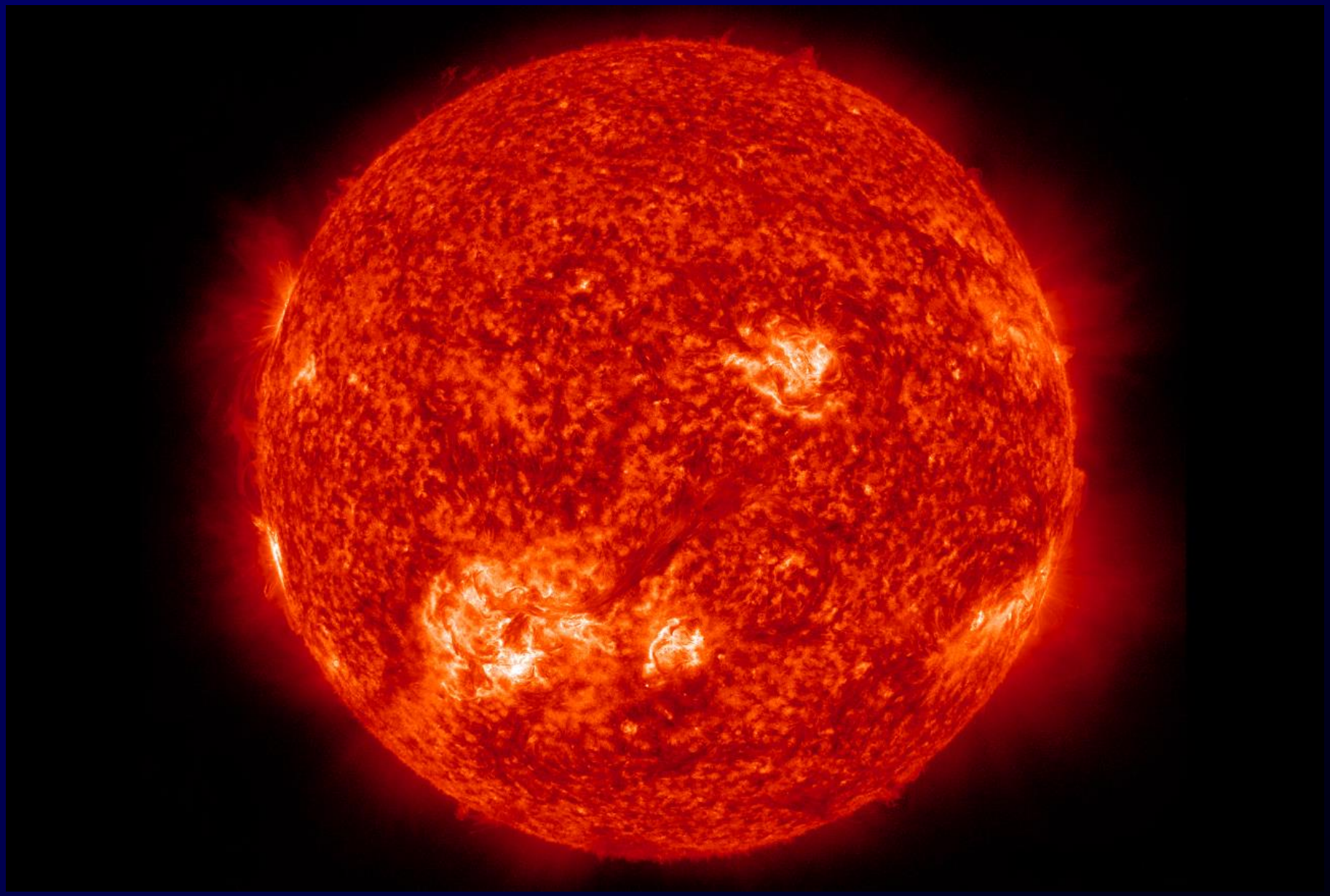
It has been spotted
in Sun spots spectra


2001/03/29 09:36 UT

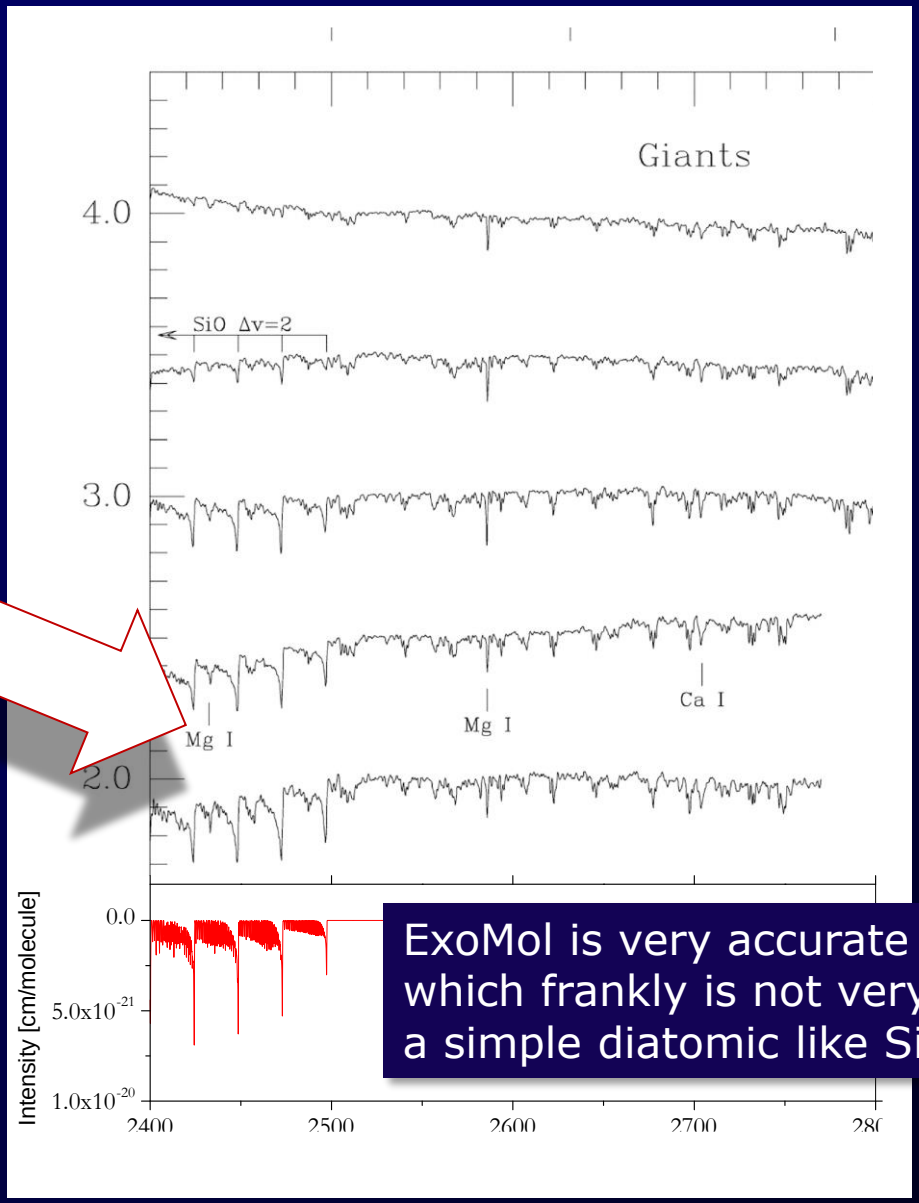

Here

SiO

and red Giants



Here are SiO bands in oxygen-rich giants and supergiants



ExoMol is very accurate
which frankly is not very difficult for
a simple diatomic like SiO

Wallace & Hinkle (2002)

Another example of SiO in K-type supergiant HD 225212

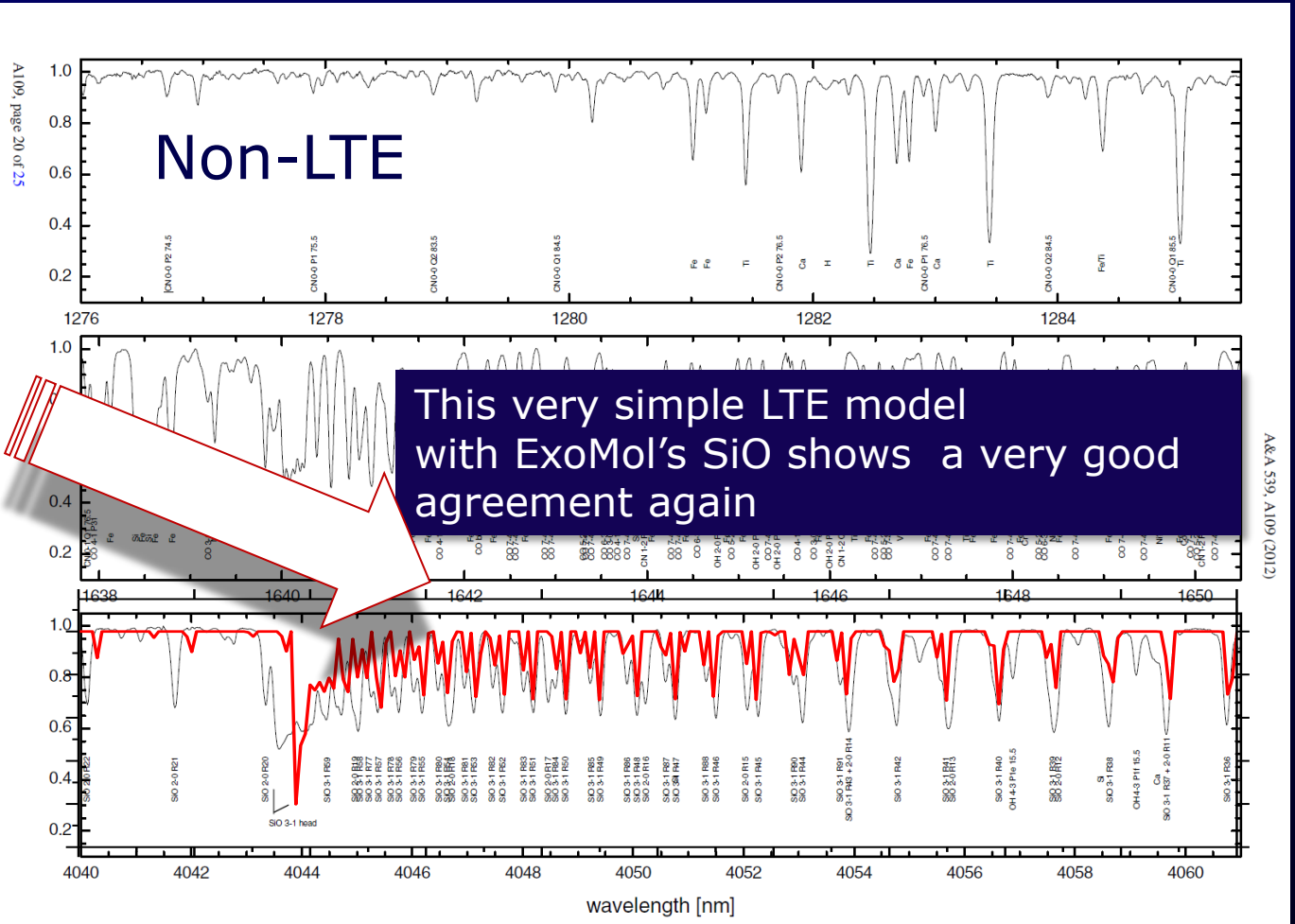


Fig. 14. Same as Fig. 3 for HD 61913 (S).

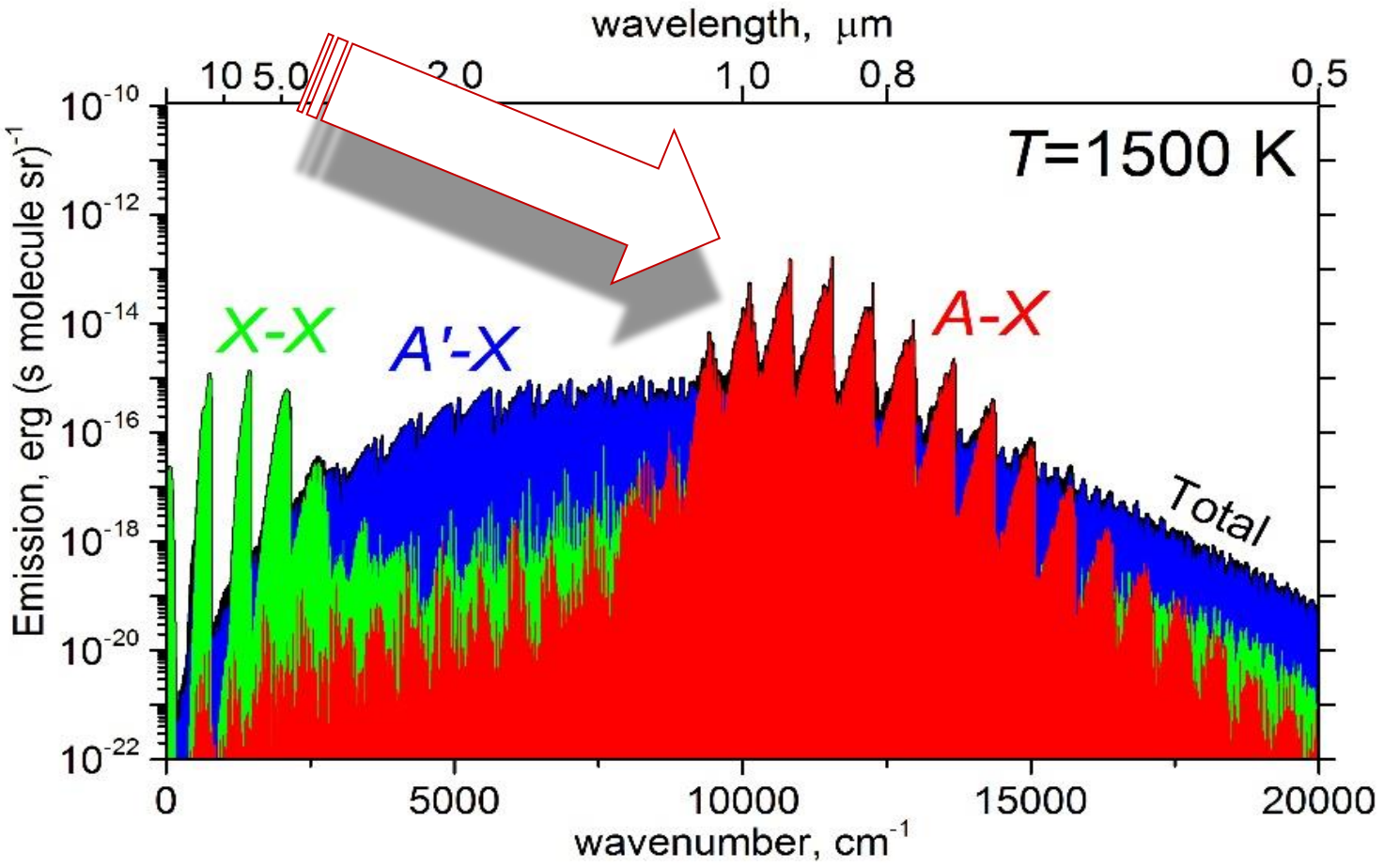
Lebzelter A&A 539, A109 (2012)
A library of high resolution spectra in the near-infrared

