UCL

ExoMol

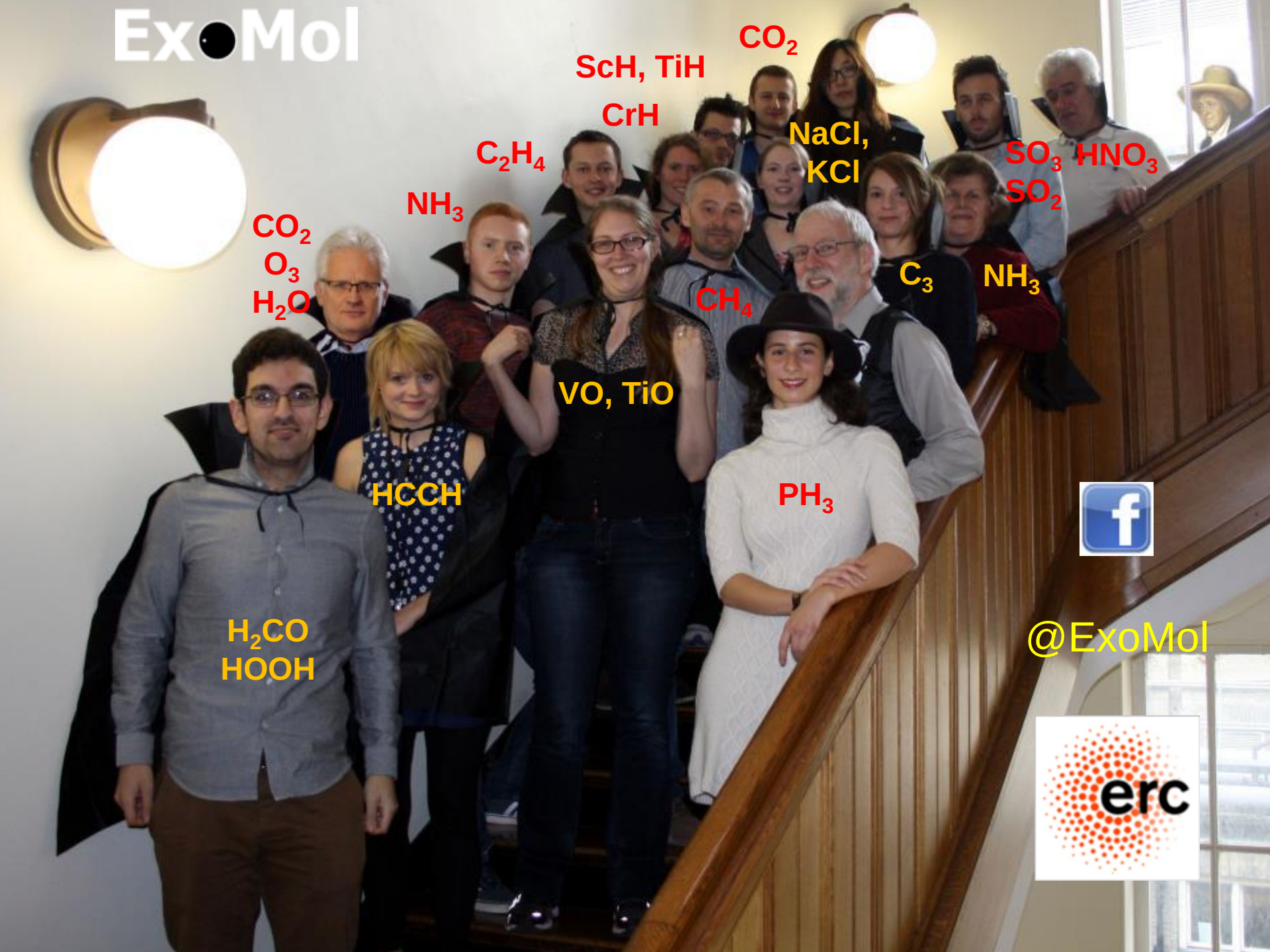
The ExoMol project: progress and perspective

Sergey Yurchenko


Science & Technology
Facilities Council


erc
European Research Council
Established by the European Commission


ExoMol
www.exomol.com
@ExoMol
erc


ExoMol
CO_2
ScH, TiH
CrH
C_2H_4
NaCl,
KCl
SO_3
HNO_3
SO_2
NH_3
CO_2
O_3
H_2O
C_3
NH_3
CH_4
VO, TiO
HCCH
PH_3
H_2CO
HOOH
@ExoMol
erc


ExoMol
Emma Barton
Emil Zak
"Zoe" Na
Anatoly Pavlyuchko
Lorenzo Lodi
Maire Gorman
Andrey Yachmenev
Dan Underwood
Phillip Coles
Afaf Al-Derzi
Renia Diamantopoulou
Oleg Polyansky
Sergey Yurchenko
Laura McKemmish
Katy Chubb
Clara Sousa-Silva
Ahmed Al-Refaie
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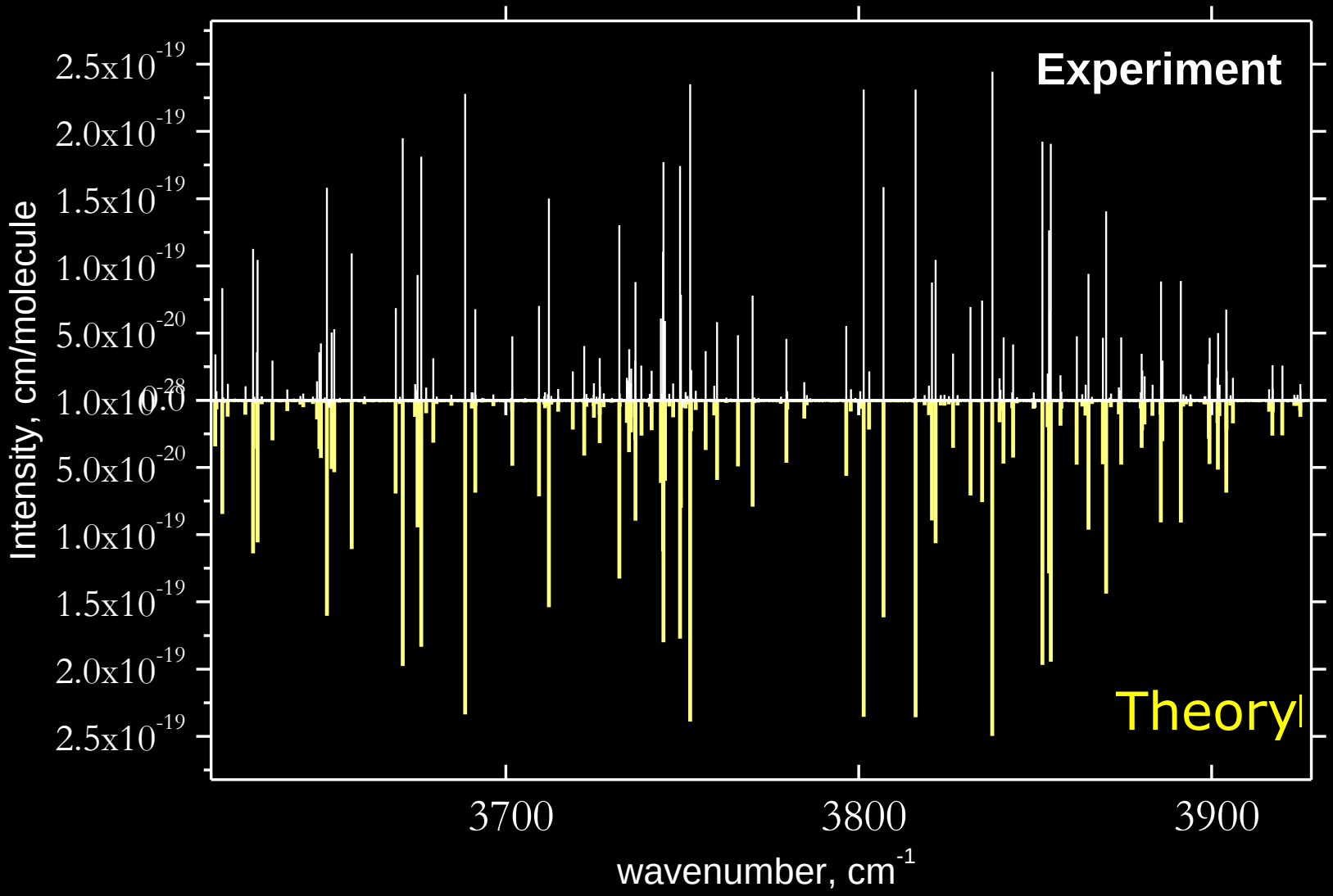
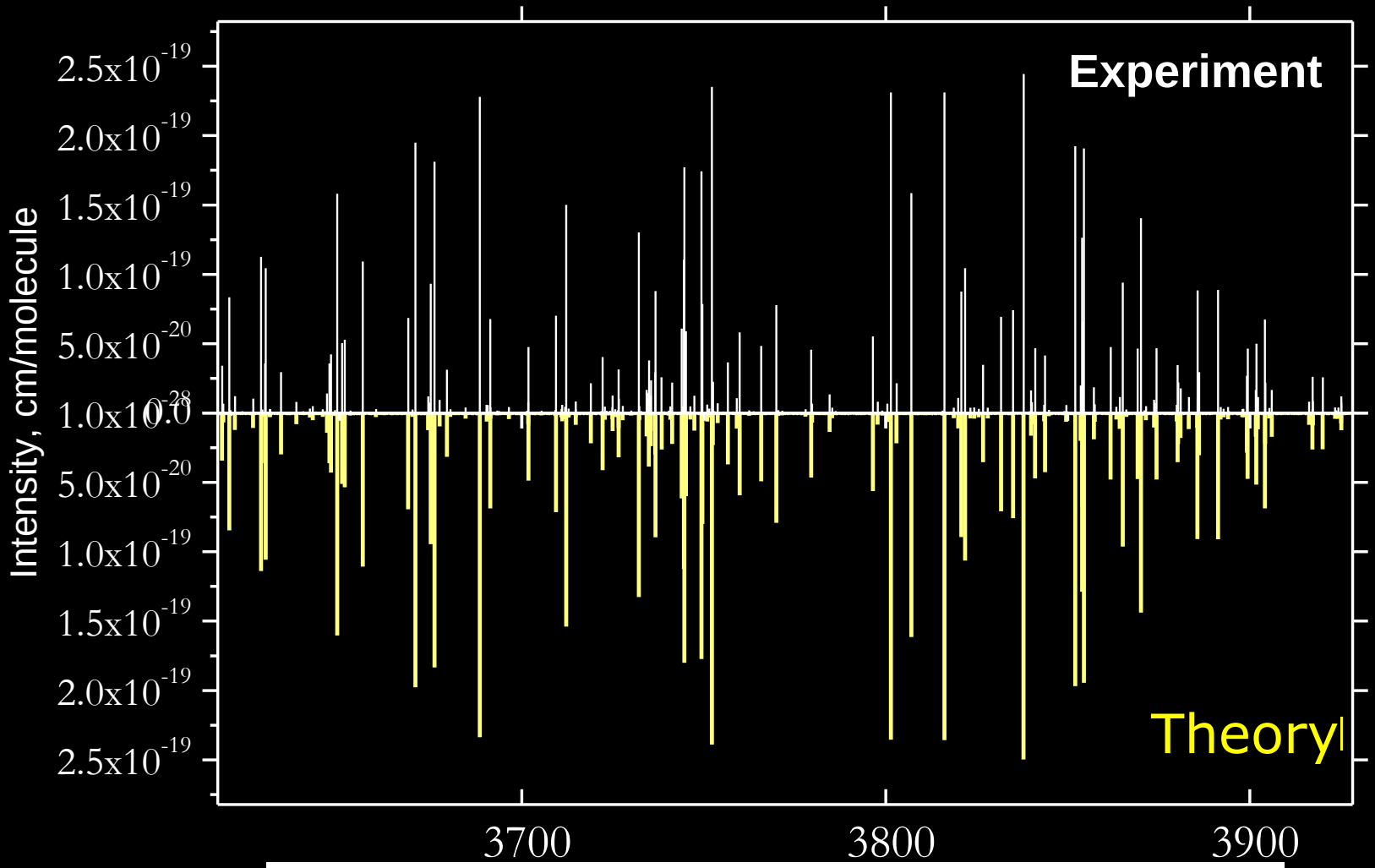
Theoretical spectroscopy



Theoretical spectroscopy



This is our 2018-line list for water

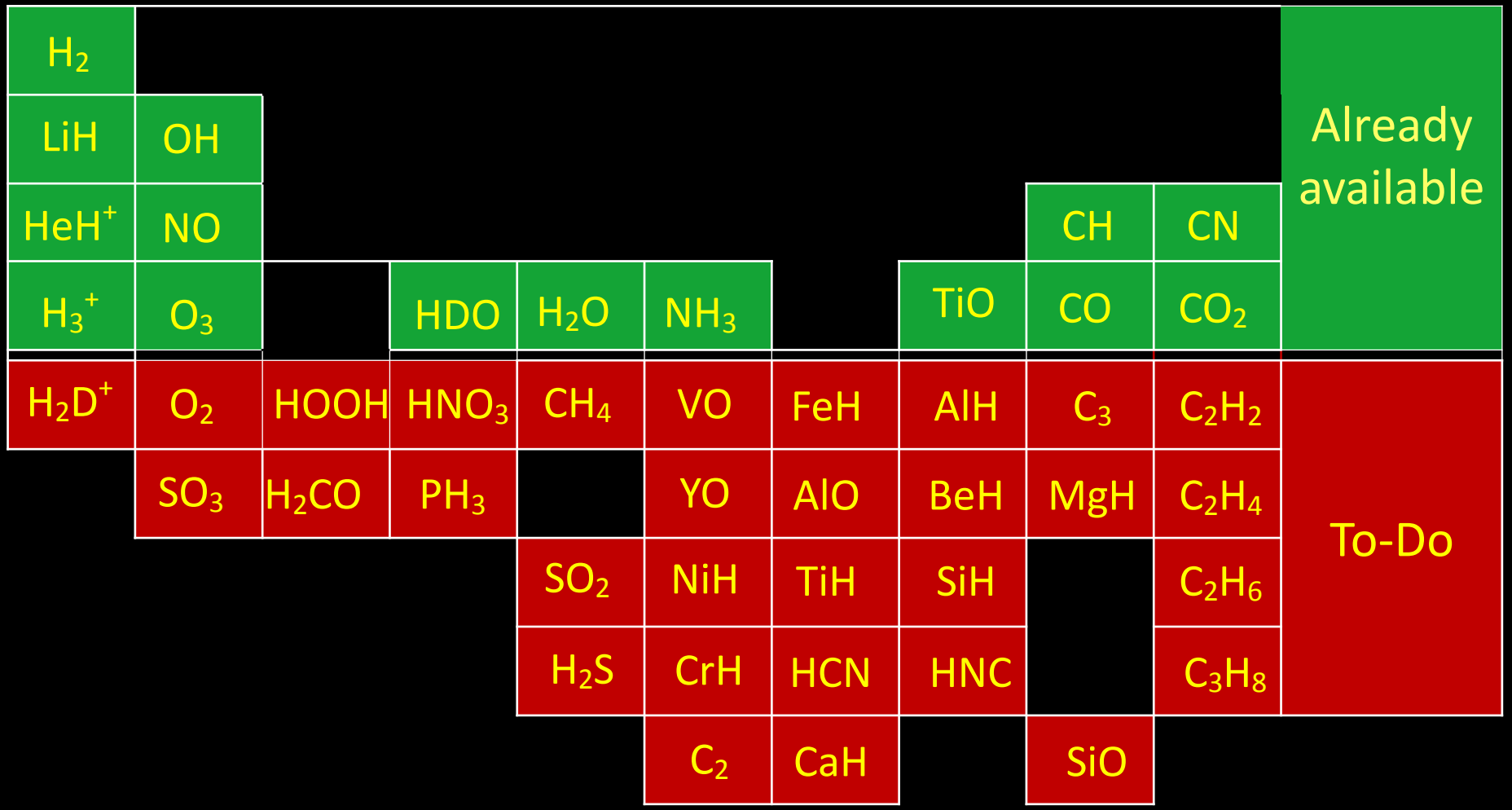
We have constructed an efficient machinery for accurate production of molecular spectra

We have constructed an efficient machinery for accurate production of molecular spectra

for atmospheric applications (stars and exoplantes)

This is where we started

2011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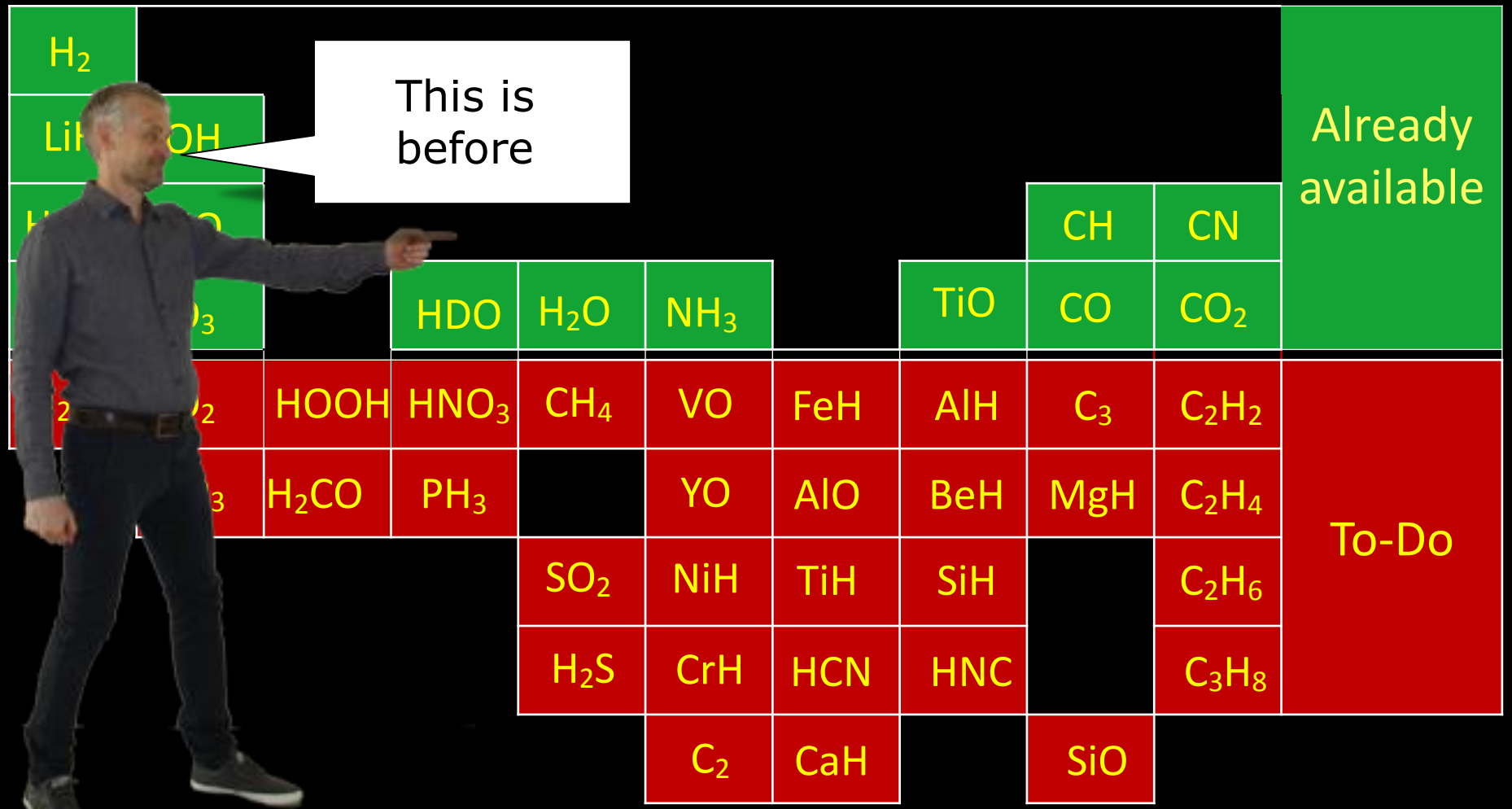
LiH
OH
HeH^+
NO
CH
CN
H_3^+
O_3
HDO
H_2O
NH_3
TiO
CO
CO_2
Already available
H_2D^+
O_2
HOOH
HNO_3
CH_4
VO
FeH
AlH
C_3
C_2H_2
SO_3
H_2CO
PH_3
YO
AlO
BeH
MgH
C_2H_4
SO_2
NiH
TiH
SiH
C_2H_6
H_2S
CrH
HCN
HNC
C_3H_8
To-Do
C_2
CaH
SiO

2011


H_2
LiH
OH
O_3
O_2
H_3
This is before
HDO
H_2O
NH_3
TiO
CH
CN
CO
CO_2
Already available
HOOH
HNO_3
CH_4
VO
FeH
AlH
C_3
C_2H_2
H_2CO
PH_3
YO
AlO
BeH
MgH
C_2H_4
To-Do
SO_2
NiH
TiH
SiH
C_2H_6
H_2S
CrH
HCN
HNC
C_3H_8
C_2
CaH
SiO

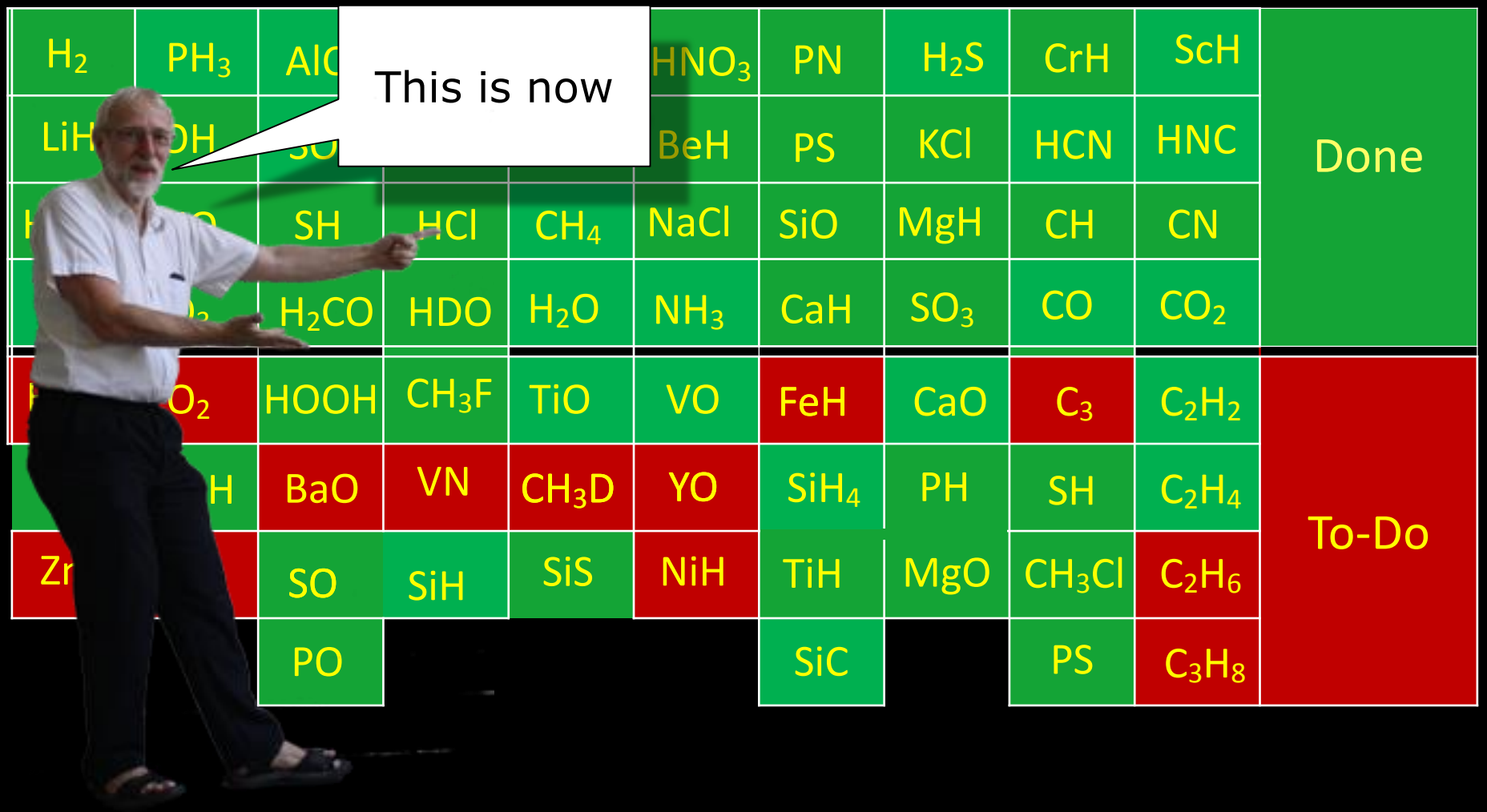
2018

ExoMol

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	Done
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	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	CH_3F	TiO	VO	FeH	CaO	C_3	C_2H_2	To-Do
NS	NaH	BaO	VN	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
ZnS	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6	
		PO				SiC		PS	C_3H_8	

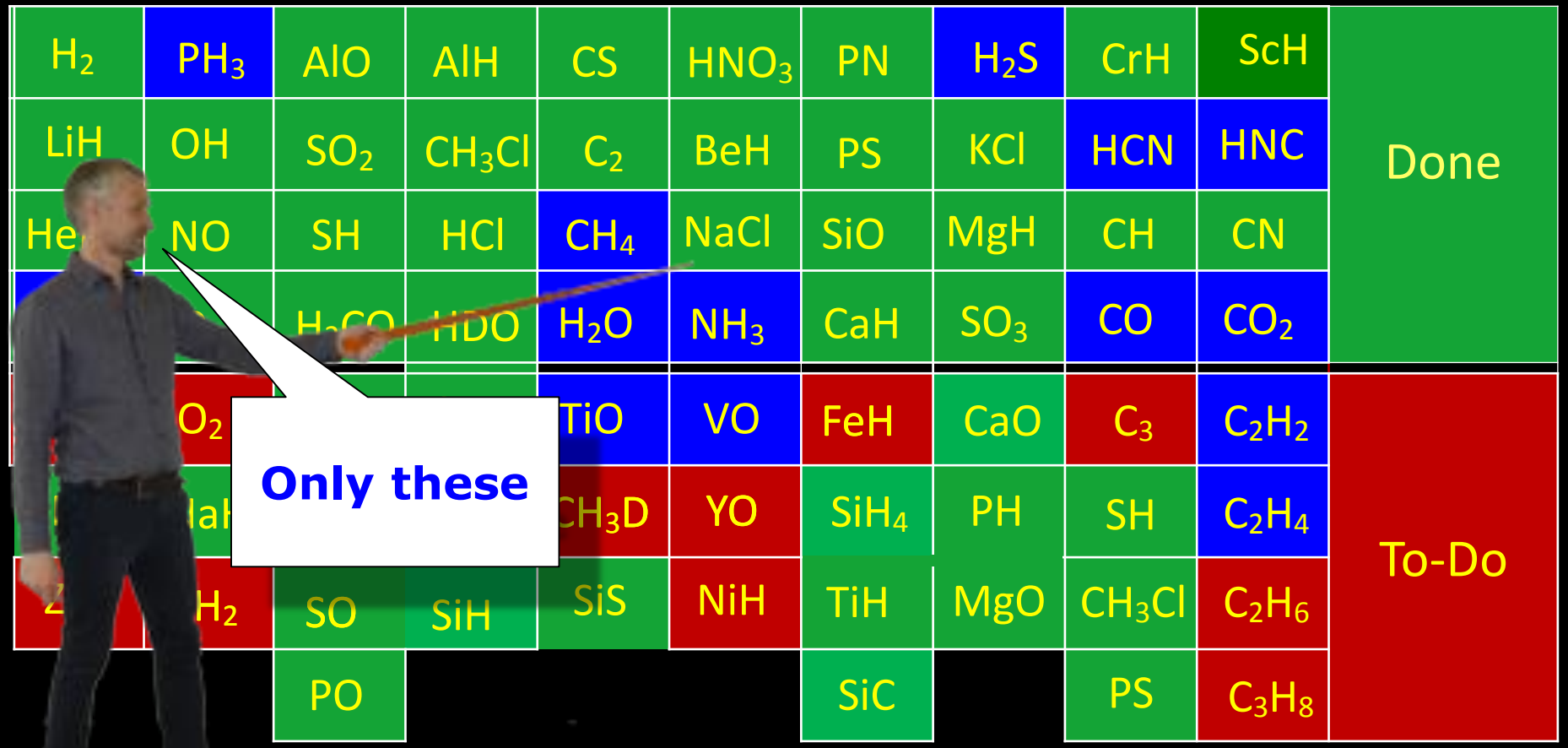
2018

ExoMol


This is now
H_2
PH_3
AlO
HNO_3
PN
H_2S
CrH
ScH
LiH
OH
BeH
PS
KCl
HCN
HNC
SH
HCl
CH_4
NaCl
SiO
MgH
CH
CN
H_2CO
HDO
H_2O
NH_3
CaH
SO_3
CO
CO_2
O_2
HOOH
CH_3F
TiO
VO
FeH
CaO
C_3
C_2H_2
H
BaO
VN
CH_3D
YO
SiH_4
PH
SH
C_2H_4
Zr
SO
SiH
SiS
NiH
TiH
MgO
CH_3Cl
C_2H_6
PO
SiC
PS
C_3H_8
Done
To-Do

Not all of them are actively used for retrievals yet

ExoMol 2018


H2
PH3
AlO
AlH
CS
HNO3
PN
H2S
CrH
ScH
LiH
OH
SO2
CH3Cl
C2
BeH
PS
KCl
HCN
HNC
Done
He
NO
SH
HCl
CH4
NaCl
SiO
MgH
CH
CN
H2CO
HDO
H2O
NH3
CaH
SO3
CO
CO2
O2
TiO
VO
FeH
CaO
C3
C2H2
Only these
CH3D
YO
SiH4
PH
SH
C2H4
H2
SO
SiH
SiS
NiH
TiH
MgO
CH3Cl
C2H6
To-Do
PO
SiC
PS
C3H8

Which is a shame

For example, consider hot rocky planets

Lava-planets

Post impact plalnets

… with atmospheres
(according to models)
consisting of vaporised water
and vaporised rocks

… the material will evaporate

… the material will evaporate

and block the emission from the object

… the material will evaporate

and block the emission from the object

at some specific wavelengths

… with a lot of other species predicted

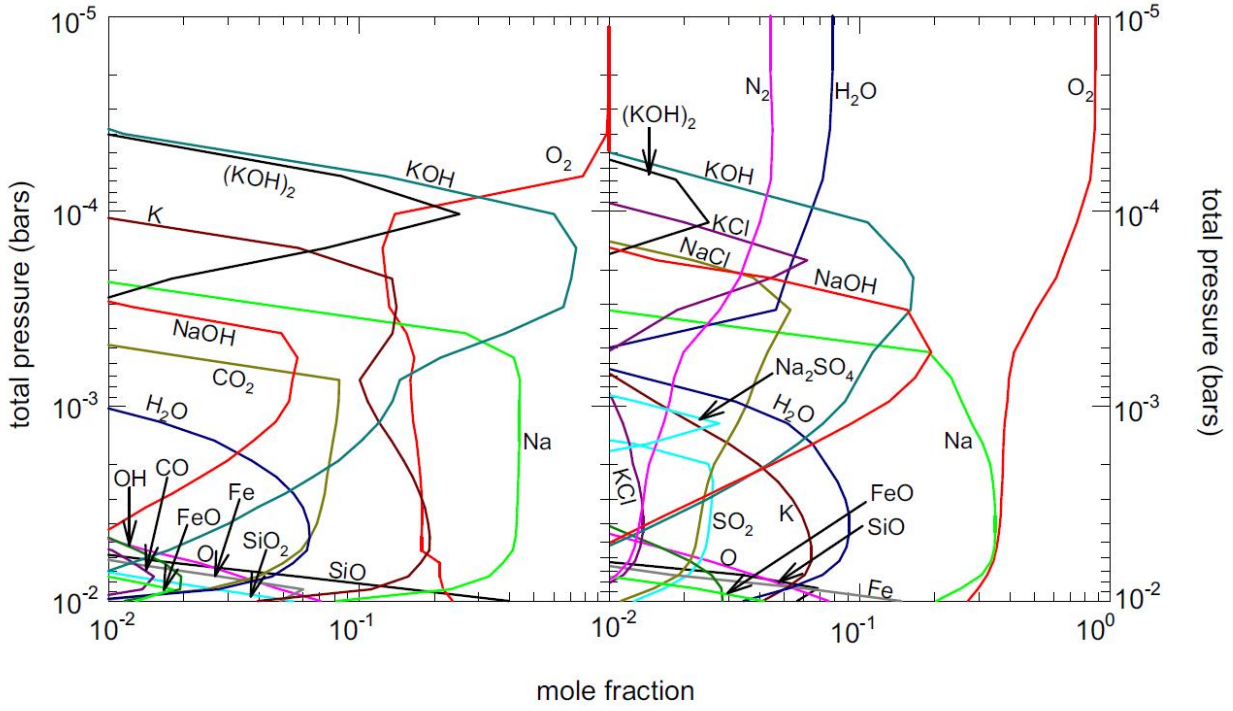


Figure 1: Atmospheric composition for a planet similar to CoRoT-7b. Starting compositions were taken for the continental crust (left) and the bulk silicate Earth (right) at 2500 K and 10^{-2} bars. Reproduced with permission from Schaefer *et al.*[42].

L. Schaefer, K. Lodders, B. Fegley, Jr., Vaporization of the earth: 55 Application to exoplanet atmospheres, Astrophys. J. 755 (2012) 41.

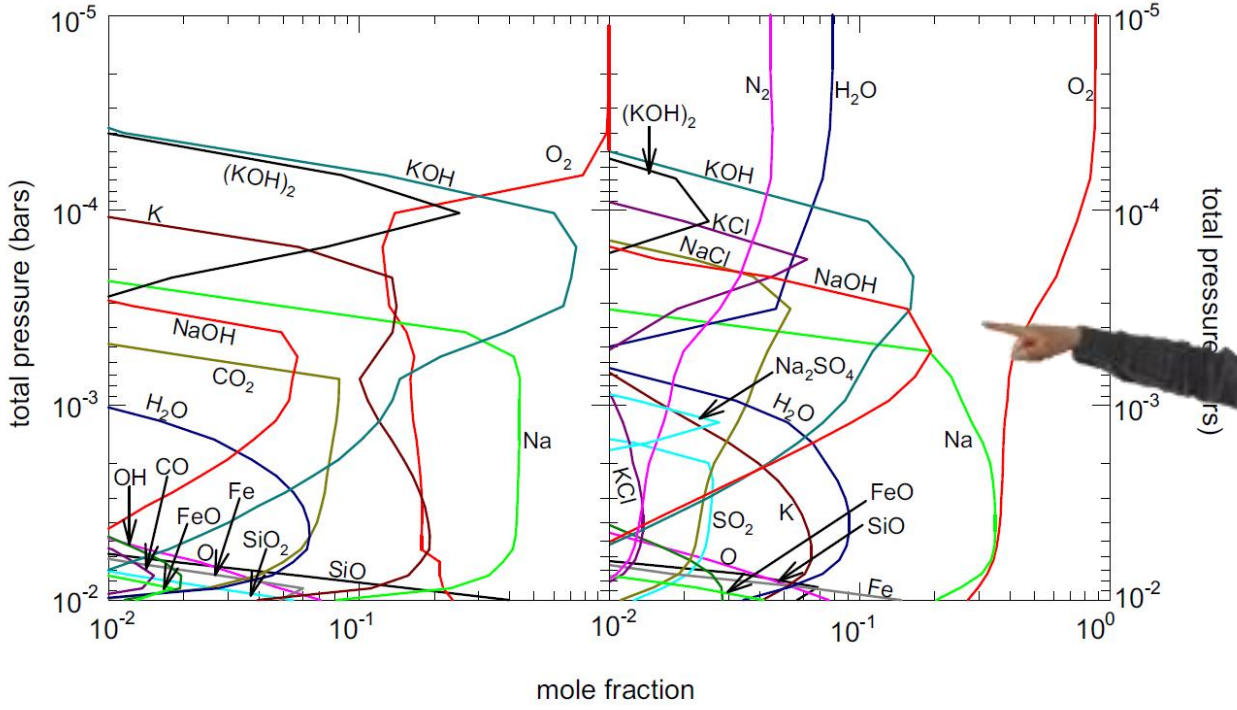
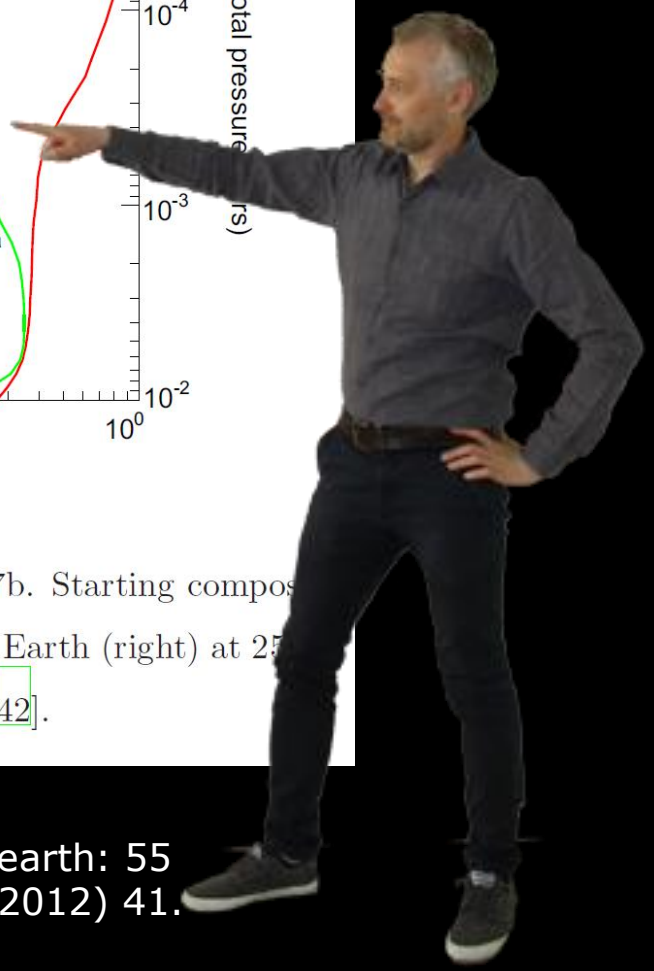


Figure 1: Atmospheric composition for a planet similar to CoRoT-7b. Starting compos
tions were taken for the continental crust (left) and the bulk silicate Earth (right) at 25
K and 10^{-2} bars. Reproduced with permission from Schaefer *et al.*[42].



L. Schaefer, K. Lodders, B. Fegley, Jr., Vaporization of the earth: 55
Application to exoplanet atmospheres, Astrophys. J. 755 (2012) 41.

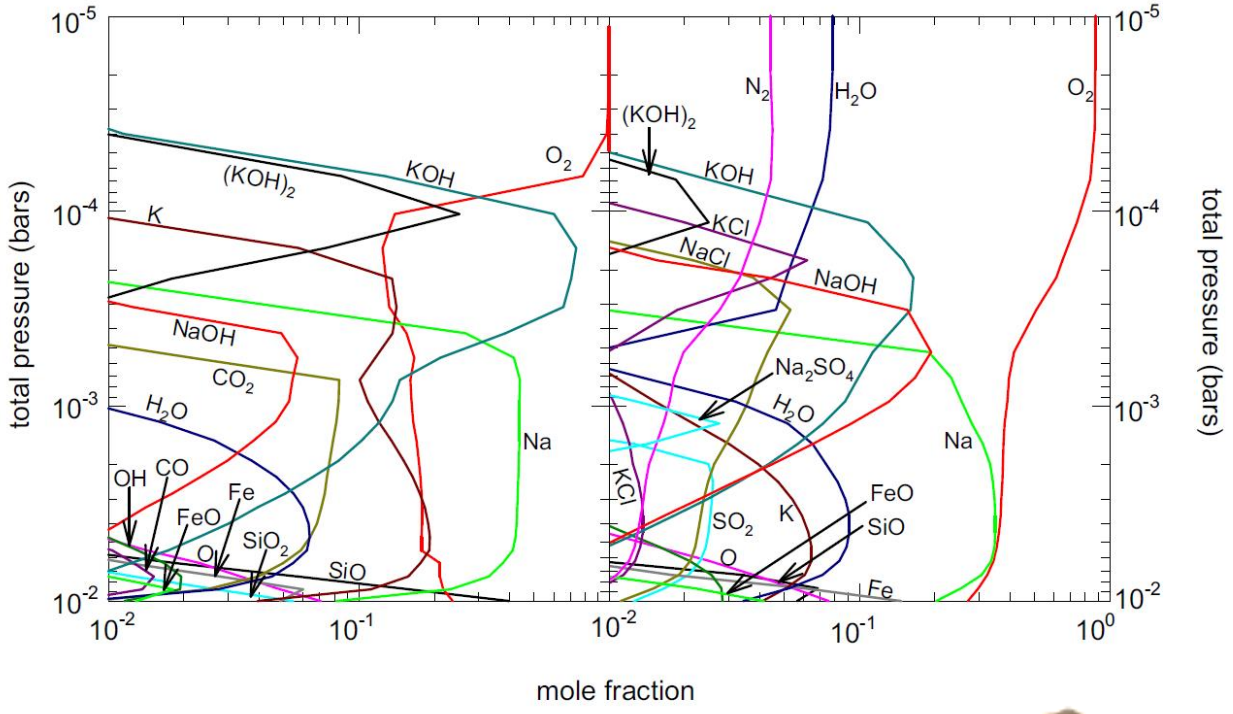


Figure 1: Atmospheric composition for a planet similar to CoRoT-7b. Starting compositions were taken for the continental crust (left) and the bulk silicate Earth (right) at 2500 K and 10^{-2} bars. Reproduced with permission from Schaefer *et al.*[42].

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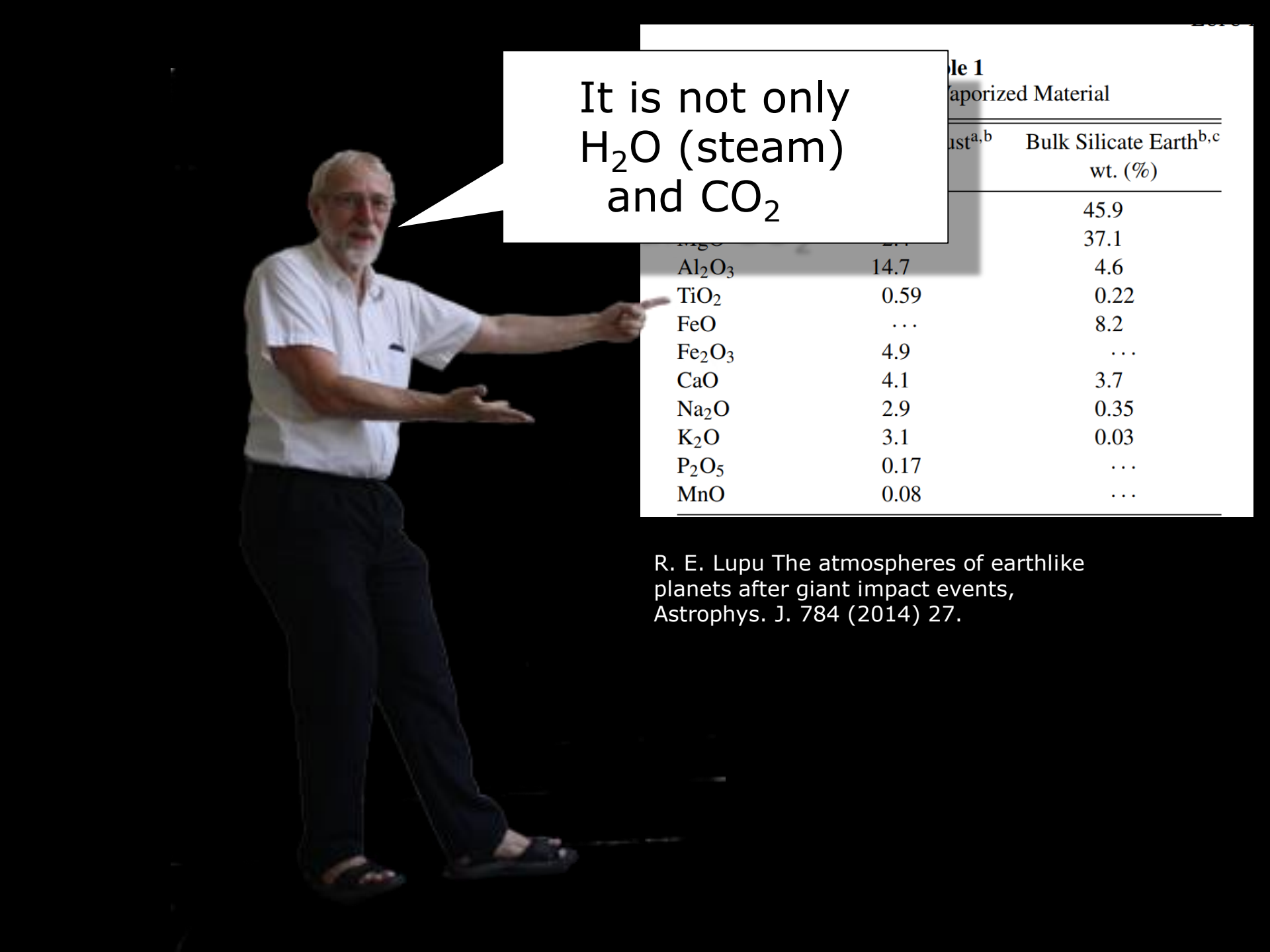
Hot rocky exoplanets

Table 1
Composition of Vaporized Material

Compound	Continental Crust[a,b] wt. (%)	Bulk Silicate Earth[b,c] wt. (%)
SiO_2	64.0	45.9
MgO	2.4	37.1
Al_2O_3	14.7	4.6
TiO_2	0.59	0.22
FeO	...	8.2
Fe_2O_3	4.9	...
CaO	4.1	3.7
Na_2O	2.9	0.35
K_2O	3.1	0.03
P_2O_5	0.17	...
MnO	0.08	...