CaO – new line list

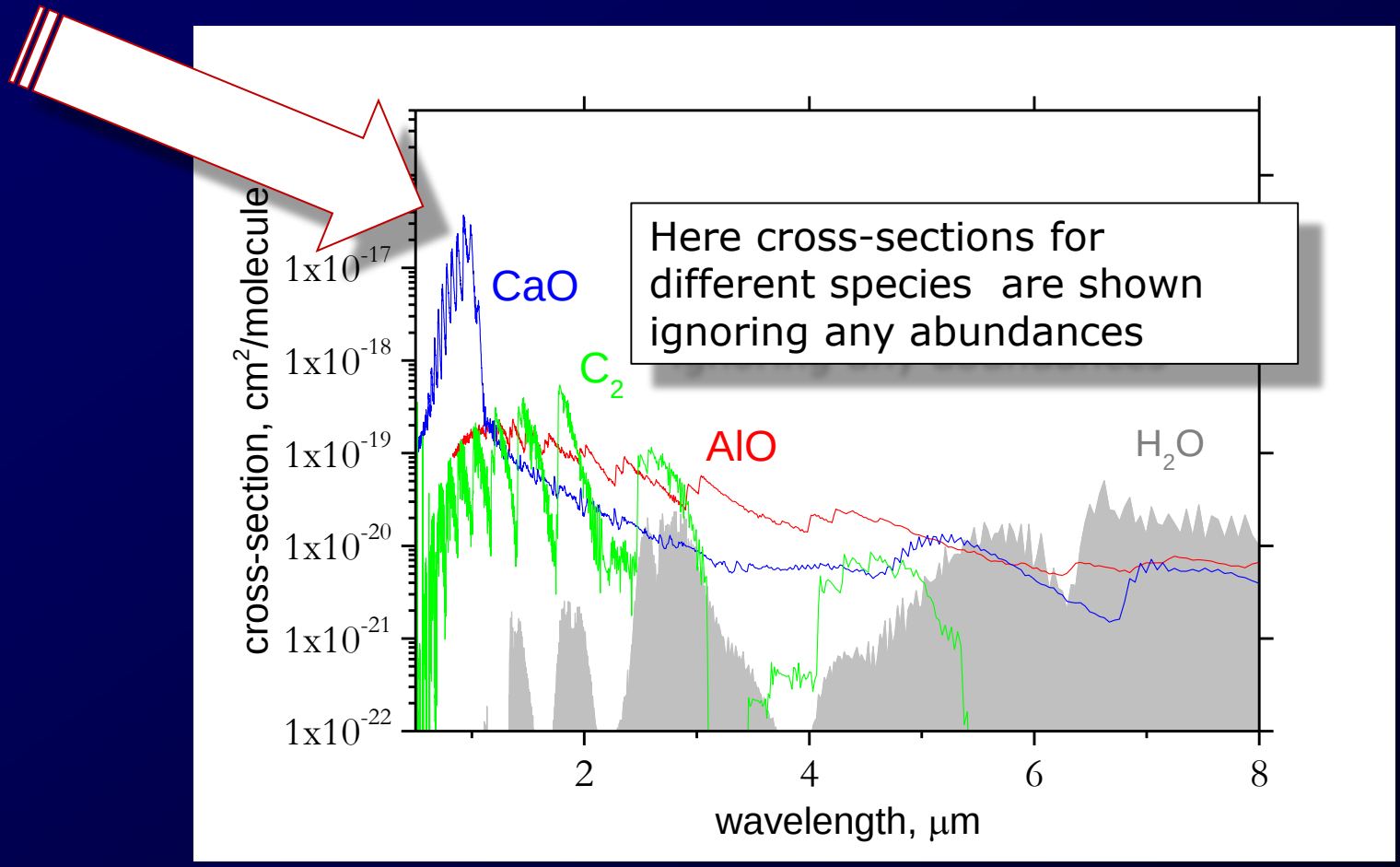
It is a possible constituent of rocky type exoplanets, CaO has not been detected astrophysically.

CaO – new line list

Here different bands are shown with the strongest at 1 μm



CaO has a huge dipole and a nice feature at 1 μm



Can these oxides be important for absorption/radiative cooling of *Lava planets?*

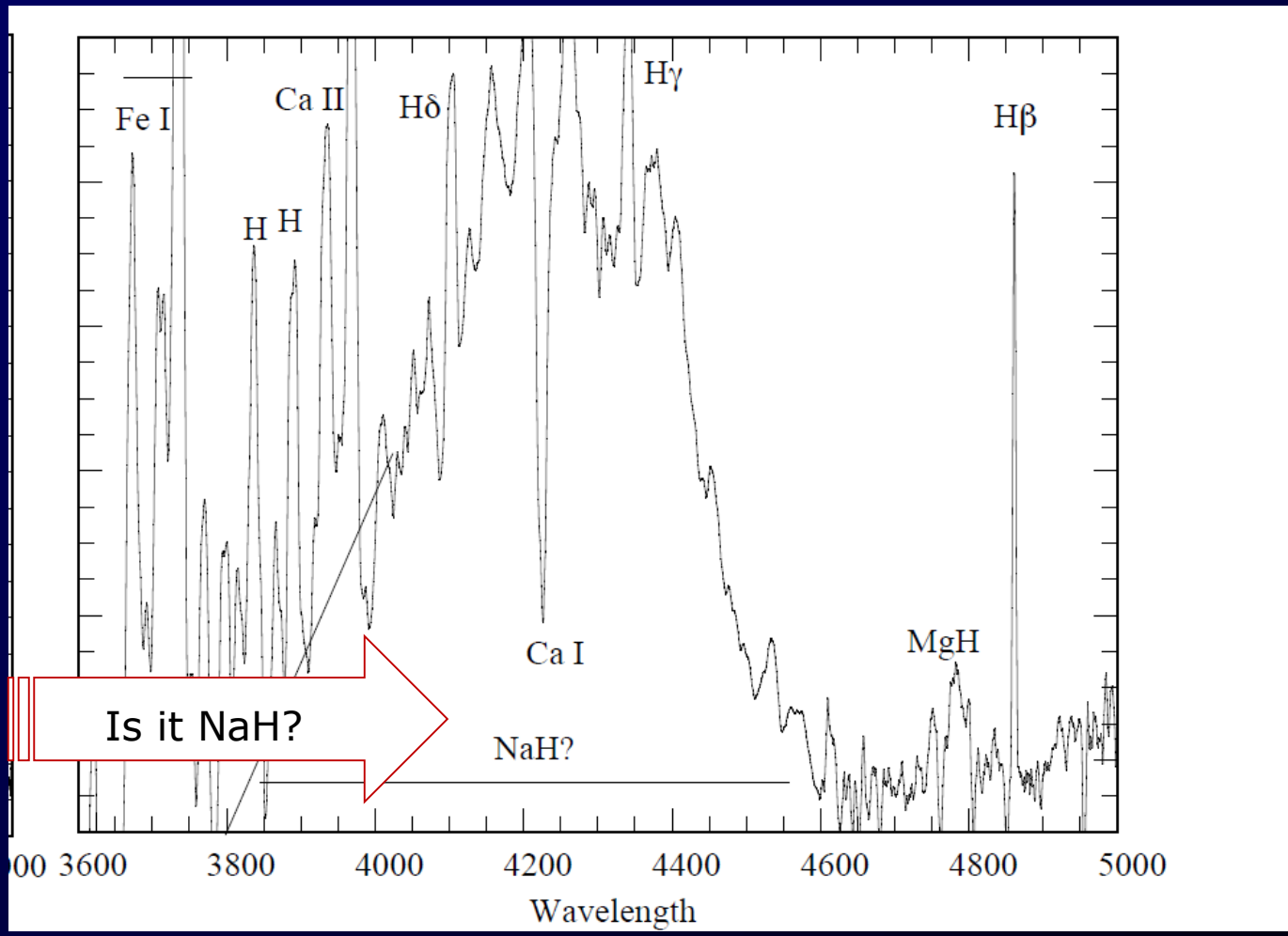
New line list for NaH

which is also to be detected, but
expected for M-type objects

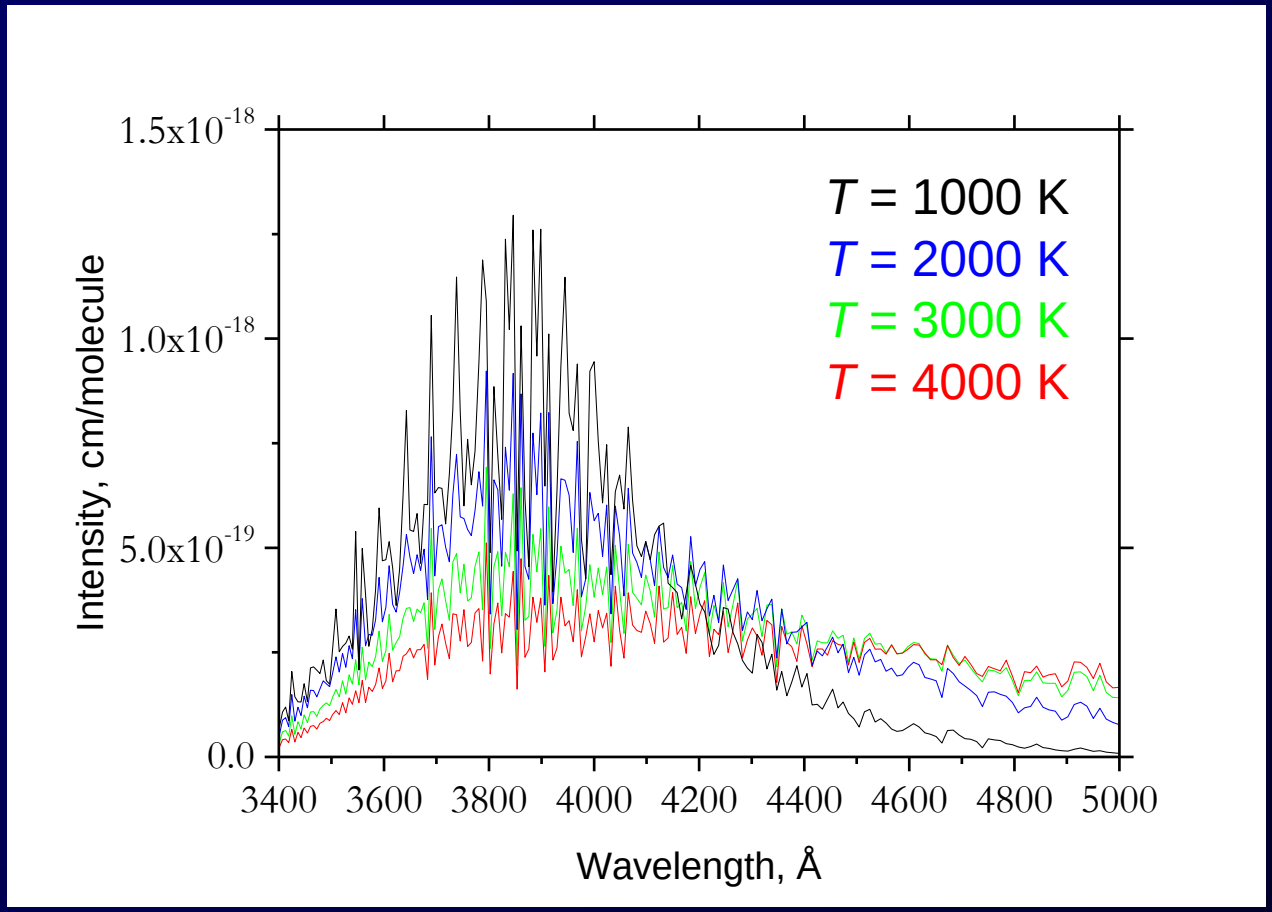
NaH

For example it was suggested for GJ 551

Here is the observed data of GJ 551 (Mike Bessell)

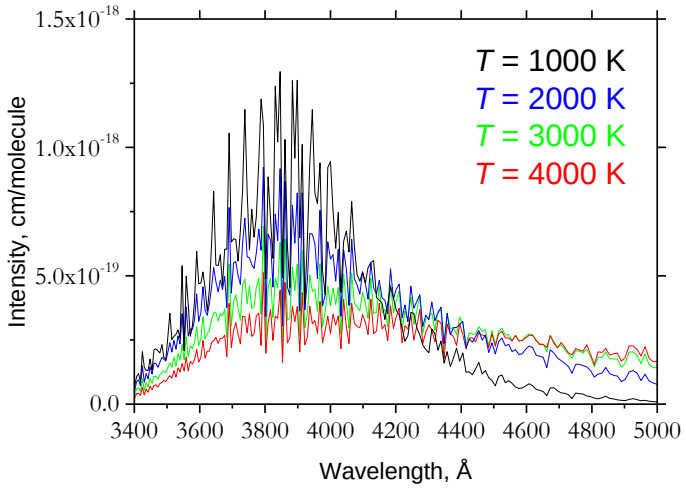


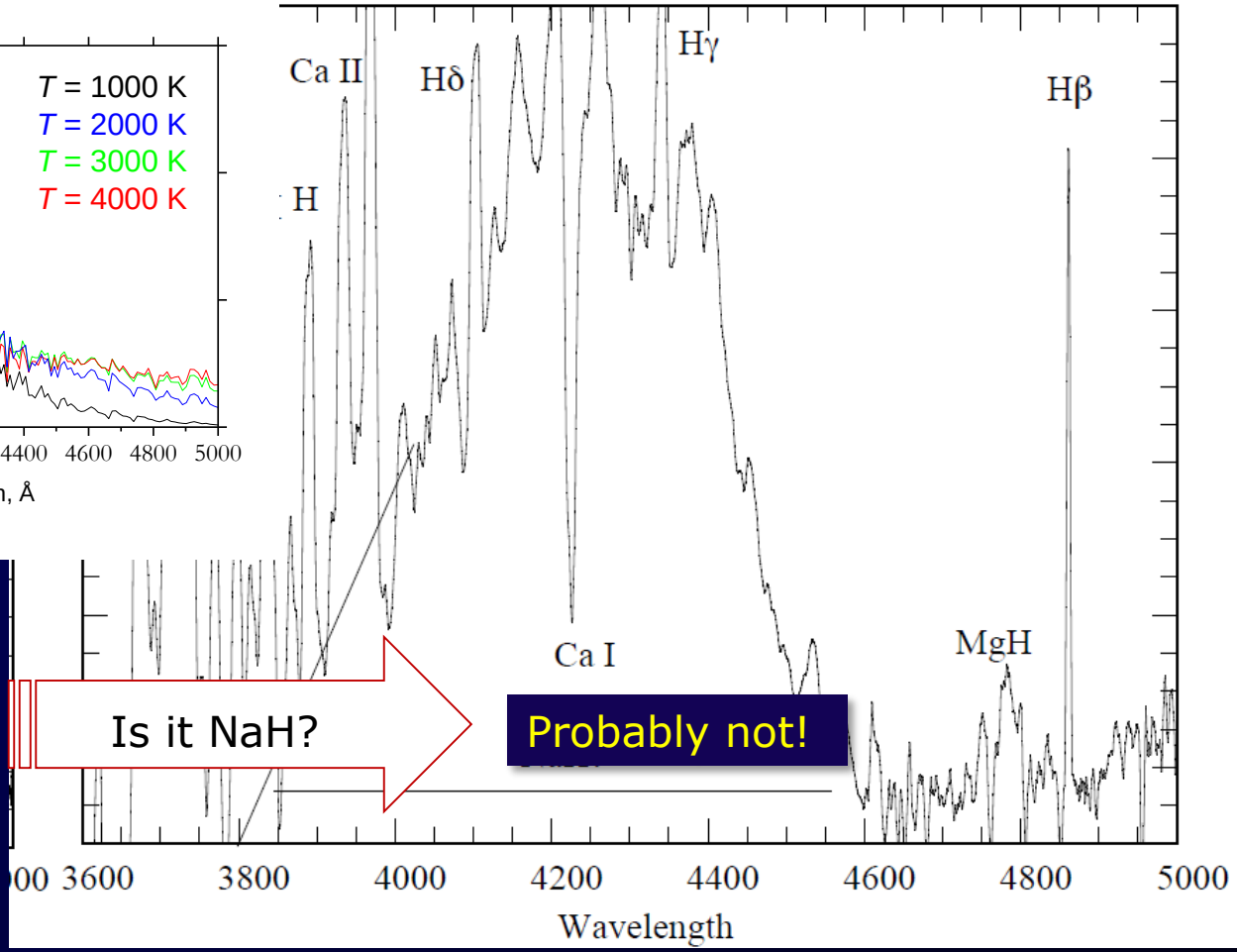
Courtesy Mike Bessell



And Exomol spectrum of NaH is very flat is broad

Here is the observed data of GJ 551 (Mike Bessell)



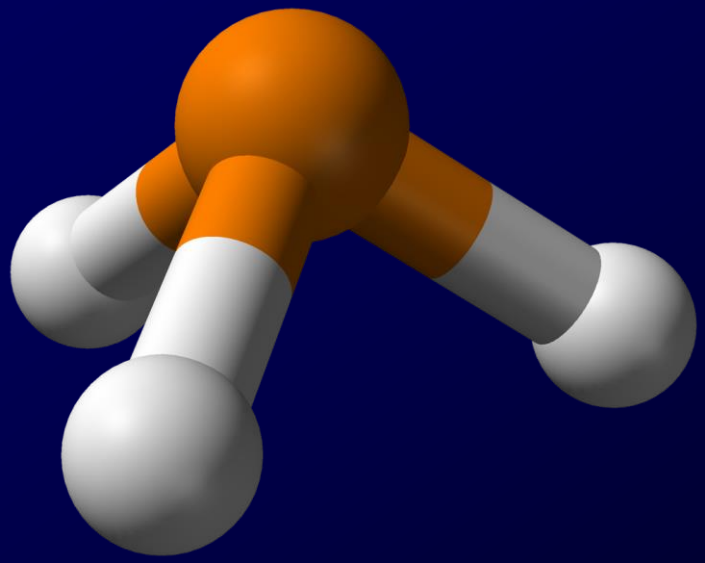


Courtesy Mike Bessell

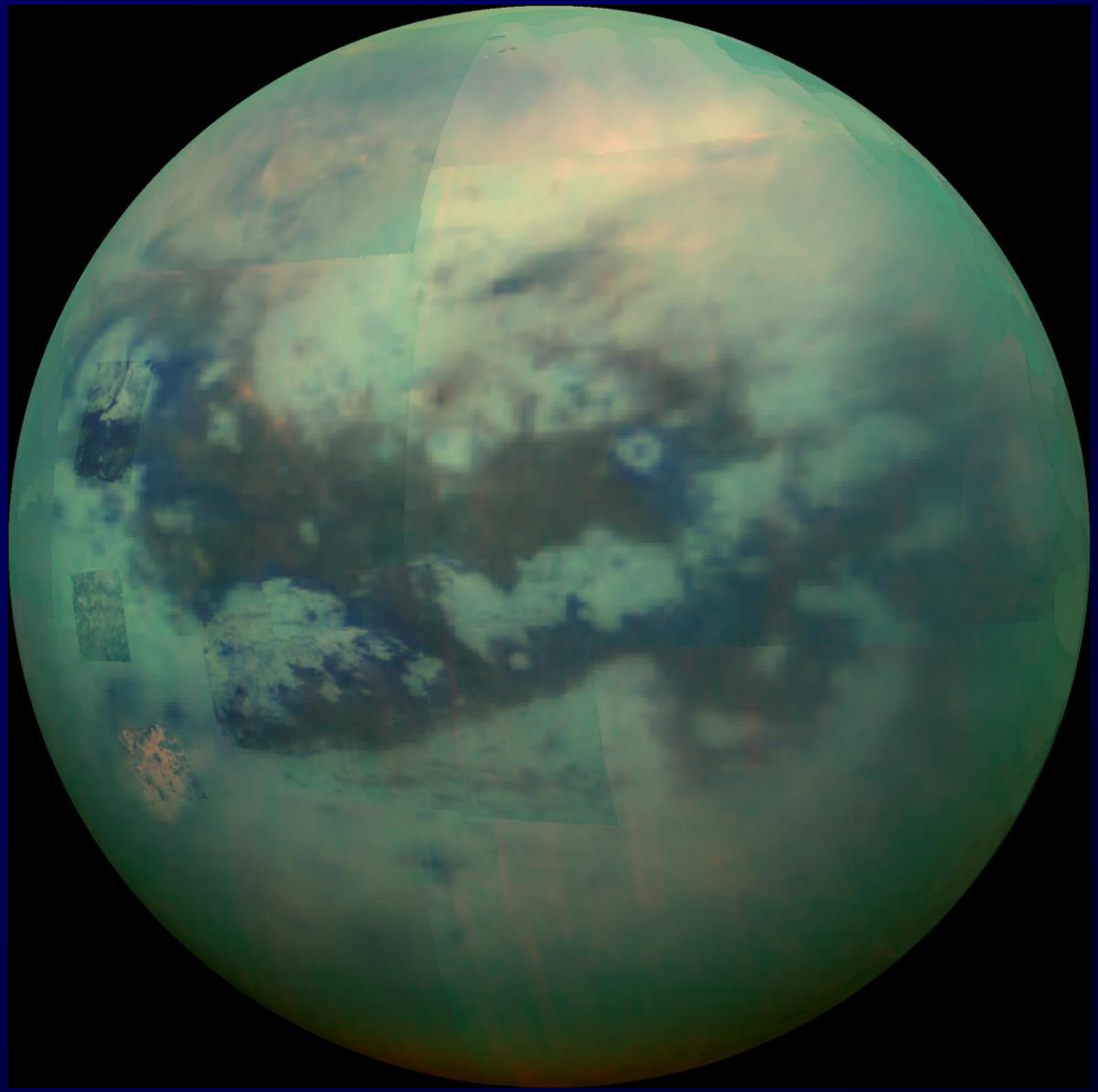
Some polyatomics

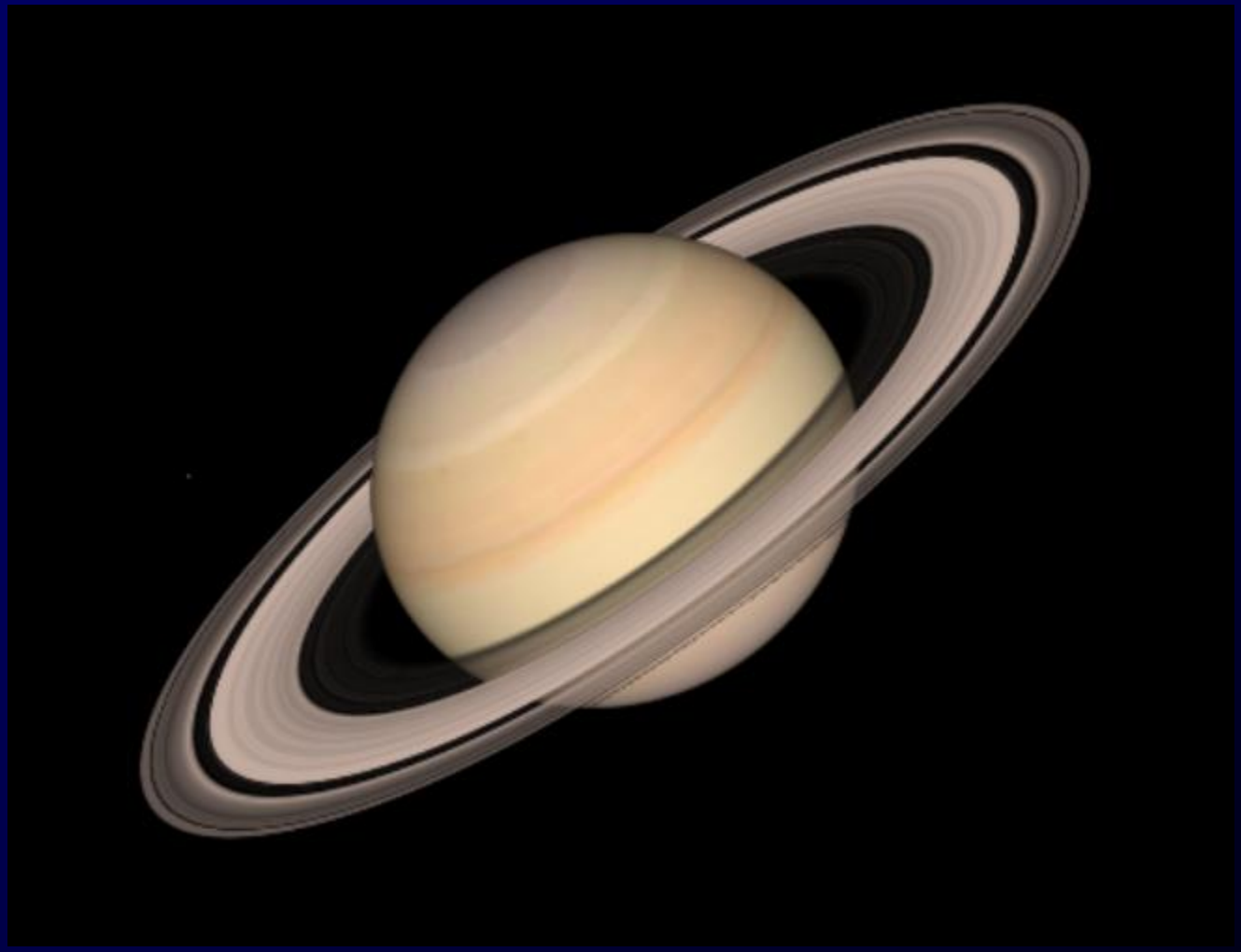
PH_3 (Phosphine)

ExoMol line list was computed
by Clara Souosa Silva
containing more than 10 billion lines