R. E. Lupu The atmospheres of earthlike planets after giant impact events, Astrophys. J. 784 (2014) 27.



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Vaporized Material

ust[a,b]	Bulk Silicate Earth[b,c] wt. (%)
	45.9
	37.1
Al_2O_3 14.7	4.6
TiO_2 0.59	0.22
FeO ...	8.2
Fe_2O_3 4.9	...
CaO 4.1	3.7
Na_2O 2.9	0.35
K_2O 3.1	0.03
P_2O_5 0.17	...
MnO 0.08	...

R. E. Lupu The atmospheres of earthlike planets after giant impact events, Astrophys. J. 784 (2014) 27.

Example of 55 Cancri e

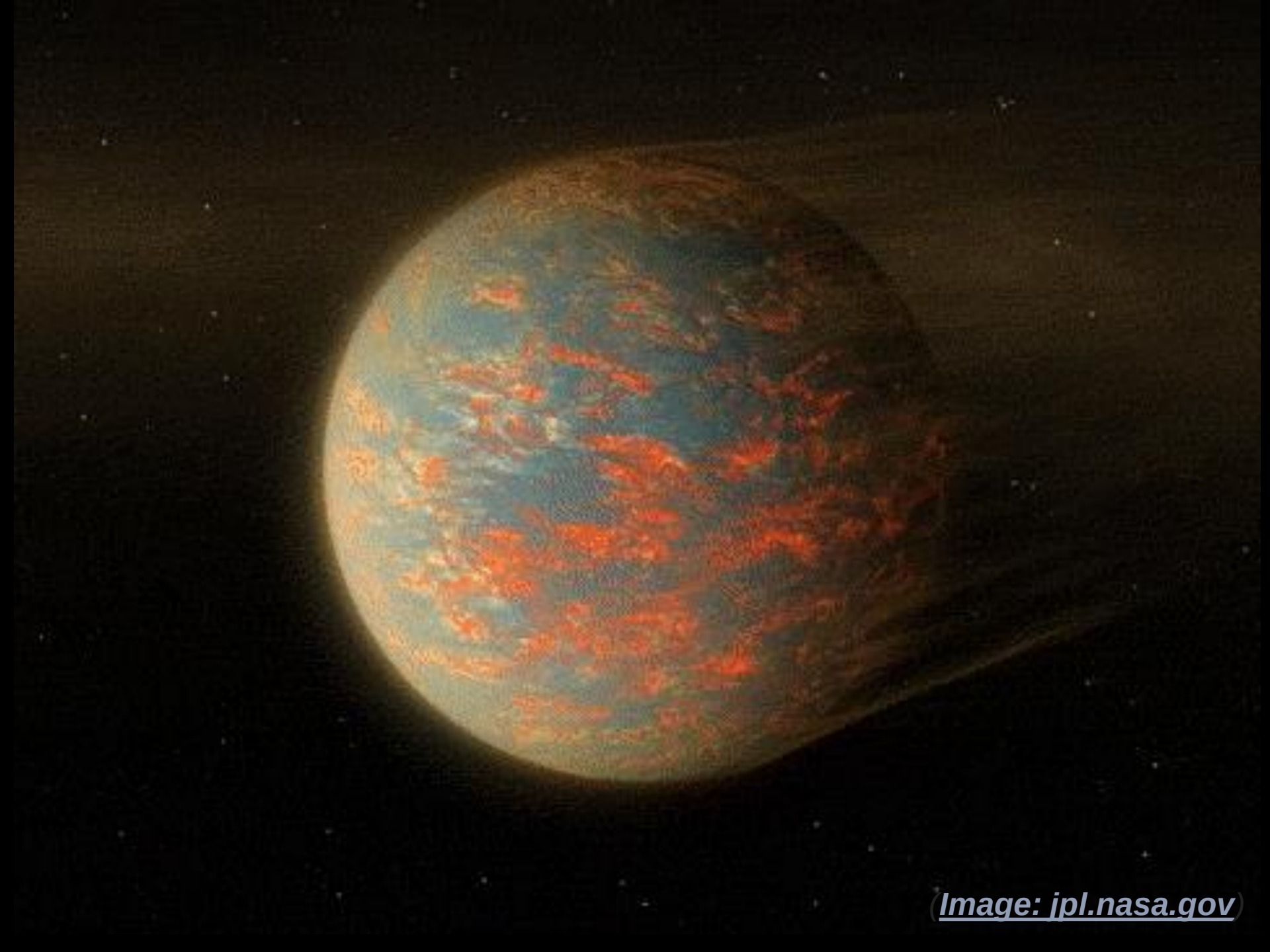

Image: jpl.nasa.gov

… attracted lots of exciting studies

LETTER

doi:10.1038/nature17169

A map of the large day–night temperature gradient of a super-Earth exoplanet

Brice-Olivier Demory[1], Michael Gillon[2], Julien de Wit[3], Nikku Madhusudhan[4], Emeline Bolmont[5], Kevin Heng[6], Tiffany Kataria[7], Nikole Lewis[8], Renyu Hu[9,10], Jessica Krick[11], Vlada Stamenković[9,10], Björn Benneke[10], Stephen Kane[12] & Didier Queloz[1]

Over the past decade, observations of giant exoplanets (Jupiter-

of the detector evolves with time and allows further improvement to the

Draft version October 11, 2017
Typeset using LaTeX **twocolumn** style in AASTeX61

LINKING THE CLIMATE AND THERMAL PHASE CURVE OF 55 CANCRI E

Mark Hammond[1] and Raymond Pierrehumbert[1]

[1] *University of Oxford*

(Accepted 10/10/17)

Submitted to ApJ

ABSTRACT

The thermal phase curve of 55 Cancri e is the first measurement of the temperature distribution of a tidally locked Super-Earth, but raises a number of puzzling questions about the planet's climate. The phase curve has a high

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Submitted to ApJ

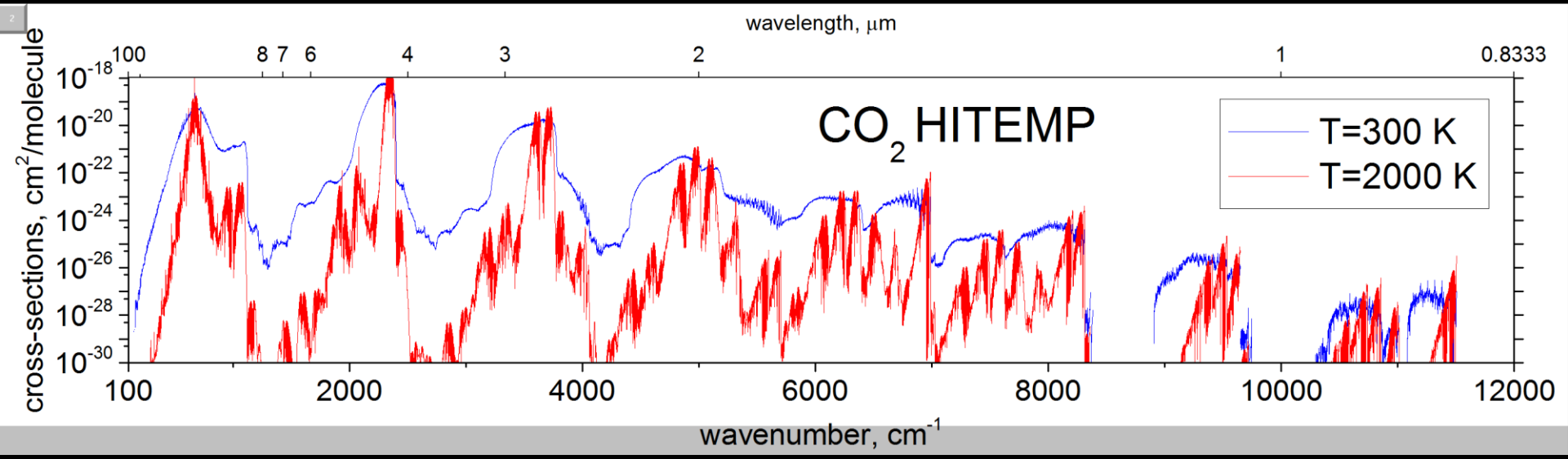
ABSTRACT

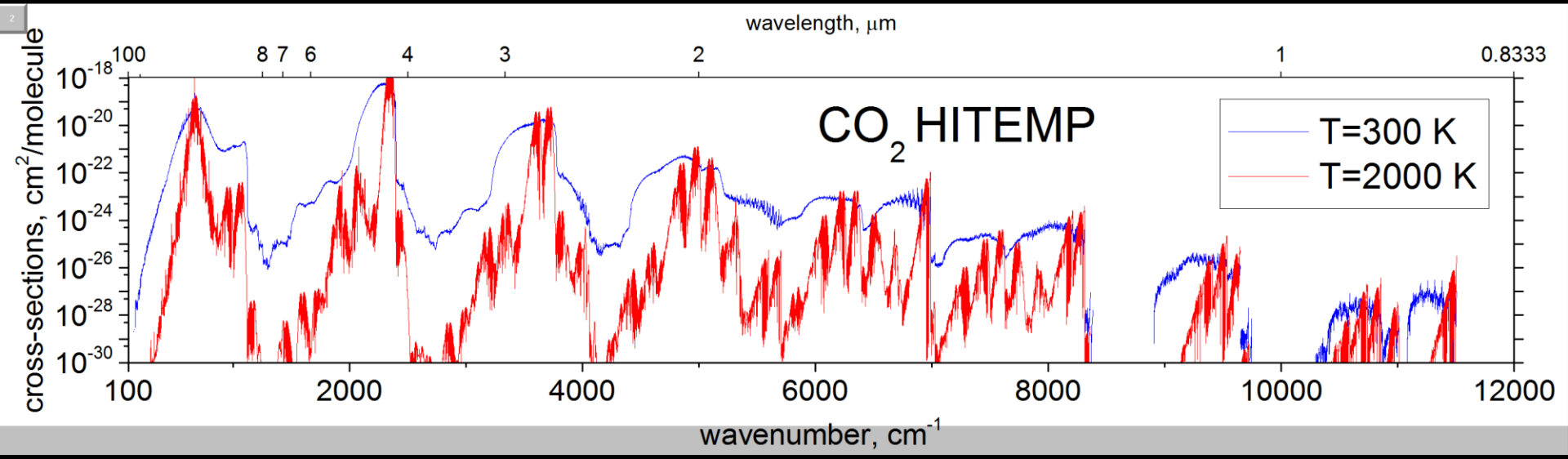
The thermal phase curve of 55 Cancri e is the first measurement of the temperature distribution of a tidally locked Super-Earth and raises a number of puzzling questions about the planet's climate. The phase curve has a high

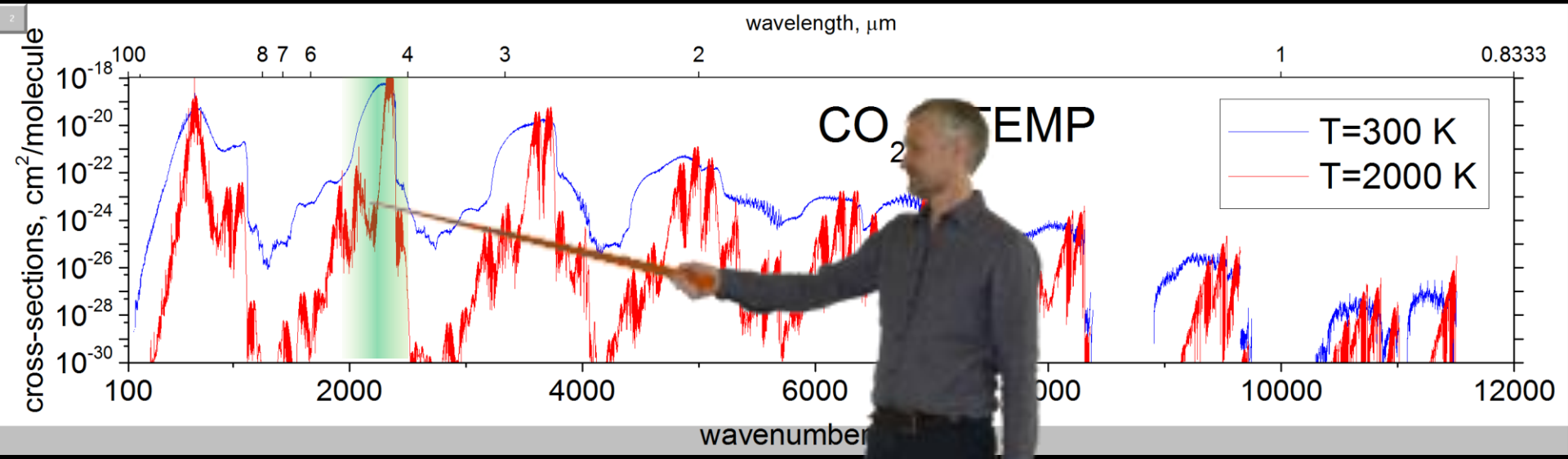
Largely based on the Spitzer photometry at 4.5 μm

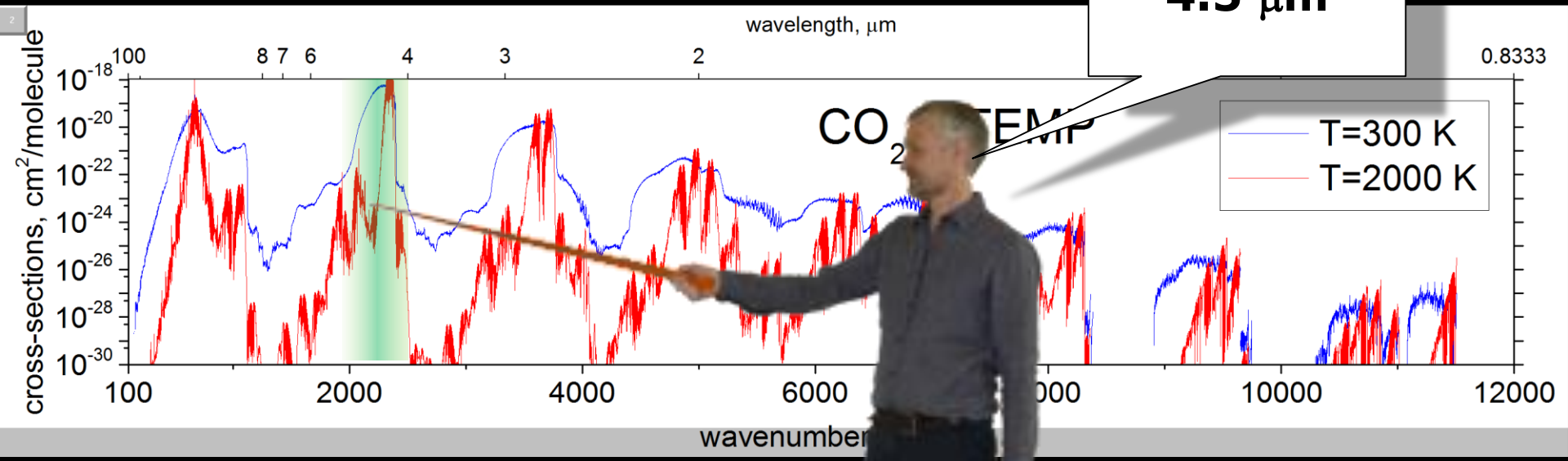
All those lava-planet molecules are ignored, except CO_2, H_2, H_2O

Well, the CO_2 band seems to be an obvious absorber in this region

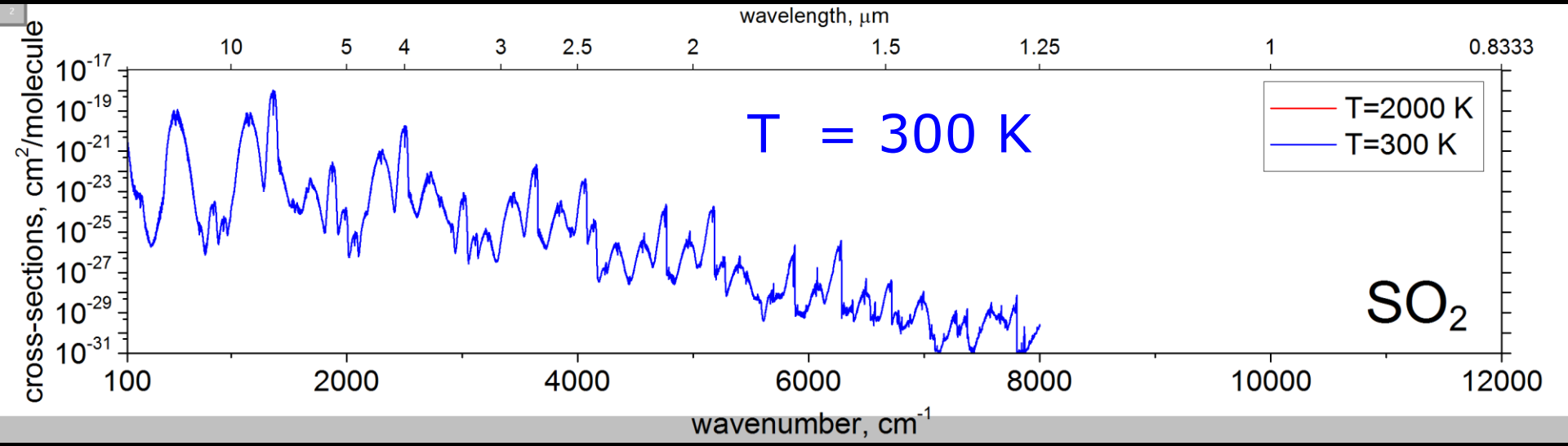

wavelength, μm
100
8 7 6
4
3
2
1
0.8333
cross-sections, cm²/molecule
10⁻¹⁸
10⁻²⁰
10⁻²²
10⁻²⁴
10⁻²⁶
10⁻²⁸
10⁻³⁰
CO2 HITEMP
T=300 K
T=2000 K
100
2000
4000
6000
8000
10000
12000
wavenumber, cm⁻¹

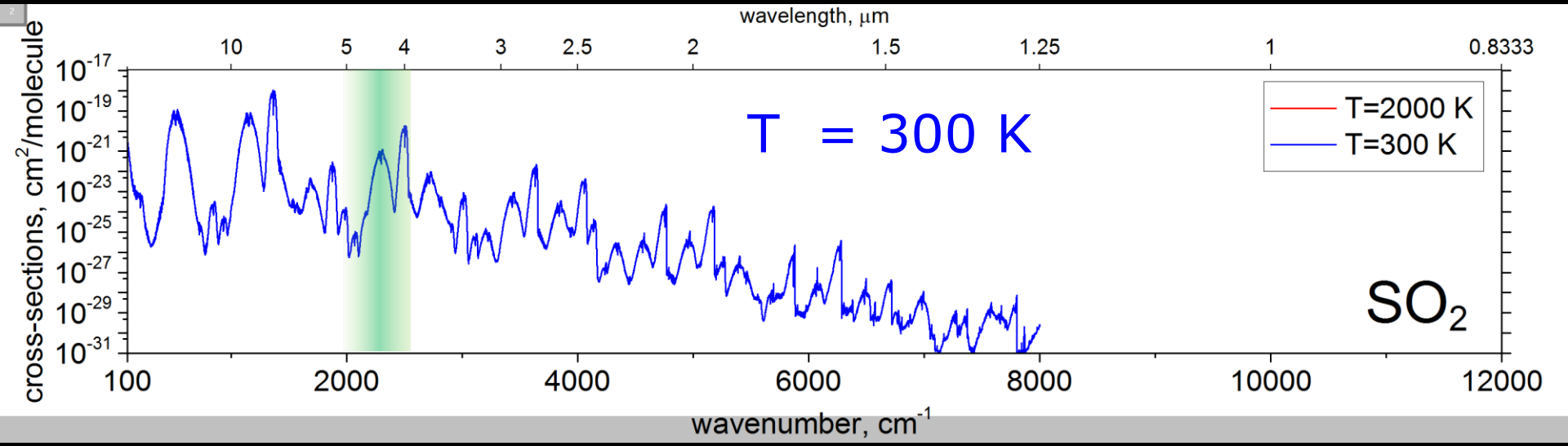

wavelength, μm
100
8 7 6
4
3
2
1
0.8333
cross-sections, cm²/molecule
10⁻¹⁸
10⁻²⁰
10⁻²²
10⁻²⁴
10⁻²⁶
10⁻²⁸
10⁻³⁰
CO2 HITEMP
T=300 K
T=2000 K
100
2000
4000
6000
8000
10000
12000
wavenumber, cm⁻¹

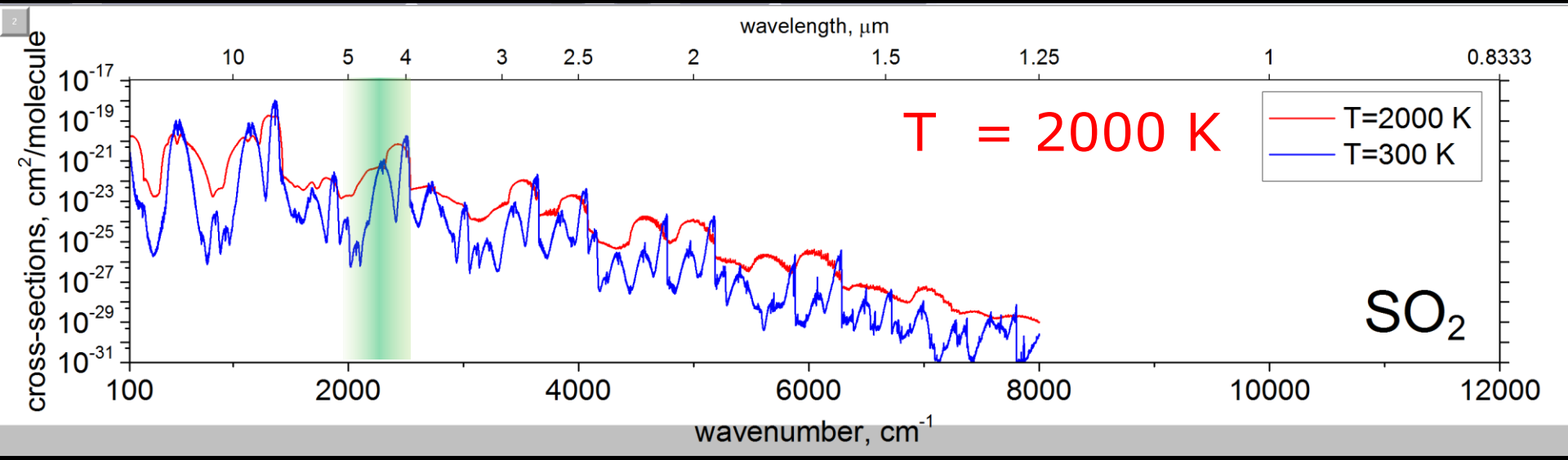

wavelength, μm
100
8 7 6
4
3
2
1
0.8333
cross-sections, cm²/molecule
10^-18
10^-20
10^-22
10^-24
10^-26
10^-28
10^-30
CO2 TEMP
T=300 K
T=2000 K
100
2000
4000
6000
10000
12000
wavenumber

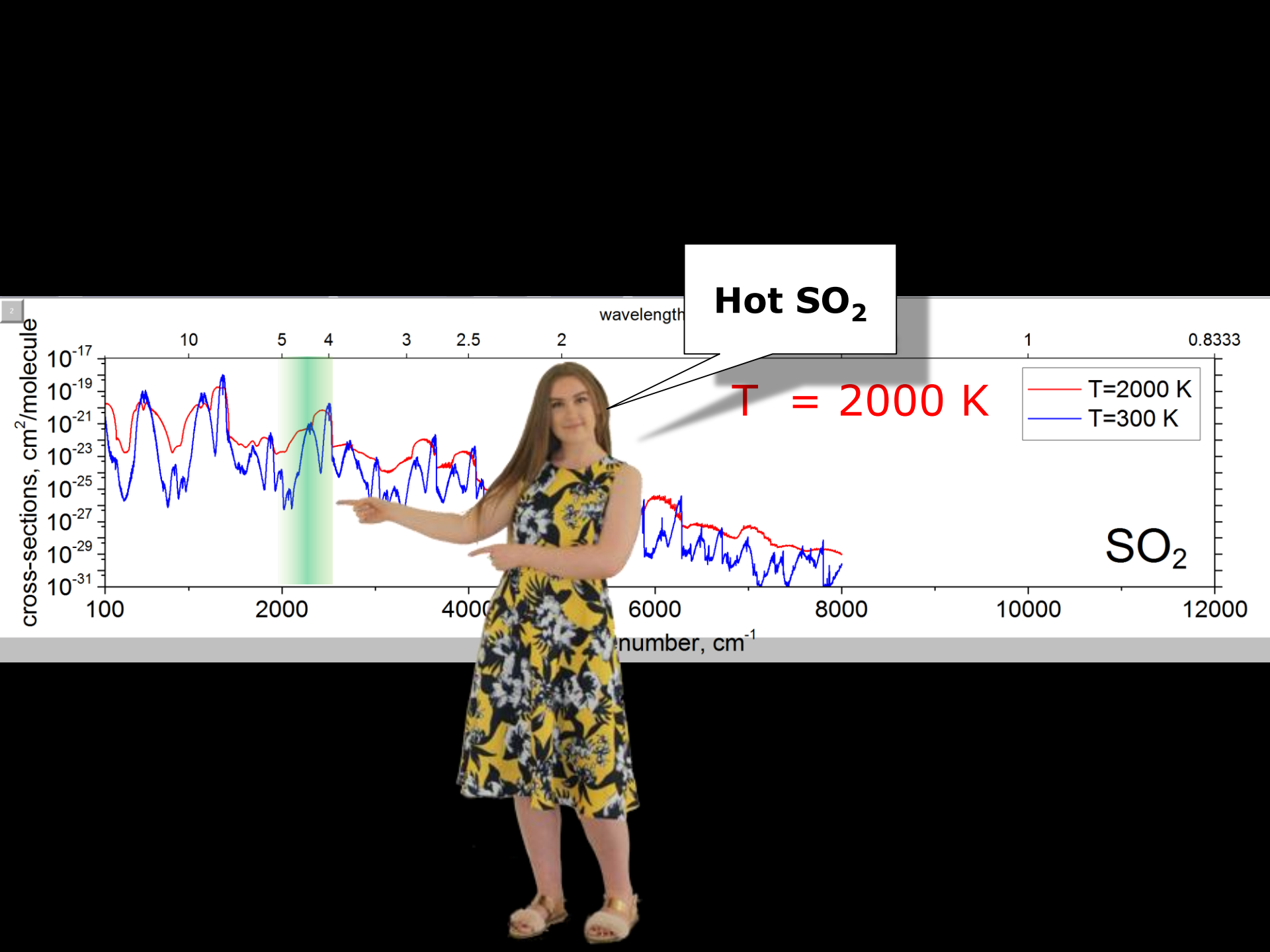

4.5 μm
wavelength, μm
100
8 7 6
4
3
2
0.8333
cross-sections, cm²/molecule
10^-18
10^-20
10^-22
10^-24
10^-26
10^-28
10^-30
CO2
T=300 K
T=2000 K
100
2000
4000
6000
10000
12000
wavenumber

What about other molecules?

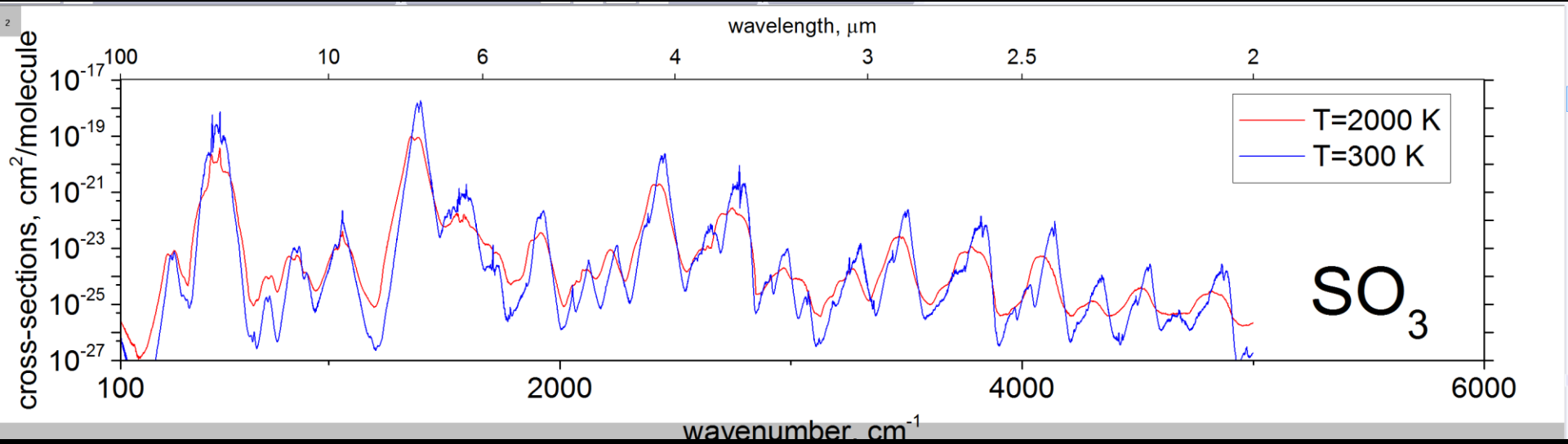

wavelength, μm
10
5
4
3
2.5
2
1.5
1.25
1
0.8333
cross-sections, cm2/molecule
10-17
10-19
10-21
10-23
10-25
10-27
10-29
10-31
T = 300 K
T=2000 K
T=300 K
SO2
100
2000
4000
6000
8000
10000
12000
wavenumber, cm-1


wavelength, μm
10
5
4
3
2.5
2
1.5
1.25
1
0.8333
cross-sections, cm²/molecule
10^-17
10^-19
10^-21
10^-23
10^-25
10^-27
10^-29
10^-31
T = 300 K
T=2000 K
T=300 K
SO2
100
2000
4000
6000
8000
10000
12000
wavenumber, cm^-1

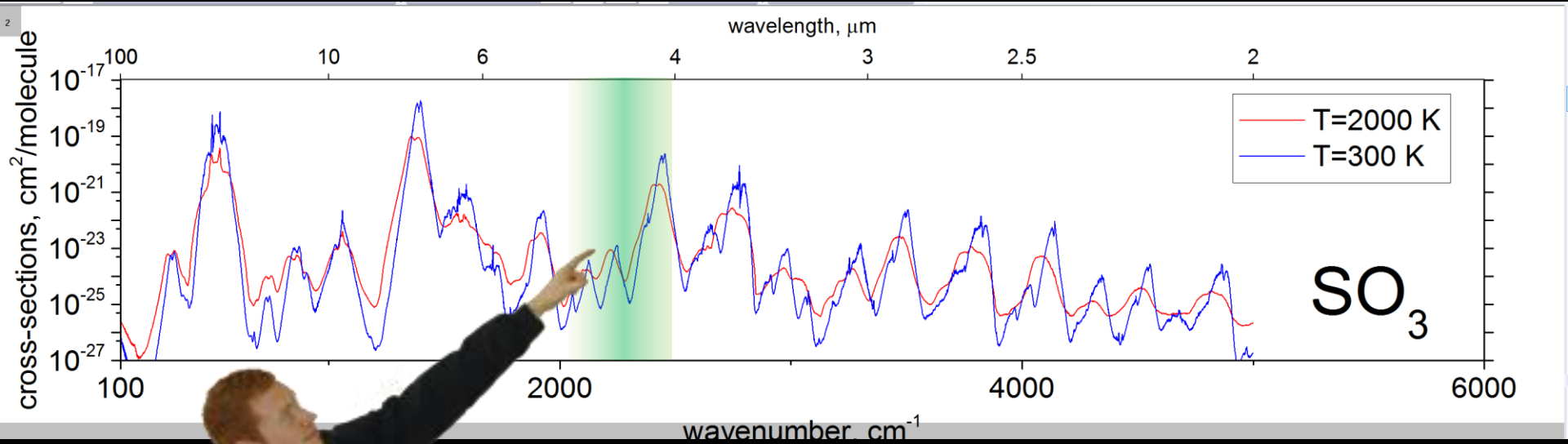

wavelength, μm
10
5
4
3
2.5
2
1.5
1.25
1
0.8333
cross-sections, cm²/molecule
10⁻¹⁷
10⁻¹⁹
10⁻²¹
10⁻²³
10⁻²⁵
10⁻²⁷
10⁻²⁹
10⁻³¹
T = 2000 K
T=2000 K
T=300 K
SO2
100
2000
4000
6000
8000
10000
12000
wavenumber, cm⁻¹


Hot SO_2
T = 2000 K
wavelength
10
5
4
3
2.5
2
1
0.8333
cross-sections, cm^2/molecule
10^{-17}
10^{-19}
10^{-21}
10^{-23}
10^{-25}
10^{-27}
10^{-29}
10^{-31}
100
2000
4000
6000
8000
10000
12000
number, cm^{-1}
T=2000 K
T=300 K
SO_2

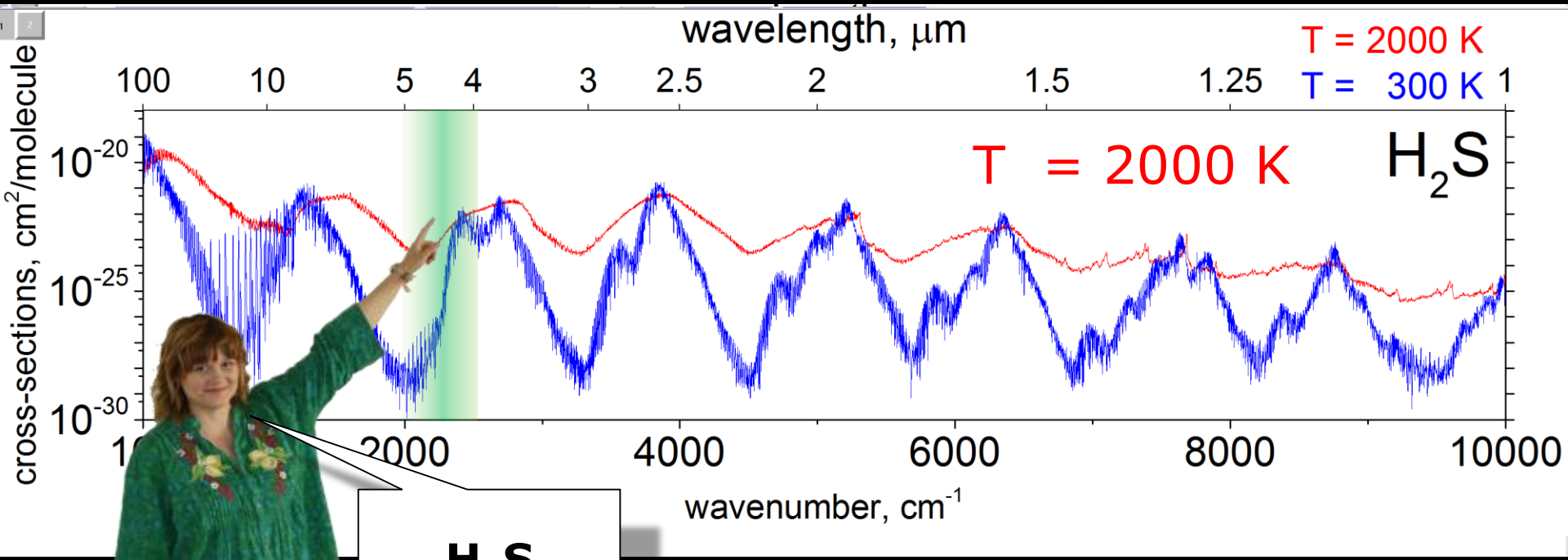
T = 2000 K

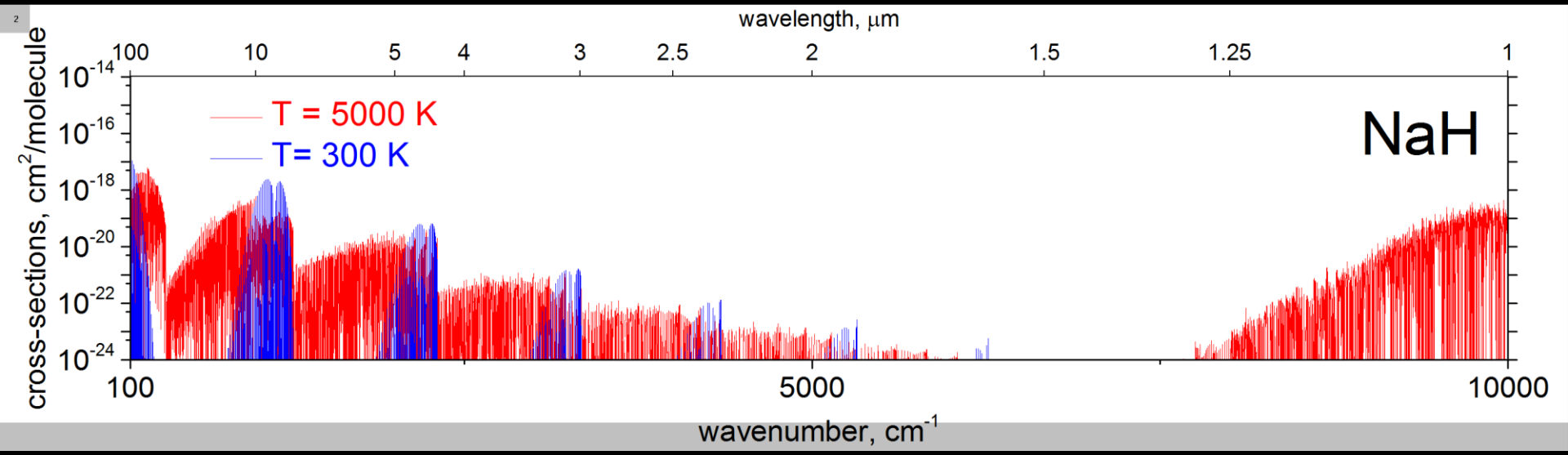

wavelength, μm
100
10
6
4
3
2.5
2
cross-sections, cm²/molecule
10⁻¹⁷
10⁻¹⁹
10⁻²¹
10⁻²³
10⁻²⁵
10⁻²⁷
T=2000 K
T=300 K
SO3
100
2000
4000
6000
wavenumber, cm⁻¹

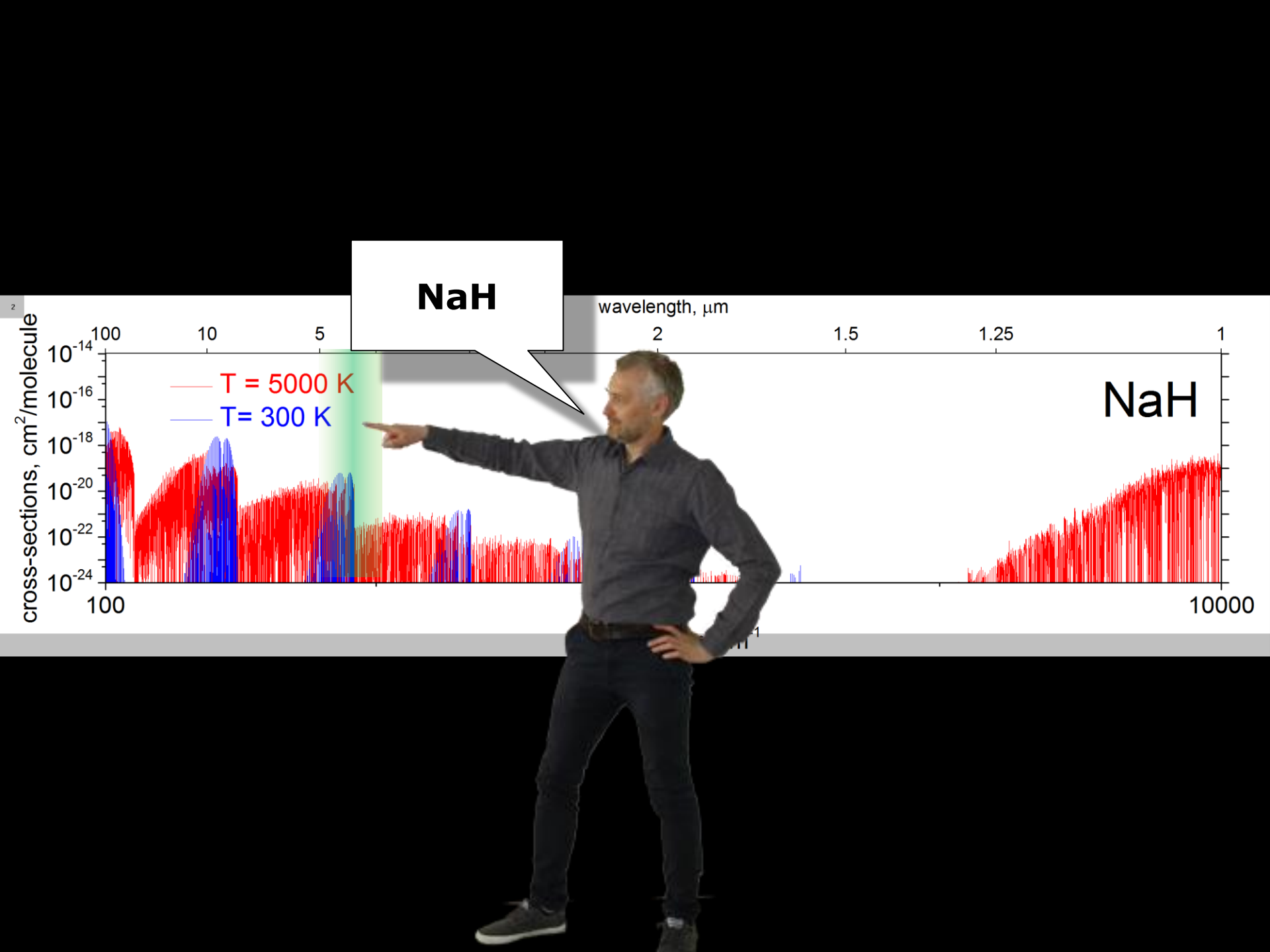
T = 2000 K


wavelength, μm
100
10
6
4
3
2.5
2
cross-sections, cm²/molecule
10⁻¹⁷
10⁻¹⁹
10⁻²¹
10⁻²³
10⁻²⁵
10⁻²⁷
T=2000 K
T=300 K
SO3
100
2000
4000
6000
wavenumber, cm⁻¹


SO3


wavelength, μm
100
10
5
4
3
2.5
2
1.5
1.25
1
T = 2000 K
T = 300 K
T = 2000 K
H2S
cross-sections, cm2/molecule
10-20
10-25
10-30
2000
4000
6000
8000
10000
wavenumber, cm-1
H2S


wavelength, μm
100
10
5
4
3
2.5
2
1.5
1.25
1
cross-sections, cm²/molecule
10⁻¹⁴
10⁻¹⁶
10⁻¹⁸
10⁻²⁰
10⁻²²
10⁻²⁴
T = 5000 K
T= 300 K
NaH
100
5000
10000
wavenumber, cm⁻¹


NaH
wavelength, μm
100
10
5
2
1.5
1.25
1
cross-sections, cm²/molecule
10⁻¹⁴
10⁻¹⁶
10⁻¹⁸
10⁻²⁰
10⁻²²
10⁻²⁴
T = 5000 K
T= 300 K
NaH
100
10000

Should not all these molecules to be also included, not only water and CO_2?