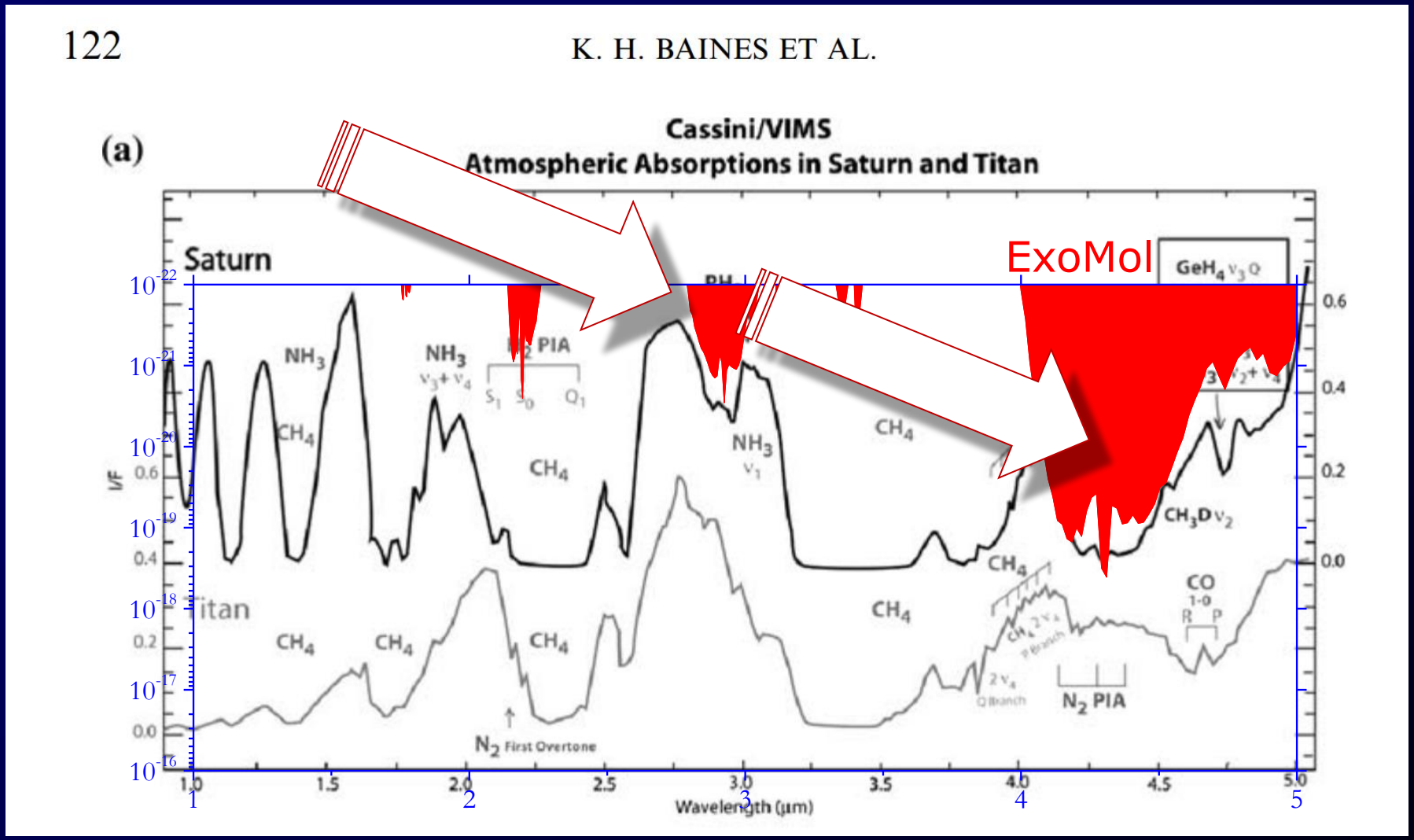


Phosphine
was found spectroscopically
in the Solar system





Here is the Cassini spectrum of Saturn and Titan, where many molecules have been detected incl PH_3



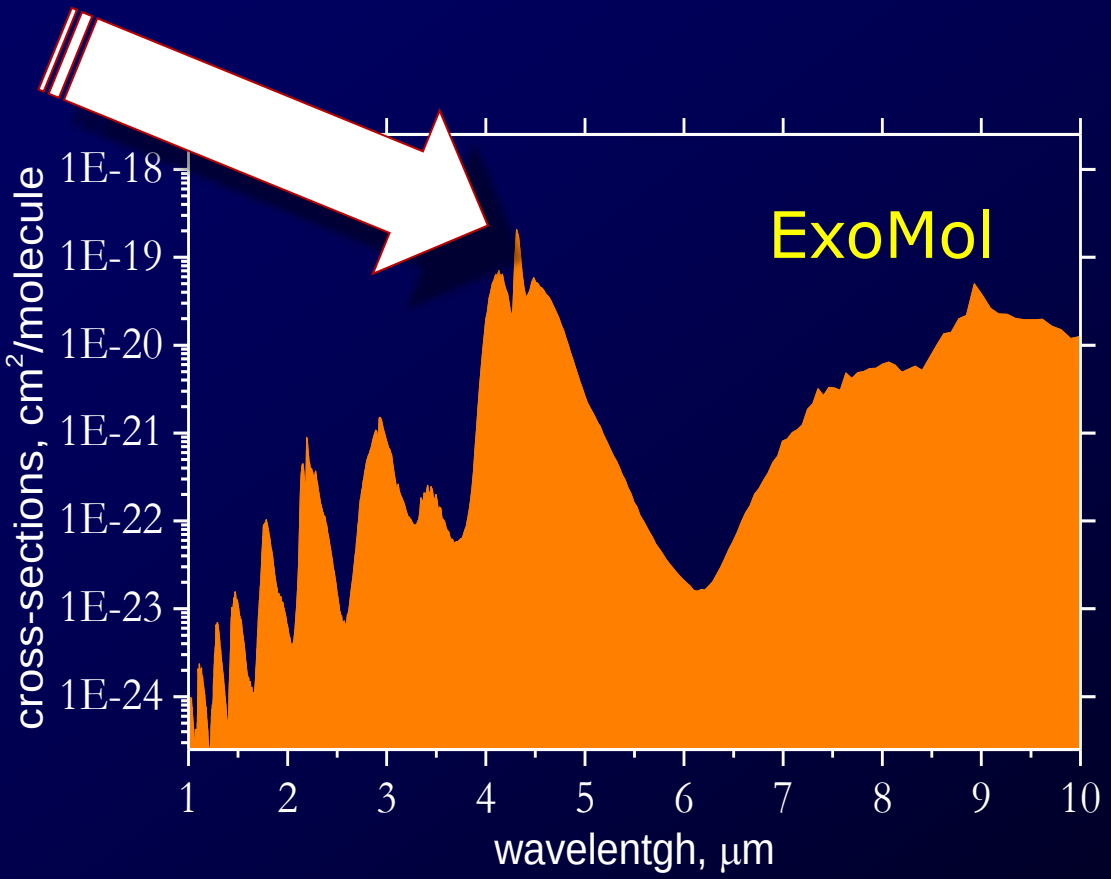
Baines et al , Earth, Moon, and Planets 96, 119 (2005)

More excitingly: Clara figured out that due to spontaneously flammable and extremely toxic PH_3

…. and since it can be produced by organic sources, it be suggested as a chemically sound biosignature for fire breathing *dragons*

C. Sousa-Silva et al (ExoMol) MNRAS 446, 2337 (2015)

It also has a nice strong feature at 4.5 μm



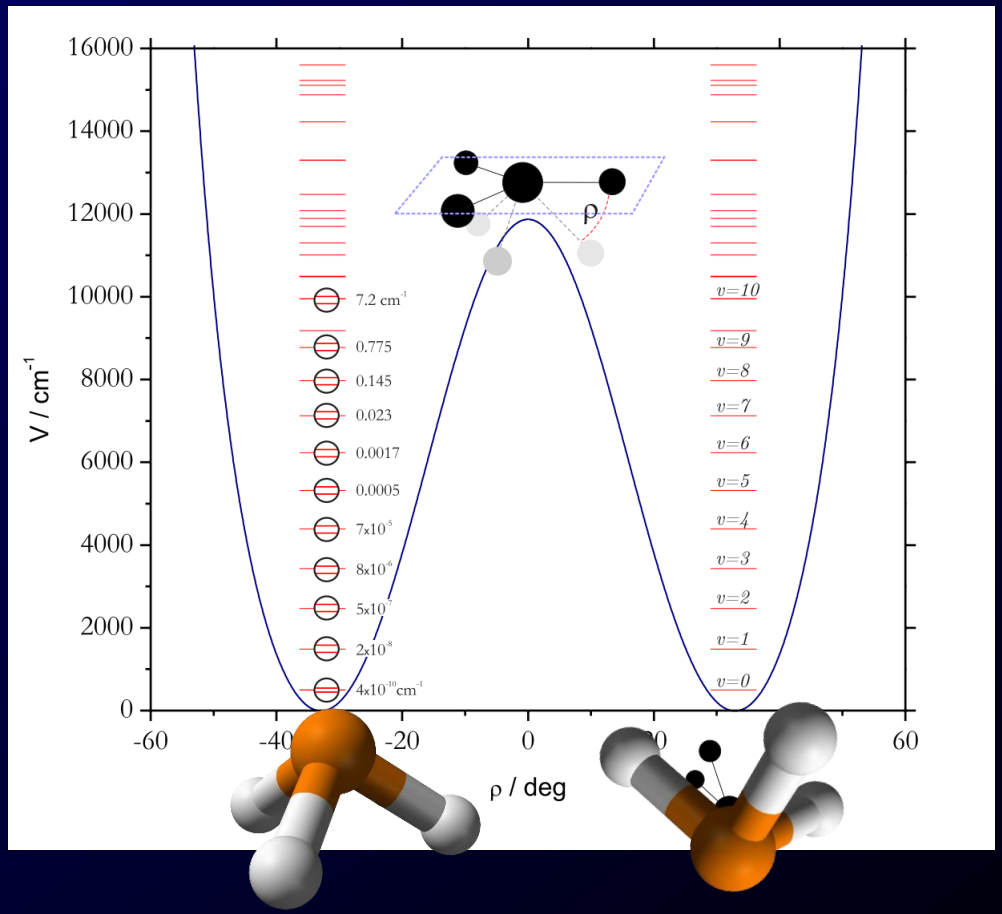
Another exciting Clara's idea is inversion splitting of PH_3

Just like Ammonia it has a pyramid structure

… but with large barrier to the planarity. Here is the double-well potential

The splitting at the bottom of about 1 Hz

We just need to convince experimental people to do the observations



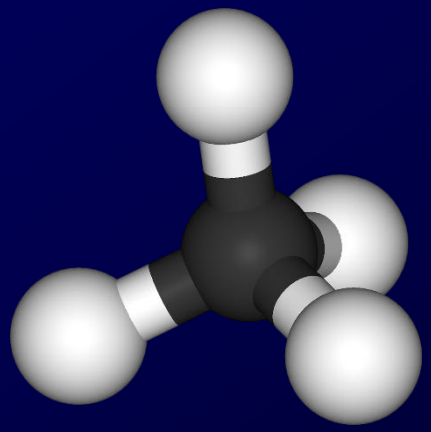
So far - no one is interested in Phosphine gas


T+

Methane (CH_4)

ExoMol line list: 10 billion lines 10to10

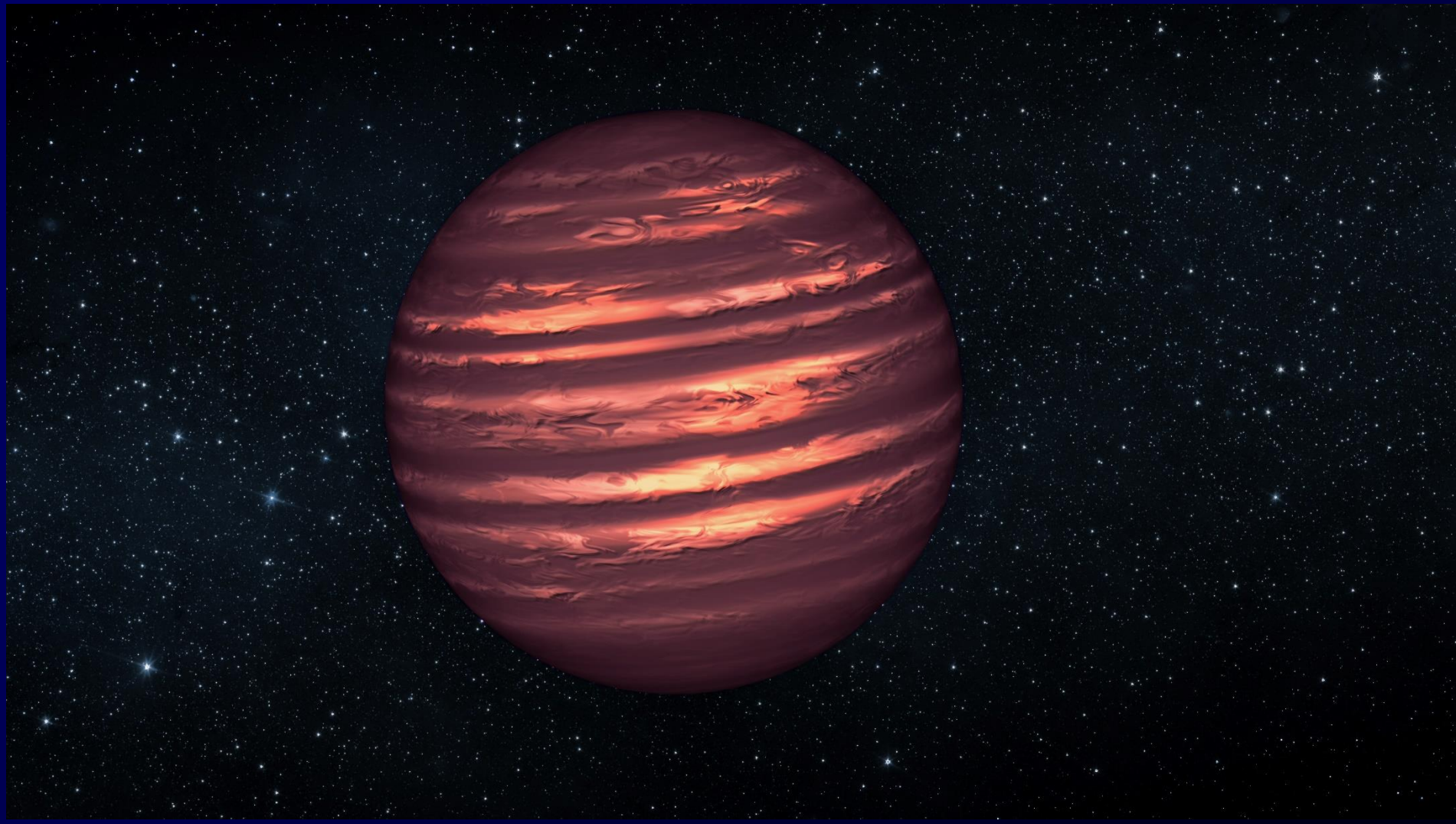
CH_4 is the most important molecule for the project

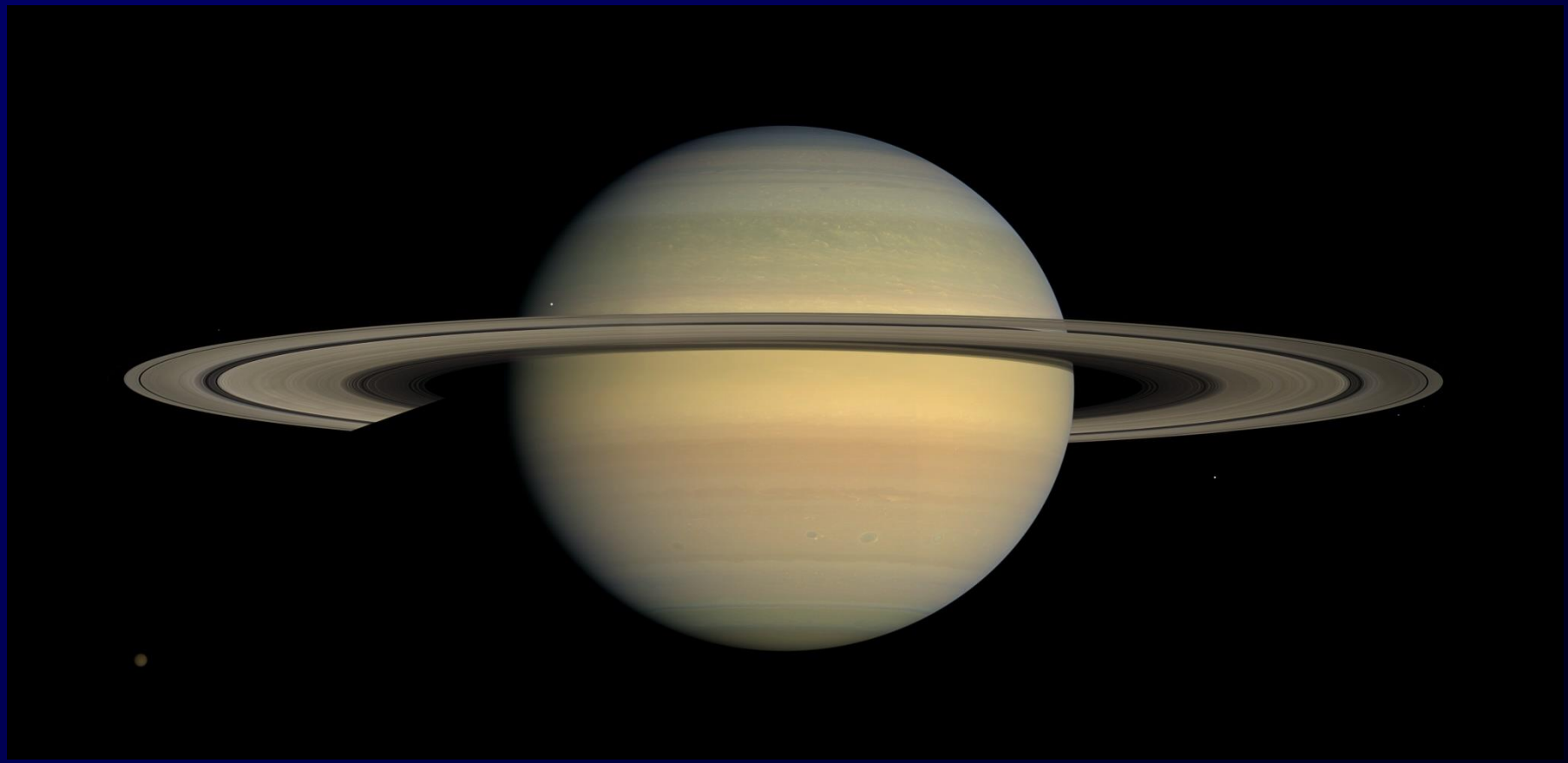


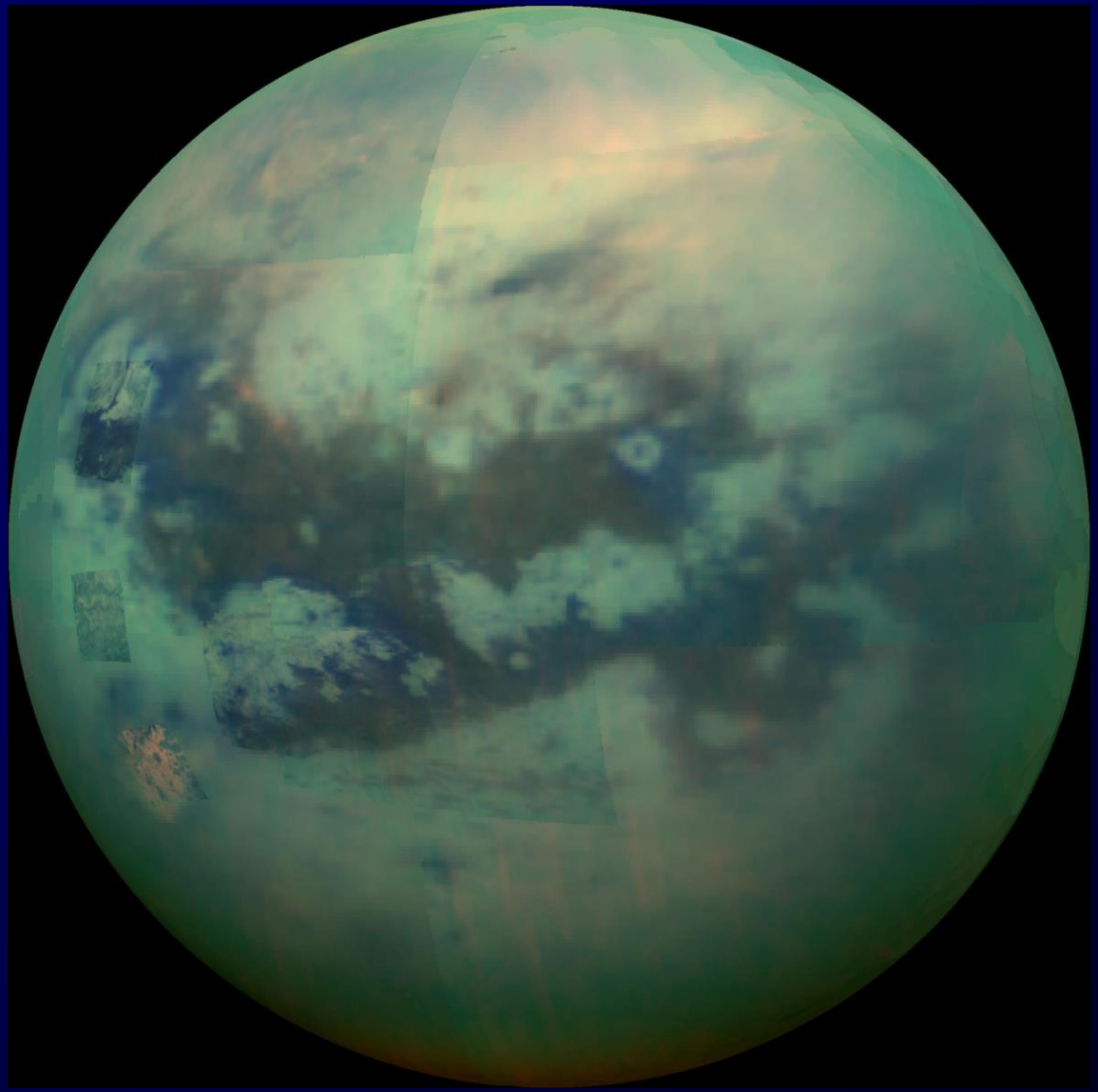
Methane
ExoMol line list ~~10 billion~~ 35 billion lines

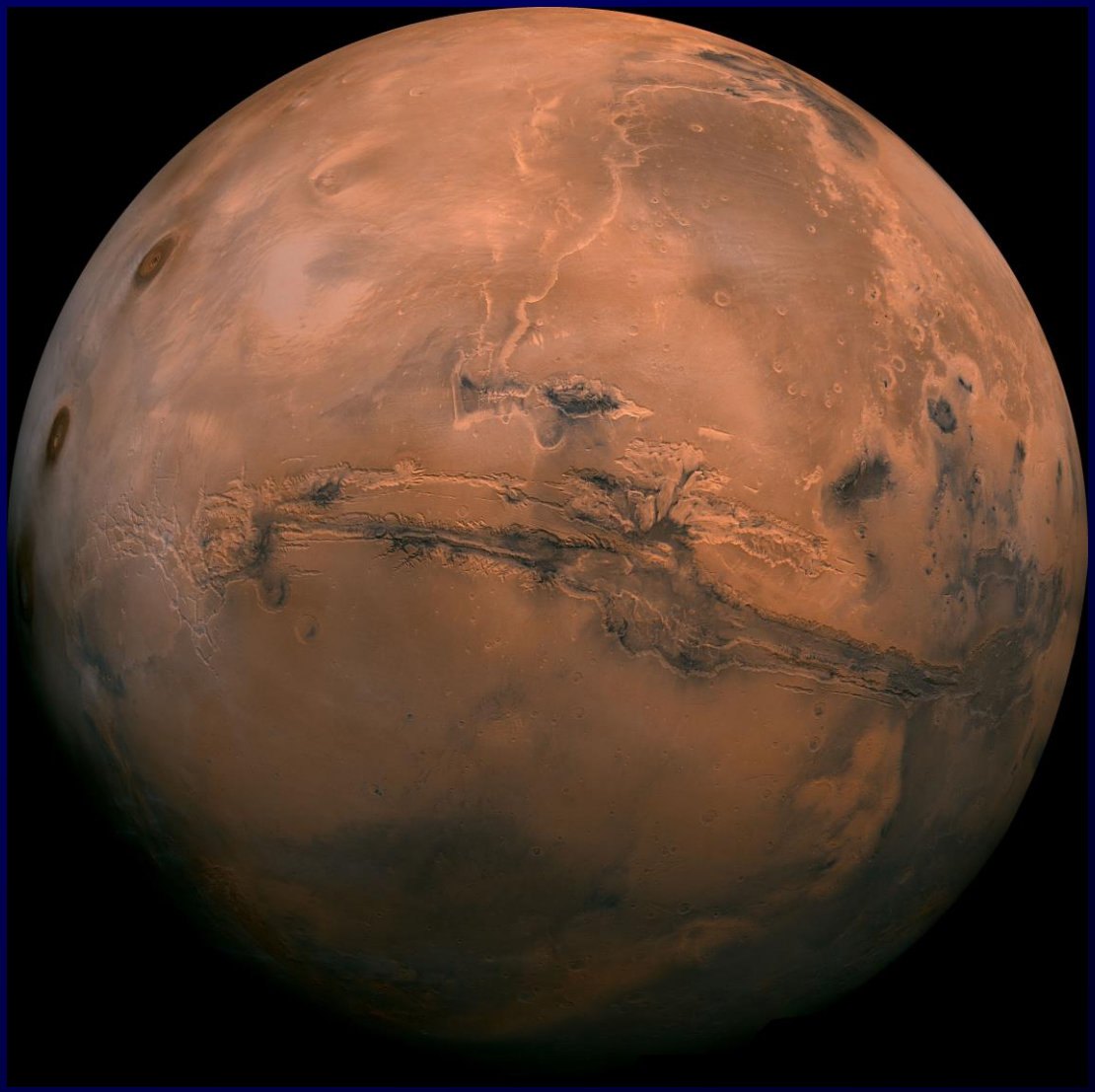
which took 4.5 million CPUh
DiRAC HPC (COSMOS and Darwin)
and about 6 months of the human time

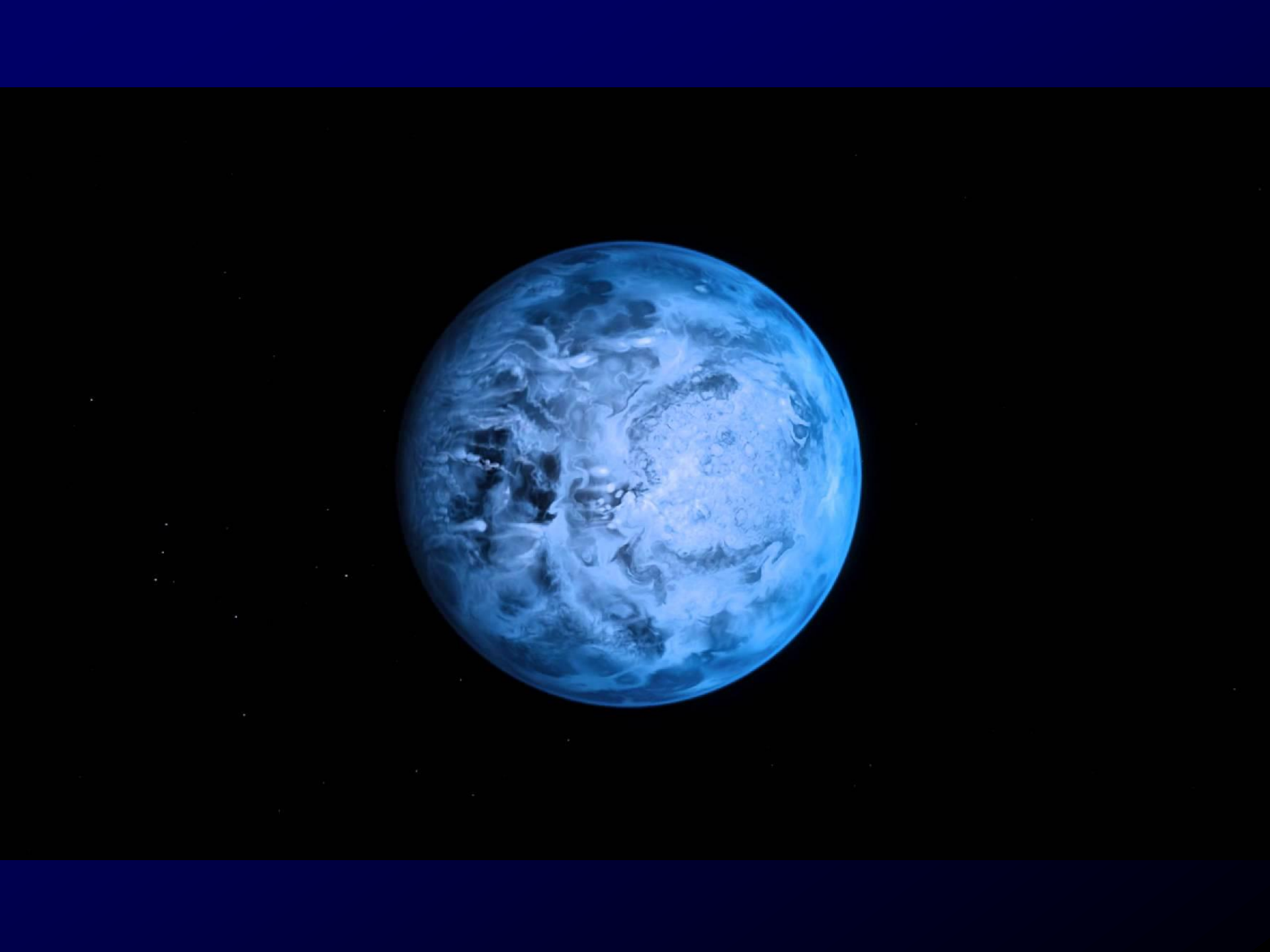
CH_4 has been detected in many objects.