BTW, these spectra images are from our recent ExoMol Atlas of spectra of exoplanets

BTW, these spectra images are from our recent ExoMol Atlas of spectra of exoplanets

atoms

MDPI

Article

The ExoMol Atlas of Molecular Opacities

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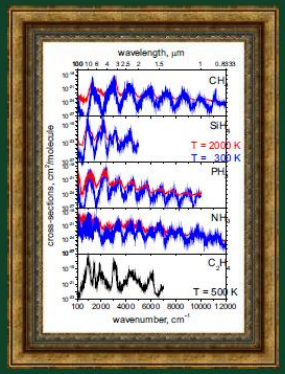
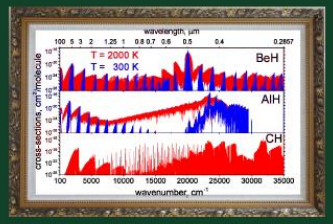
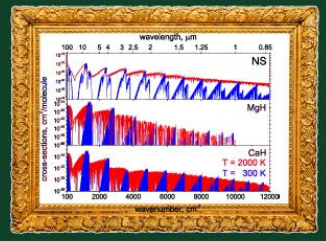
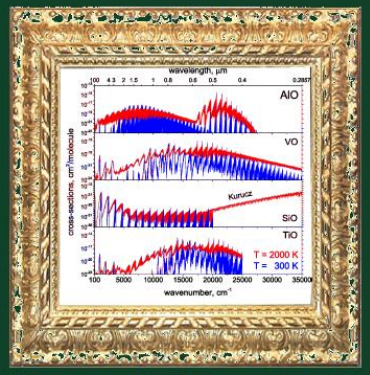
* Correspondence: j.tennyson@ucl.ac.uk

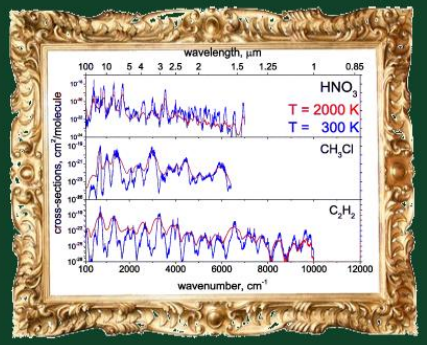
Spectral gallery for exoplanets

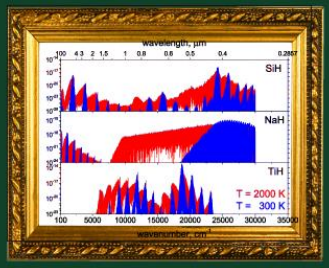


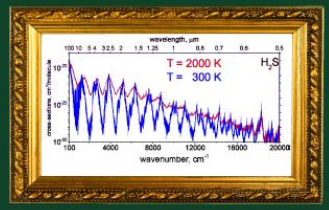


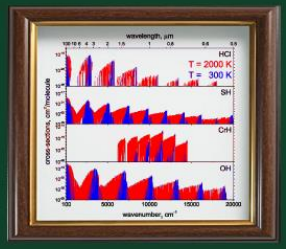


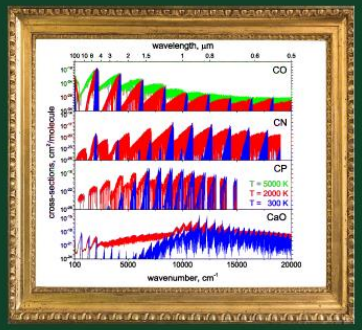


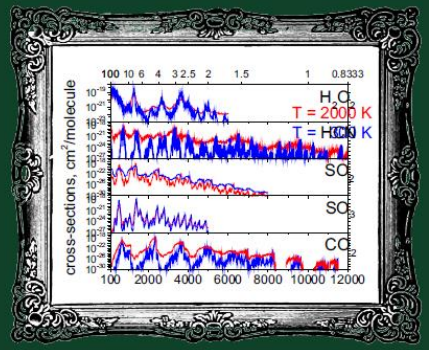


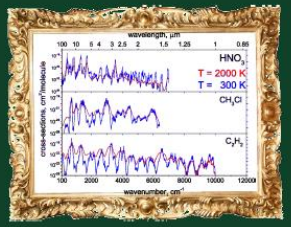


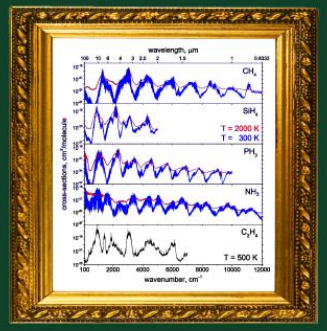


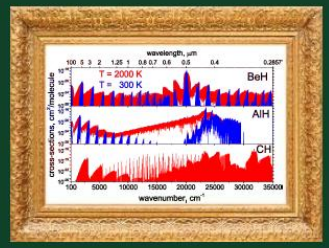


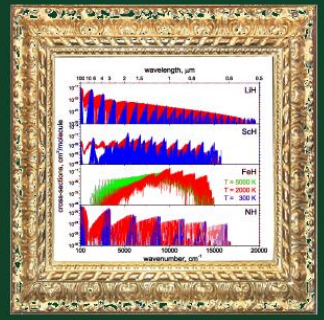


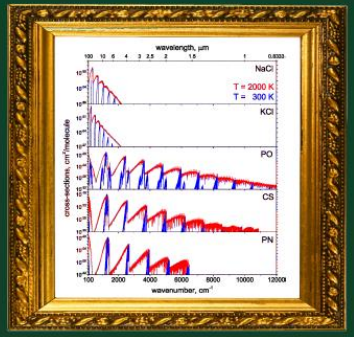


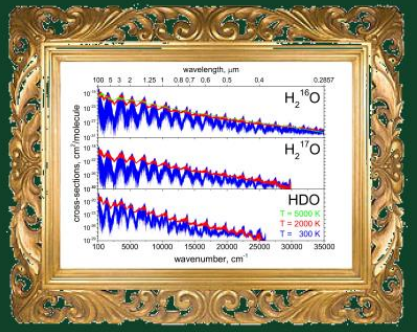


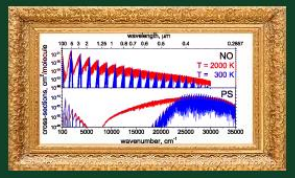




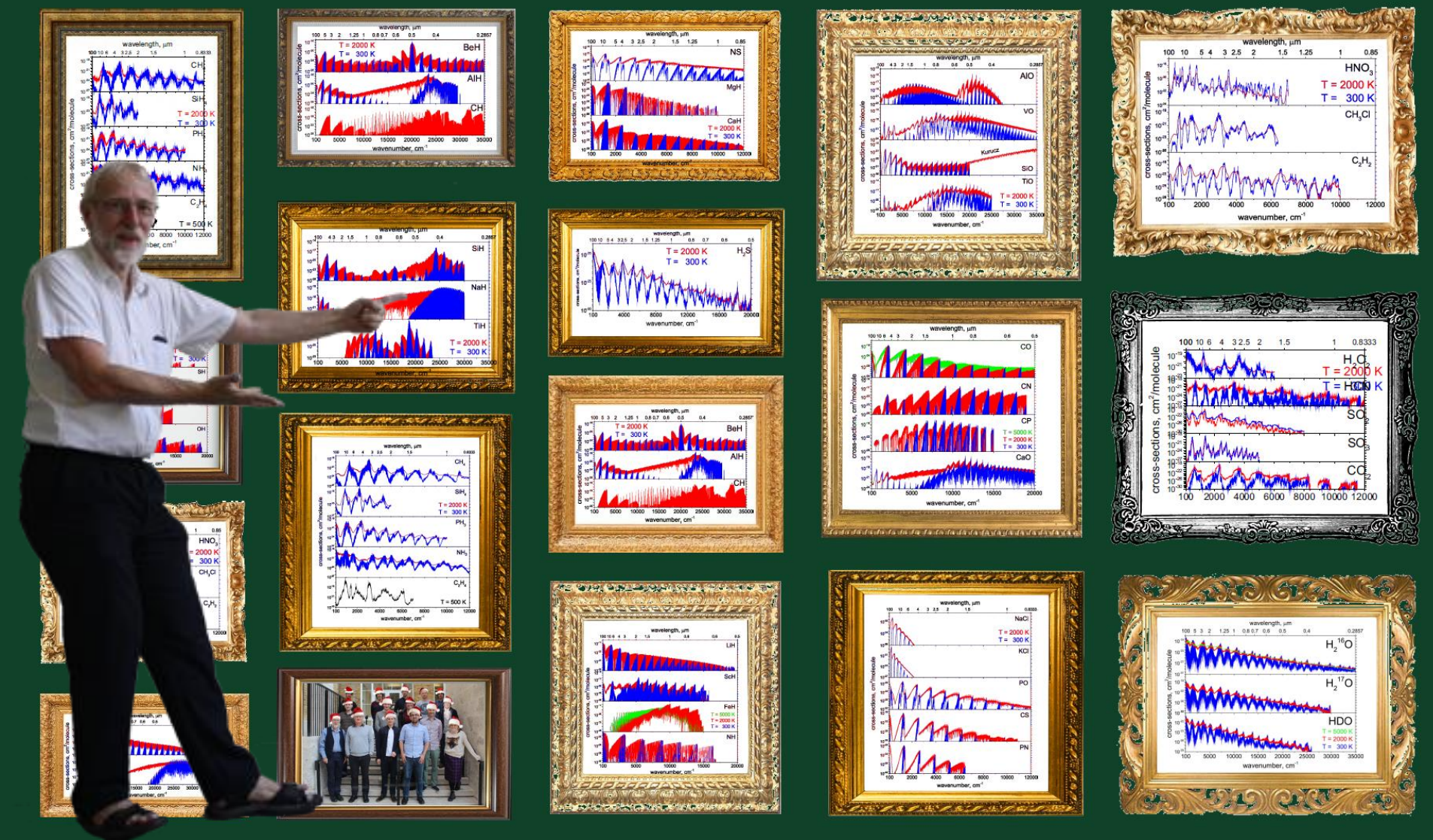








Spectral gallery for exoplanets

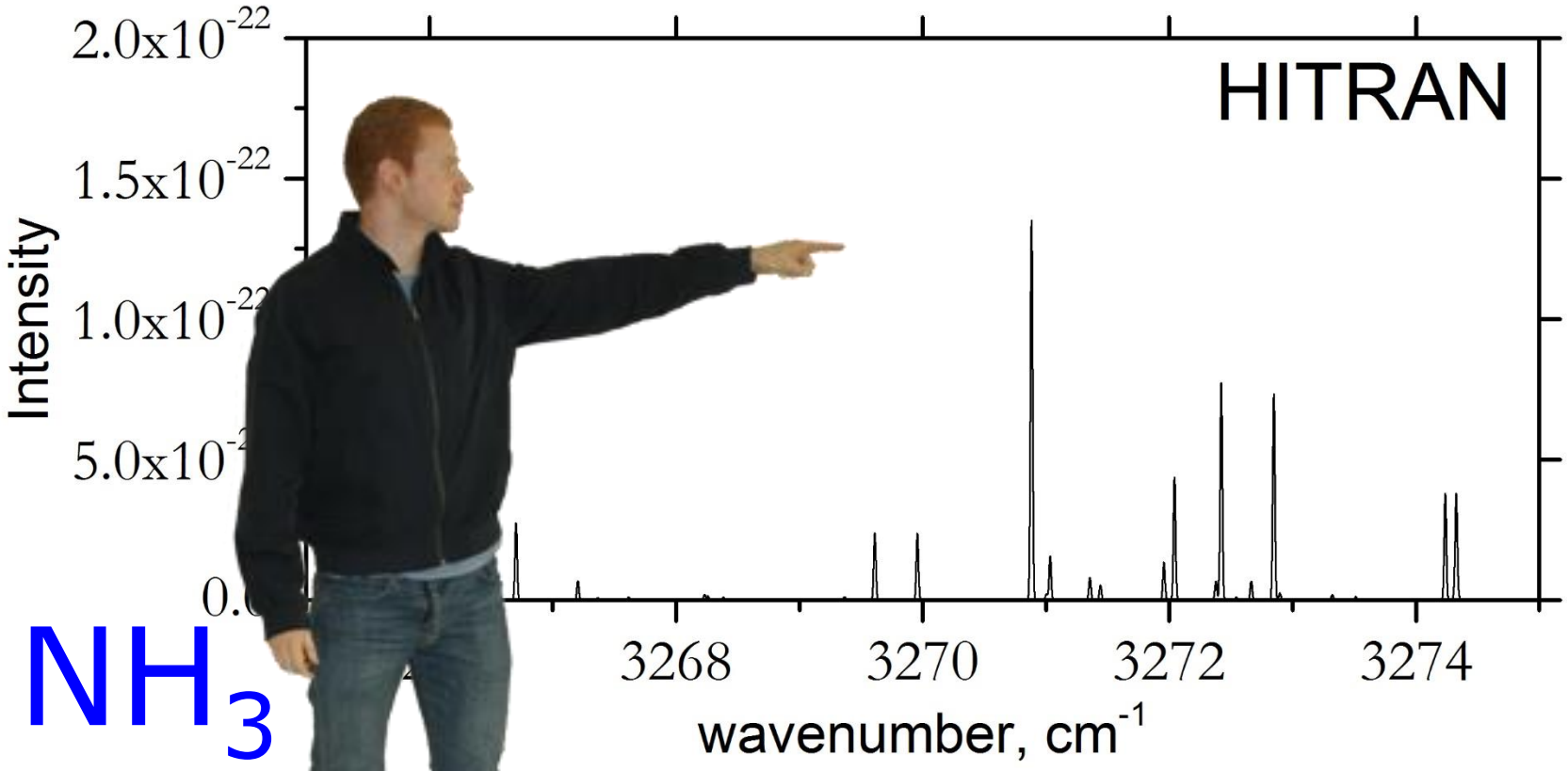


High Resolution spectroscopy of Exoplanets: some questions

Two important points:
Accuracy and (relative) completeness

Let’s take Ammonia as an example

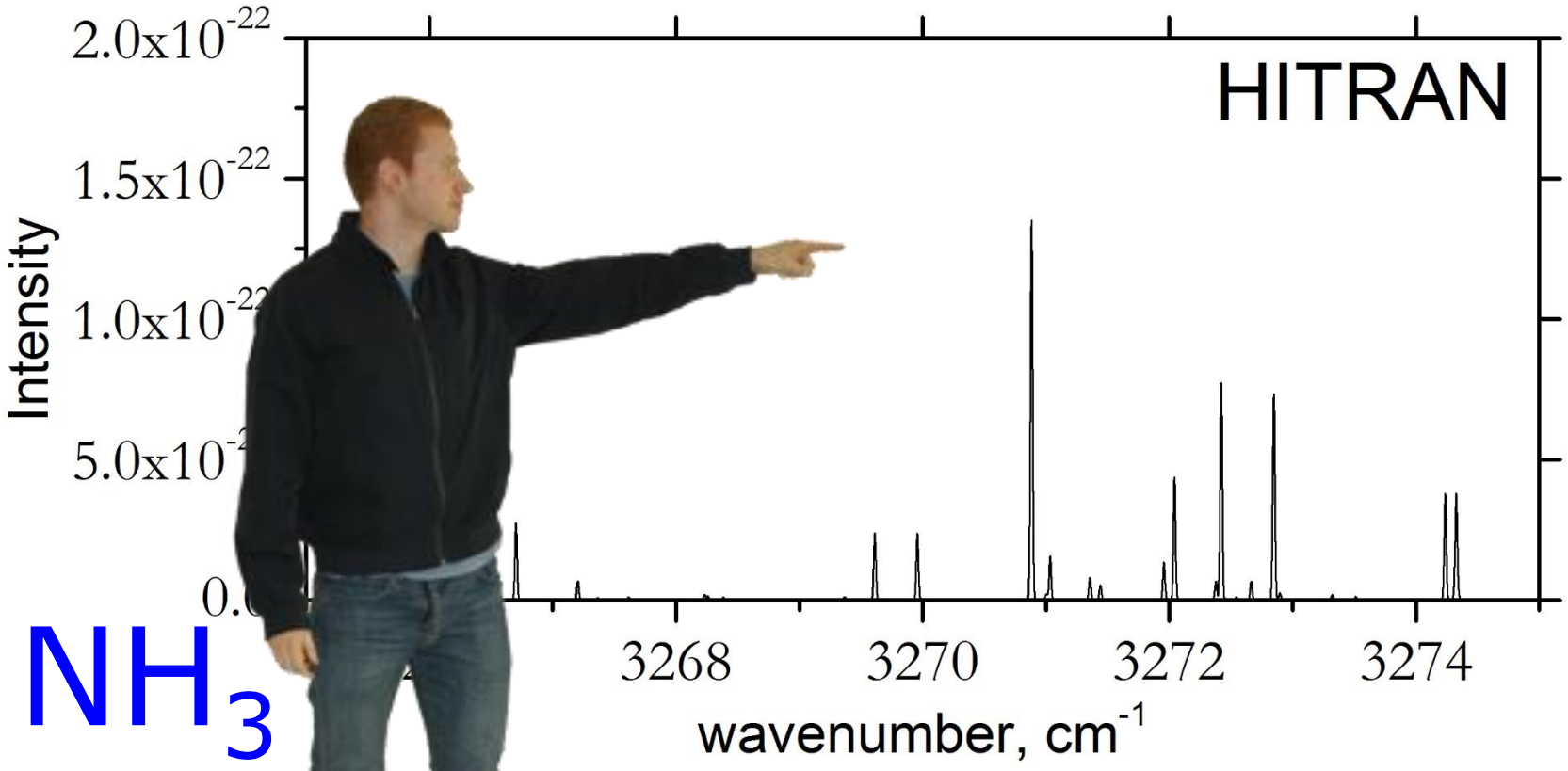
3.06 μm 3.058 μm 3.054 μm



NH_3

T = 300 K

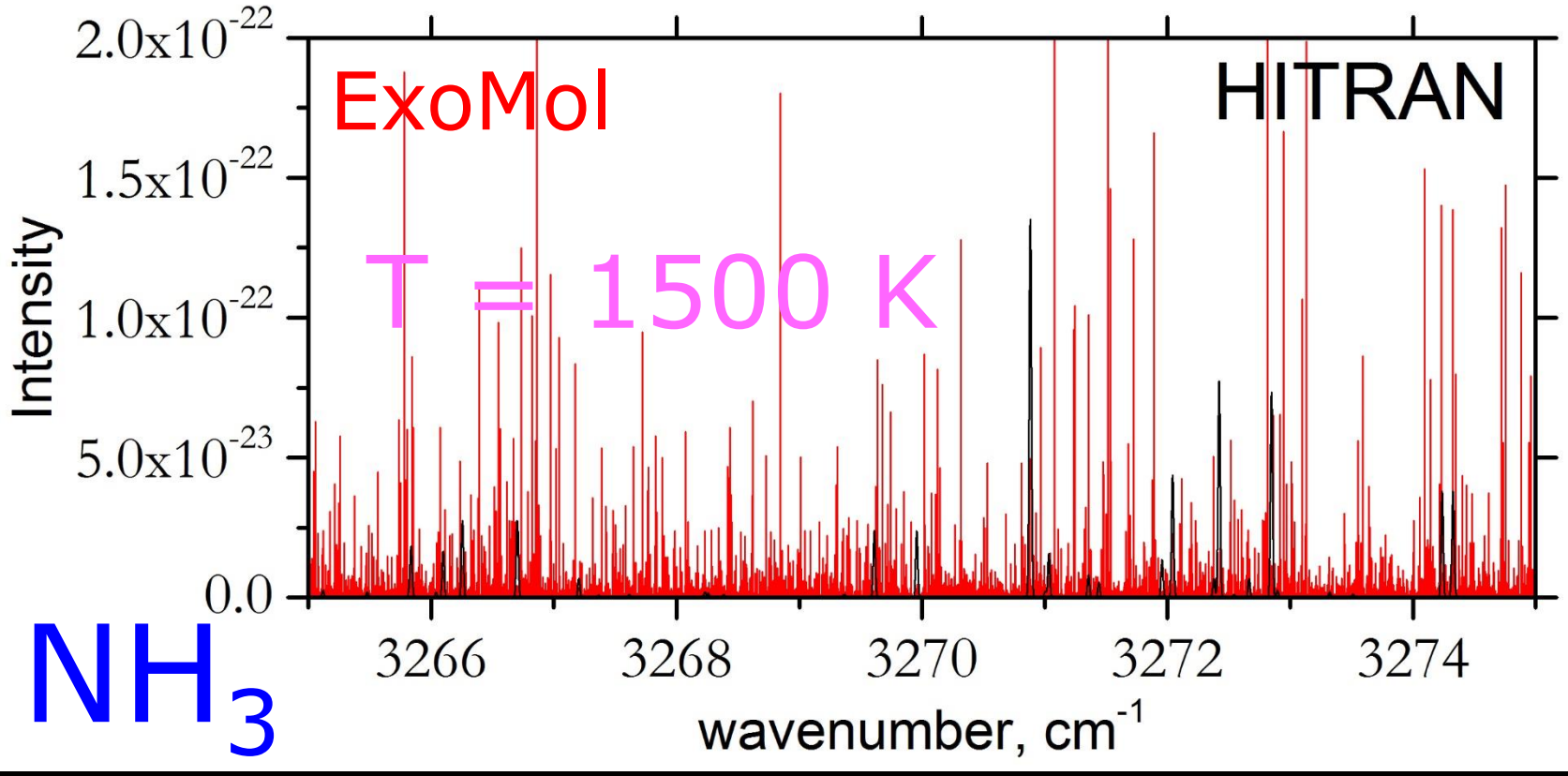
3.06 μm 3.058 μm 3.054 μm



NH_3

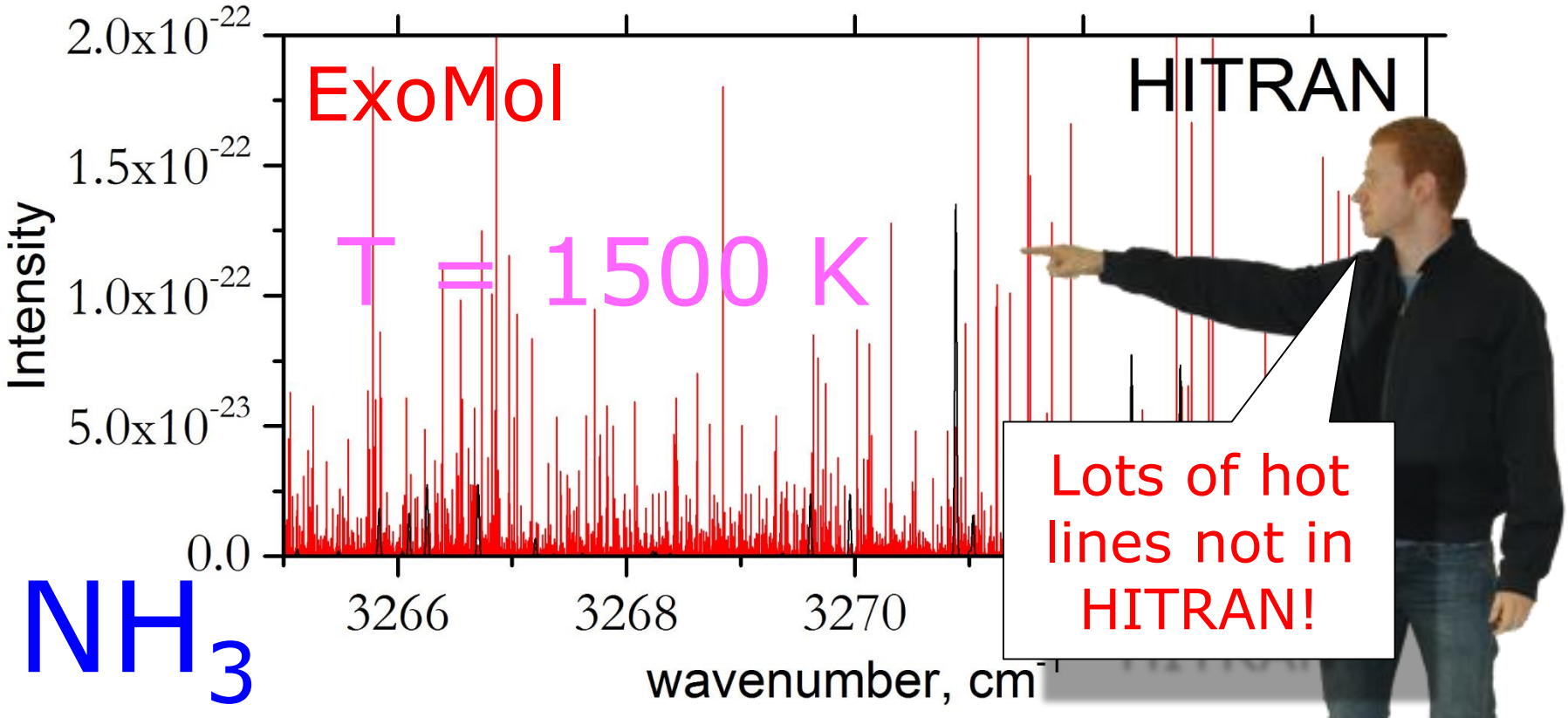
T = 300 K

3.06 μm 3.058 μm 3.054 μm



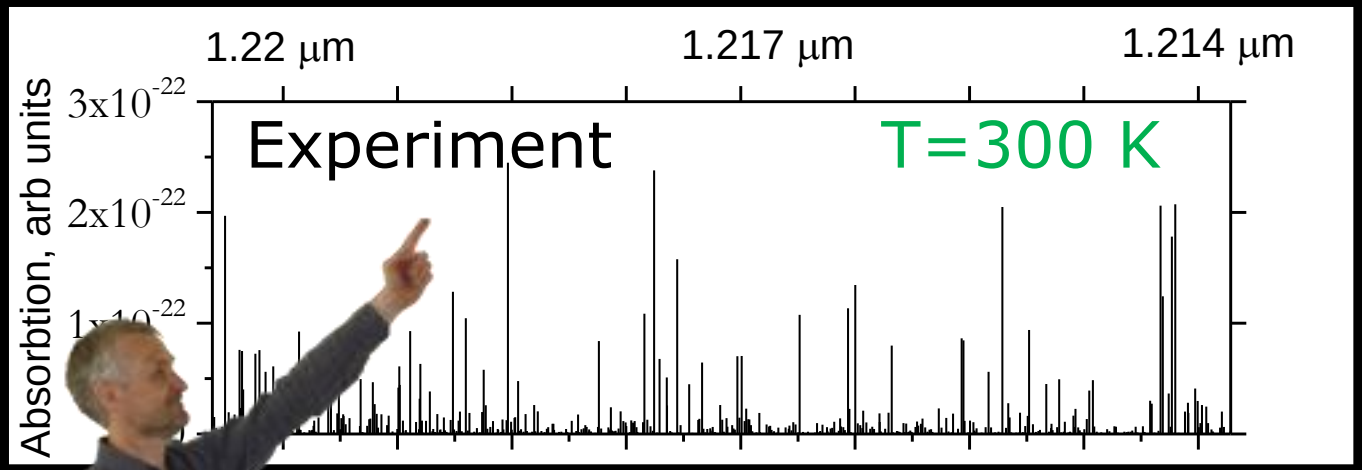
NH_3

3.06 μm 3.058 μm 3.054 μm

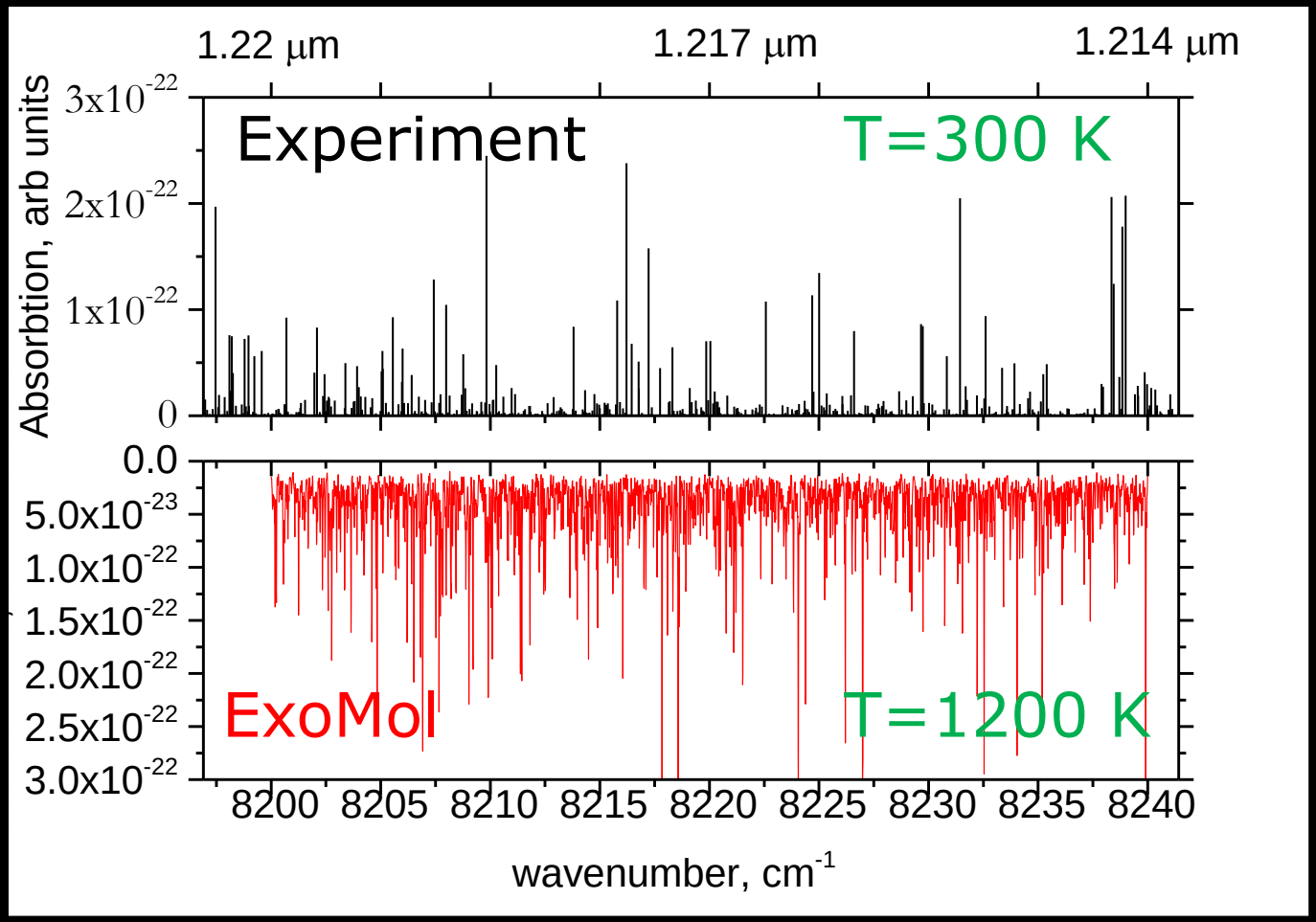


A different region: 1.27 μm

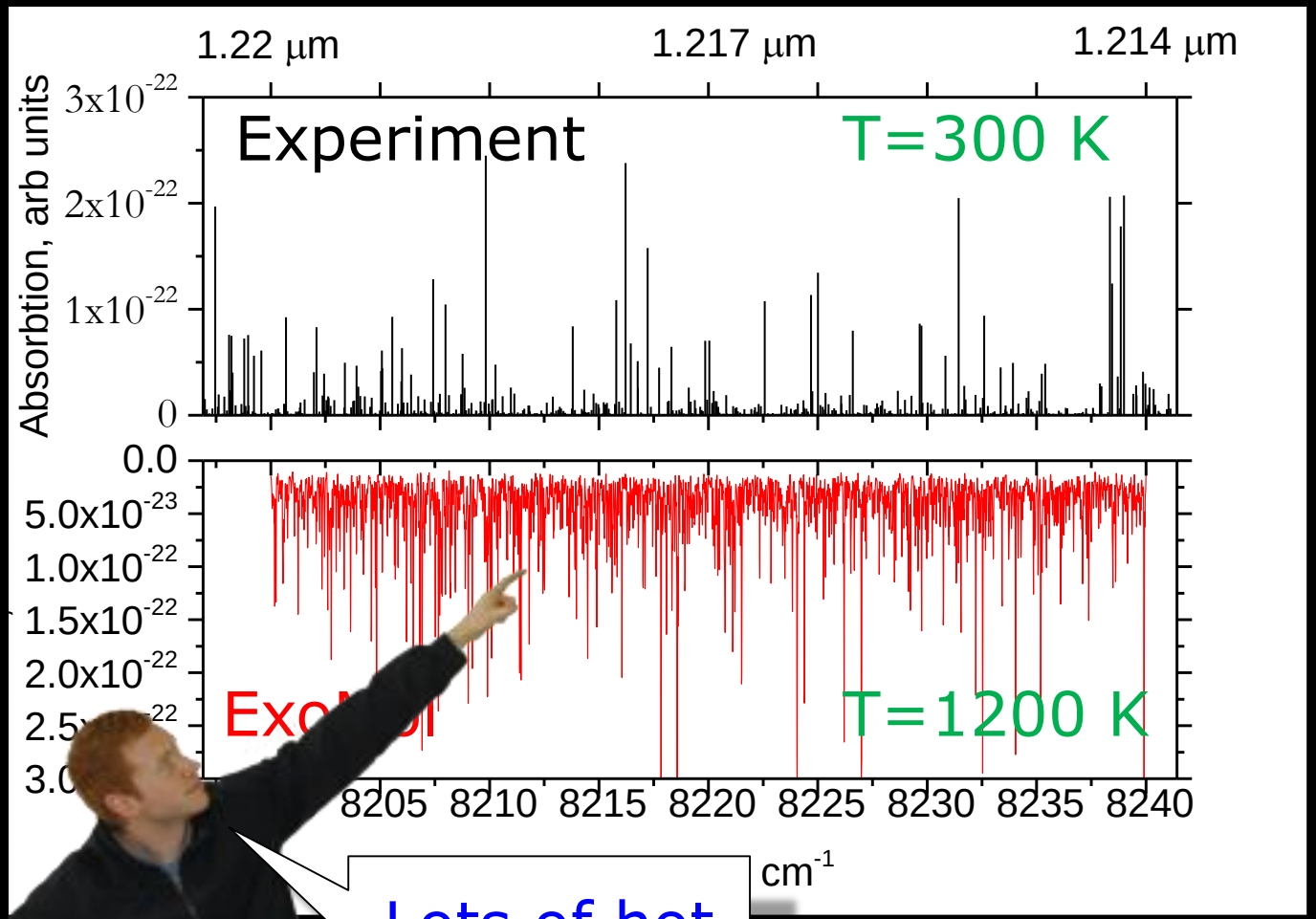
NH_3


1.22 μm
1.217 μm
1.214 μm
Absorbtion, arb units
3x10-22
2x10-22
Experiment
T=300 K

NH_3


1.22 μm
1.217 μm
1.214 μm
Absorbtion, arb units
3x10-22
2x10-22
1x10-22
0
Experiment
T=300 K
0.0
5.0x10-23
1.0x10-22
1.5x10-22
2.0x10-22
2.5x10-22
3.0x10-22
ExoMol
T=1200 K
8200 8205 8210 8215 8220 8225 8230 8235 8240
wavenumber, cm-1

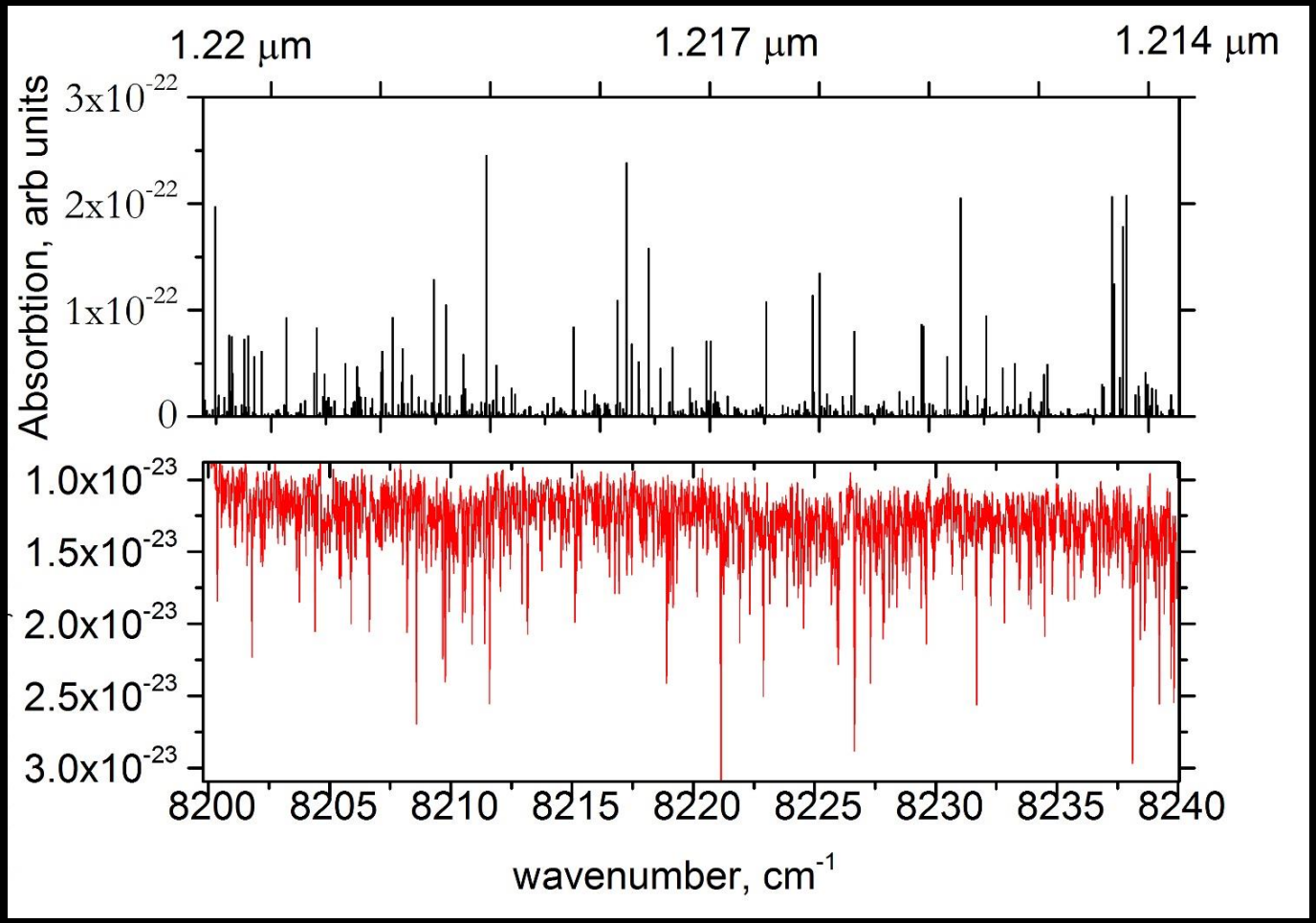
NH_3



Lots of hot lines

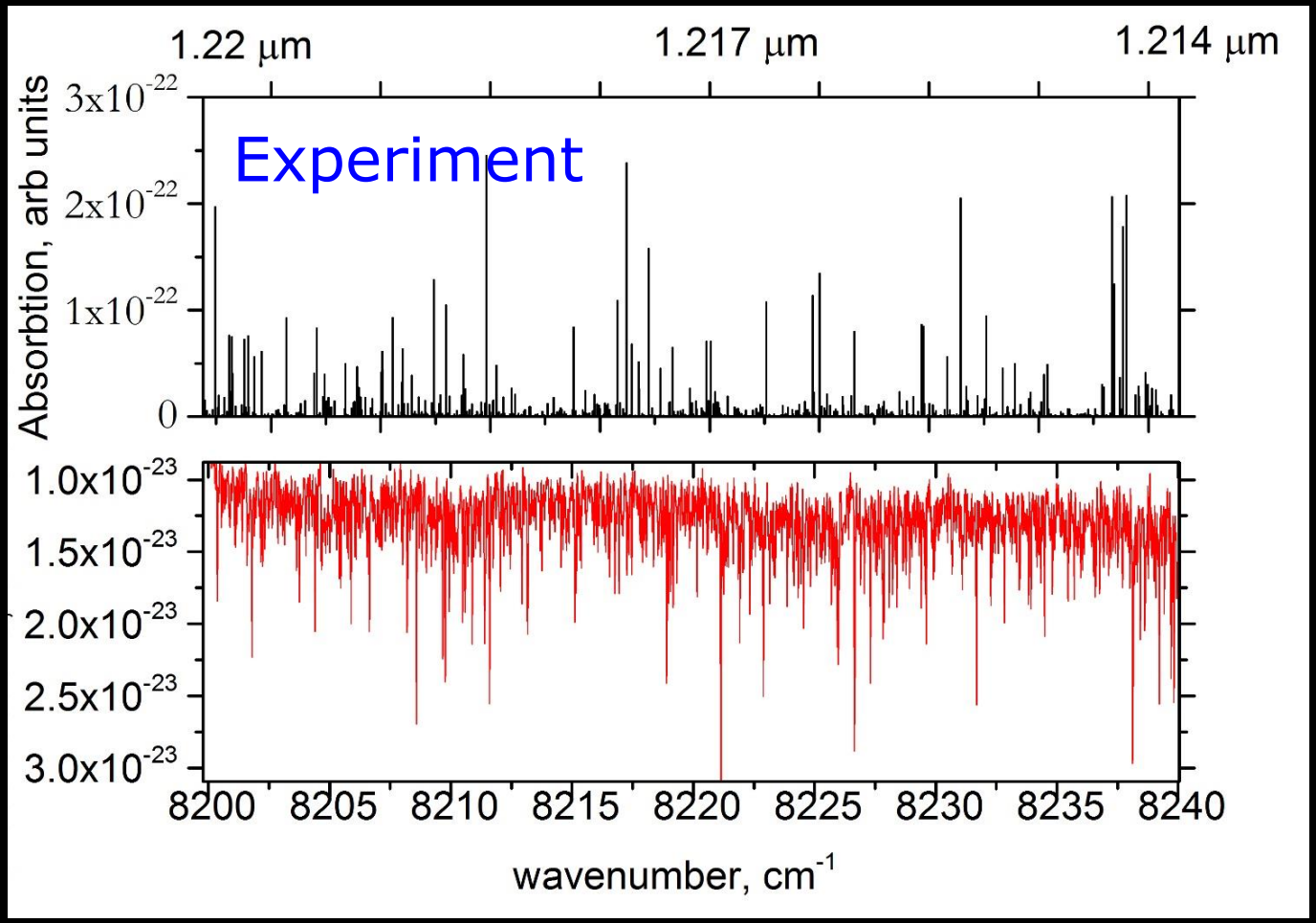
What about methane lines in this region?

NH_3


1.22 μm
1.217 μm
1.214 μm
Absorbtion, arb units
3x10-22
2x10-22
1x10-22
0
1.0x10-23
1.5x10-23
2.0x10-23
2.5x10-23
3.0x10-23
8200
8205
8210
8215
8220
8225
8230
8235
8240
wavenumber, cm-1

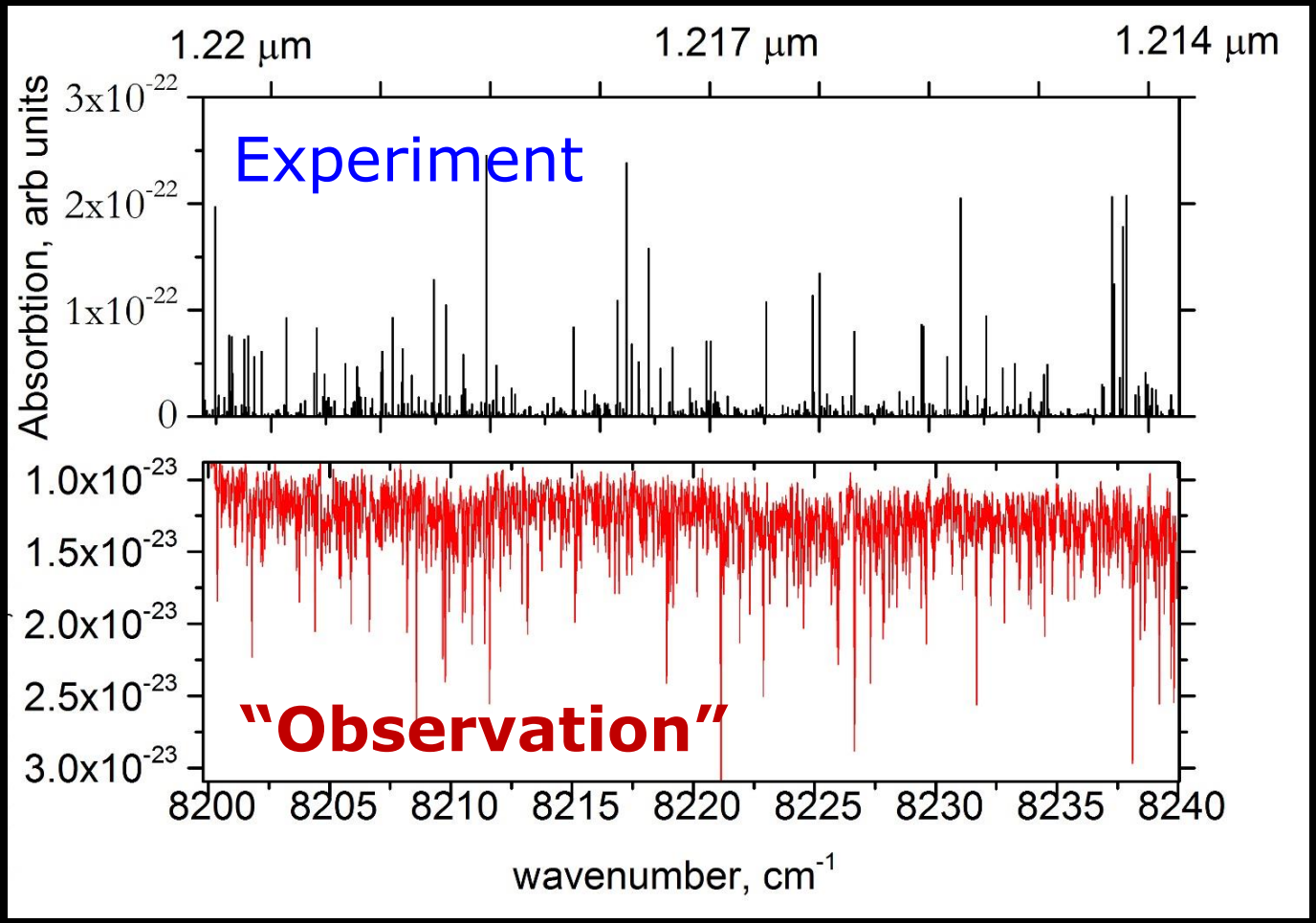
CH_4

NH_3


1.22 μm
1.217 μm
1.214 μm
Experiment
Absorbtion, arb units
3x10-22
2x10-22
1x10-22
0
1.0x10-23
1.5x10-23
2.0x10-23
2.5x10-23
3.0x10-23
8200
8205
8210
8215
8220
8225
8230
8235
8240
wavenumber, cm-1

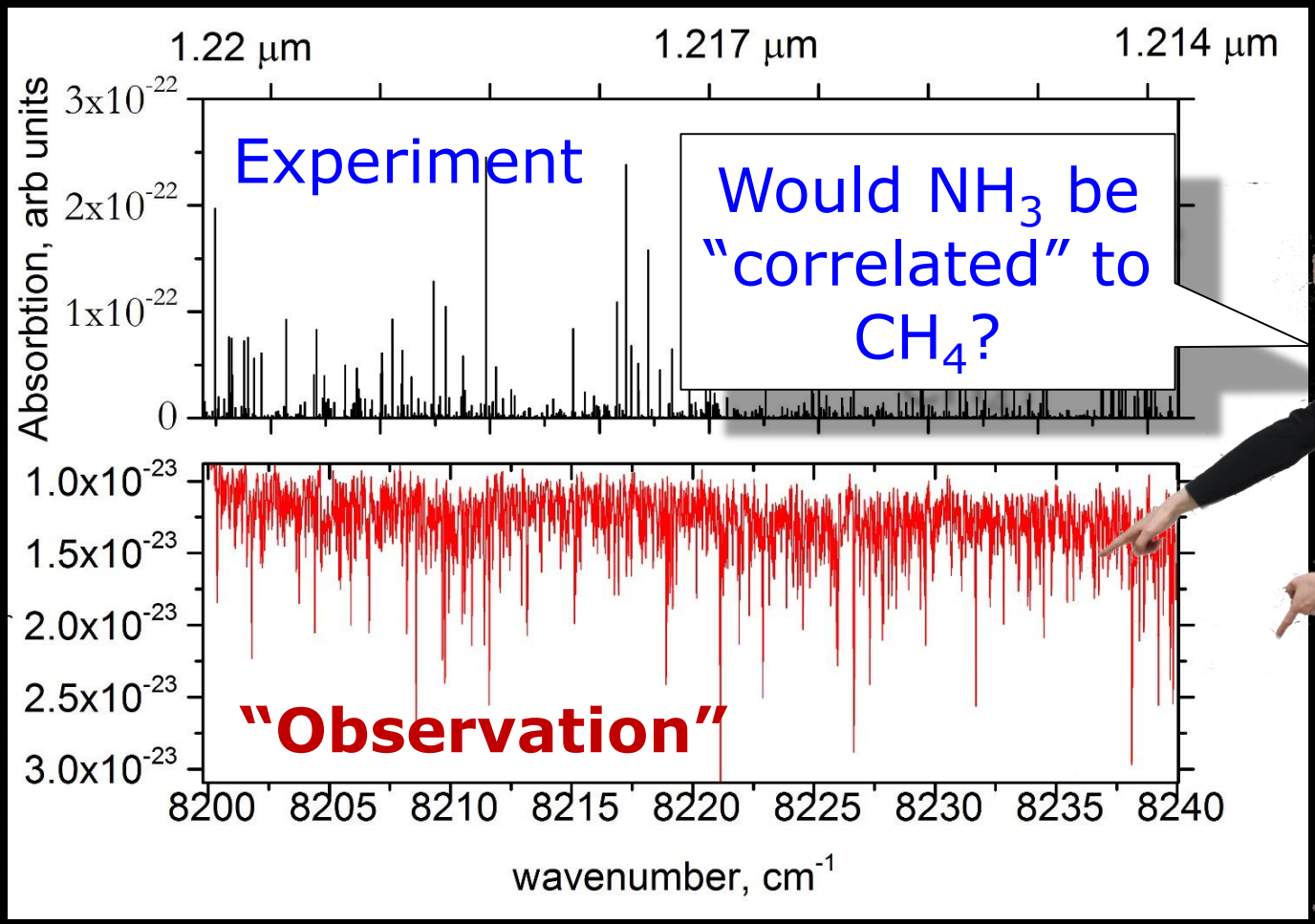
CH_4

NH_3


1.22 μm
1.217 μm
1.214 μm
Absorbtion, arb units
3x10-22
2x10-22
1x10-22
0
Experiment
1.0x10-23
1.5x10-23
2.0x10-23
2.5x10-23
3.0x10-23
"Observation"
8200
8205
8210
8215
8220
8225
8230
8235
8240
wavenumber, cm-1

CH_4

NH_3


1.22 μm
1.217 μm
1.214 μm
Absorbtion, arb units
3x10-22
2x10-22
1x10-22
0
Experiment
Would NH3 be "correlated" to CH4?
1.0x10-23
1.5x10-23
2.0x10-23
2.5x10-23
3.0x10-23
"Observation"
8200
8205
8210
8215
8220
8225
8230
8235
8240
wavenumber, cm-1

CH_4


I have a naive question

Is there a risk of “detecting” a wrong molecule?