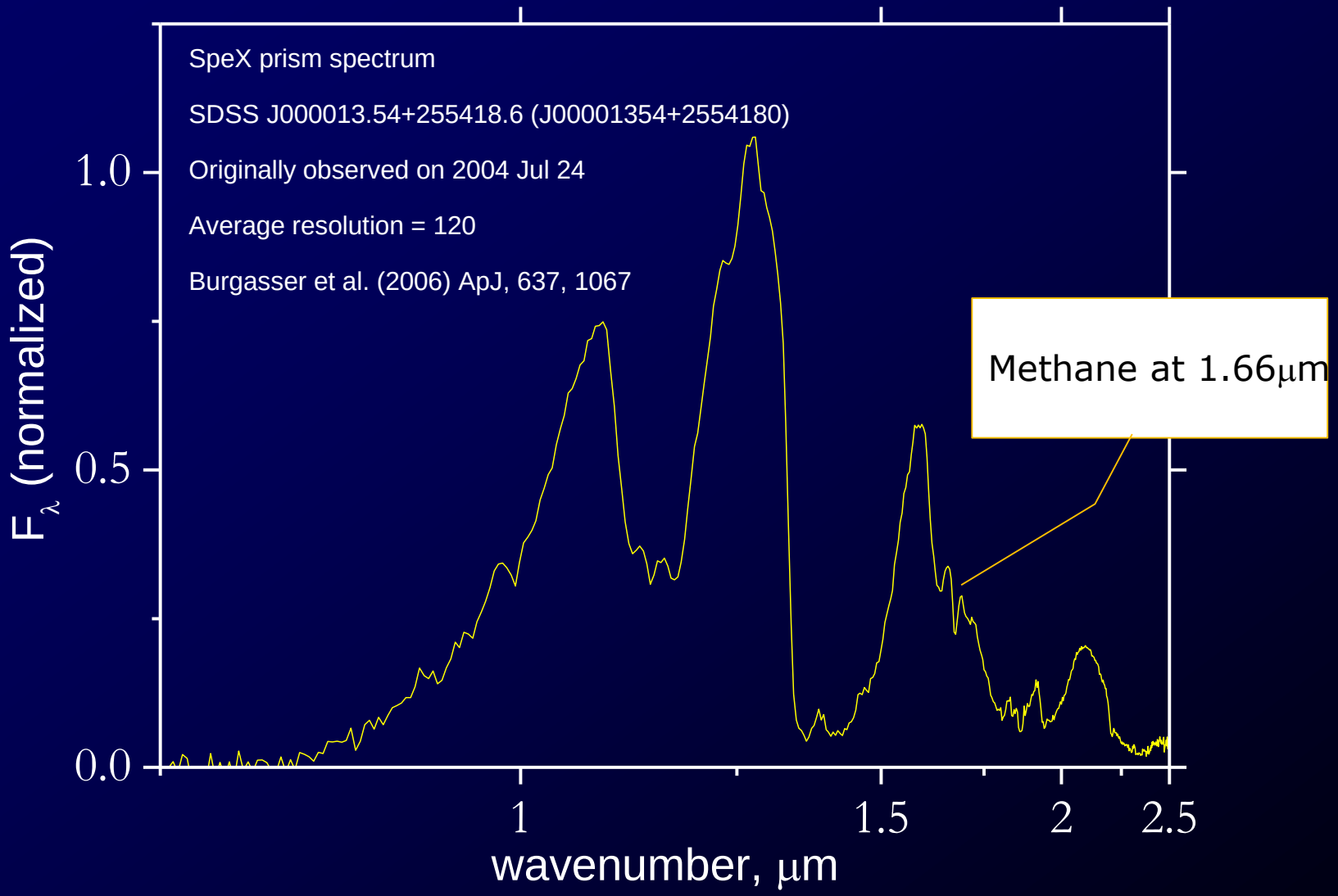






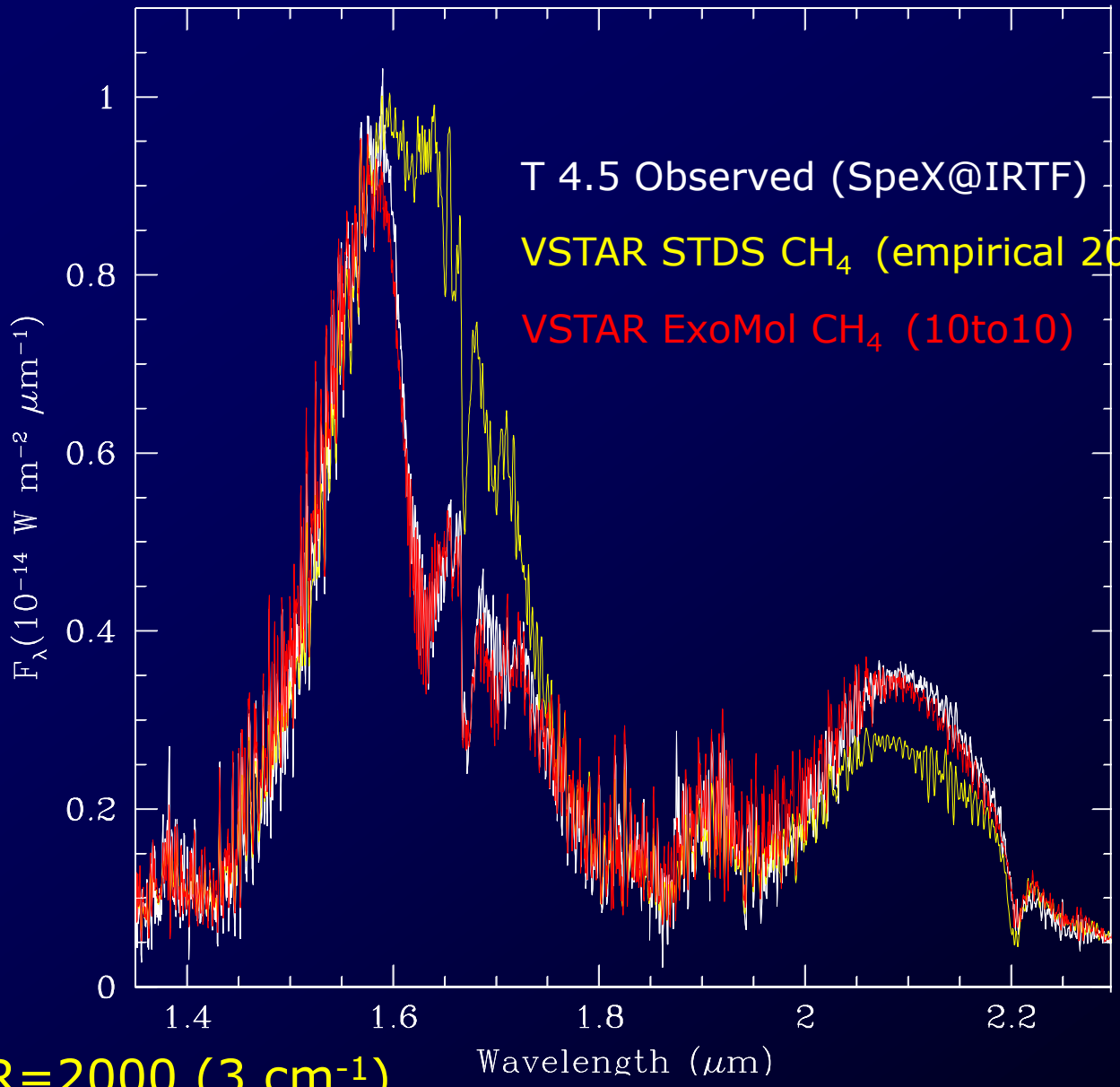
CH_4 is detectable even at low resolution

Here is the Brown dwarf spectrum at R=120



In fact the feature at 1.61 μm is very important and it was difficult to model before ExoMol

Here is the T 4.5 dwarf spectrum and our solution to that



2MASS 0559-14

Yurchenko et al PNAS, 111, 9379 (2014)

Cushing Rayner, Vacca (2005)

R=2000 (3 cm^{-1})


It'll take your breath away! The world's


Now Salmond warns Scotland


'Could life get any better?' What


Mario Balotelli suffers racial abuse


House of horrors: Daughter tells how


Toddler, 2, rushed to hospital with

Hunt for extraterrestrial life given a boost: Methane detector can 'sniff out' a wider range of molecules to find alien organisms

- 90% of the methane in Earth's atmosphere is created by living organisms
- As a result, methane on other planets is regarded as an indicator of life
- Methane is detected by the way a planet's atmosphere absorbs starlight
- Previous models of methane were incomplete, making method inaccurate
- New model can detect methane at temperatures of up to 1,500K/1220°C
- This could increase chances of finding methane on another planet

By ELLIE ZOLFAGHARIFARD

PUBLISHED: 20:01, 16 June 2014 | UPDATED: 20:35, 16 June 2014

A powerful new model to detect life on planets outside our solar system has been developed by British-Australian researchers.

The new model focuses on methane, the simplest organic molecule on Earth, widely acknowledged to be a sign of potential life.

At least 90 per cent of the methane in Earth's atmosphere is created by living organisms. As a

Anyways, it has been now
used by many groups

Tau-Rex

NEMESIS

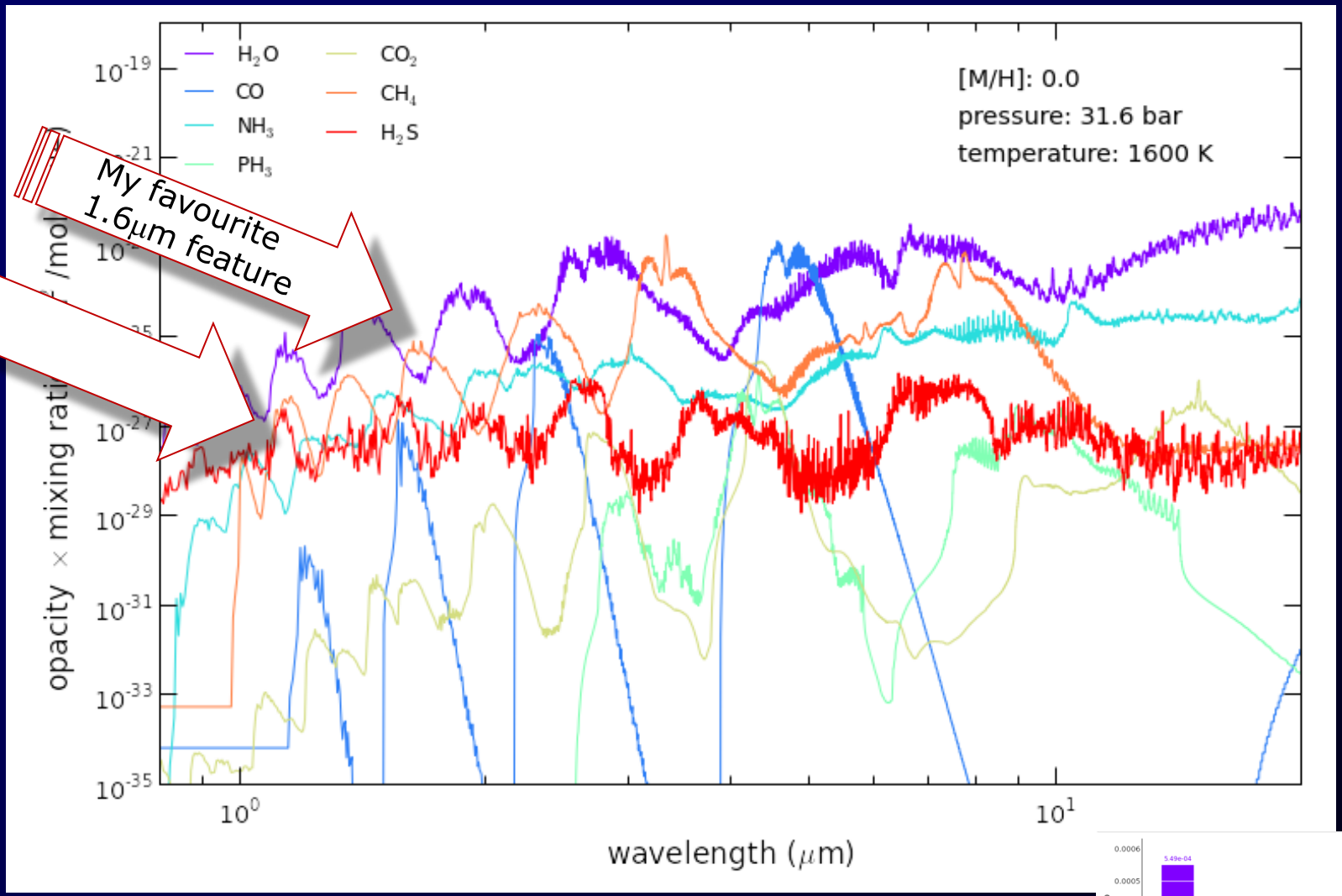
Met Office

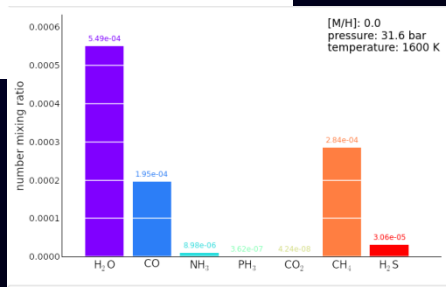
NASA Ames

However it is not perfect ☹
and we are now working on
Methane 2.0

The main problem is that it is incomplete and inaccurate at $< 0.9\ \mu m$

It may appear weak on this graph but it is known to be important



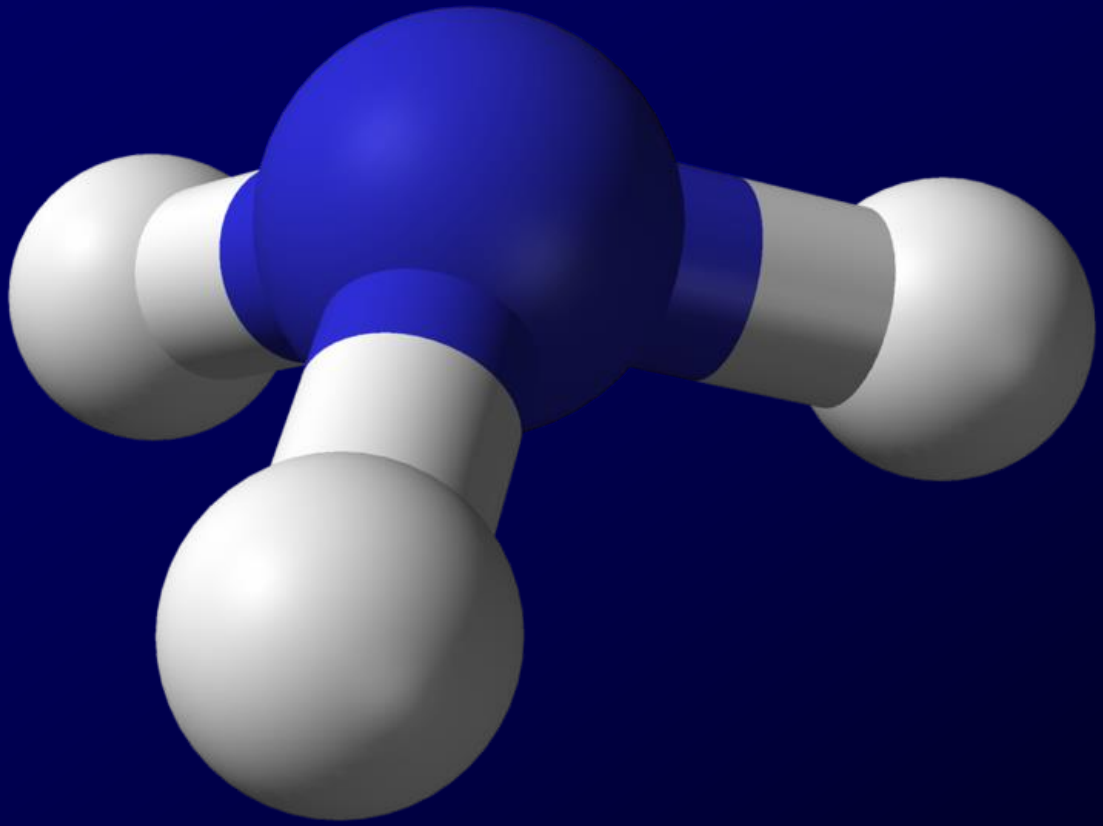


Opacity Wizard tool by Caroline Morley, NASA AMES

The methane line list is also too big (35 billion lines) for line-by-line modeling

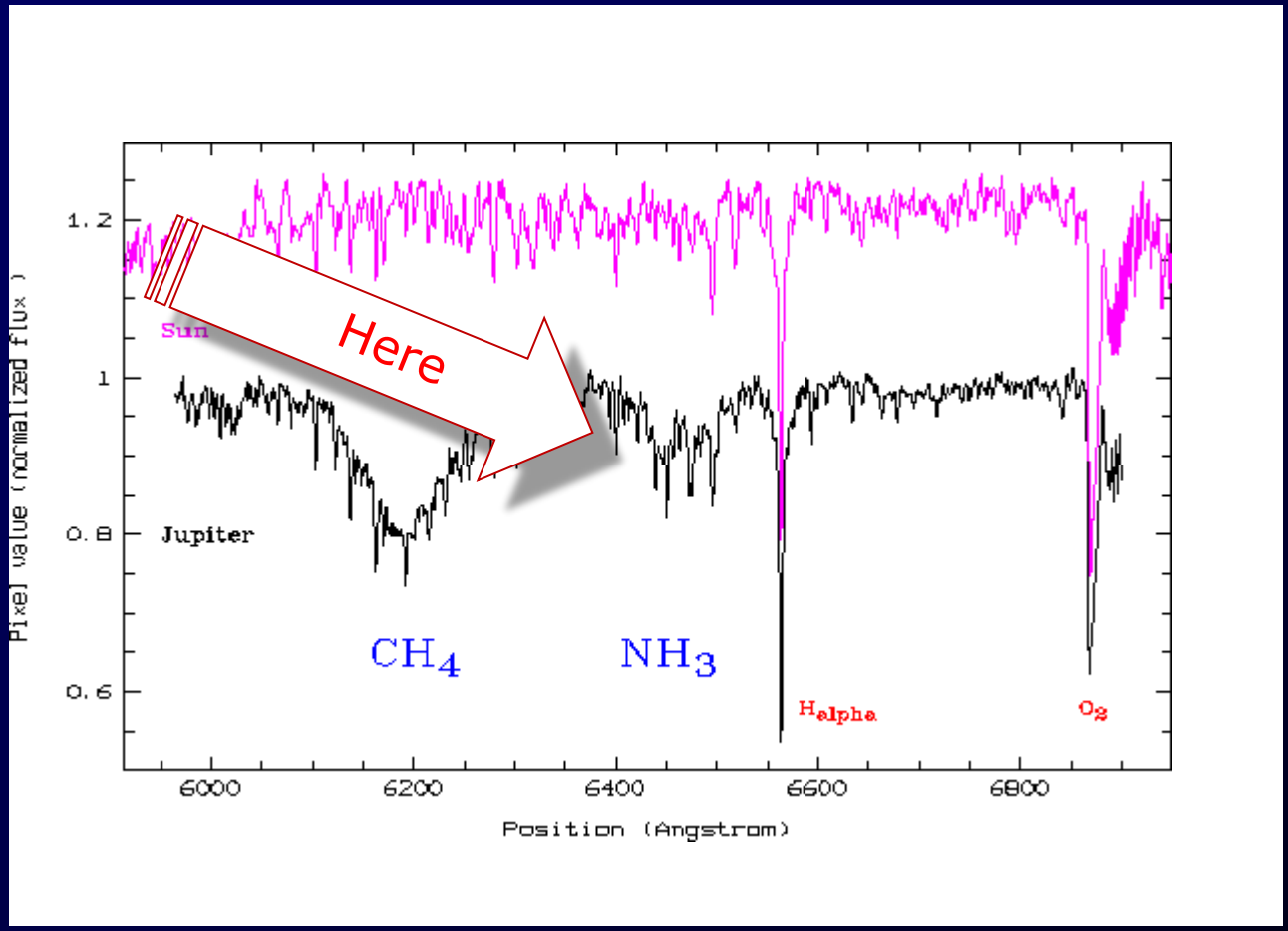
We are working on it
with help by
David Amundsen and Isabelle Baraffe

Ammonia (NH_3)



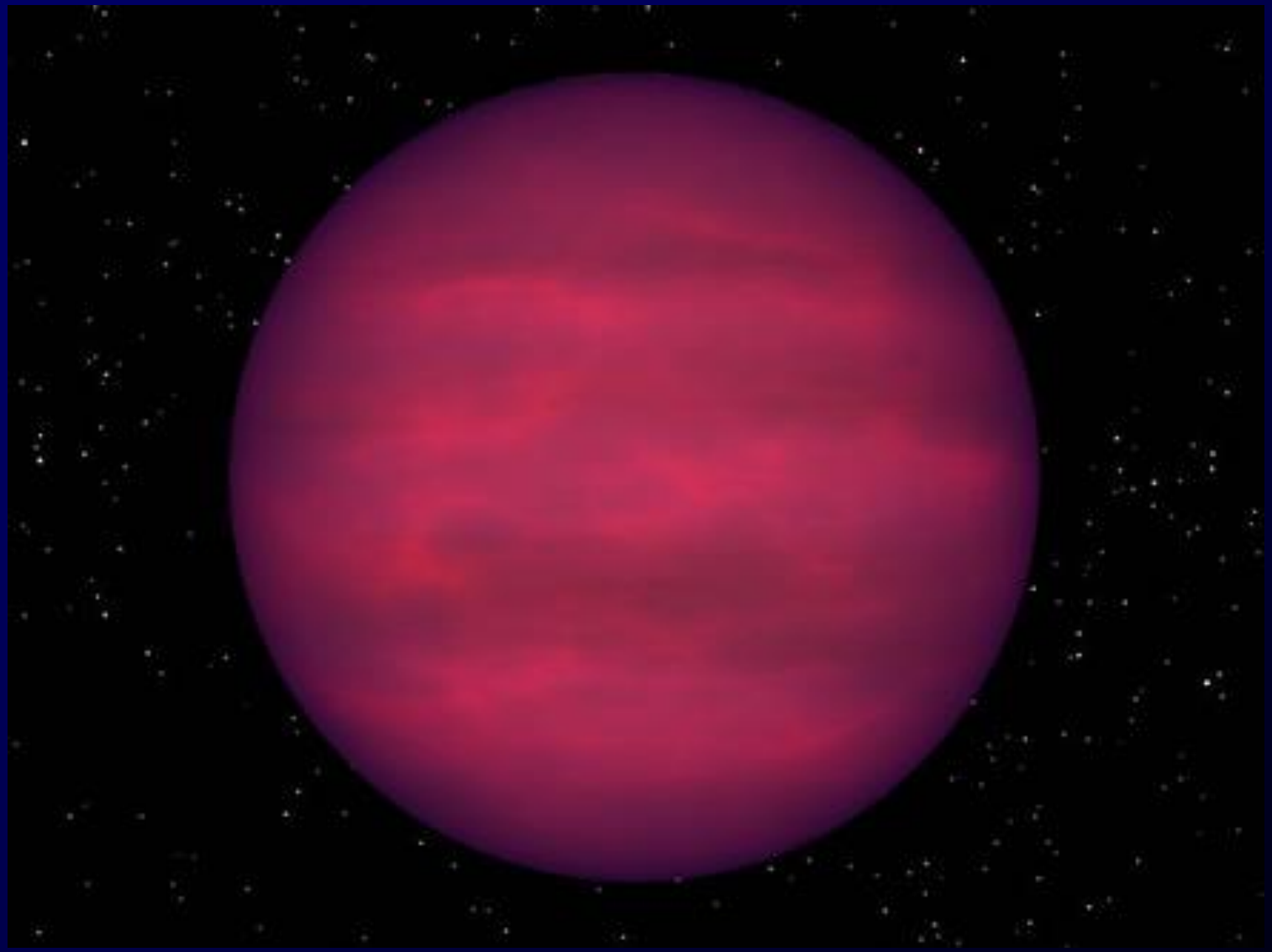
Ammonia (NH_3)

Known to be on Jupiter

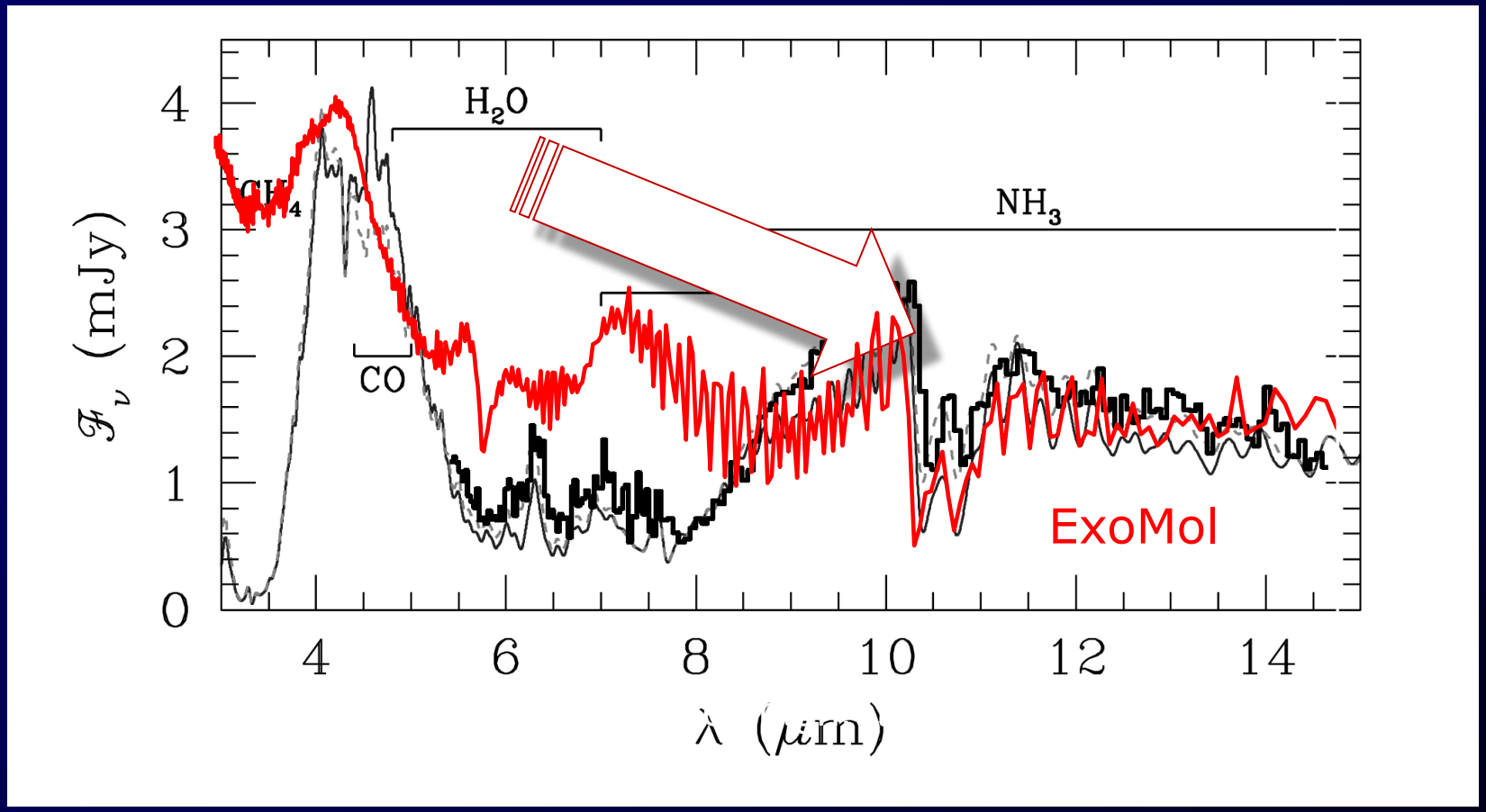

Here
Sun
Jupiter
CH_4
NH_3
H_{alpha}
O_2
1.2
1
0.8
0.6
6000
6200
6400
6600
6800
Position (Angstrom)
Pixel value (normalized flux)

Ammonia

Exiting detections on (cold)
Brown dwarfs



Here is an example of Dwarf Gl 570D by Adam Burgasser et al. (2003)