Anyways… ExoMol

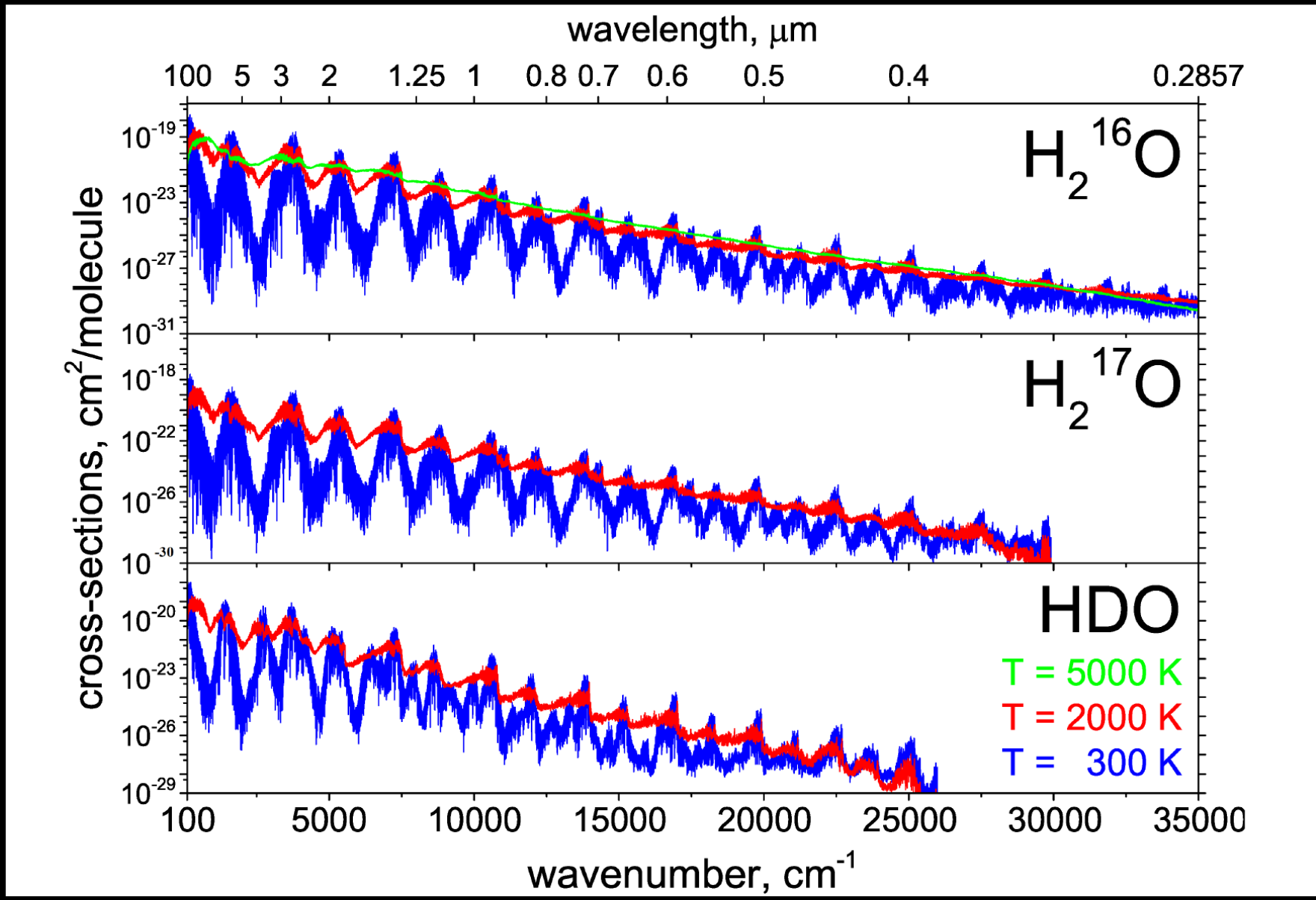
We have produced a new water line list POKAZATEL, fully complete and more accurate

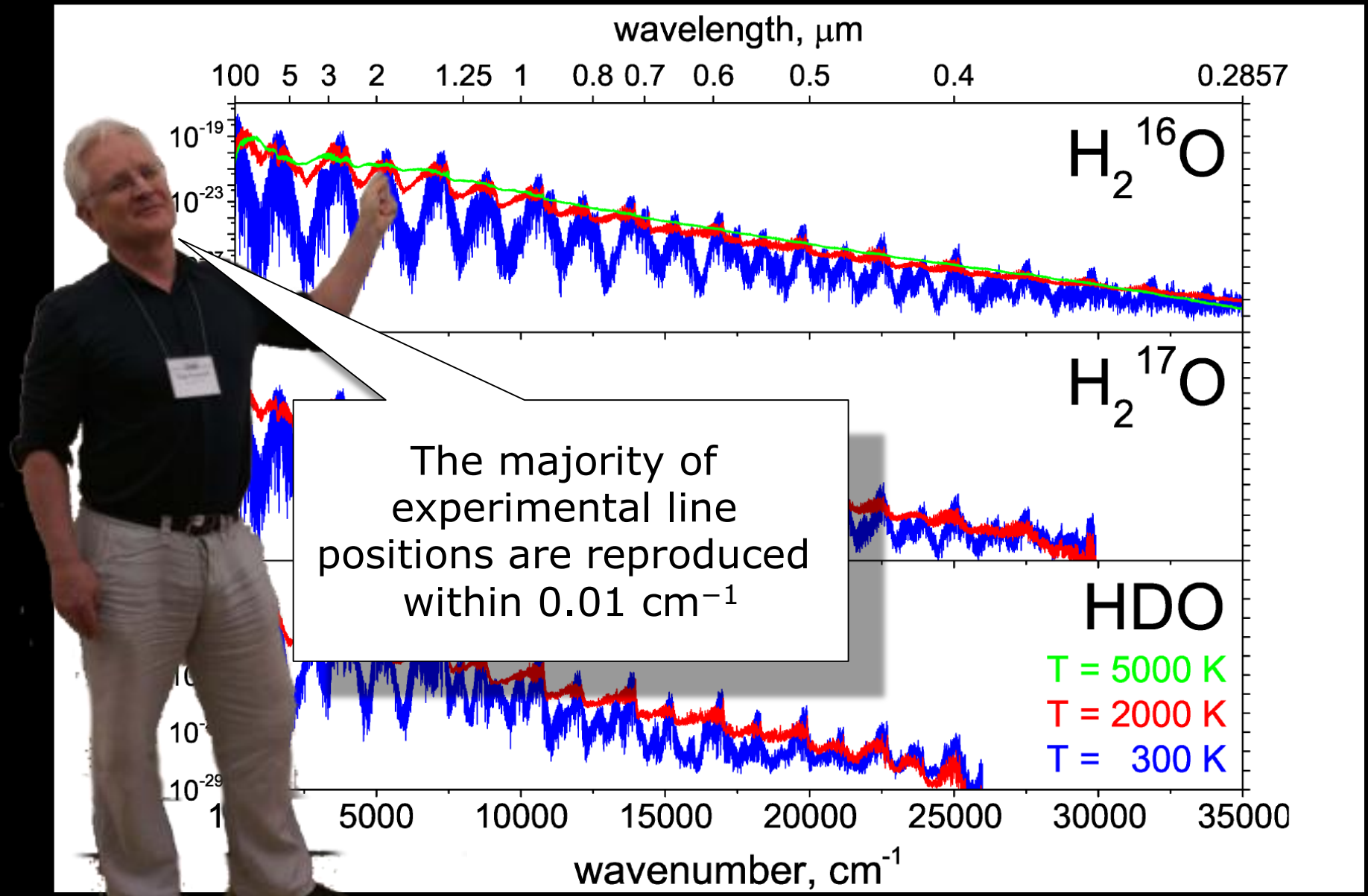
Oleg Polyansky et al (now at)
MNRAS (2018)

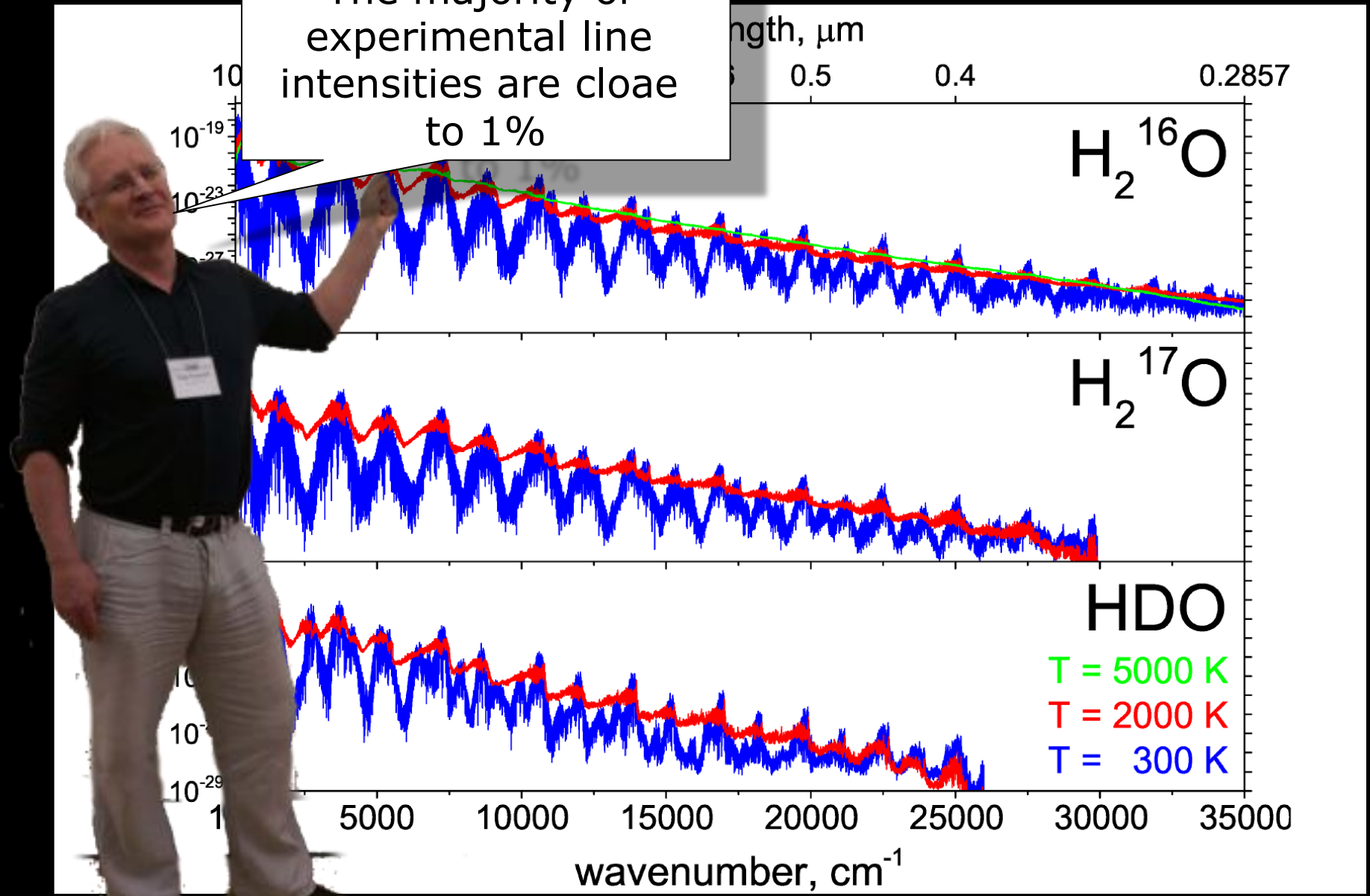
Q: How many states to inbnlcude into a line list

Q: How many states to inbnlcude into a line list

All bound states up to dissociation


wavelength, μm
100 5 3 2 1.25 1 0.8 0.7 0.6 0.5 0.4 0.2857
cross-sections, cm²/molecule
H2 16O
H2 17O
HDO
T = 5000 K
T = 2000 K
T = 300 K
100 5000 10000 15000 20000 25000 30000 35000
wavenumber, cm-1


wavelength, μm
100 5 3 2 1.25 1 0.8 0.7 0.6 0.5 0.4 0.2857
$H_2{}^{16}O$
$H_2{}^{17}O$
HDO
T = 5000 K
T = 2000 K
T = 300 K
The majority of experimental line positions are reproduced within 0.01 cm^{-1}
5000 10000 15000 20000 25000 30000 35000
wavenumber, cm^{-1}


The majority of experimental line intensities are cloae to 1%
ngth, μm
0.5
0.4
0.2857
$H_2{}^{16}O$
$H_2{}^{17}O$
HDO
T = 5000 K
T = 2000 K
T = 300 K
5000
10000
15000
20000
25000
30000
35000
wavenumber, cm^{-1}

This summarises our main goals…

Accurate line positions

Accurate line intensities

To be complete for high excitations and hot spectra

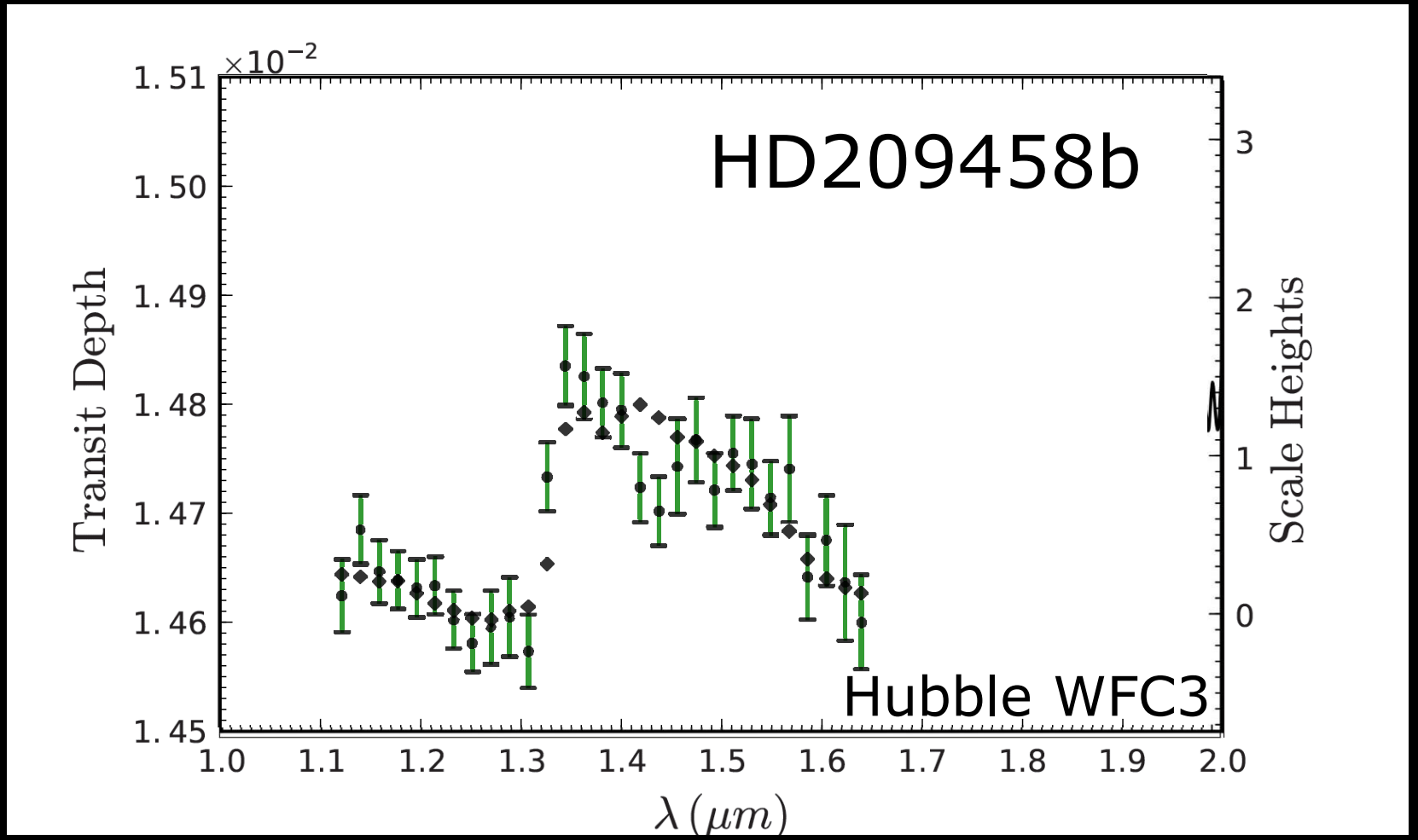
These goals however are not always compatible

It is too difficult or even impossible to be accurate and complete

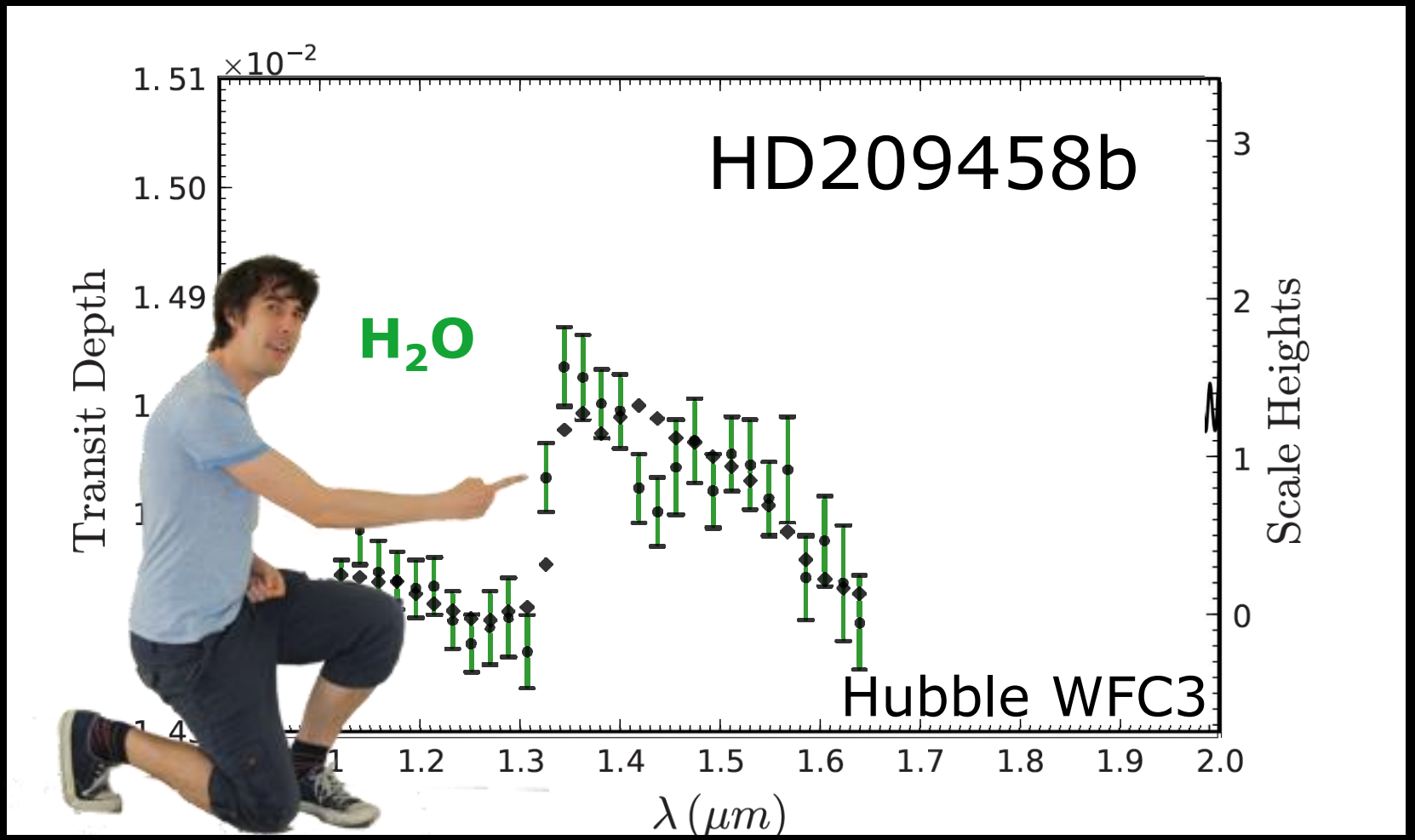
Luckily, most of applications require to be either accurate or complete

For example, the Doppler high resolution stuff must be accurate but not so much complete

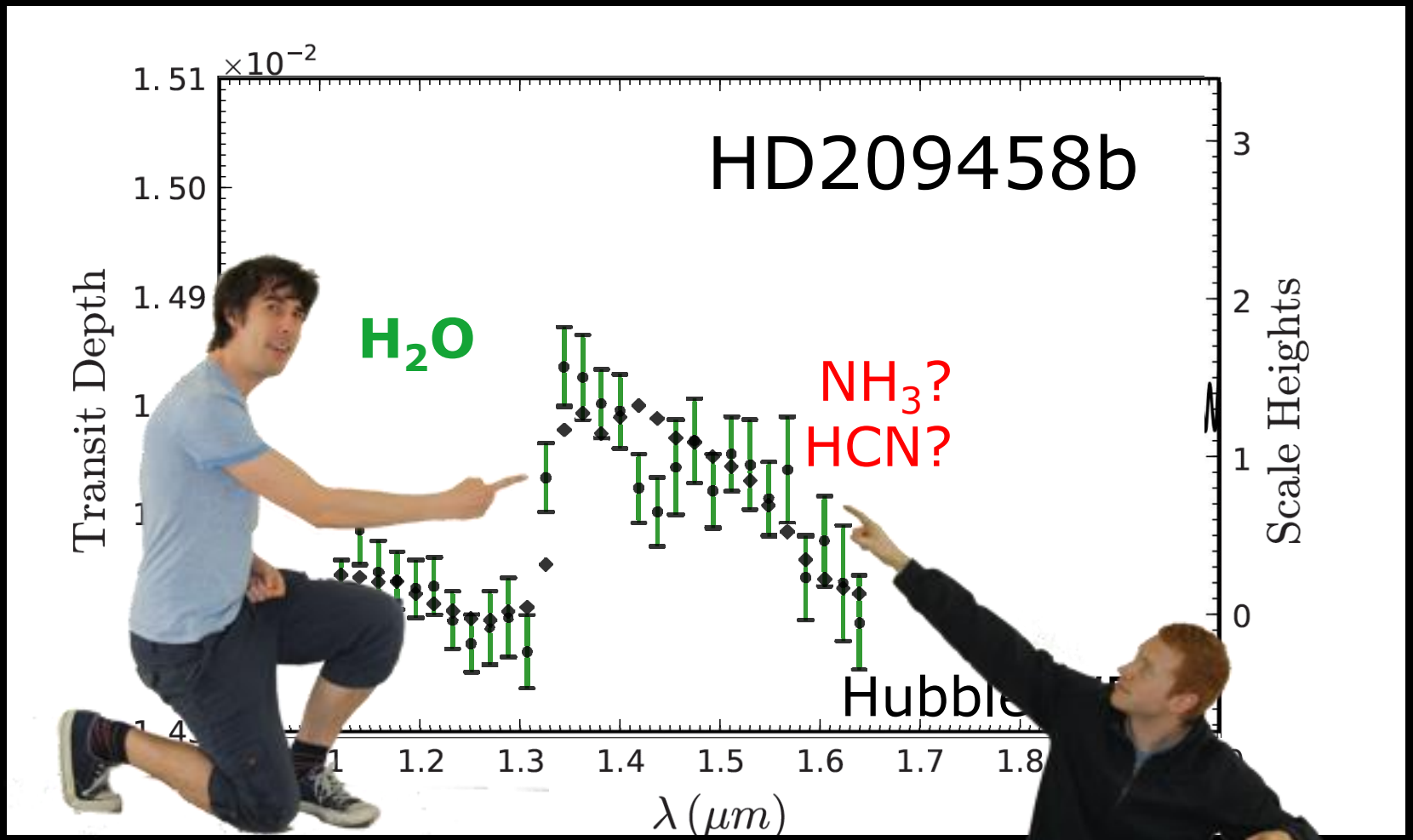
Most of the opacity applications (atmospheric retrievals) require to be complete not so much accurate



MacDonald and Madhusudhan (2017)



MacDonald and Madhusudhan (2017)

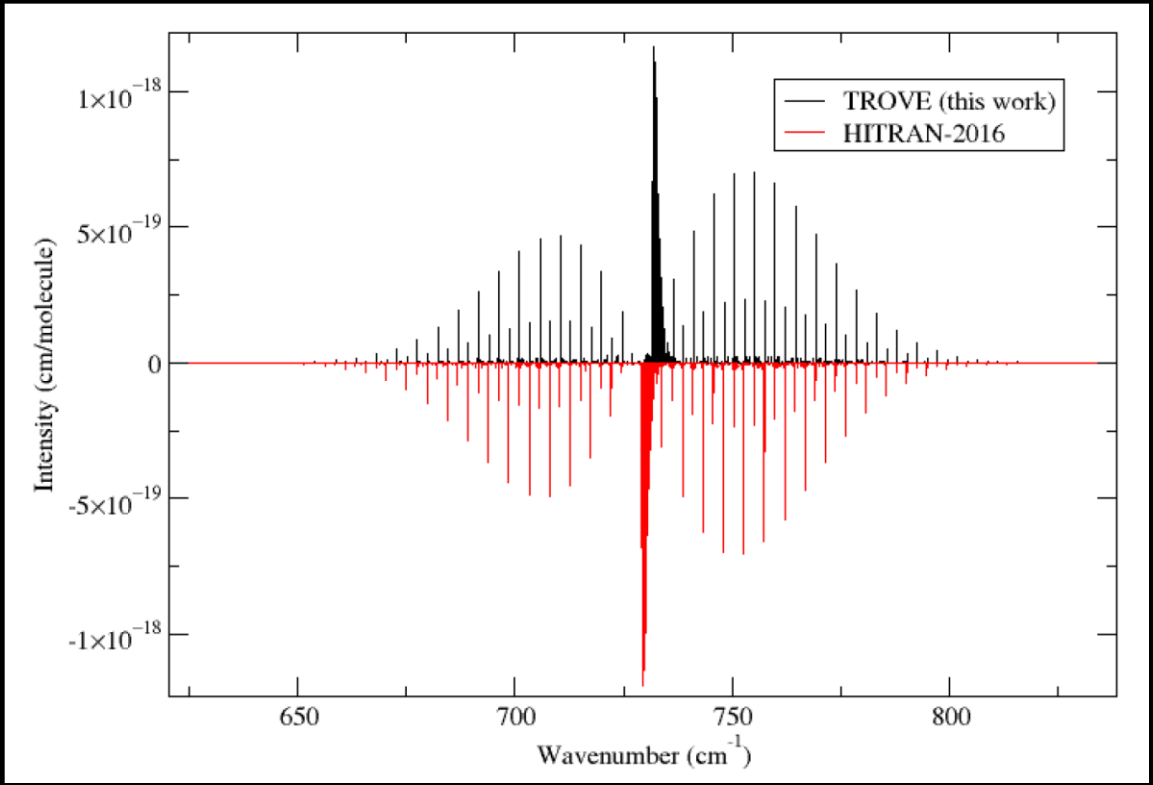


MacDonald and Madhusudhan (2017)

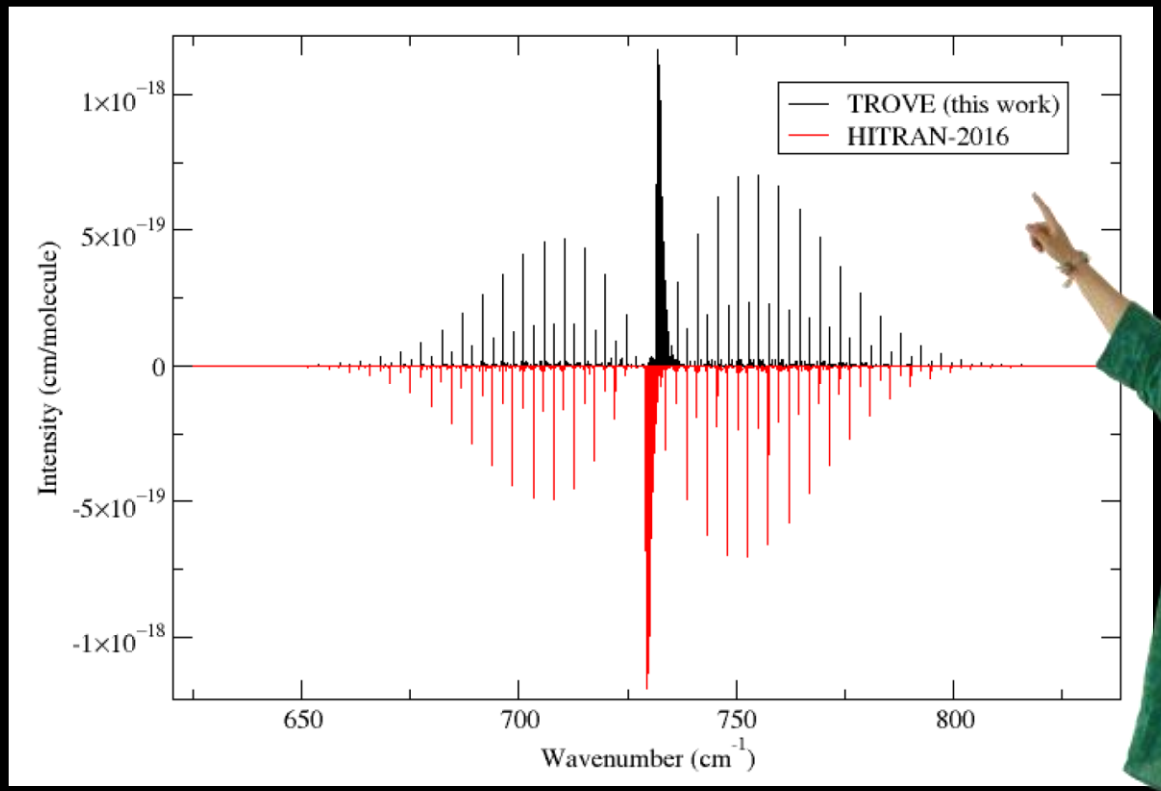
Our accuracy

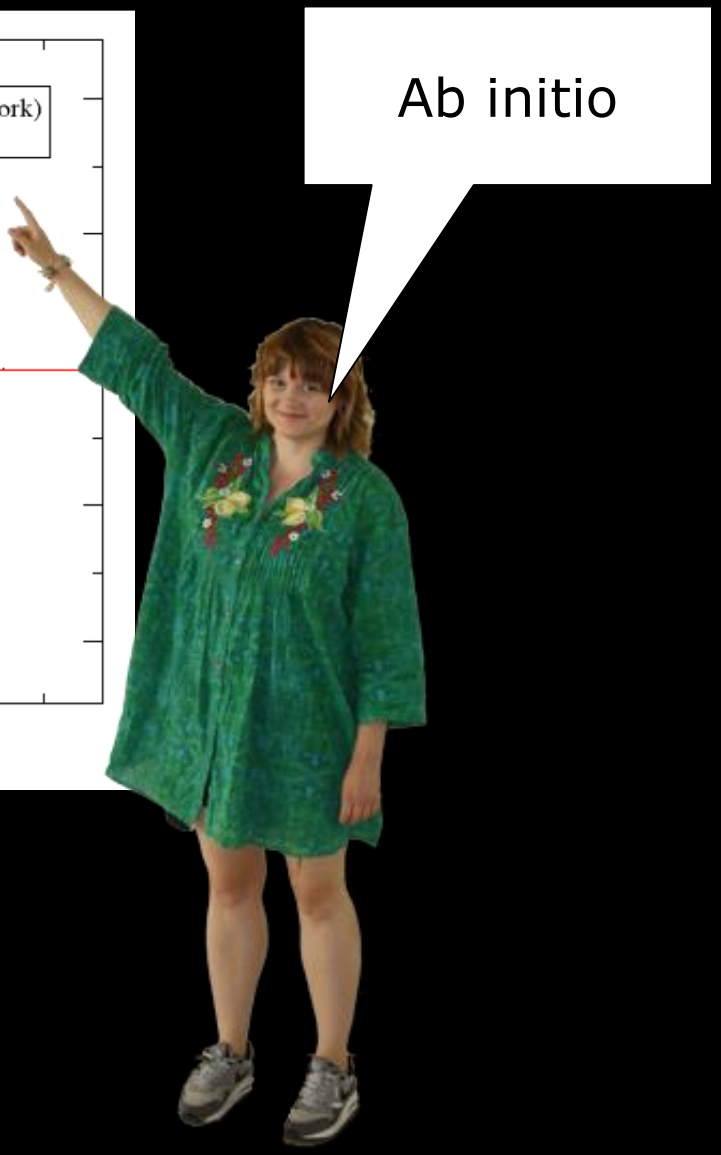
We (almost) always have to refine our ab initio model to experiment

C_2H_2

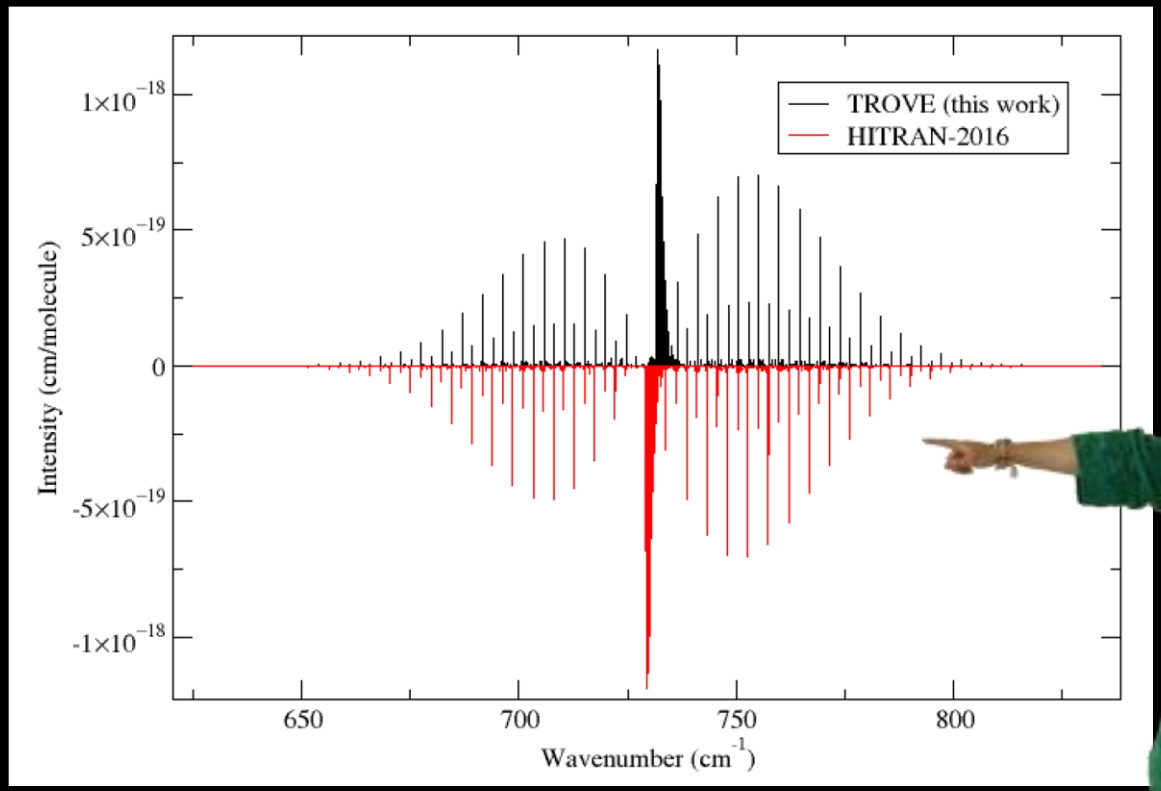

TROVE (this work)
HITRAN-2016
1×10^-18
5×10^-19
0
-5×10^-19
-1×10^-18
Intensity (cm/molecule)
650
700
750
800
Wavenumber (cm^-1)

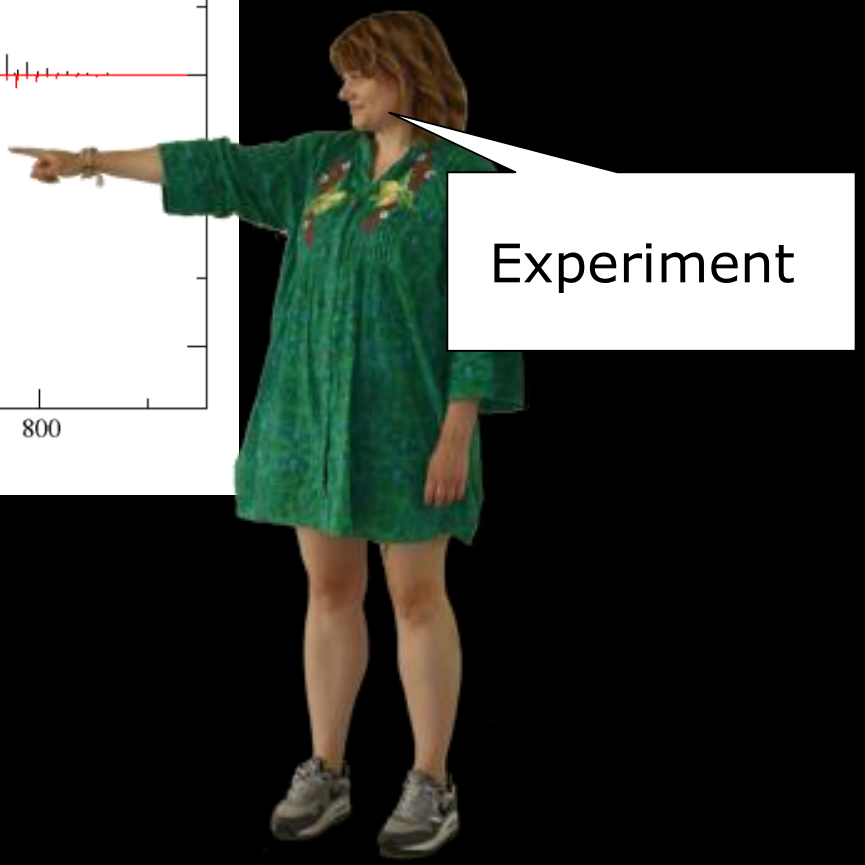
C_2H_2


TROVE (this work)
HITRAN-2016
1×10⁻¹⁸
5×10⁻¹⁹
0
-5×10⁻¹⁹
-1×10⁻¹⁸
Intensity (cm/molecule)
650
700
750
800
Wavenumber (cm⁻¹)


Ab initio

C_2H_2


TROVE (this work)
HITRAN-2016
1×10^-18
5×10^-19
0
-5×10^-19
-1×10^-18
Intensity (cm/molecule)
650
700
750
800
Wavenumber (cm^-1)

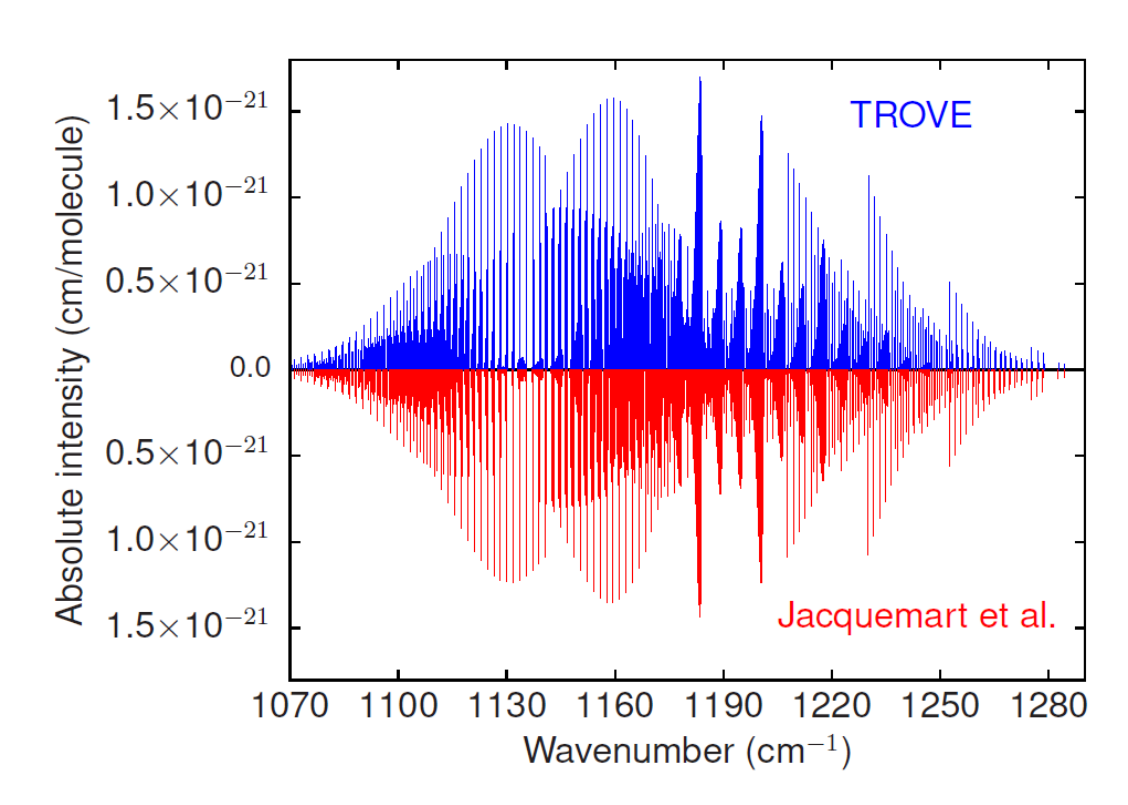

Experiment

… which is typically 1-5 cm^{-1}
for the fundamentals

You can do a better ab initio if
you push really hard …

… for example pure ab initio (no cheating) spectrum of CH_3F

CH_3F



PCCP

PAPER

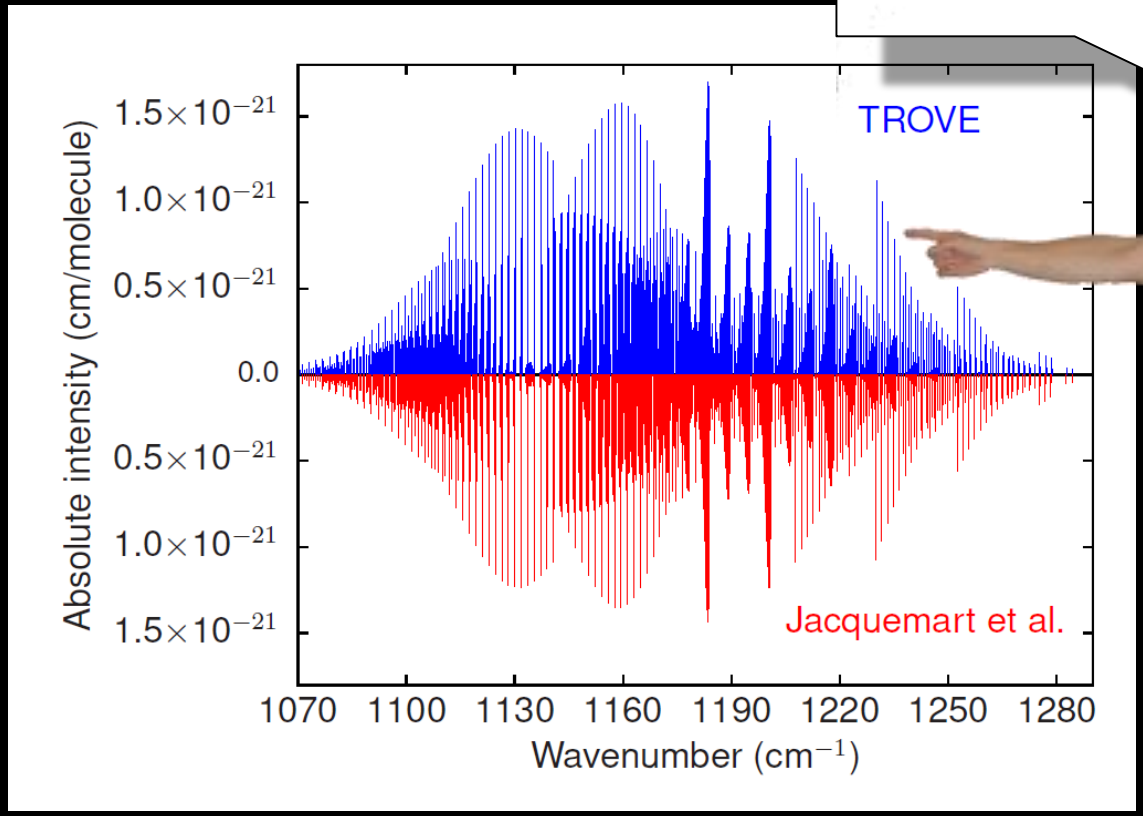
The rotation–vibration spectrum of methyl fluoride from first principles†

Cite this: DOI: 10.1039/c8cp01721b

Alec Owens, *[ab] Andrey Yachmenev,[ab] Jochen Küpper,[abc] Sergei N. Yurchenko[d] and Walter Thiel[e]

CH_3F

Theory



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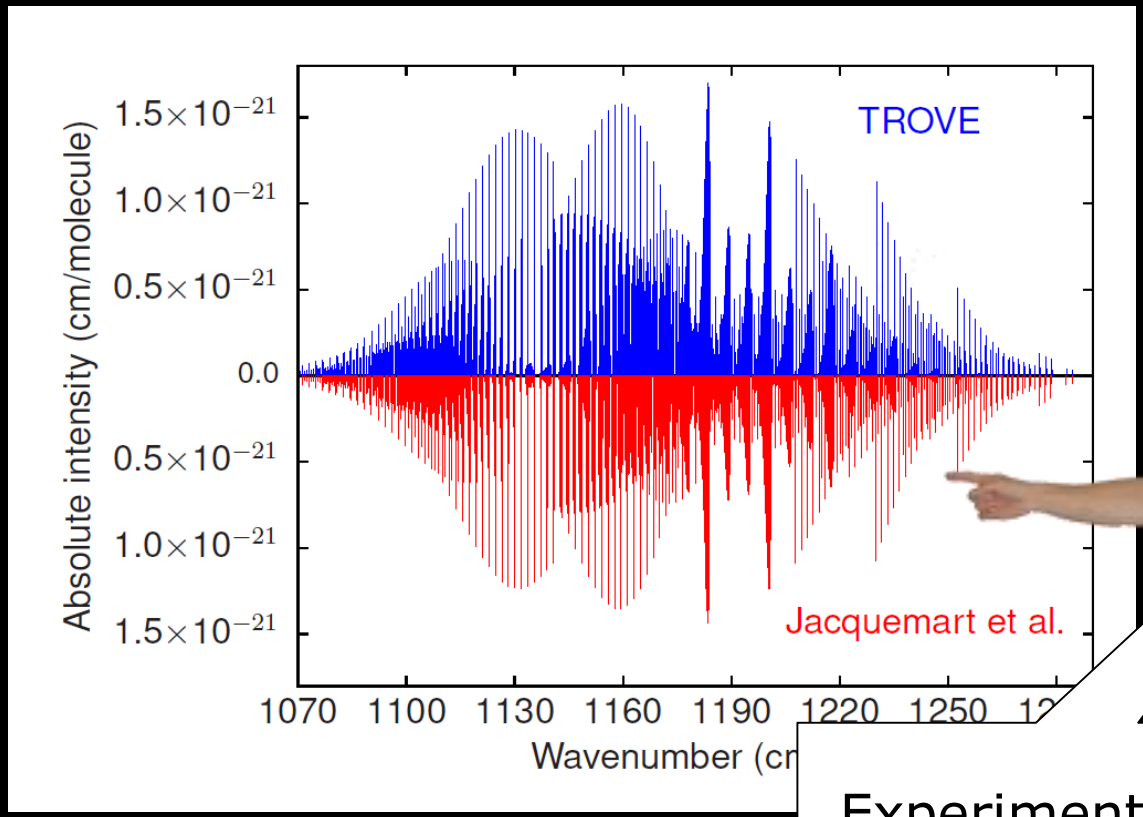
CH_3F



Experiment

PCCP

PAPER

The rotation–vibration spectrum of methyl fluoride from first principles†

Cite this: DOI: 10.1039/c8cp01721b

Alec Owens, *[ab] Andrey Yachmenev,[ab] Jochen Küpper,[abc] Sergei N. Yurchenko[d] and Walter Thiel[e]

In fact intensities are (almost)
always ab initio!

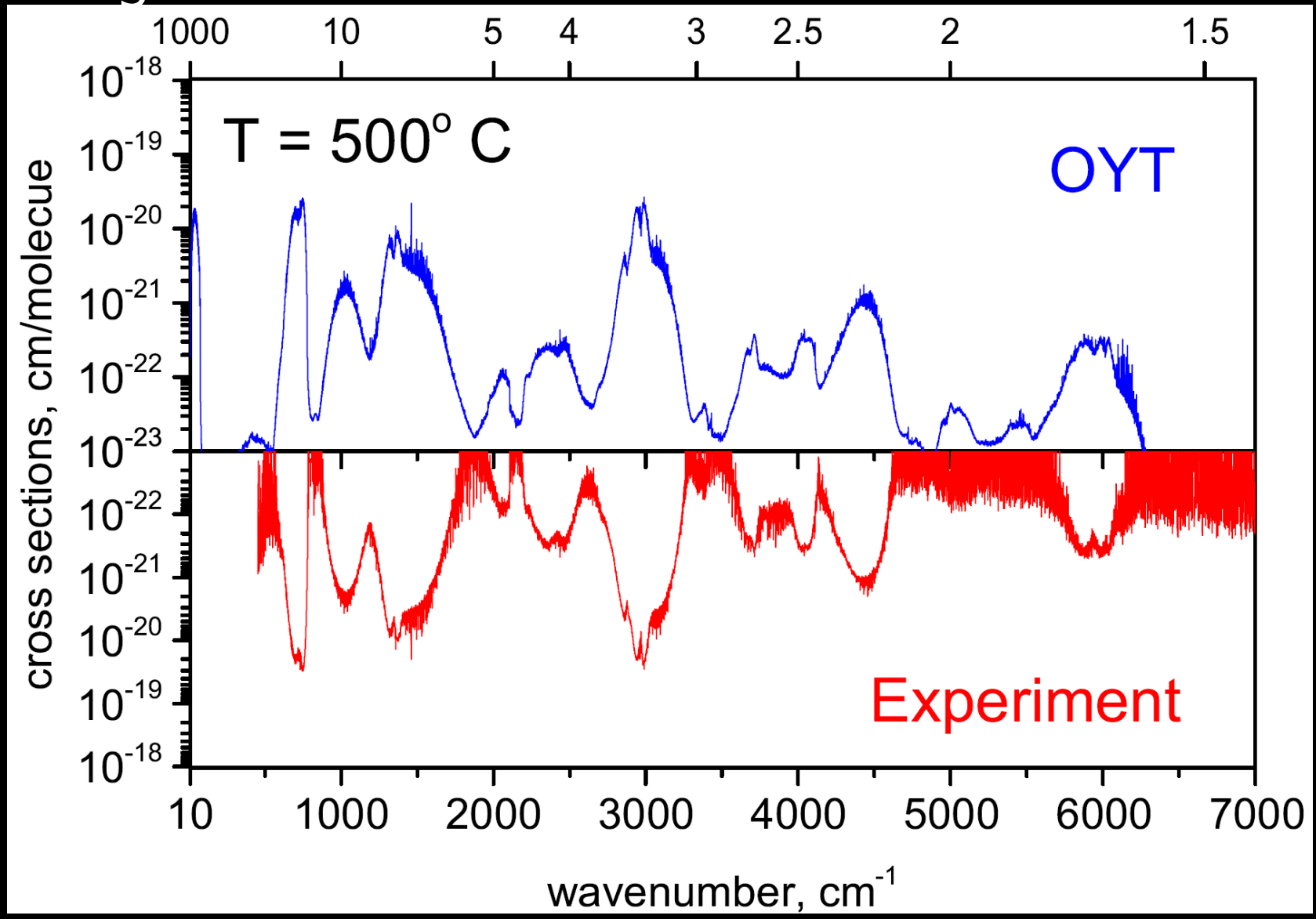
Accuracy of 10-20% is common for a reasonable level of theory

CH_3Cl

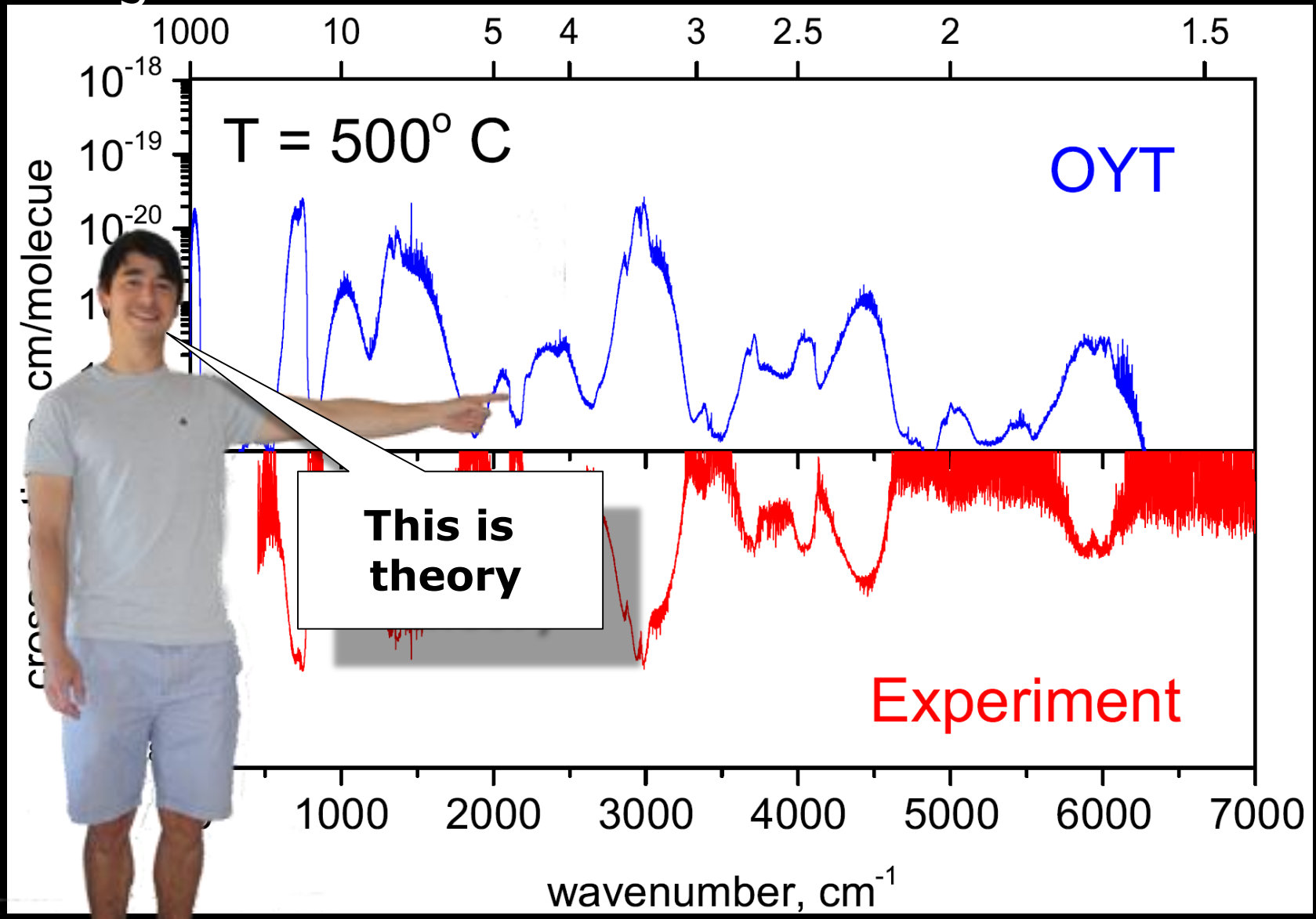
CH_3Cl

Comparing to high temperature experiments by Alex Fateev (Denmark)
T = 500°C

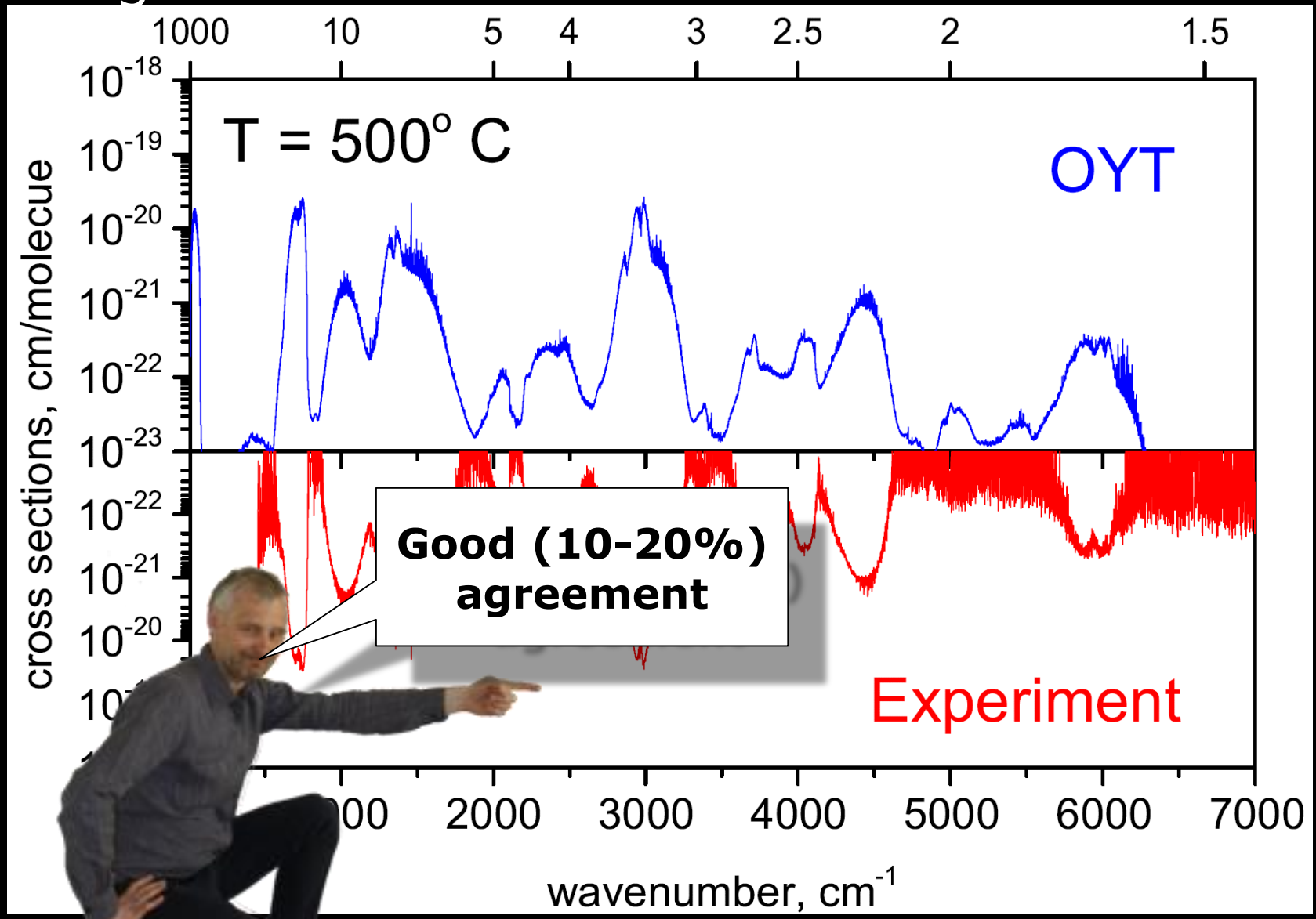
CH_3Cl


1000
10
5
4
3
2.5
2
1.5
T = 500° C
OYT
Experiment
cross sections, cm/molecue
10^-18
10^-19
10^-20
10^-21
10^-22
10^-23
10
1000
2000
3000
4000
5000
6000
7000
wavenumber, cm^-1

CH_3Cl


1000
10
5
4
3
2.5
2
1.5
10^{-18}
10^{-19}
10^{-20}
cm/molecue
T = 500° C
OYT
This is theory
Experiment
1000
2000
3000
4000
5000
6000
7000
wavenumber, cm^{-1}

CH_3Cl

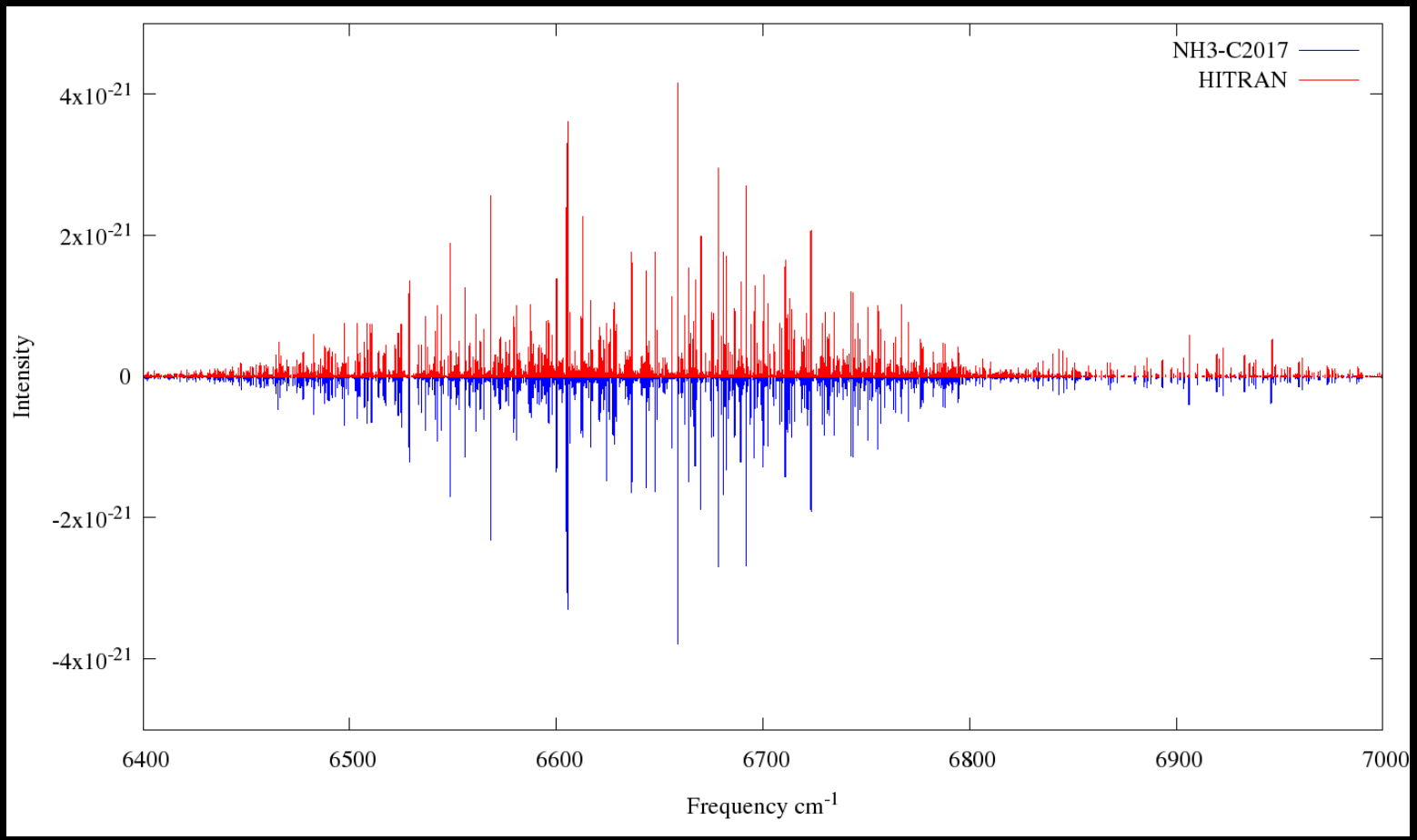

1000
10
5
4
3
2.5
2
1.5
T = 500° C
OYT
Experiment
Good (10-20%) agreement
cross sections, cm/molecue
wavenumber, cm-1
2000
3000
4000
5000
6000
7000

BTW: this is the line list
containing 320 billion lines …
~8 Tb

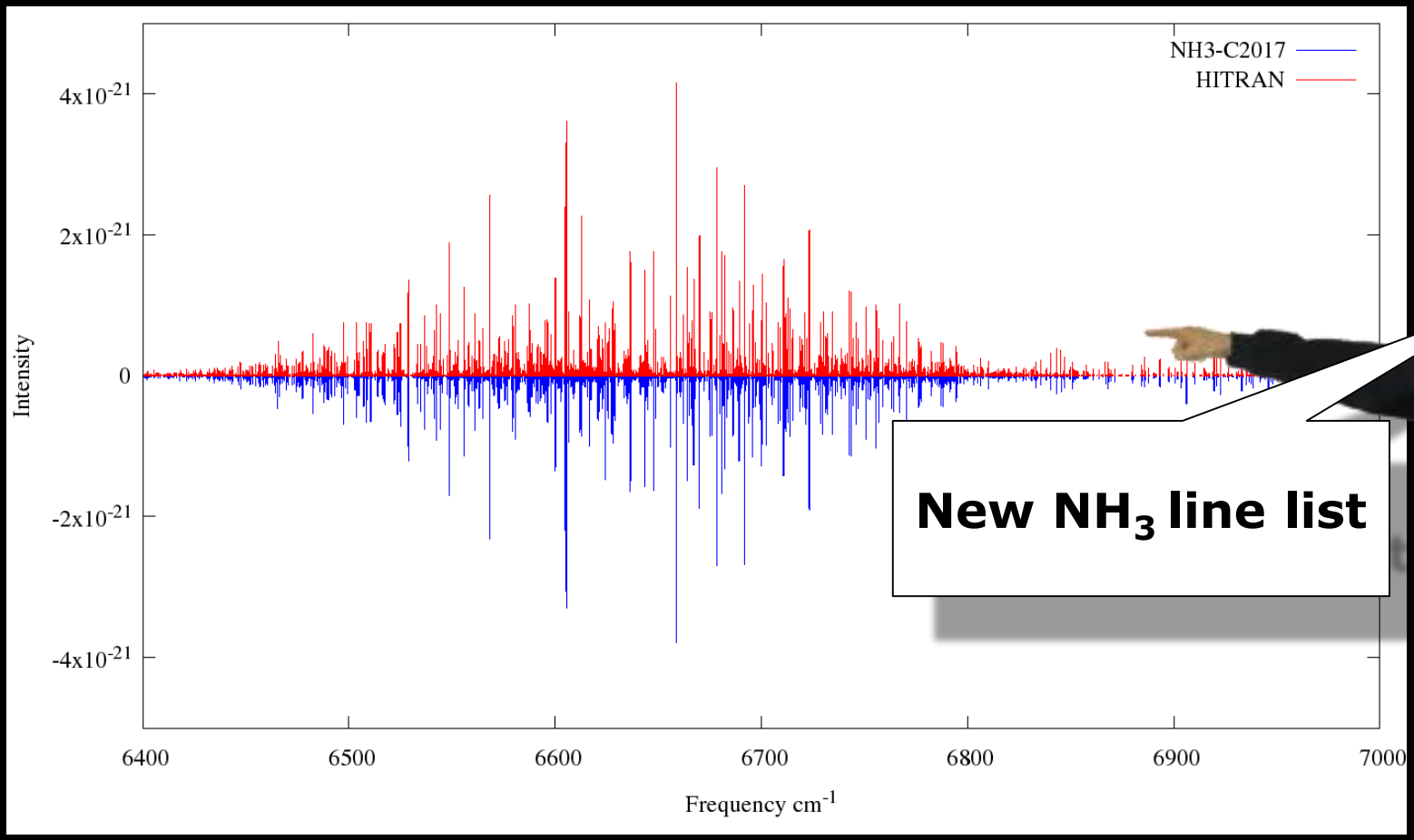
BTW: this is the line list
containing 320 billion lines ...
~8 Tb

BTW, *Olivia,*
Alex Fateev's lab can do hot temperature VUV spectra for many molecule

Accurate ro-vibrational line positions only after fitting the model to experiment

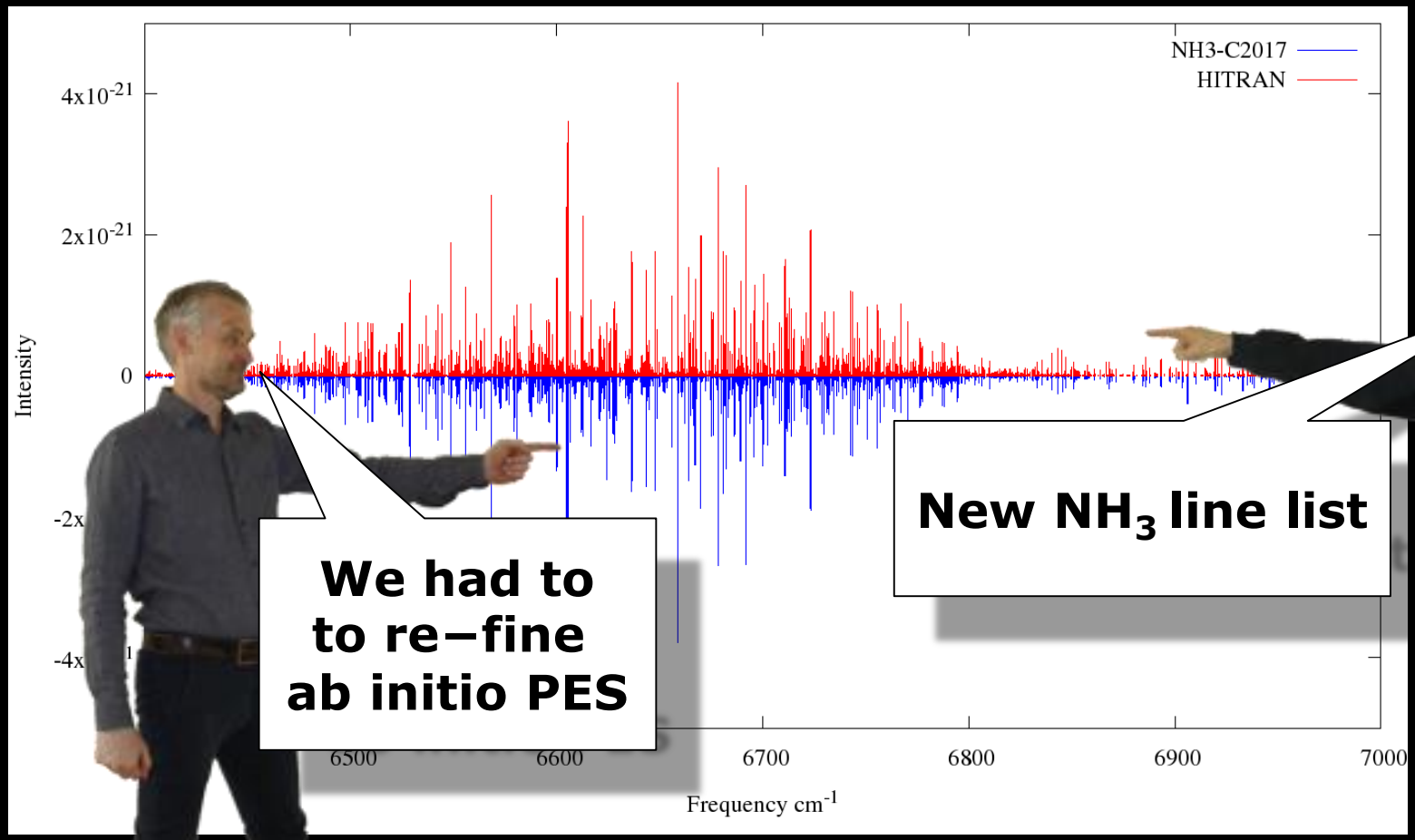

NH3-C2017
HITRAN
4x10-21
2x10-21
0
-2x10-21
-4x10-21
Intensity
6400
6500
6600
6700
6800
6900
7000
Frequency cm-1

NH_3



New NH_3 line list

NH_3

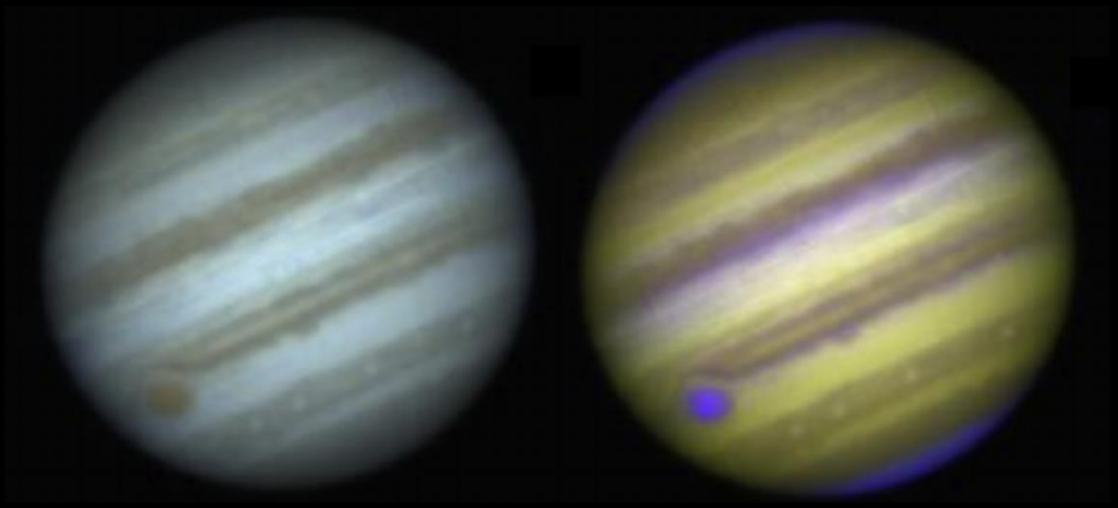


We had to to re−fine ab initio PES

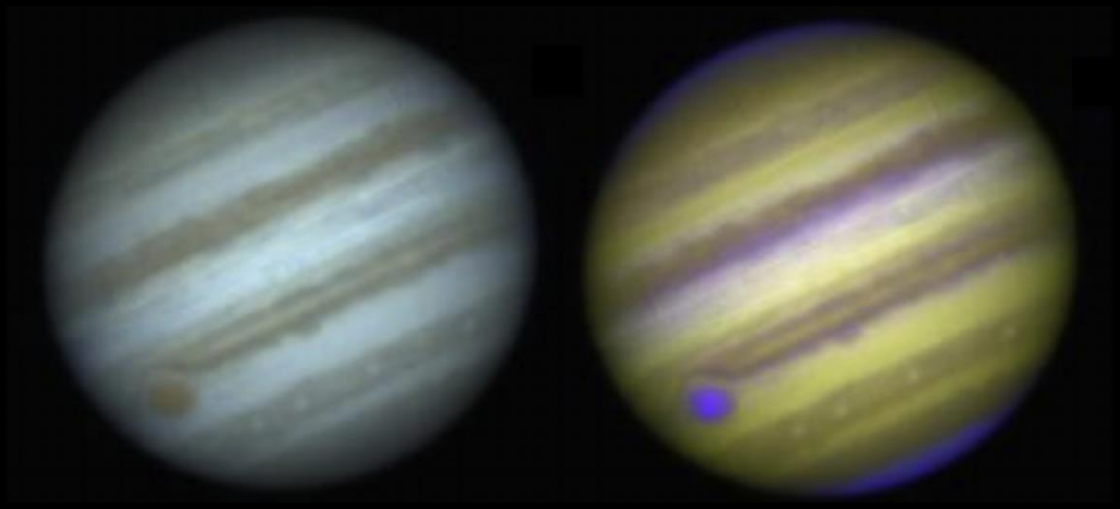
New NH_3 line list

Our Ammonia should be good enough for high resolution Doppler in IR

… and not so high resolution
in visible but still useful



Visible spectrum of Jupiter:
Ammonia bands



Visible spectrum of Jupiter: Ammonia bands

Icarus 302 (2018) 426–436

Contents lists available at ScienceDirect

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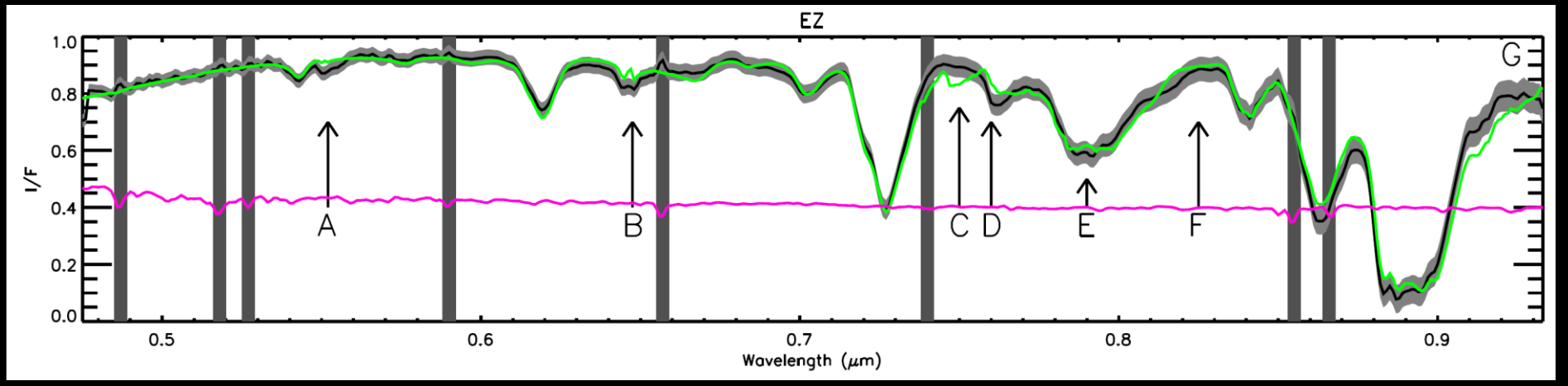
journal homepage: www.elsevier.com/locate/icarus

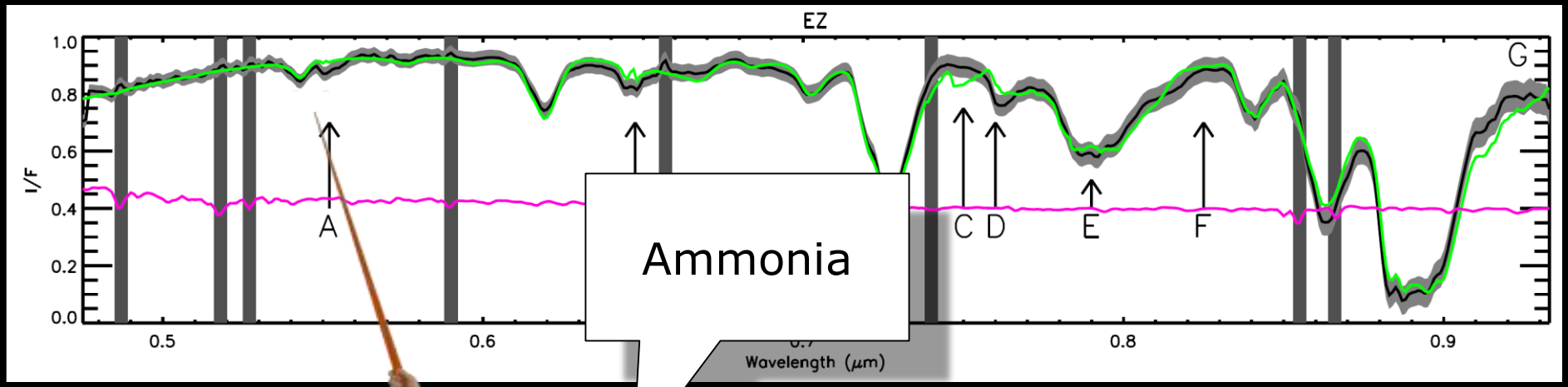
Analysis of gaseous ammonia (NH_3) absorption in the visible spectrum of Jupiter

Patrick G.J. Irwin*, Neil Bowles, Ashwin S. Braude, Ryan Garland, Simon Calcutt

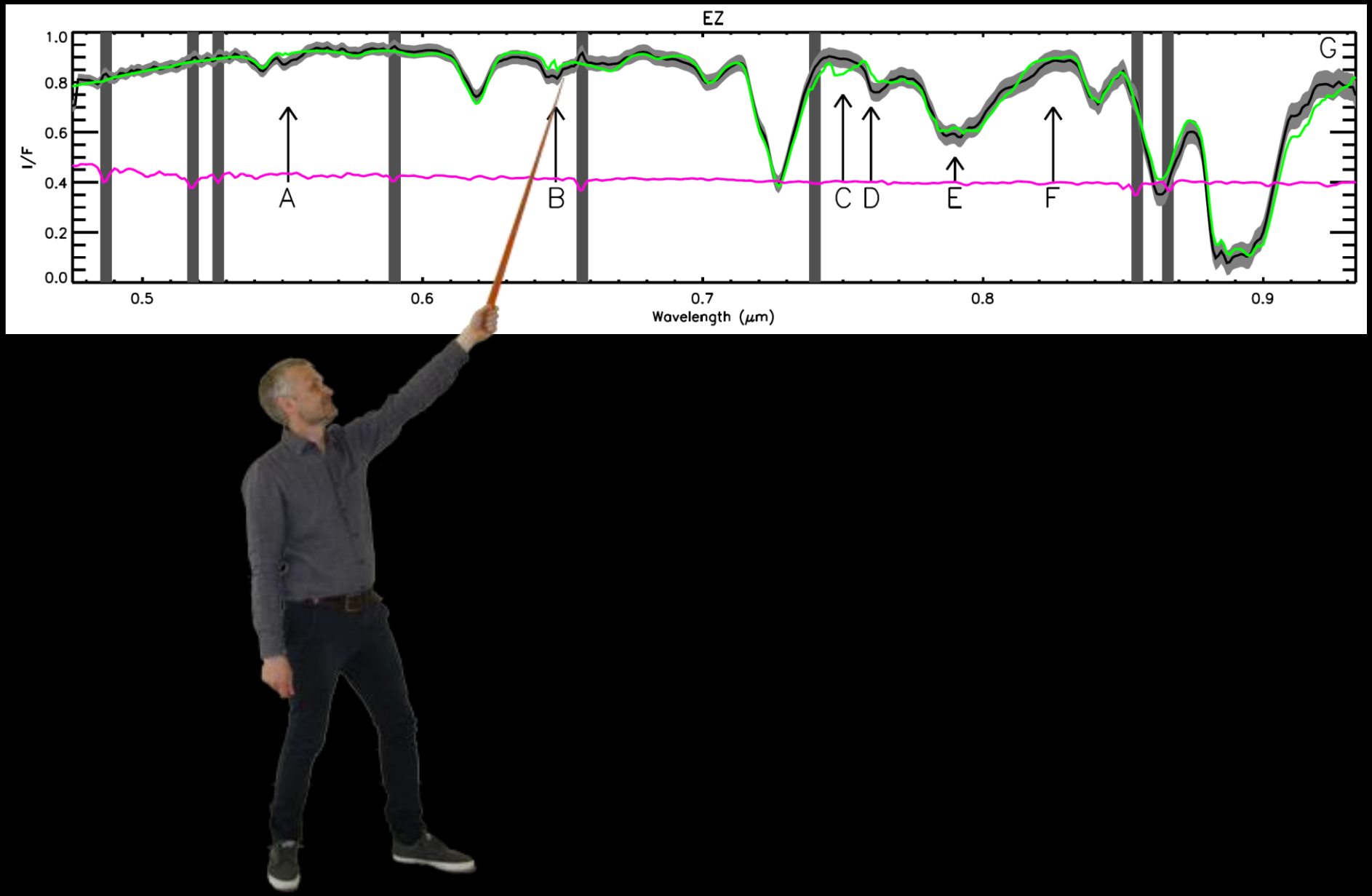
Department of Physics, University of Oxford, Parks Rd, Oxford OX1 3PU, UK

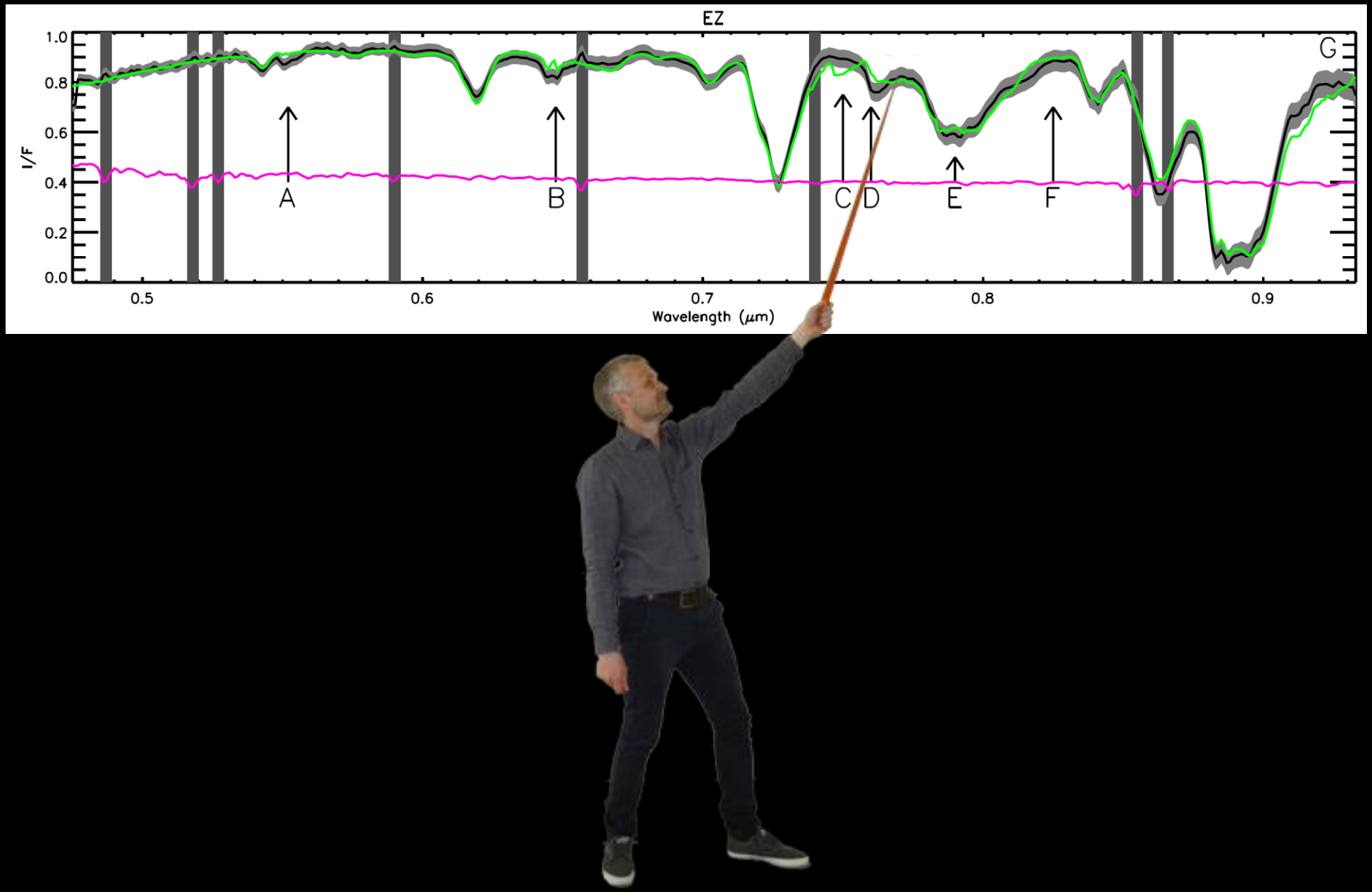
Very Large Telescope (VLT) Multi Unit Spectroscopic Explorer (MUSE) instrument in the spectral range 0.48–0.93 μm