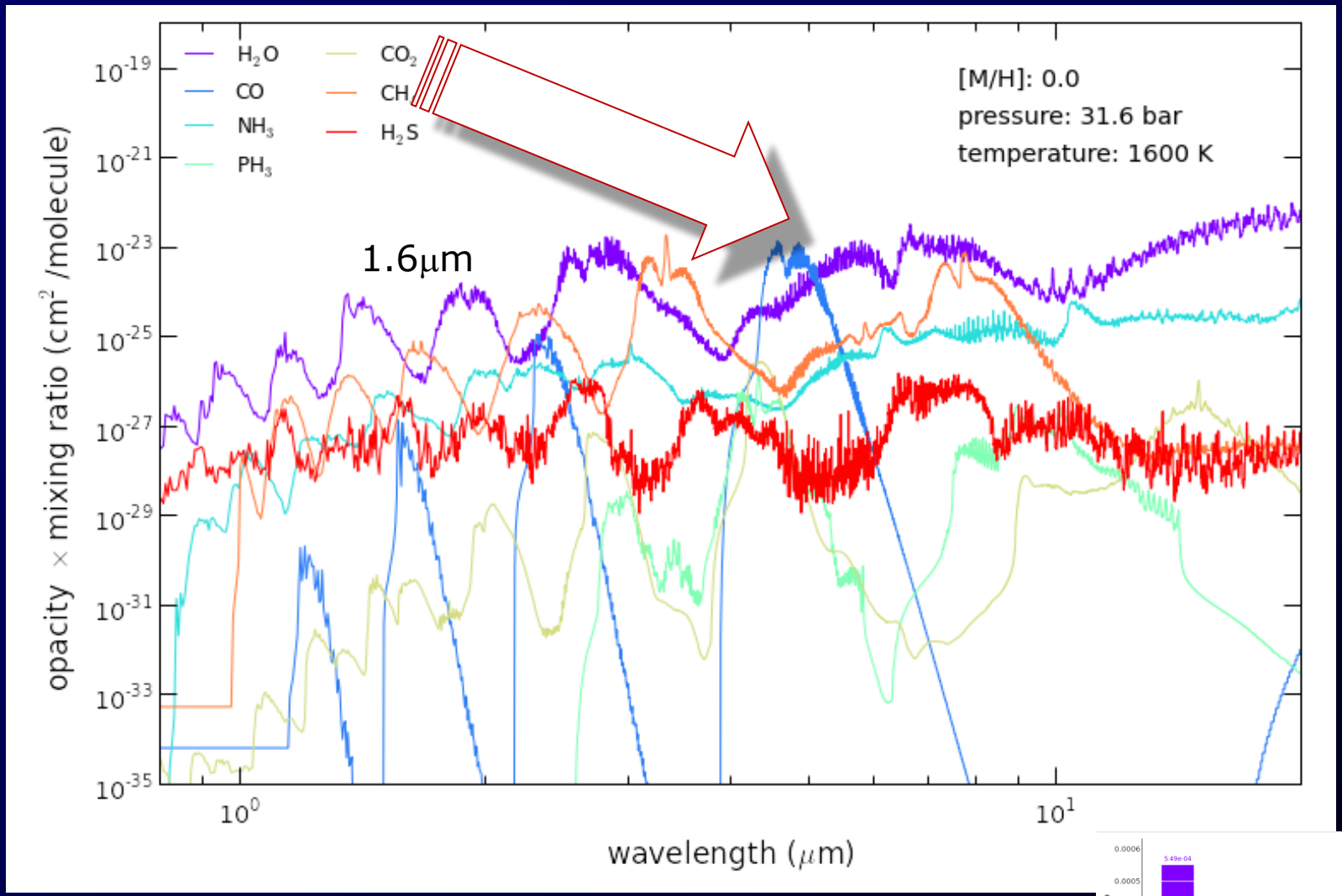
Together with model from the paper by Saumon ApJ (2006)

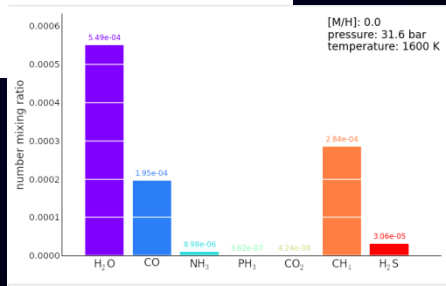
and ExoMol model on top, which agrees well for this region

Ammonia
ExoMol line list called BYTe
(1 billion transitions)

Ammonia
on exoplanets?

Why not? 11 μm feature is the most prominent





Opacity Wizard tool by Caroline Morley, NASA AMES

Other molecules

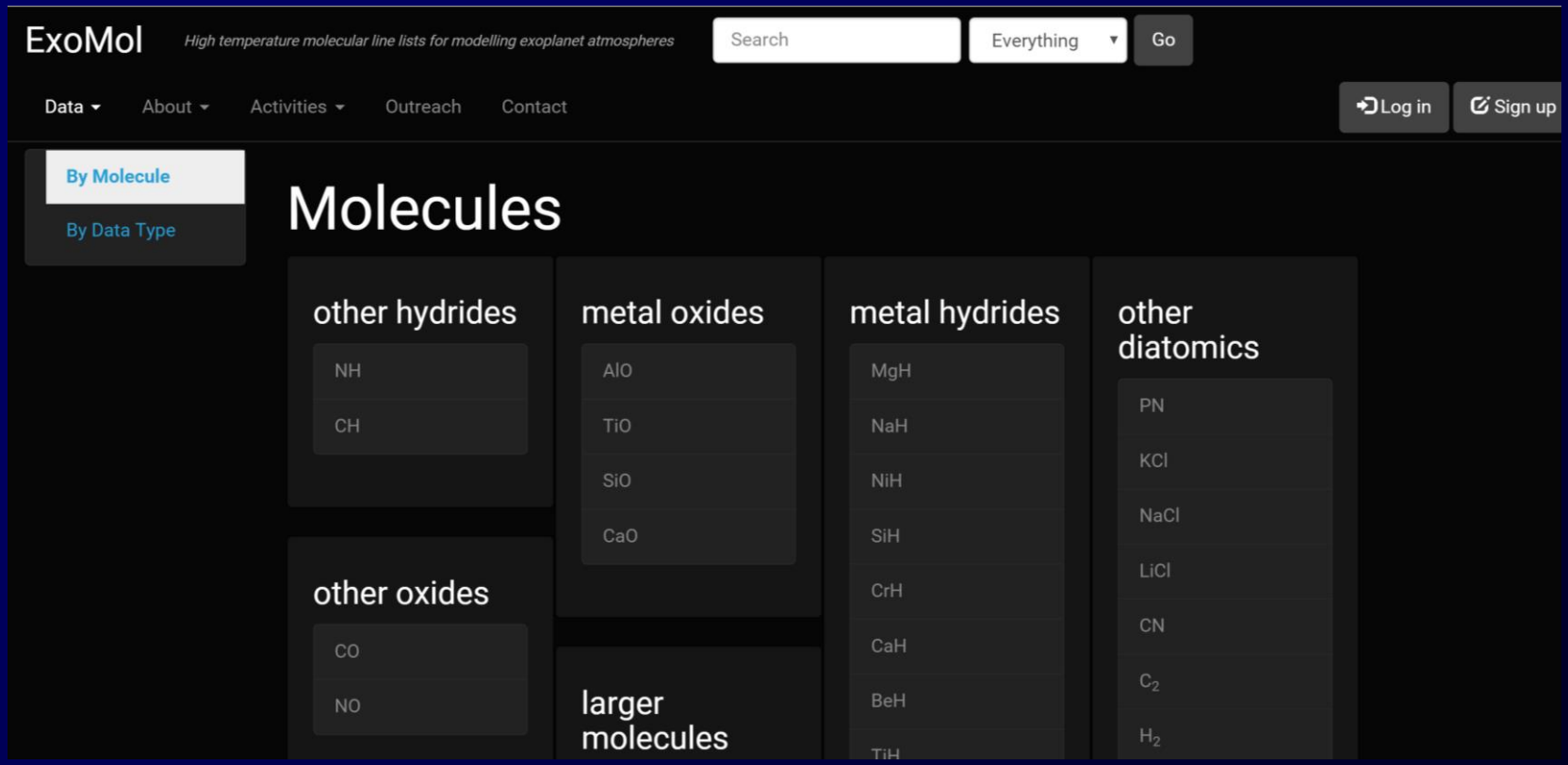
ExoMol TABLE

Molecular line lists for exoplanet & other atmospheres

ExoMol0: Tennyson and Yurchenko MNRAS (2012)

H_2	PH_3	AlO	AlH	C_3	HNO_3	PN	H_2S	CrH	ScH	Done
LiH	OH	SO_2	CH_3Cl	C_2	BeH	H_2S	KCl	HCN	HNC	
HeH^+	NO	SH	HCl	CH_4	NaCl	SiO	MgH	CH	CN	
H_3^+	O_3	H_2CO	HDO	H_2O	NH_3	CaH	SO_3	CO	CO_2	
H_2D^+	O_2	HOOH		TiO	VO	FeH	CaO	C_3	C_2H_2	To-Do
	NaH	BaO	VN	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
	P_2H_2	SO	HF		NiH	TiH	SiH	CH_3Cl	C_2H_6	
		PO				SiC		PS	C_3H_8	

ExoMol website will have a new look soon …

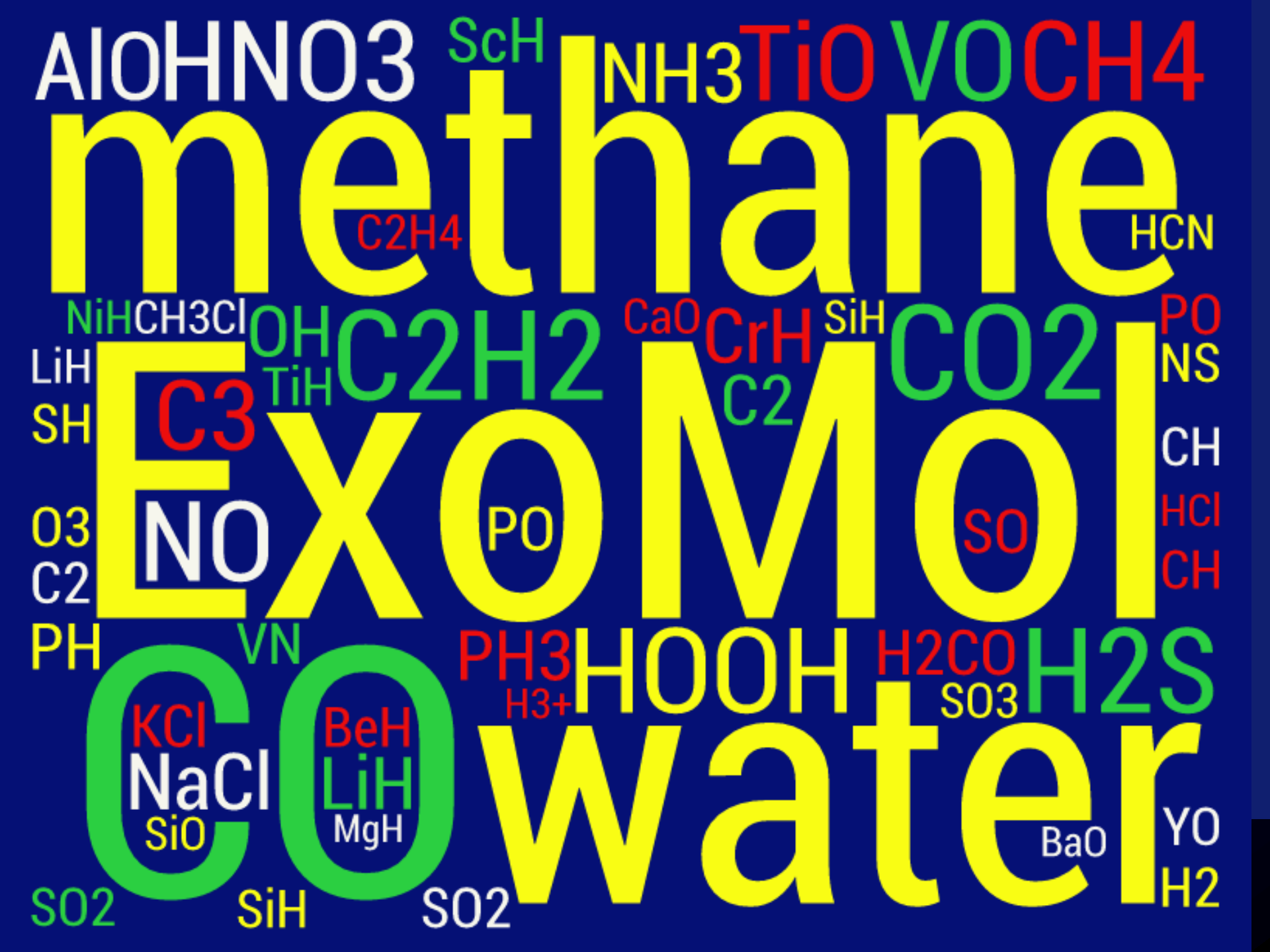

ExoMol
High temperature molecular line lists for modelling exoplanet atmospheres
Search
Everything
Go
Data
About
Activities
Outreach
Contact
Log in
Sign up
By Molecule
By Data Type
Molecules
other hydrides
NH
CH
metal oxides
AlO
TiO
SiO
CaO
metal hydrides
MgH
NaH
NiH
SiH
CrH
CaH
BeH
TiH
other diatomics
PN
KCl
NaCl
LiCl
CN
C_2
H_2
other oxides
CO
NO
larger molecules

ExoMol database with new features

1. Line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
5. K-tables
6. Lifetimes
7. Cooling functions

Constructed by these wonderful people

ExoMol: will known by their molecules


AlOHNO3
ScH
NH3
TiO
VO
CH4
methane
C2H4
HCN
NiH
CH3Cl
OH
C2H2
CaO
CrH
SiH
CO2
PO
LiH
TiH
C2
NS
SH
C3
ExoMol
CH
O3
NO
PO
SO
HCl
C2
CH
PH
VN
PH3
HOOH
H2CO
H2S
H3+
SO3
CO
KCl
NaCl
SiO
BeH
LiH
MgH
water
BaO
YO
H2
SO2
SiH
SO2