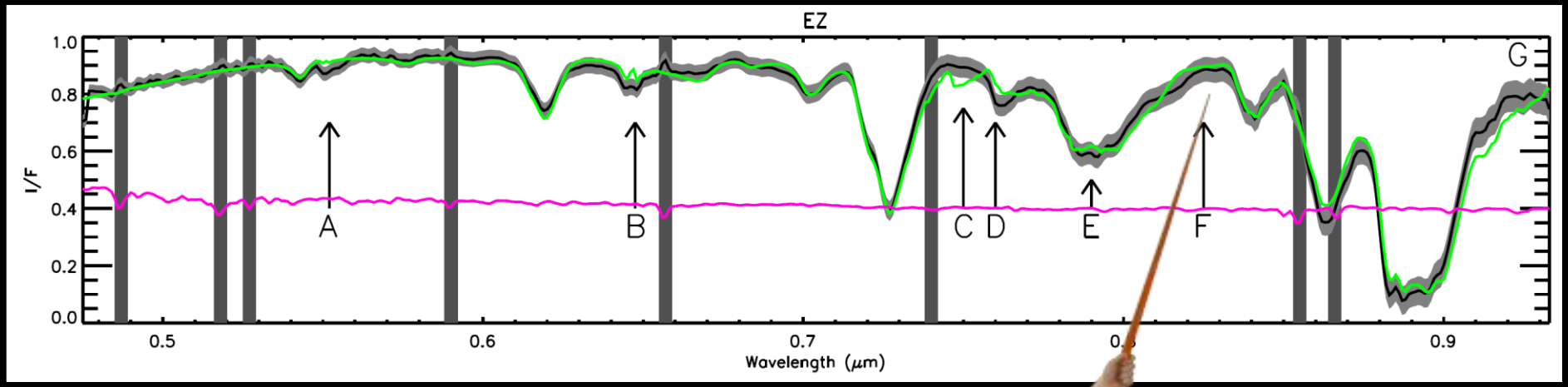

EZ
1.0
0.8
0.6
0.4
0.2
0.0
I/F
0.5
0.6
0.7
0.8
0.9
Wavelength (μm)
A
B
C
D
E
F
G

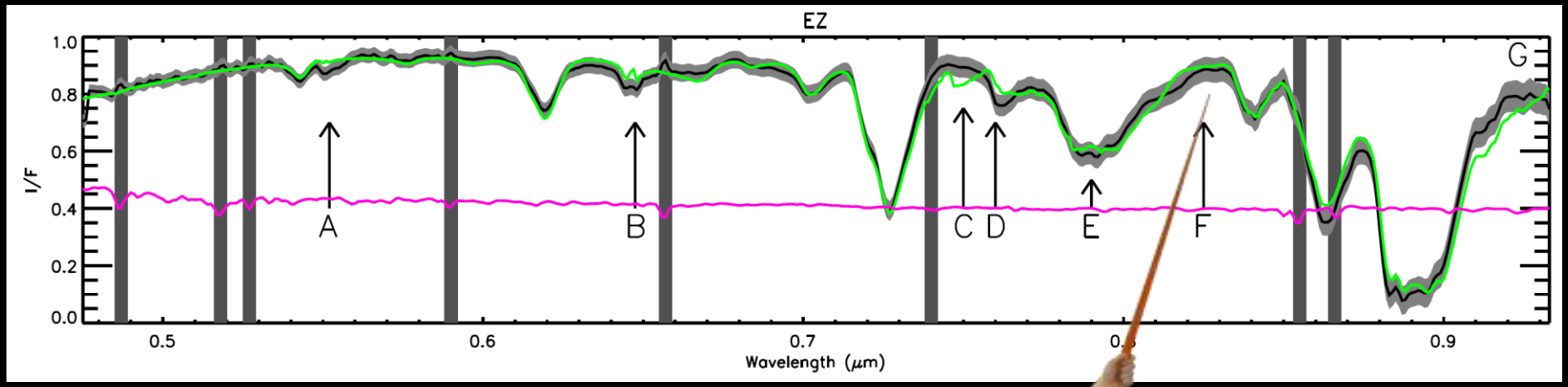


Ammonia


EZ
I/F
1.0
0.8
0.6
0.4
0.2
0.0
0.5
0.6
0.7
0.8
0.9
Wavelength (μm)
A
B
C
D
E
F
G


EZ
I/F
1.0
0.8
0.6
0.4
0.2
0.0
0.5
0.6
0.7
0.8
0.9
Wavelength (μm)
A
B
C
D
E
F
G


EZ
I/F
1.0
0.8
0.6
0.4
0.2
0.0
0.5
0.6
0.7
0.9
Wavelength (μm)
A
B
C
D
E
F
G



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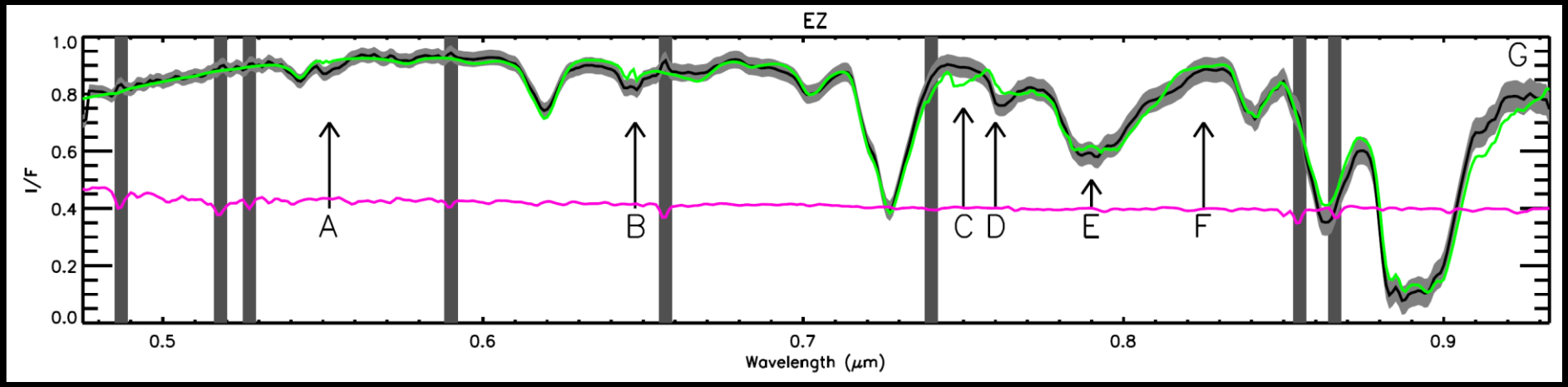
Department of Physics, University of Oxford, Parks Rd, Oxford OX1 3PU, UK



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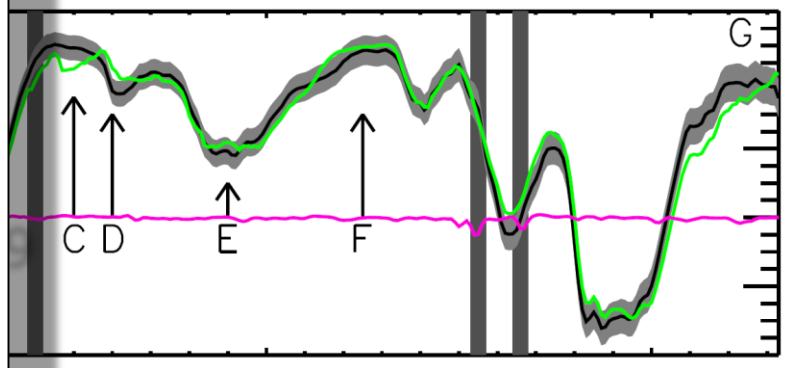
" These band data appear consistent with ExoMOL data, at wavelengths where they overlap, but ExoMol does not cover the ammonia bands at 0.79 and 0.765 μm "



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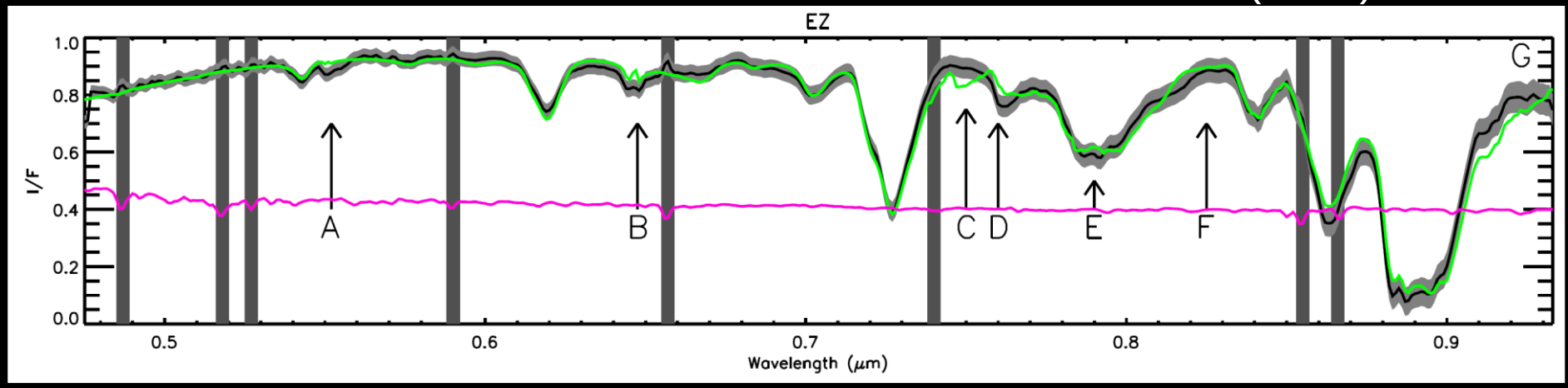
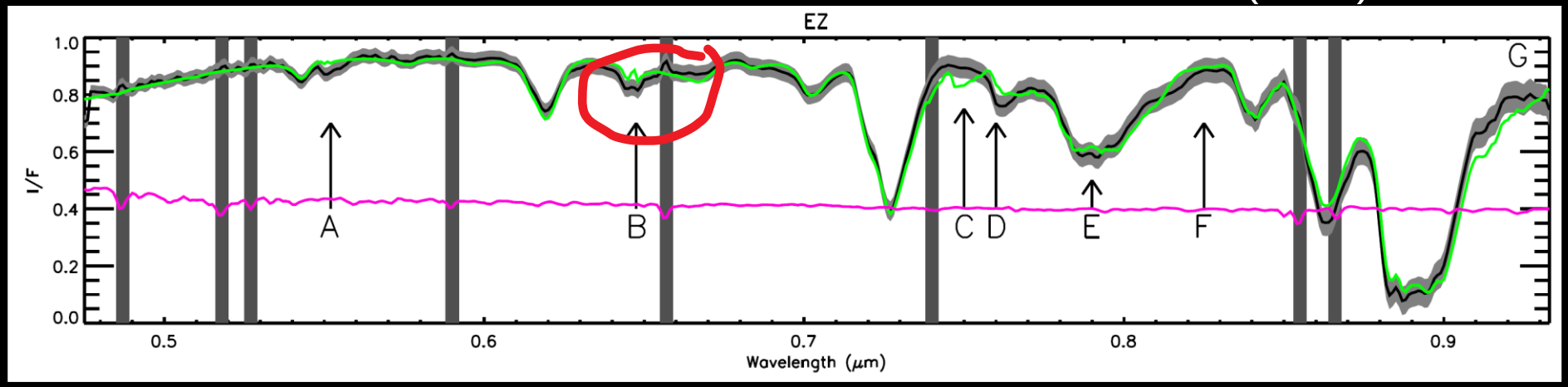
Department of Physics, University of Oxford, Parks Rd, Oxford OX1 3PU, UK

Pat Irwin is being testing our new empirical line list for NH_3

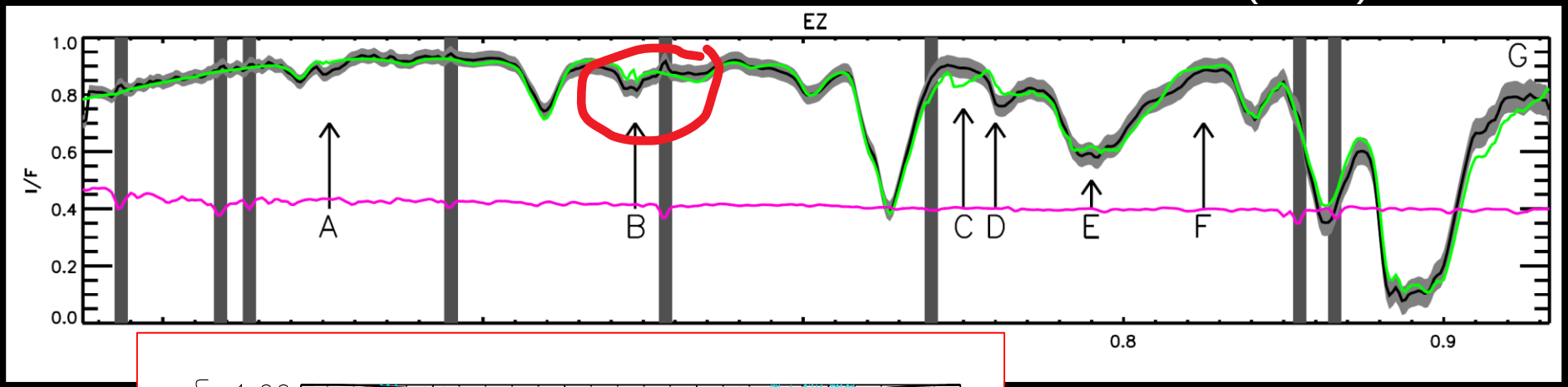
P. Irwin et. al Icarus 302 (2018) 426–436

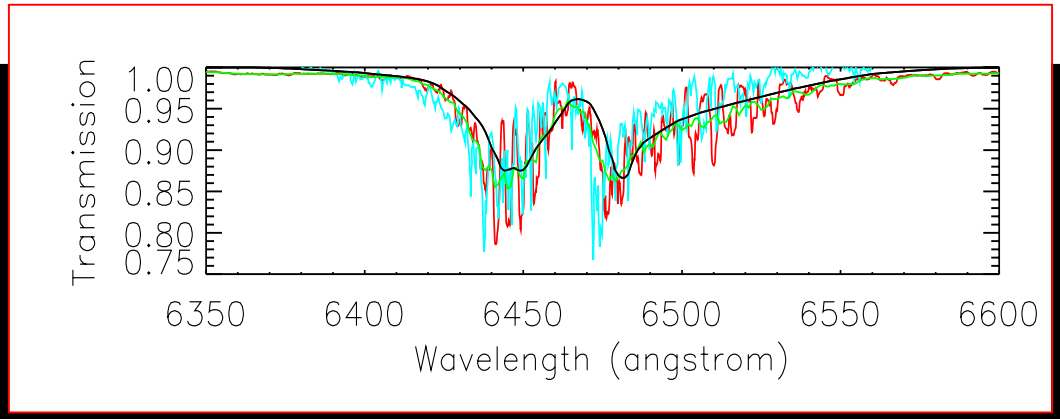


P. Irwin et. al Icarus 302 (2018) 426–436



P. Irwin et. al Icarus 302 (2018) 426–436





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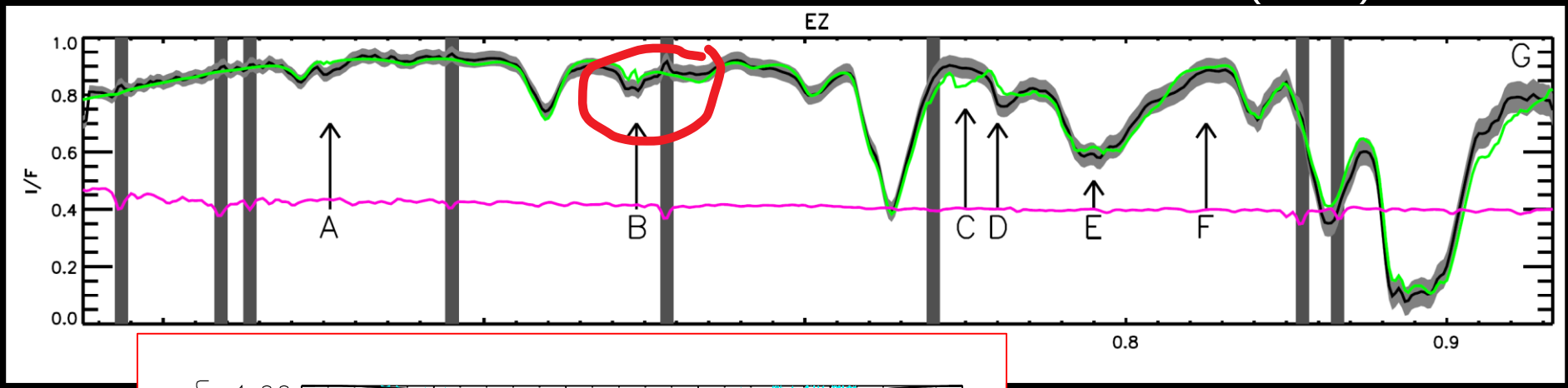
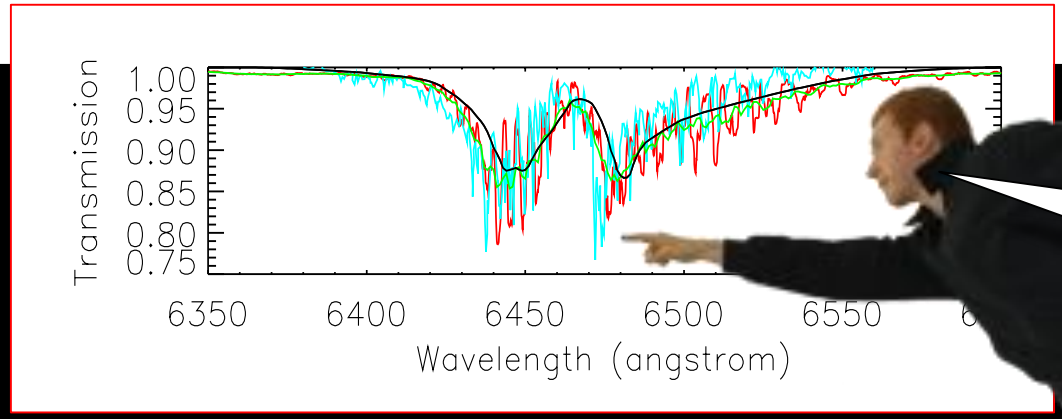
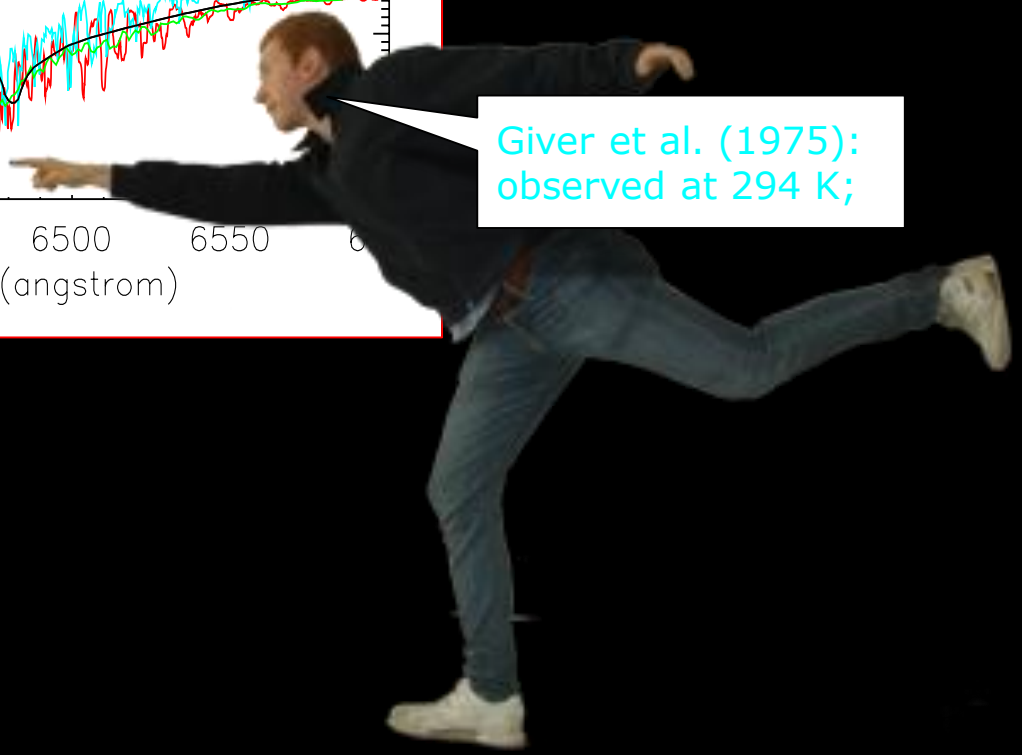
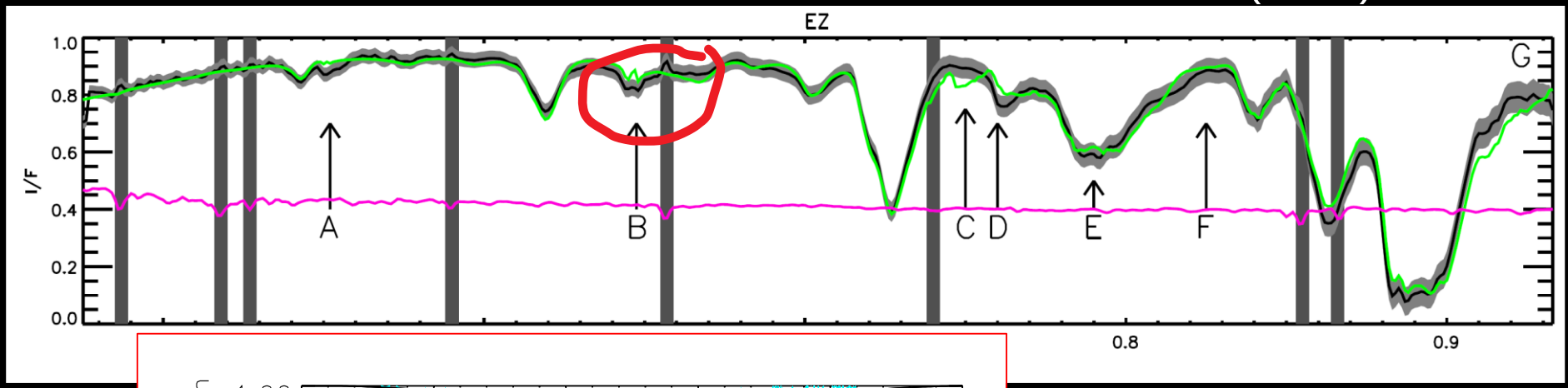


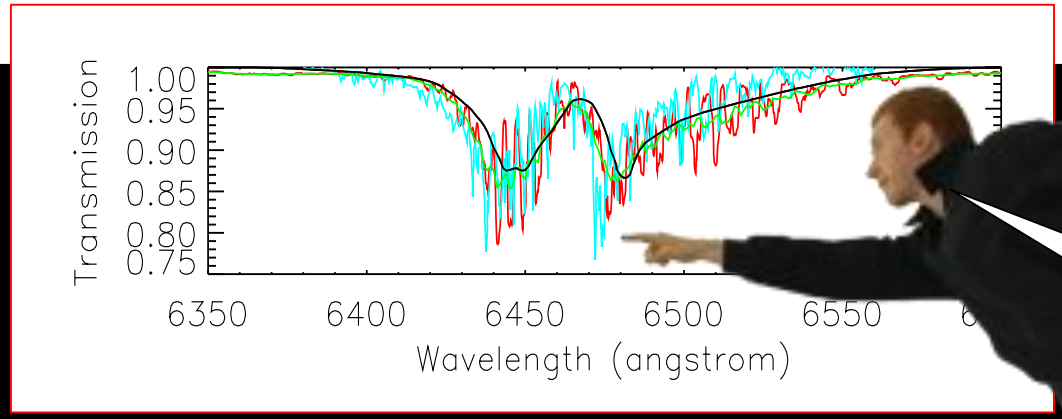




Giver et al. (1975): observed at 294 K;

P. Irwin et. al Icarus 302 (2018) 426–436





Lutz and Owen (1980): low resolution absorption coefficients.

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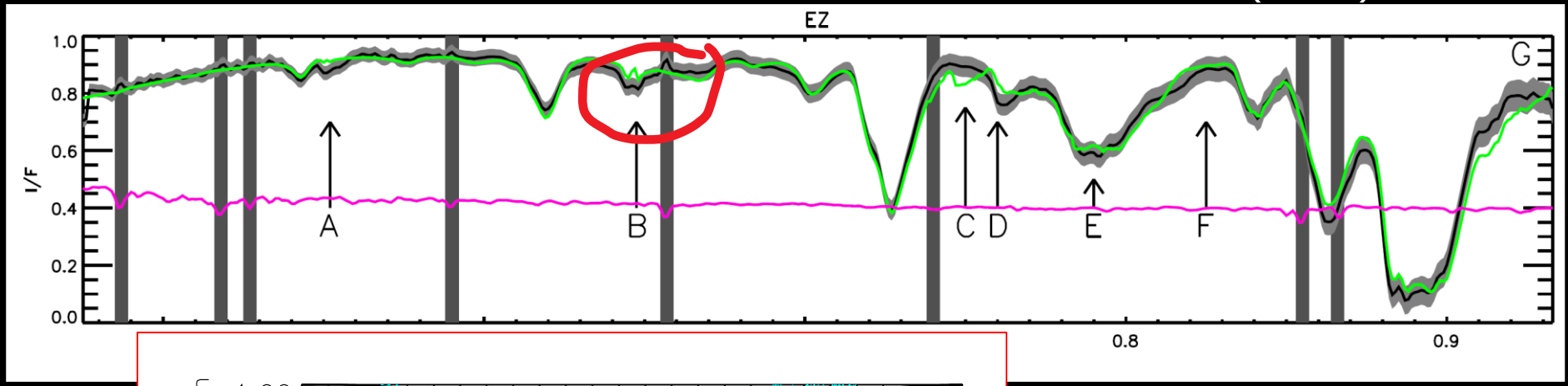
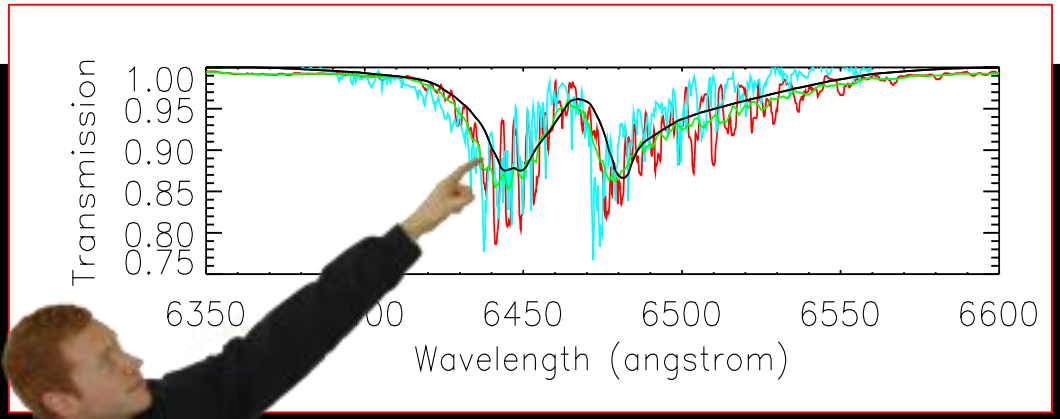




Our theoretical spectrum is represented by the green and red lines

Software

ExoCross: our open access code to generate cross sections from ExoMol, HITRAN etc

A&A 614, A131 (2018)
https://doi.org/10.1051/0004-6361/201732531

Astronomy & Astrophysics

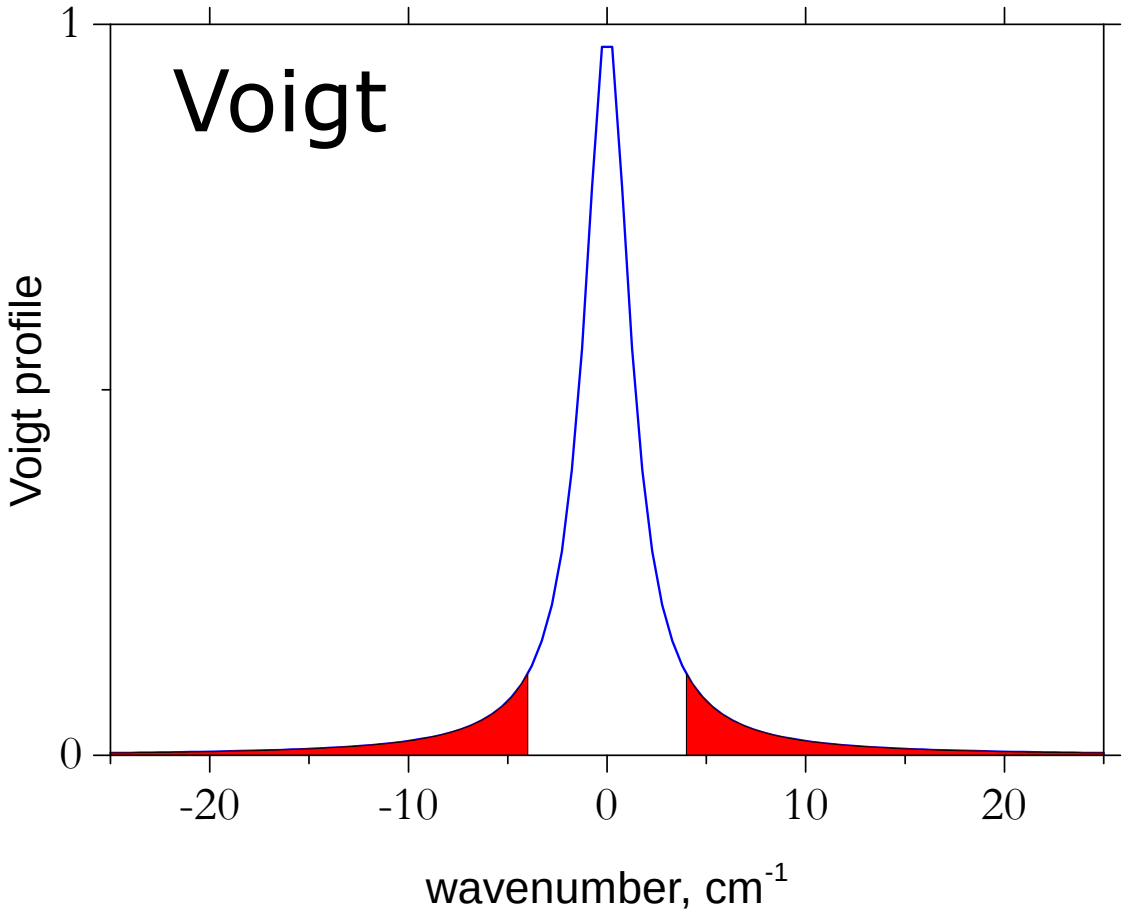
ExoCross: a general program for generating spectra from molecular line lists*

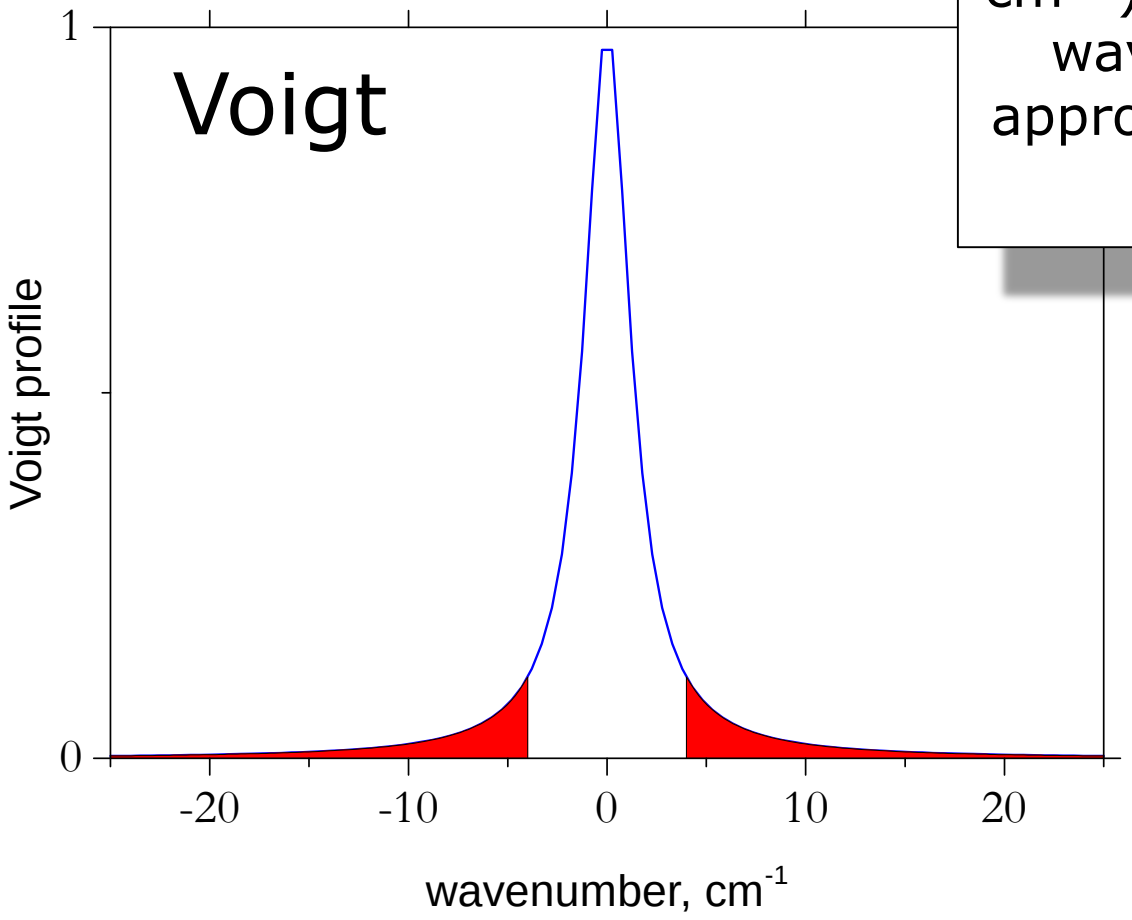
Sergei N. Yurchenko, Ahmed F. Al-Refaie, and Jonathan Tennyson

Department of Physics and Astronomy, University College London, London WC1E 6BT, UK
e-mail: s.yurchenko@ucl.ac.uk

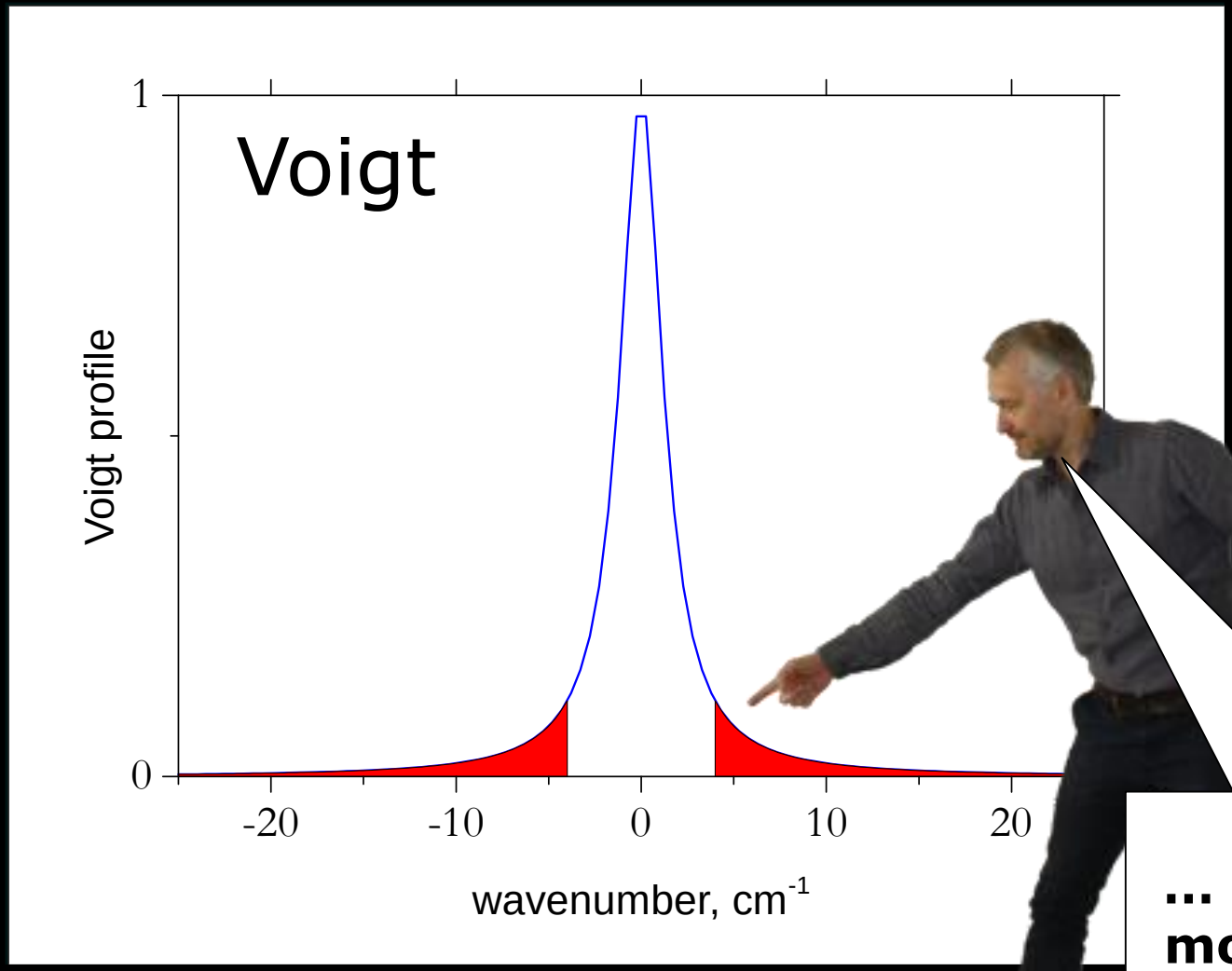
It is also fast

It uses a ‘cheating’ Voigt


Voigt
1
0
Voigt profile
-20
-10
0
10
20
wavenumber, cm-1

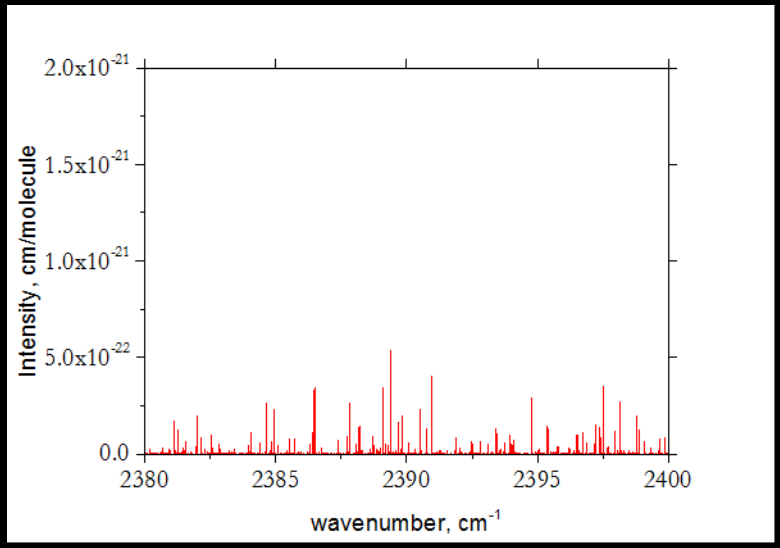


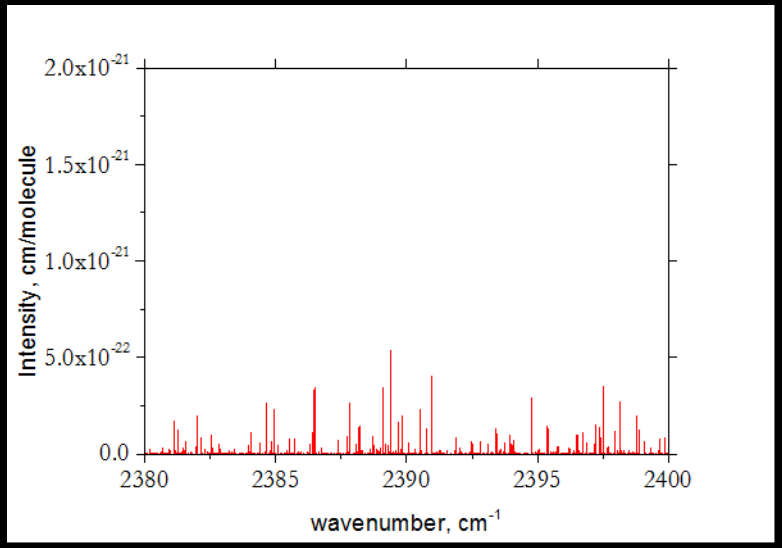
"The wings of the Vogt (>4 cm^{-1}) do not depend on the wavelength and can be approximated by the same sample profile."

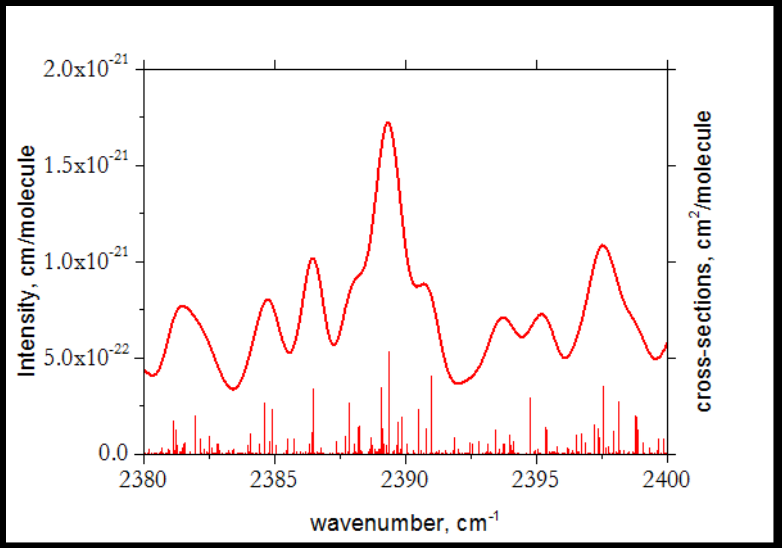


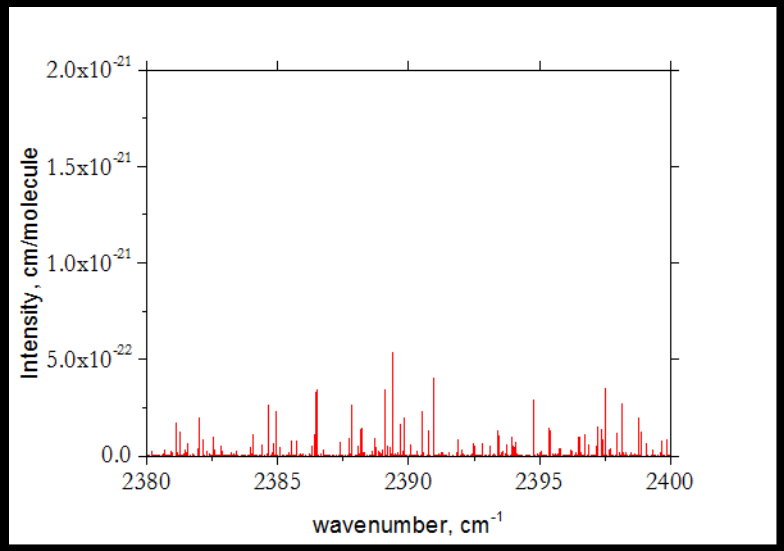
… and wings are the most expensive part

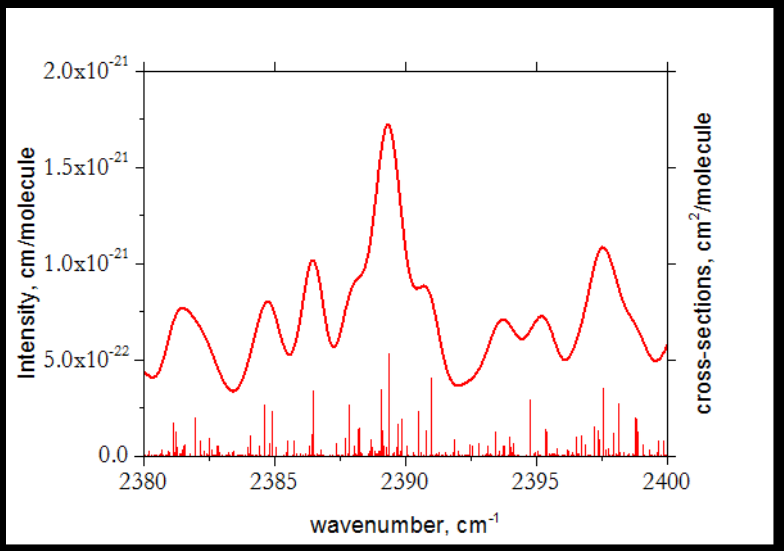
Super-lines

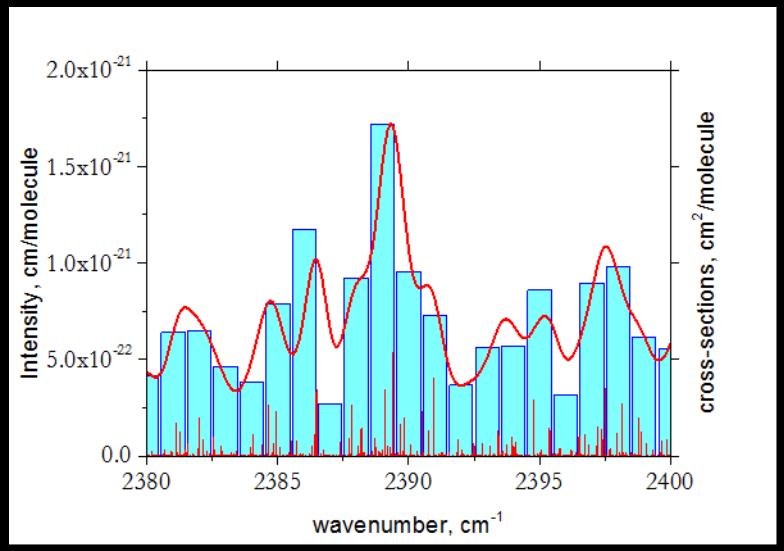

2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1

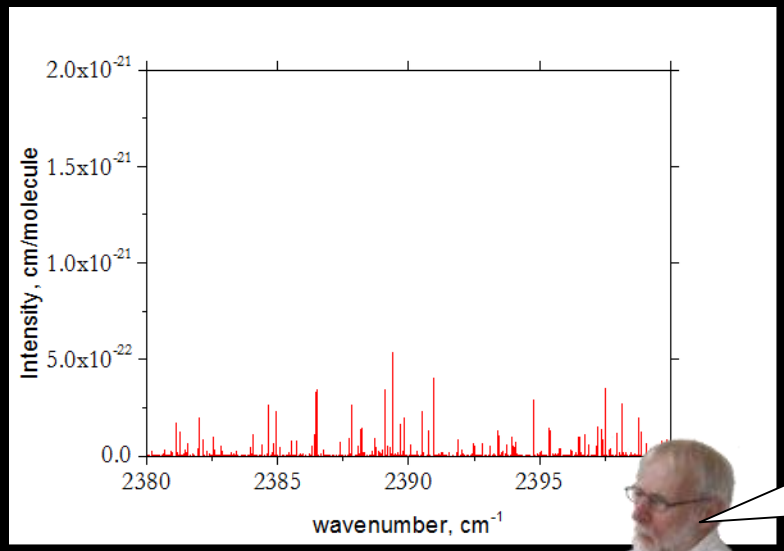

2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1

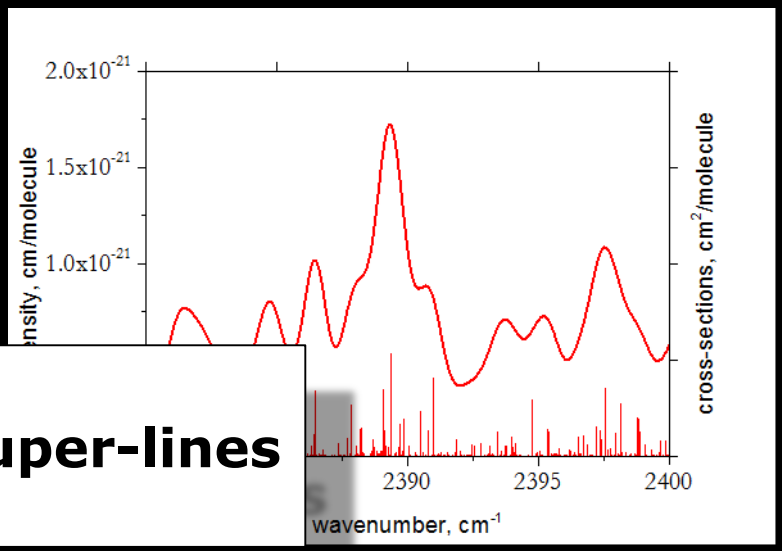

2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
cross-sections, cm2/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1


2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1

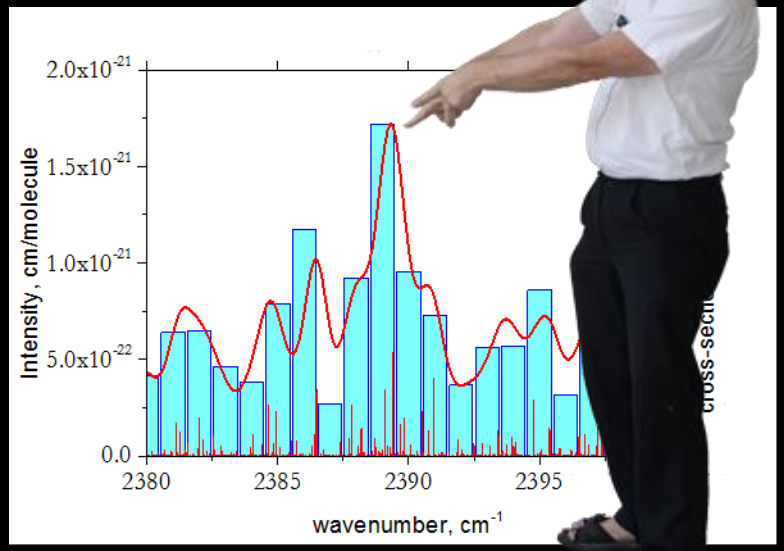

2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
cross-sections, cm2/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1

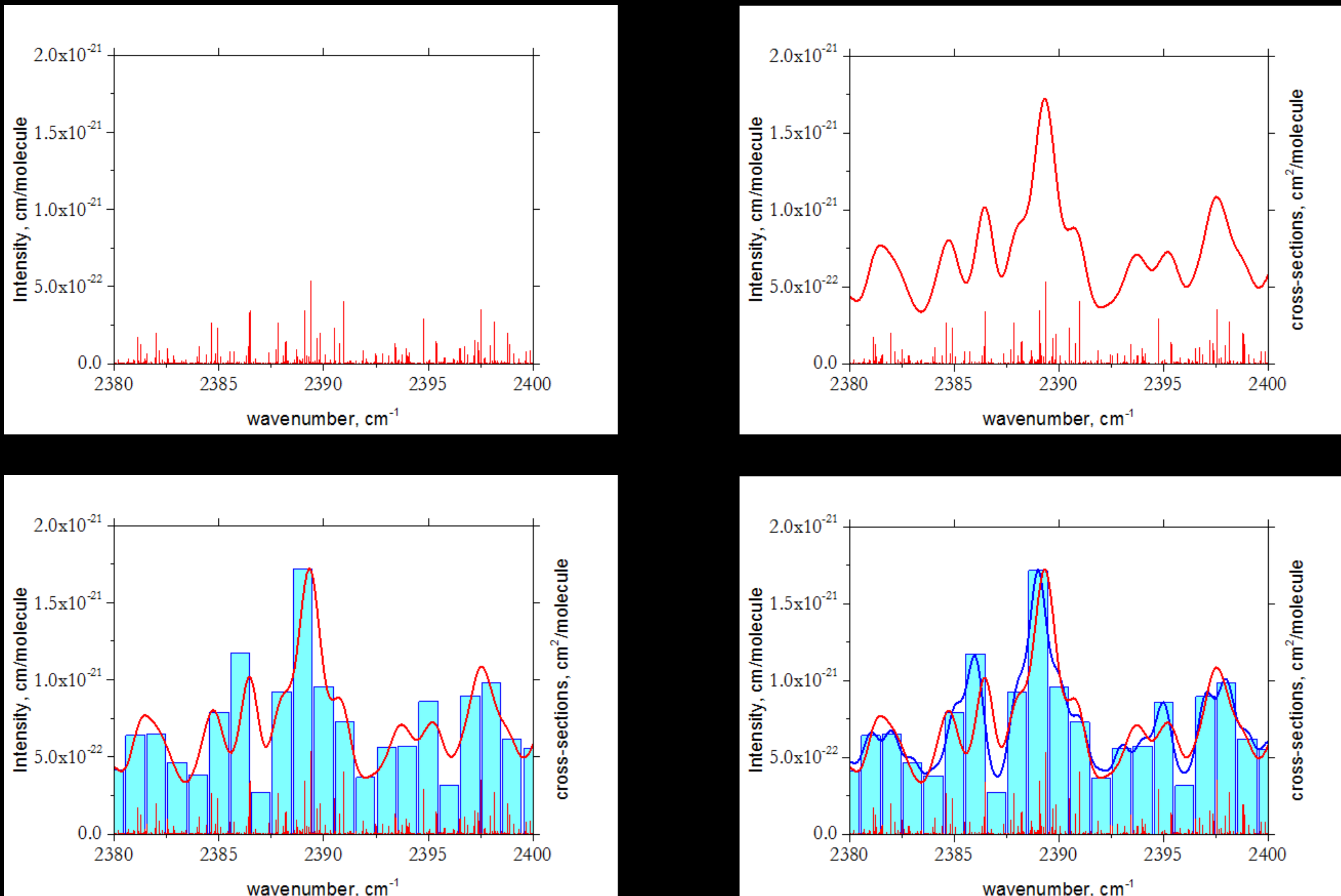

2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
cross-sections, cm2/molecule
2380
2385
2390
2395
2400
wavenumber, cm-1


2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
2380
2385
2390
2395
wavenumber, cm-1


2.0x10-21
1.5x10-21
1.0x10-21
cross-sections, cm2/molecule
2390
2395
2400
wavenumber, cm-1

Super-lines


2.0x10-21
1.5x10-21
1.0x10-21
5.0x10-22
0.0
Intensity, cm/molecule
2380
2385
2390
2395
wavenumber, cm-1


2.0x10^-21
1.5x10^-21
1.0x10^-21
5.0x10^-22
0.0
Intensity, cm/molecule
cross-sections, cm^2/molecule
2380
2385
2390
2395
2400
wavenumber, cm^-1

This speeds up the
calculations a lot

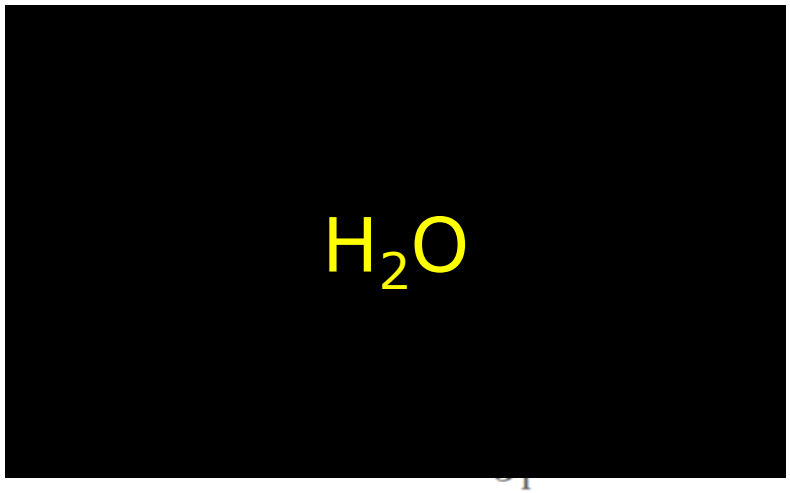
The artifact:

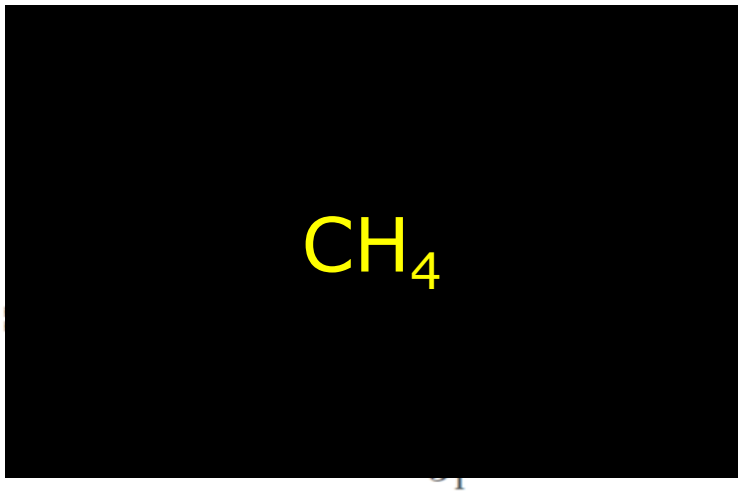
The artifact:

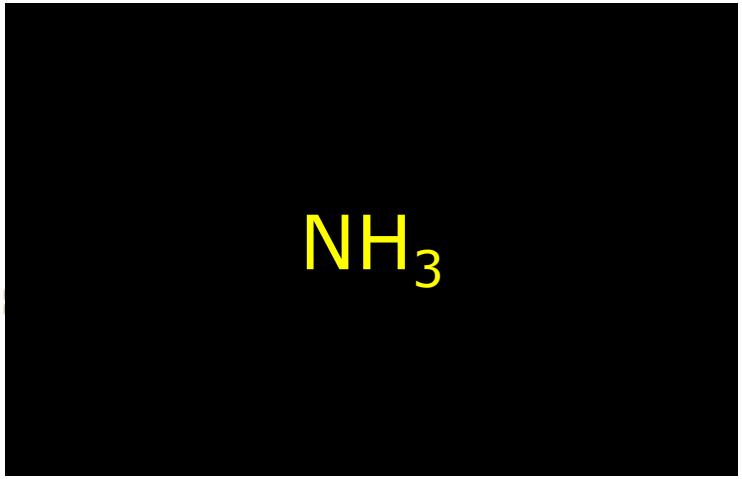
super-line profiles
cannot depend on
quantum numbers ☹

… but they do:

Voigt parameters as simple functions of *J*

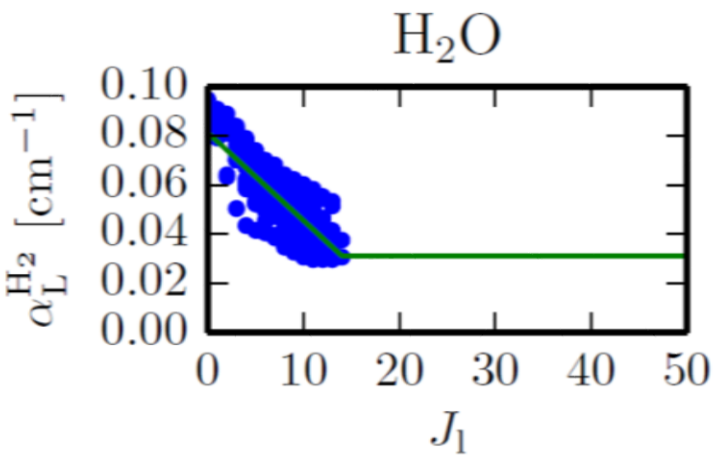






Amundsen AA (2014)

Voigt parameters as simple functions of *J*



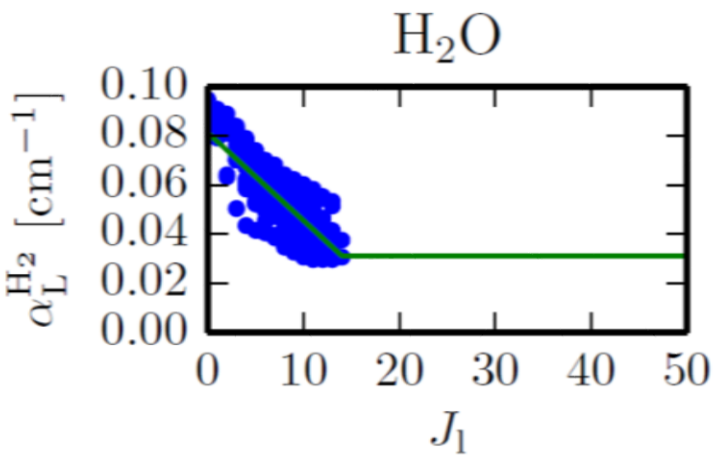
CH_4

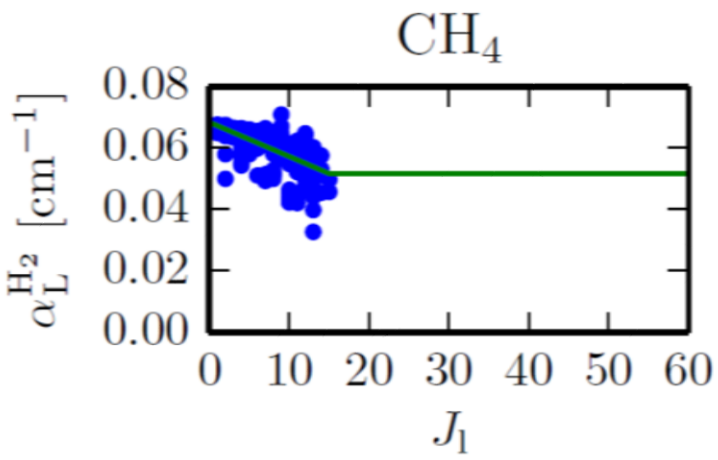
CO

NH_3

Amundsen AA (2014)

Voigt parameters as simple functions of *J*



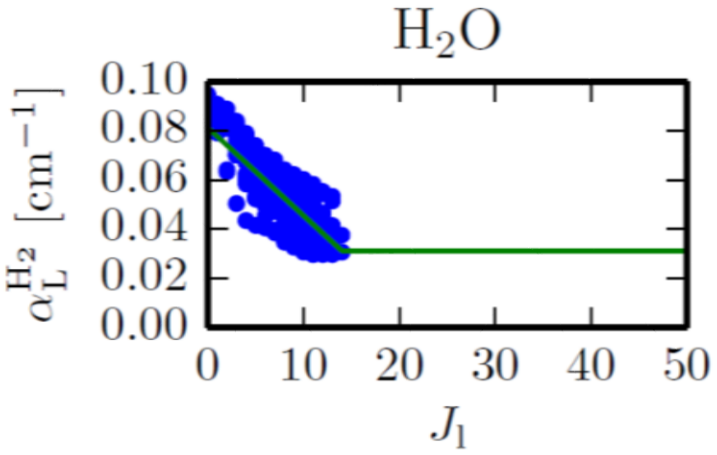


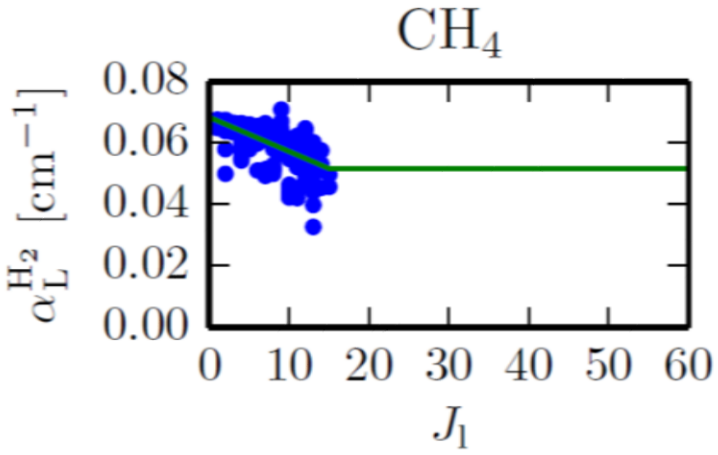
CO

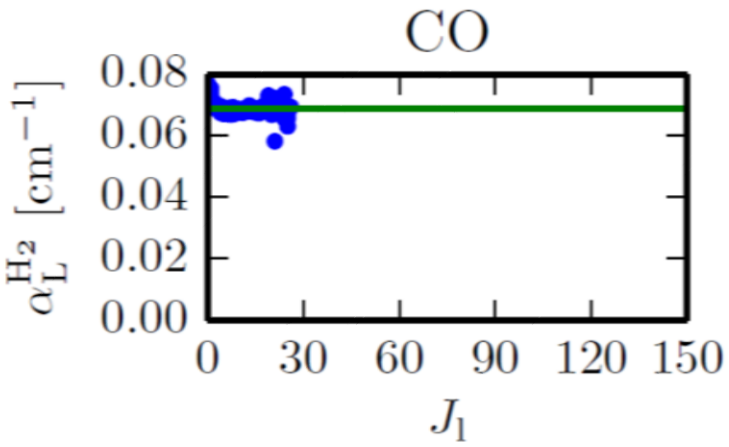
NH_3

Amundsen AA (2014)

Voigt parameters as simple functions of *J*



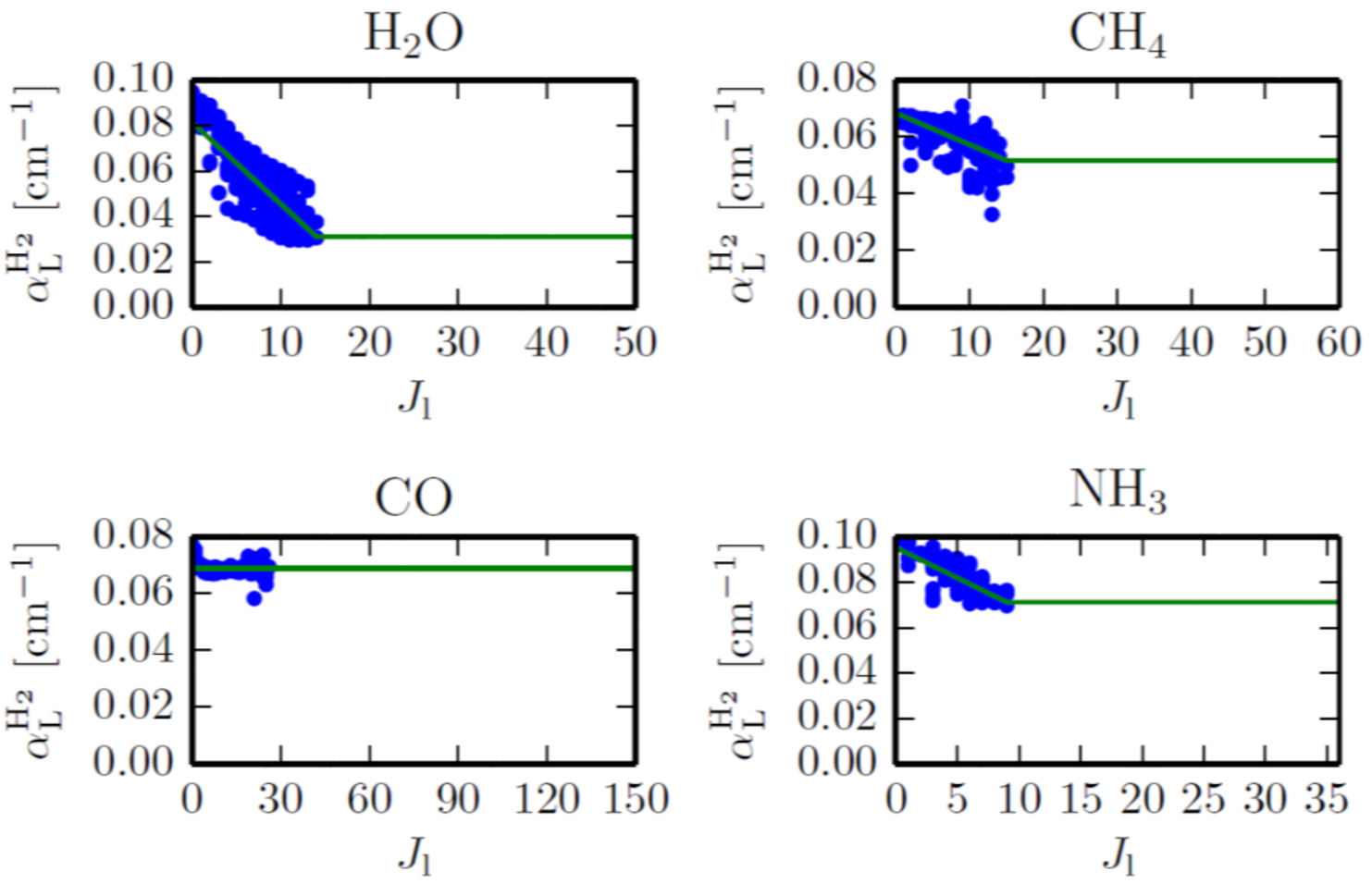




NH_3

Amundsen AA (2014)

Voigt parameters as simple functions of *J*

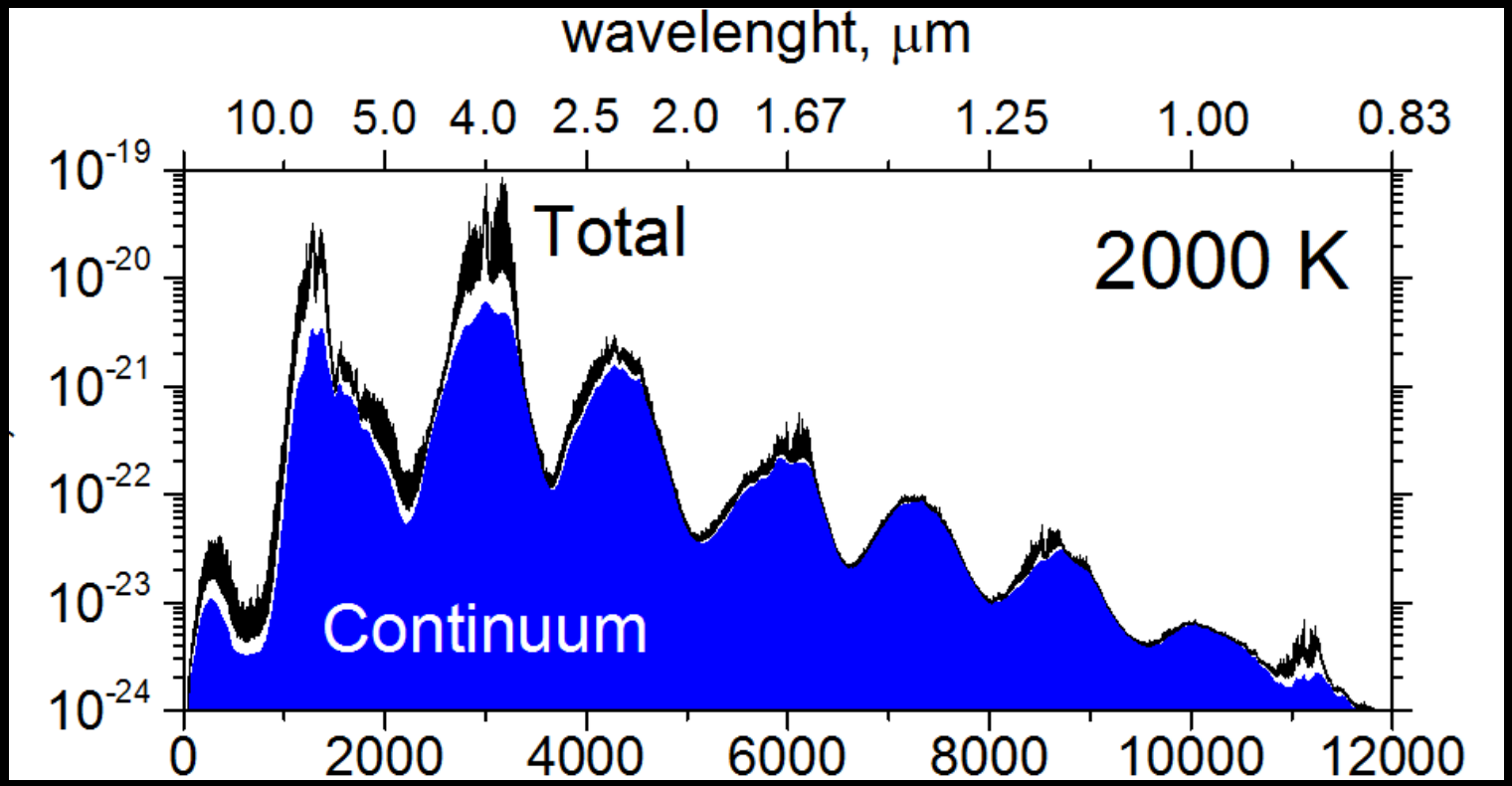


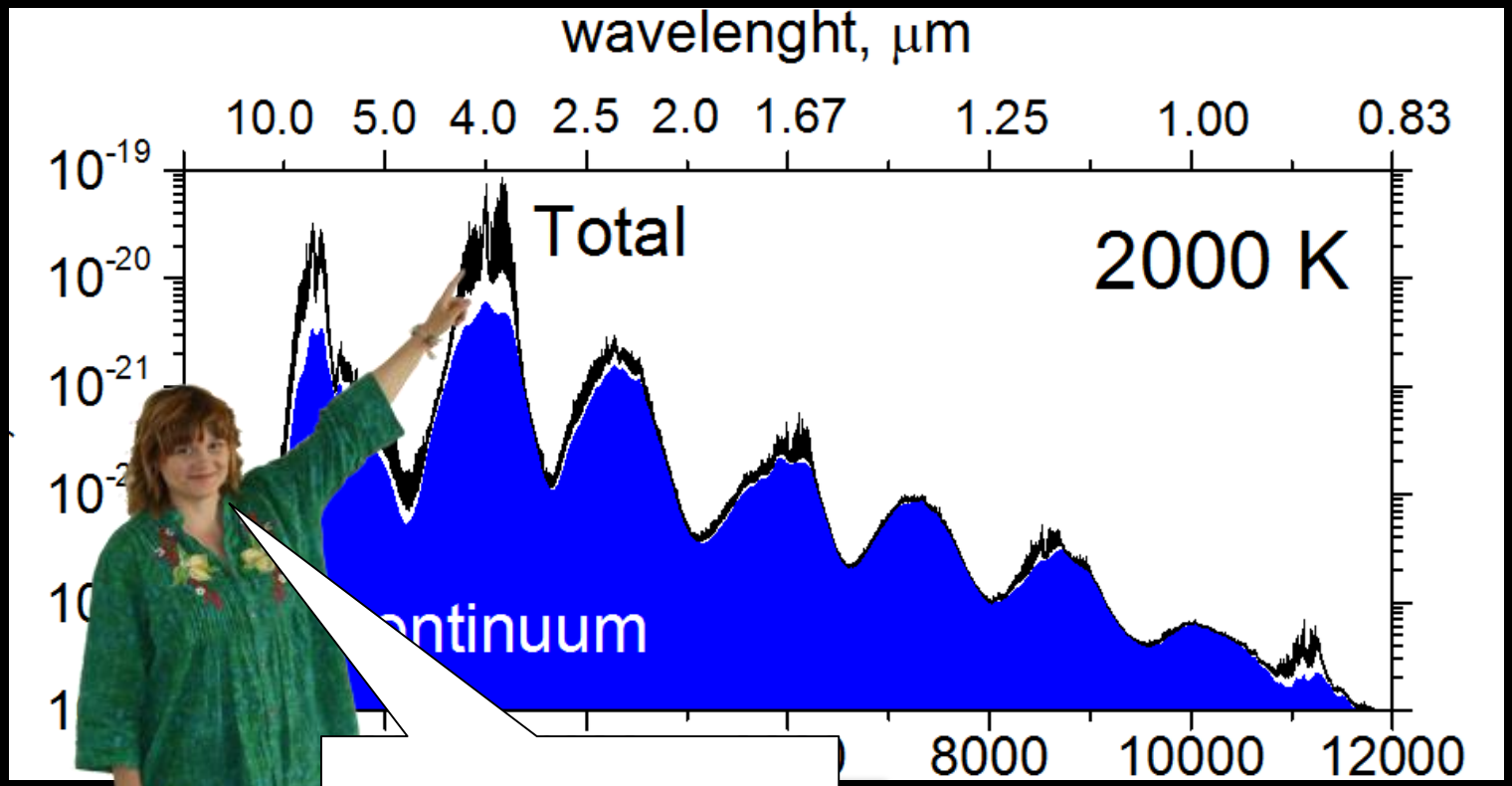
Amundsen AA (2014)

Hybrid line list:
weak continuum
and strong line list

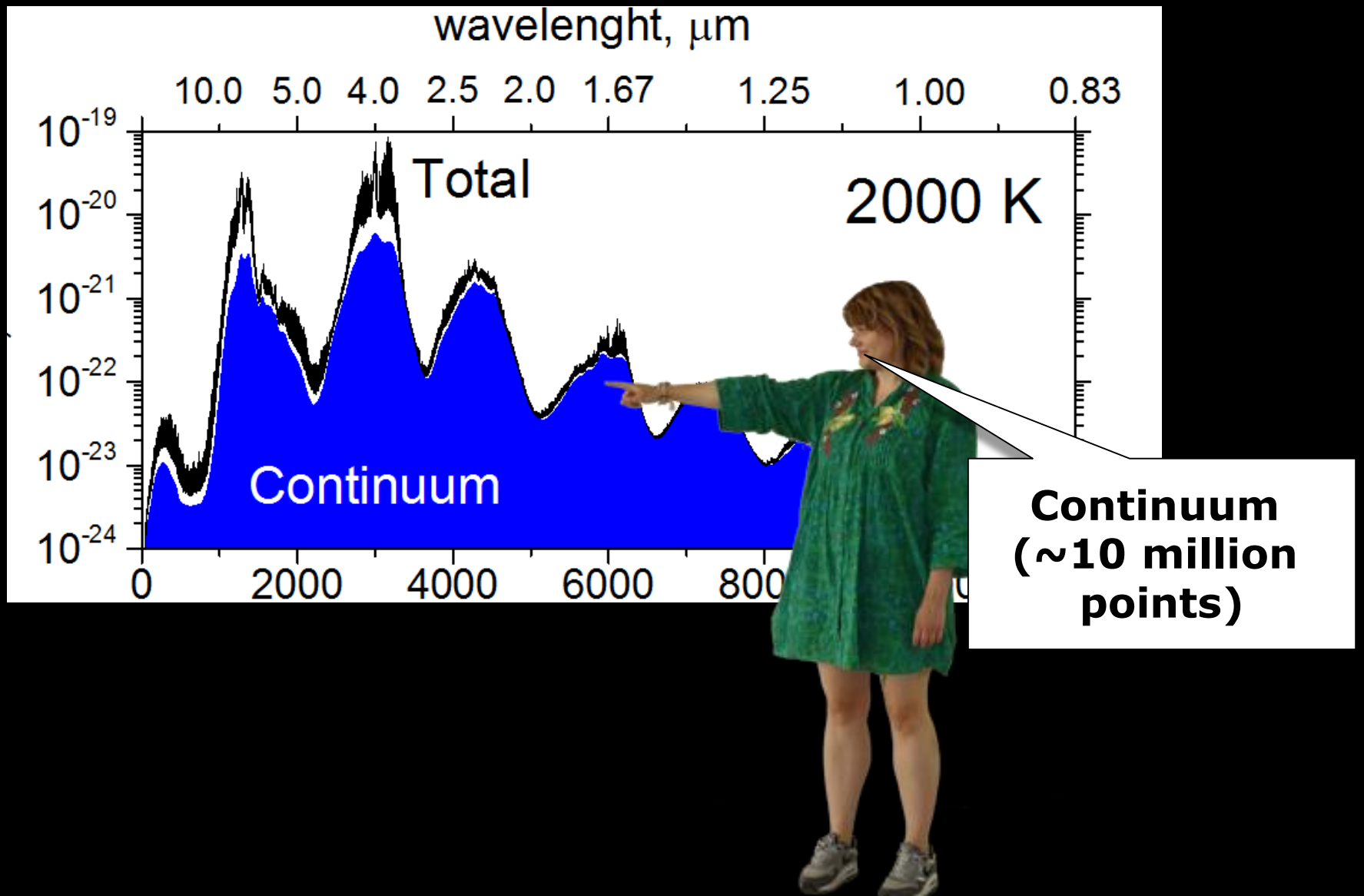
Quasi-continuum

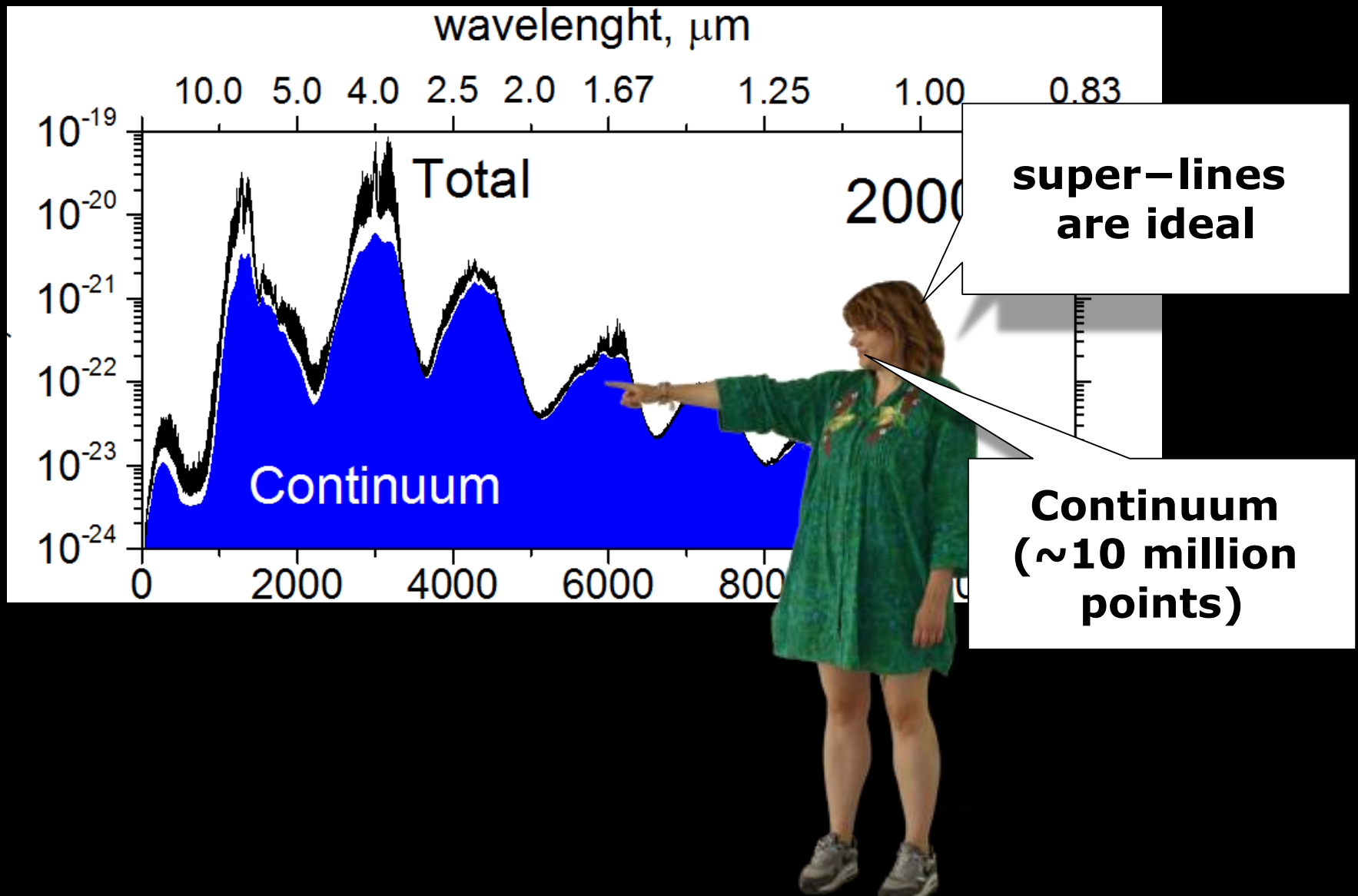
Methane: 34 billion lines


wavelenght, μm
10.0
5.0
4.0
2.5
2.0
1.67
1.25
1.00
0.83
10-19
10-20
10-21
10-22
10-23
10-24
Total
2000 K
Continuum
0
2000
4000
6000
8000
10000
12000



Strong
10 million lines


wavelenght, μm
10.0
5.0
4.0
2.5
2.0
1.67
1.25
1.00
0.83
10-19
10-20
10-21
10-22
10-23
10-24
Total
2000 K
Continuum
0
2000
4000
6000
800
Continuum (~10 million points)

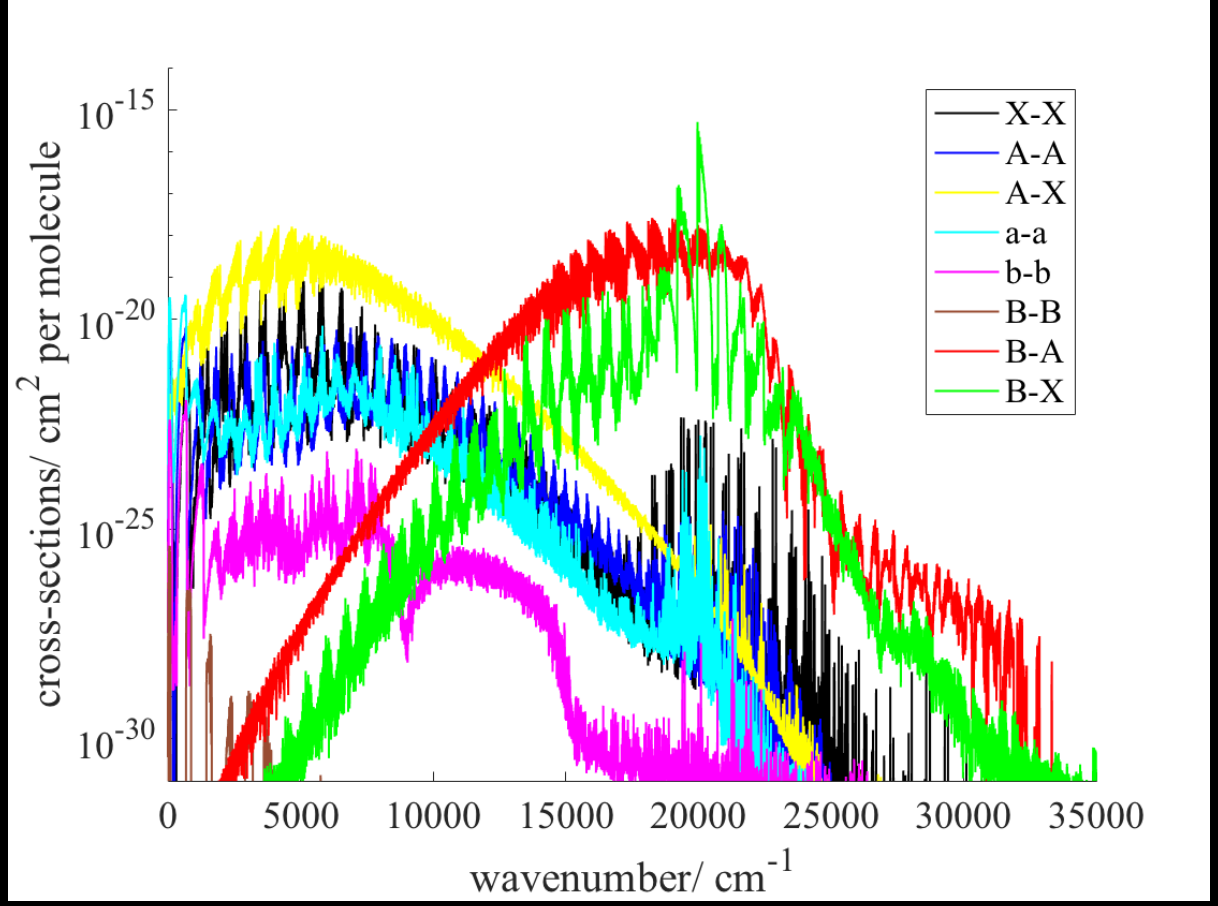

wavelenght, μm
10.0 5.0 4.0 2.5 2.0 1.67 1.25 1.00 0.83
10^-19
10^-20
10^-21
10^-22
10^-23
10^-24
Total
Continuum
0 2000 4000 6000
super−lines are ideal
Continuum (~10 million points)

Super-lines require minimum change of a cross section code

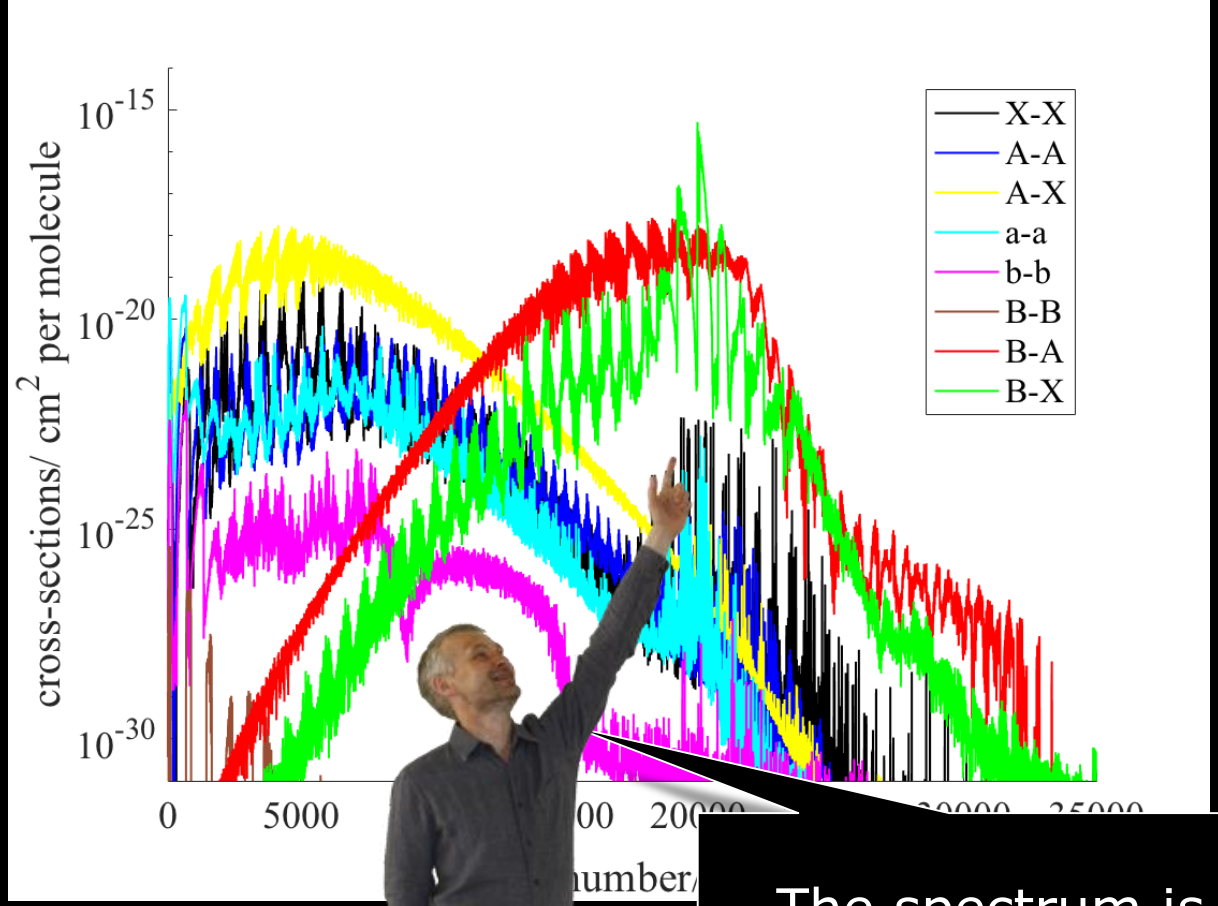
Already available for water and CH_3Cl

New diatomic line lists

We use our fully coupled code
Duo (open source + manual ;)


cross-sections/ cm^2 per molecule
10^{-15}
10^{-20}
10^{-25}
10^{-30}
0
5000
10000
15000
20000
25000
30000
35000
wavenumber/ cm^{-1}
X-X
A-A
A-X
a-a
b-b
B-B
B-A
B-X

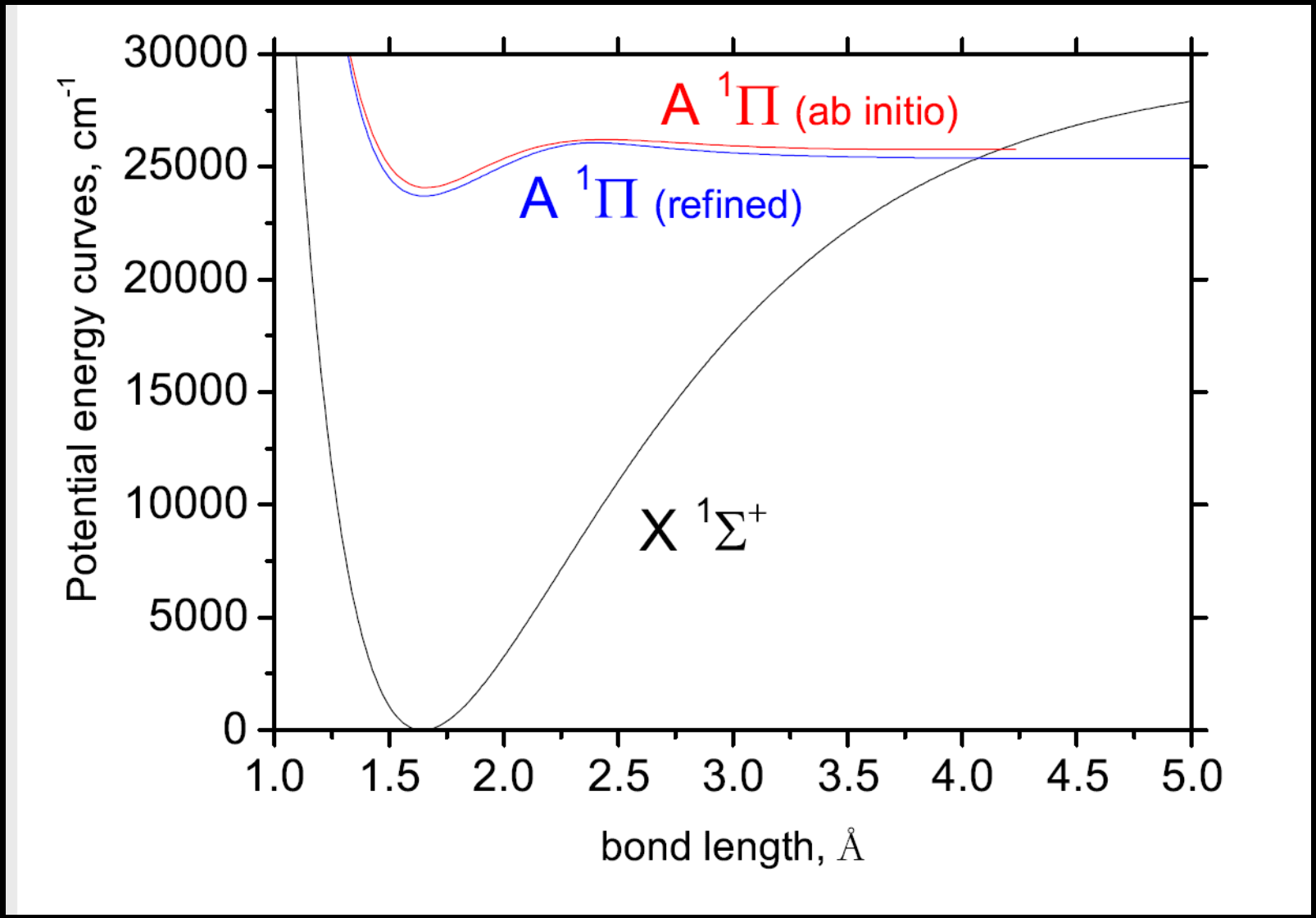
MgO

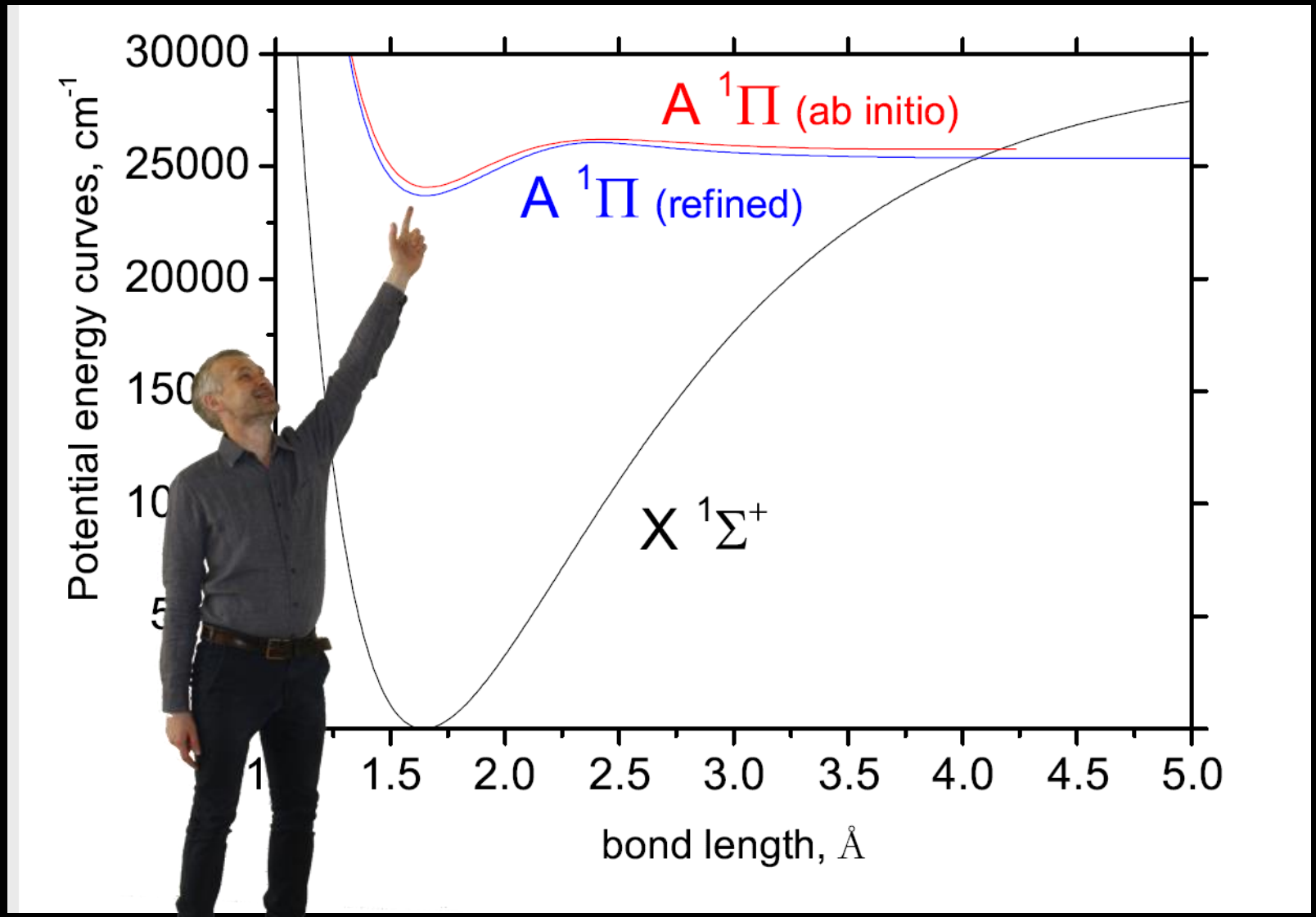


MgO

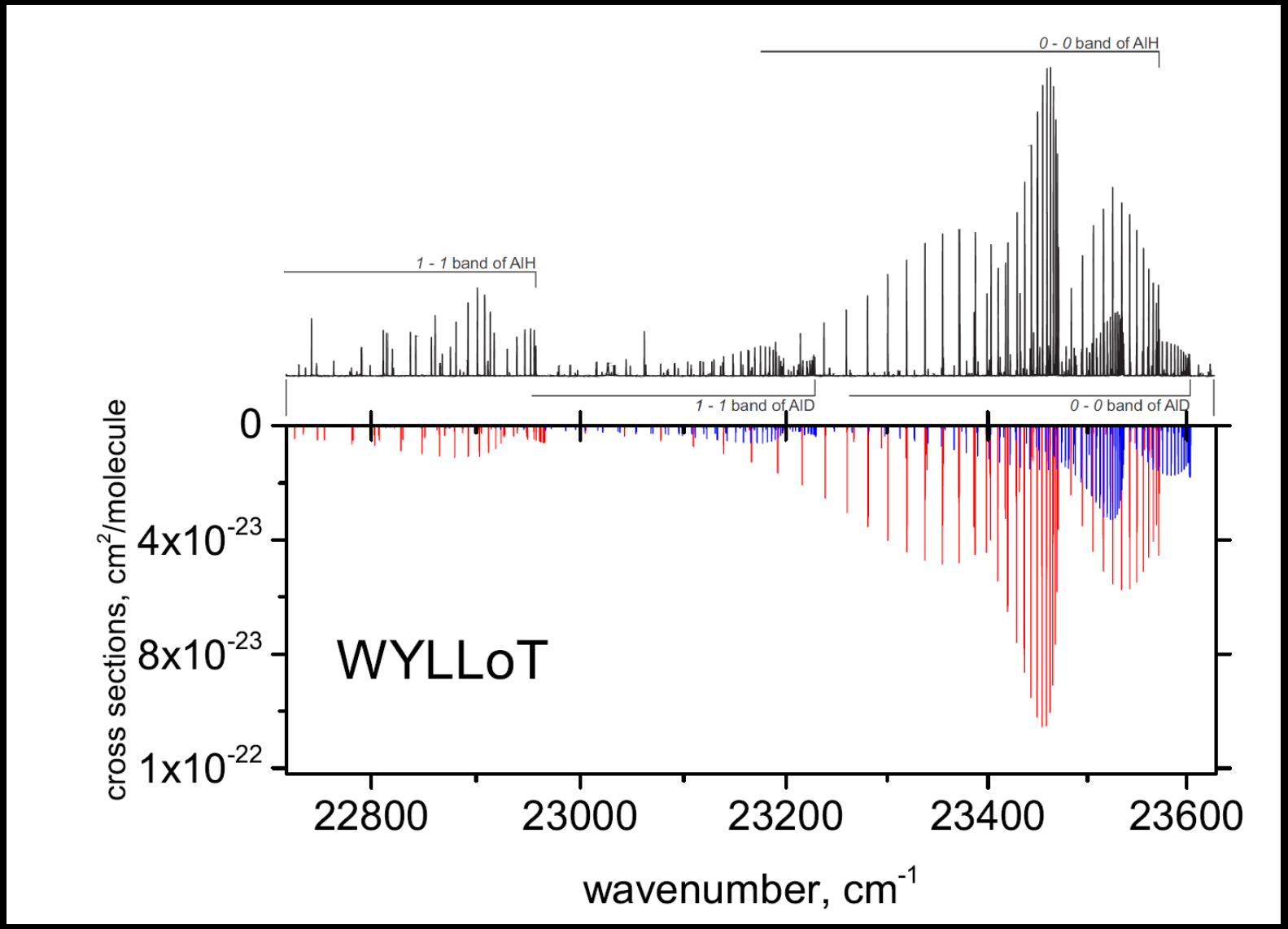
The spectrum is complex, with multiple interacting electronic bands

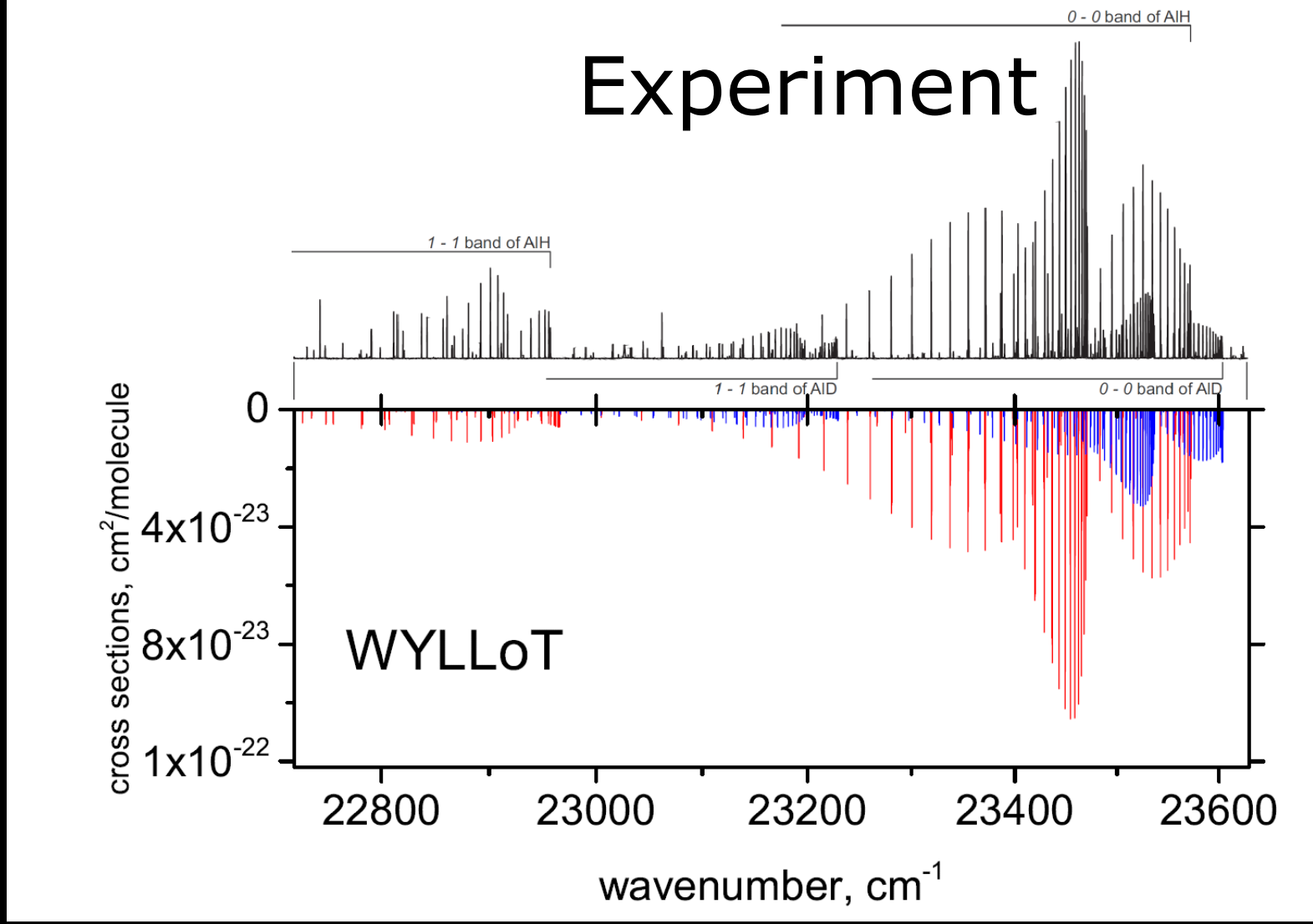
AlH:
system with strong
pre-dissociation

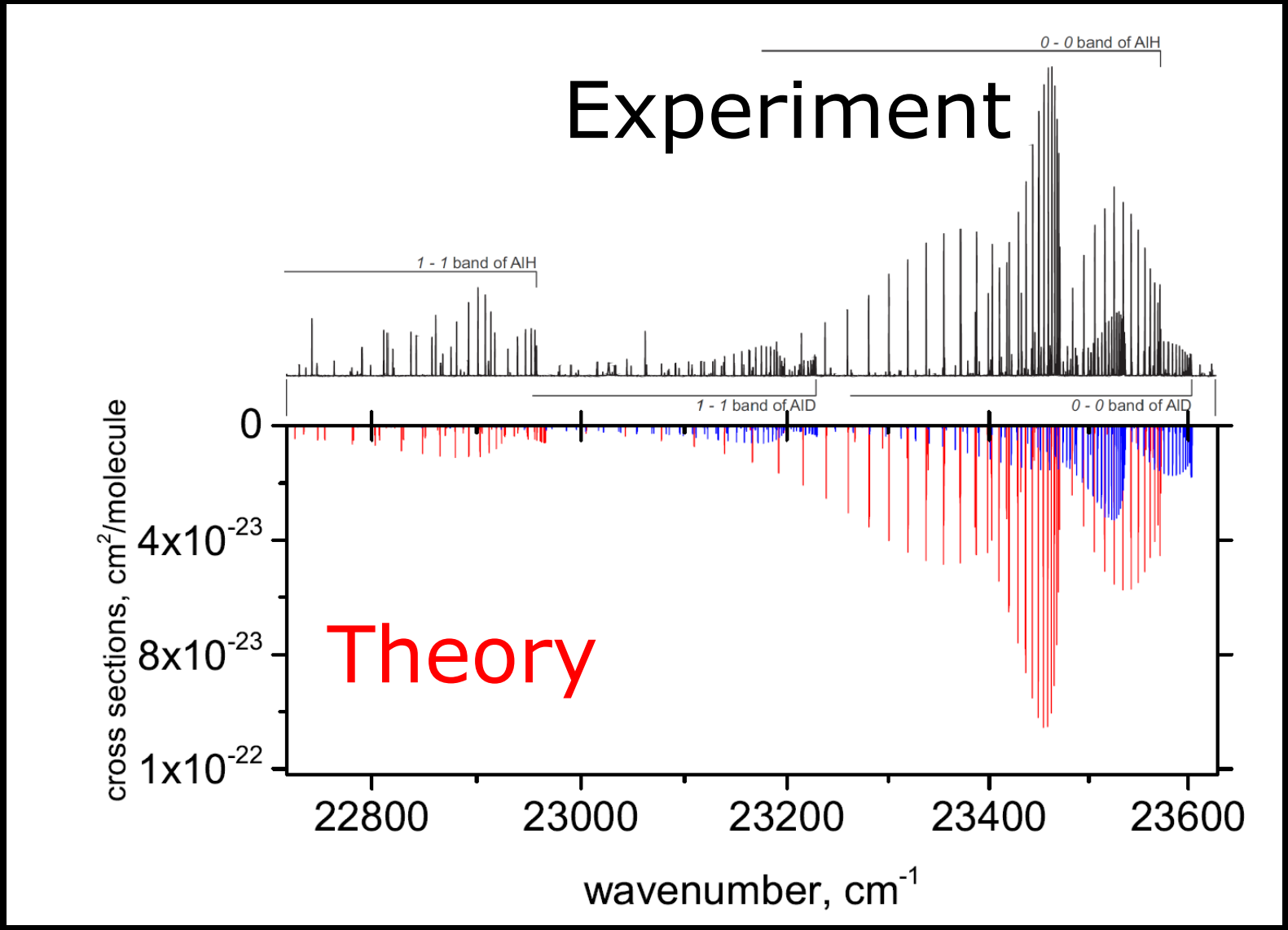

Potential energy curves, cm-1
30000
25000
20000
15000
10000
5000
0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
bond length, Å
A 1Π (ab initio)
A 1Π (refined)
X 1Σ+

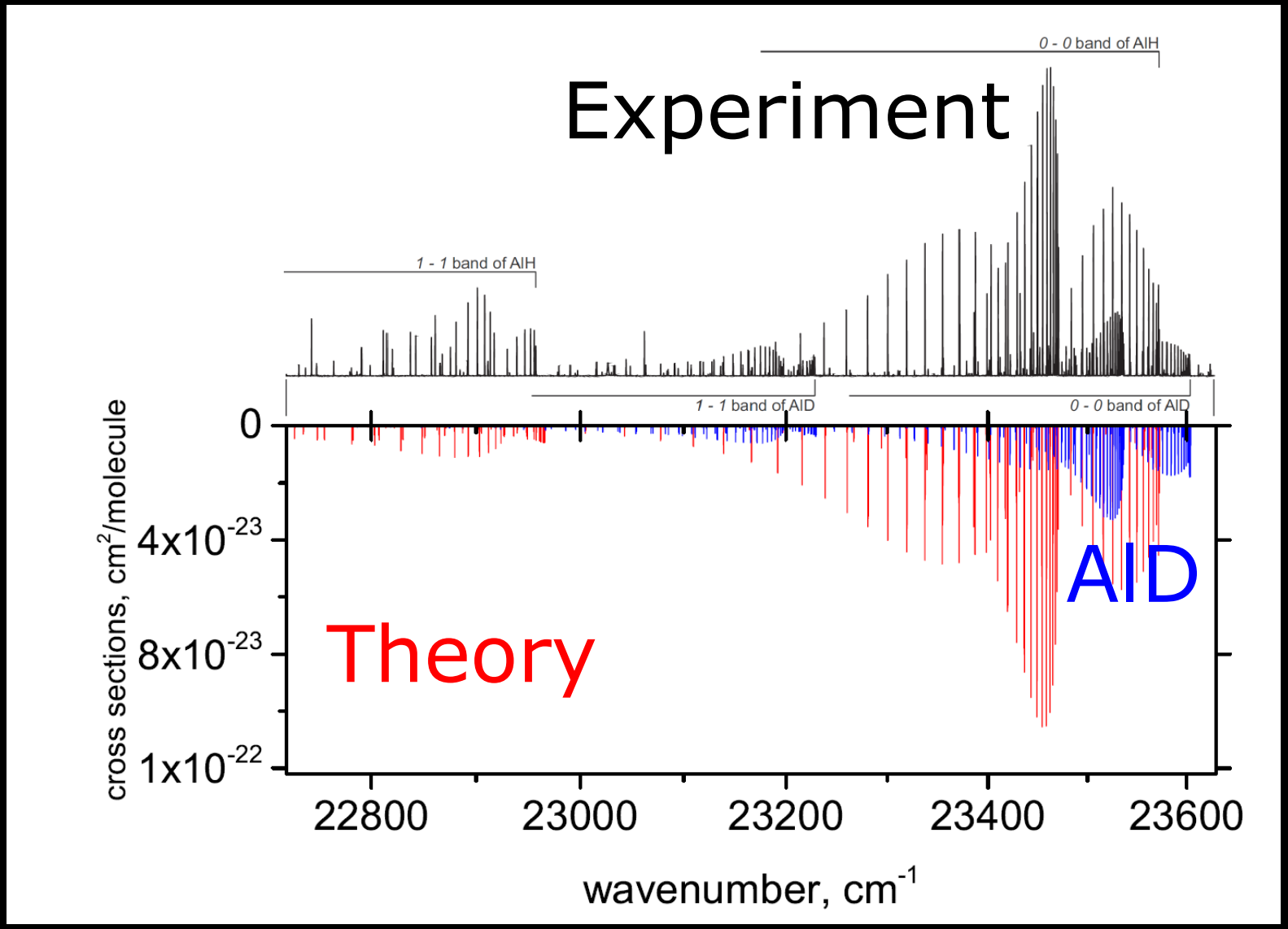

Potential energy curves, cm-1
30000
25000
20000
150
10
5
A 1Π (ab initio)
A 1Π (refined)
X 1Σ+
1
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
bond length, Å

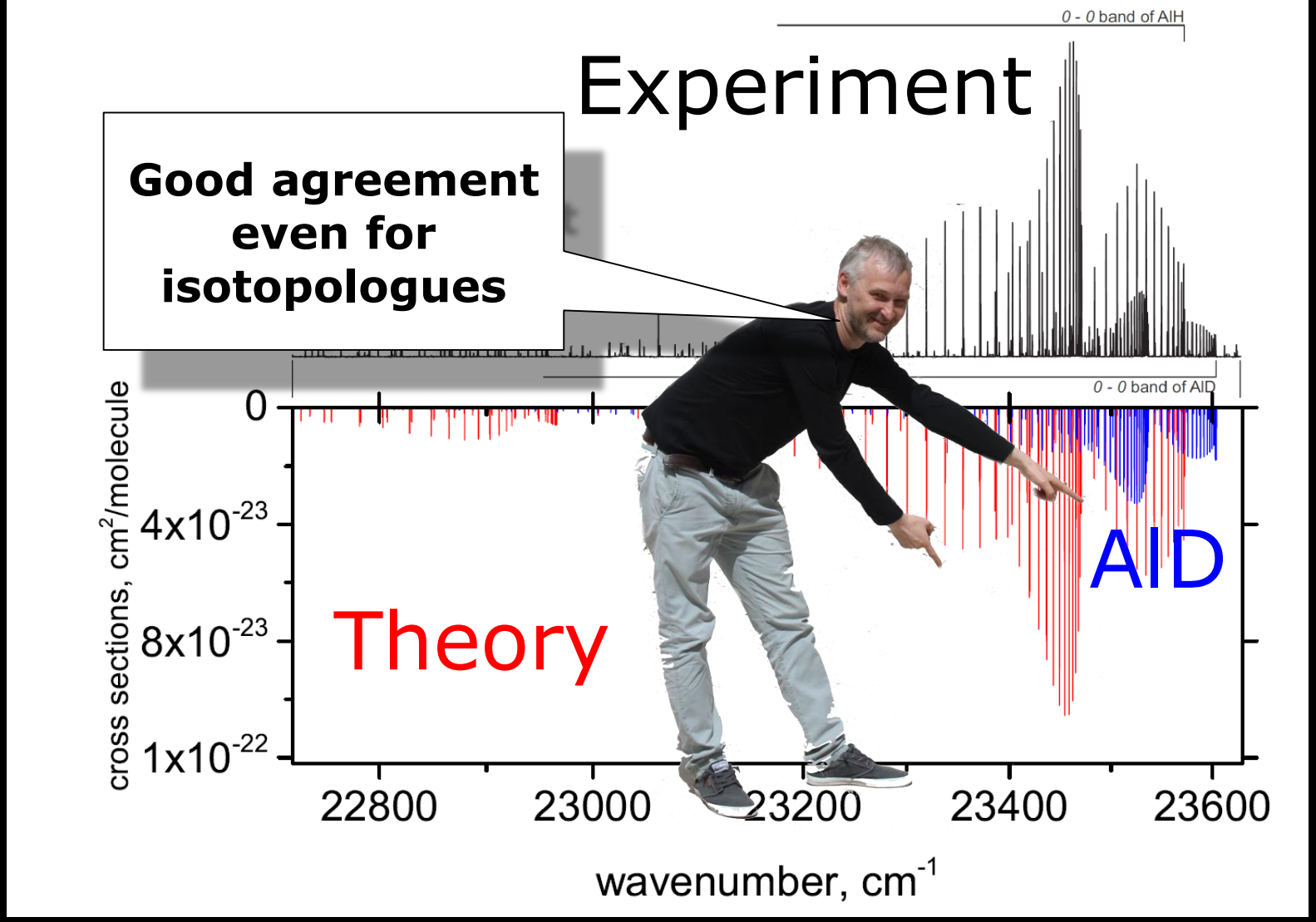
The bound spectrum is in agreement with experiment


0 - 0 band of AlH
1 - 1 band of AlH
1 - 1 band of AlD
0 - 0 band of AlD
0
4x10-23
8x10-23
1x10-22
cross sections, cm2/molecule
WYLLoT
22800
23000
23200
23400
23600
wavenumber, cm-1


Experiment
0 - 0 band of AlH
1 - 1 band of AlH
1 - 1 band of AlD
0 - 0 band of AlD
0
4x10-23
8x10-23
1x10-22
cross sections, cm2/molecule
WYLLoT
22800
23000
23200
23400
23600
wavenumber, cm-1

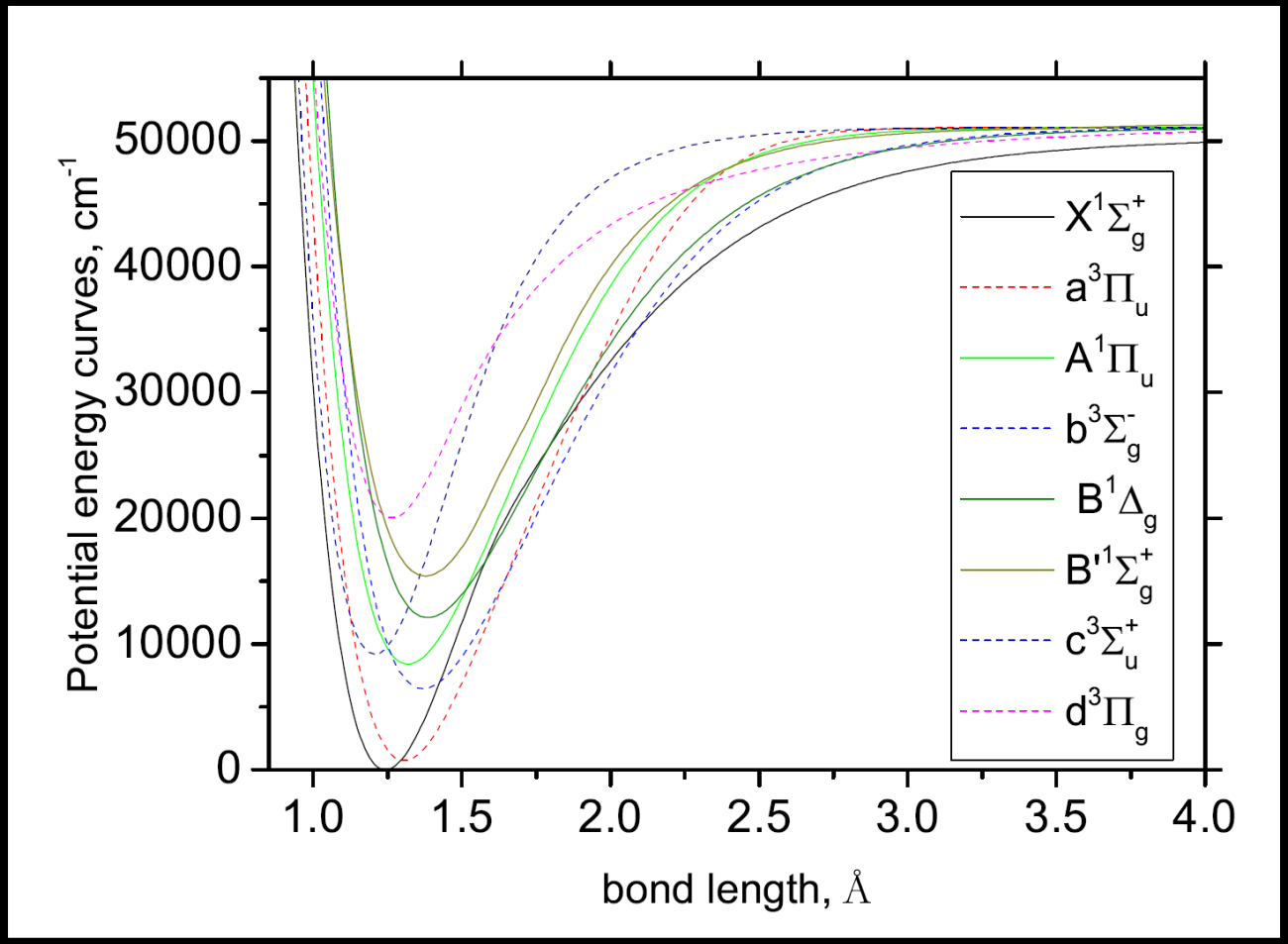

Experiment
Theory
0 - 0 band of AlH
1 - 1 band of AlH
1 - 1 band of AlD
0 - 0 band of AlD
0
4x10-23
8x10-23
1x10-22
cross sections, cm2/molecule
22800
23000
23200
23400
23600
wavenumber, cm-1

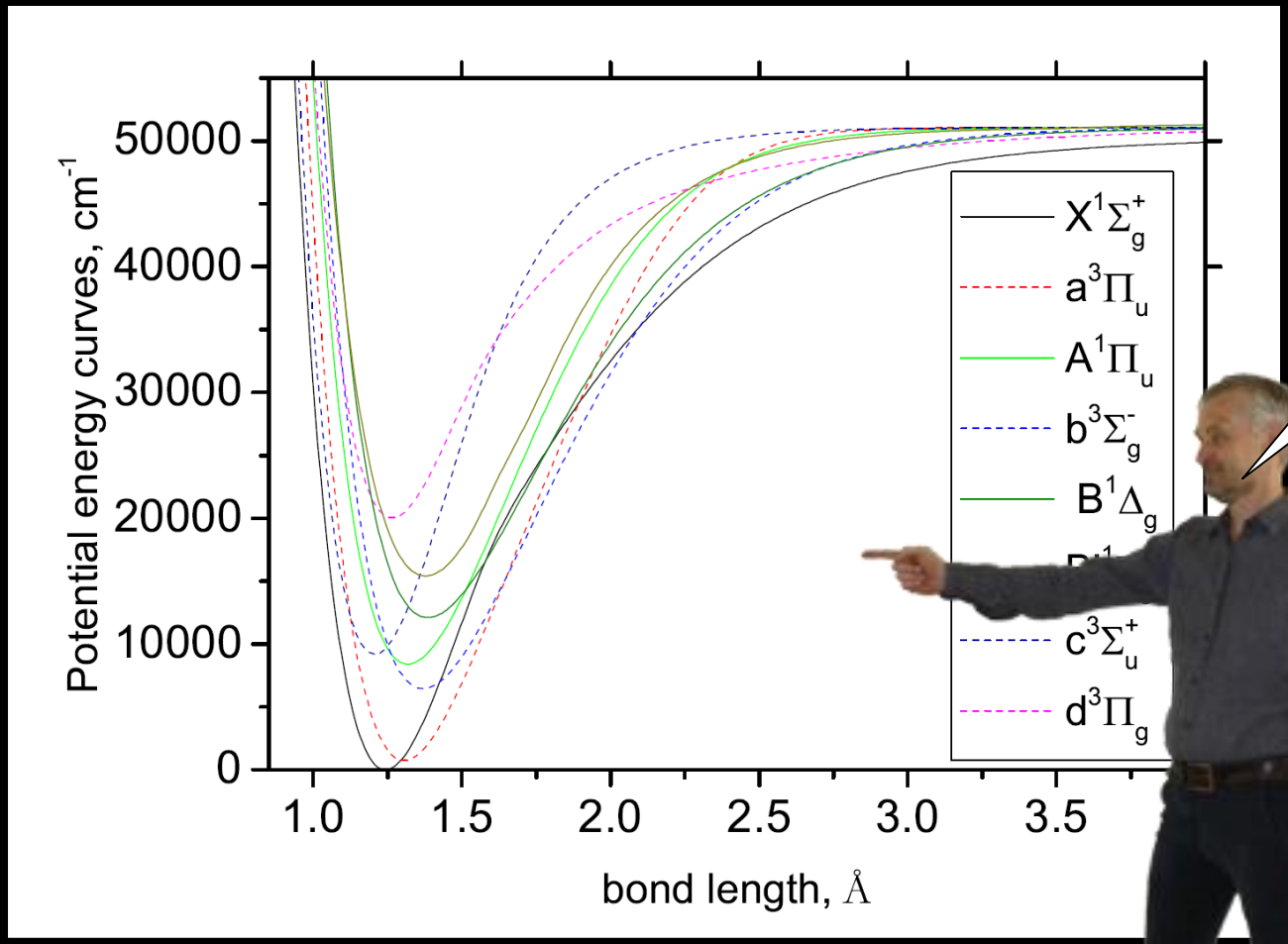

Experiment
0 - 0 band of AlH
1 - 1 band of AlH
1 - 1 band of AlD
0 - 0 band of AlD
Theory
AlD
0
4x10-23
8x10-23
1x10-22
cross sections, cm2/molecule
22800
23000
23200
23400
23600
wavenumber, cm-1


Experiment
Good agreement even for isotopologues
0 - 0 band of AlH
0 - 0 band of AlD
Theory
AlD
cross sections, cm²/molecule
0
4x10⁻²³
8x10⁻²³
1x10⁻²²
22800
23000
23200
23400
23600
wavenumber, cm⁻¹

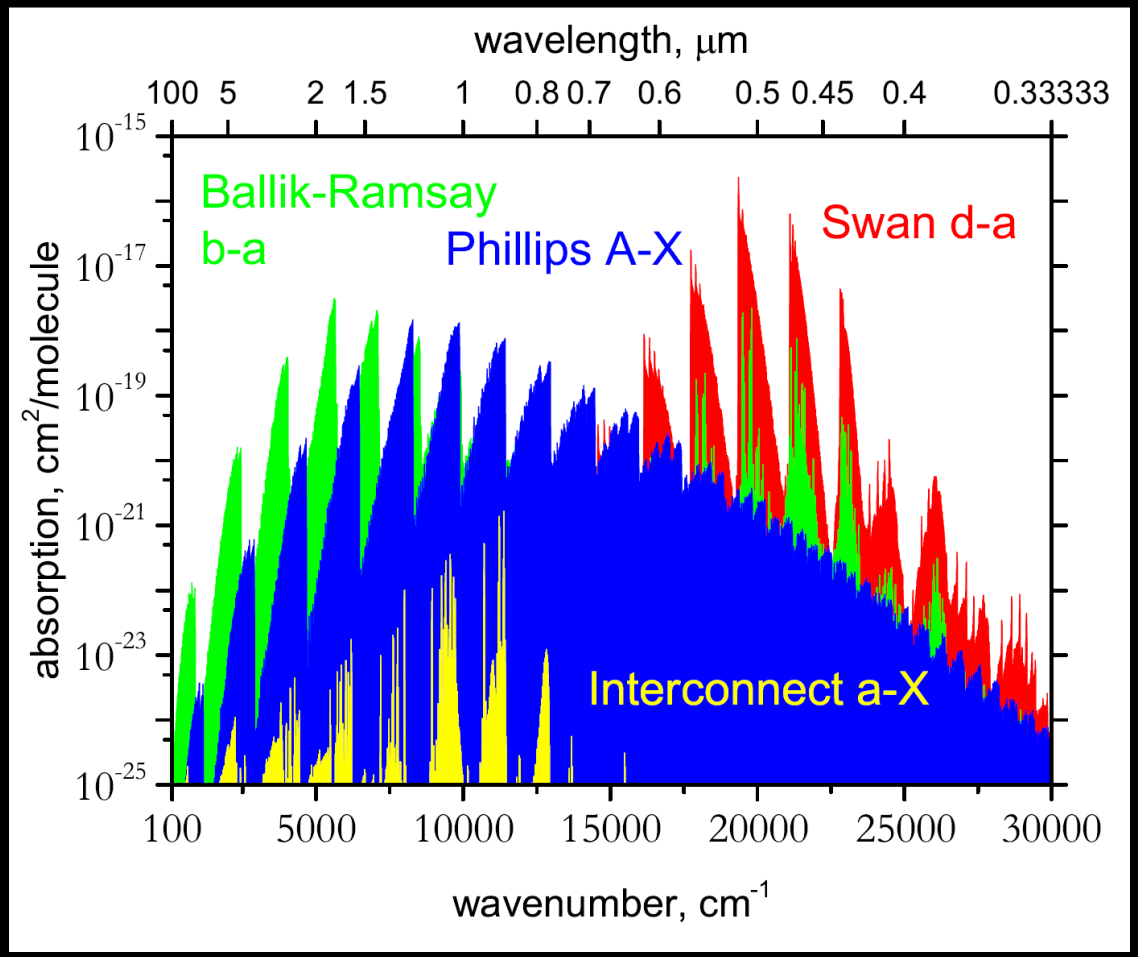
C_2 line list XXXI: submitted to MNRAS

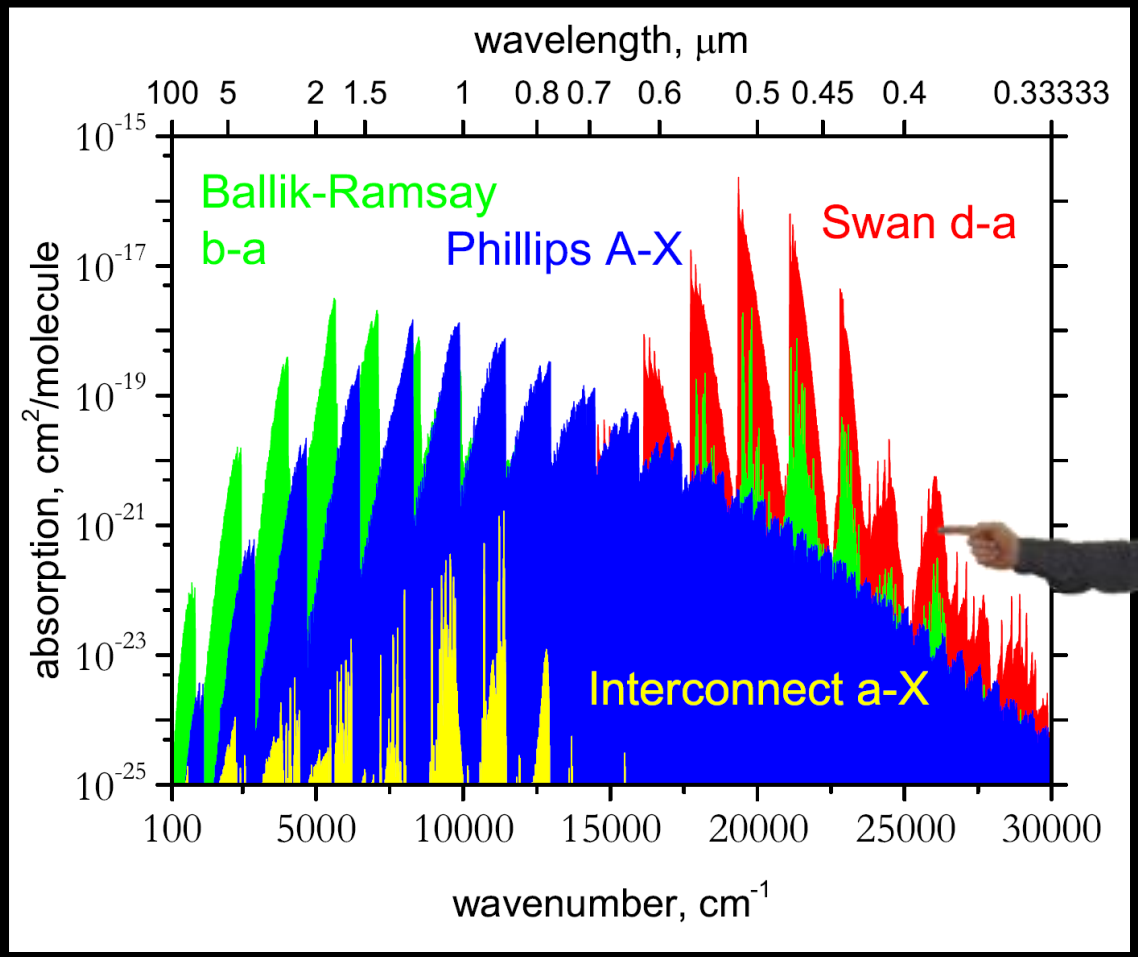
Strongly non-adiabatic curves


Potential energy curves, cm-1
50000
40000
30000
20000
10000
0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
bond length, Å
X1Σg+
a3Πu
A1Πu
b3Σg-
B1Δg
B'1Σg+
c3Σu+
d3Πg

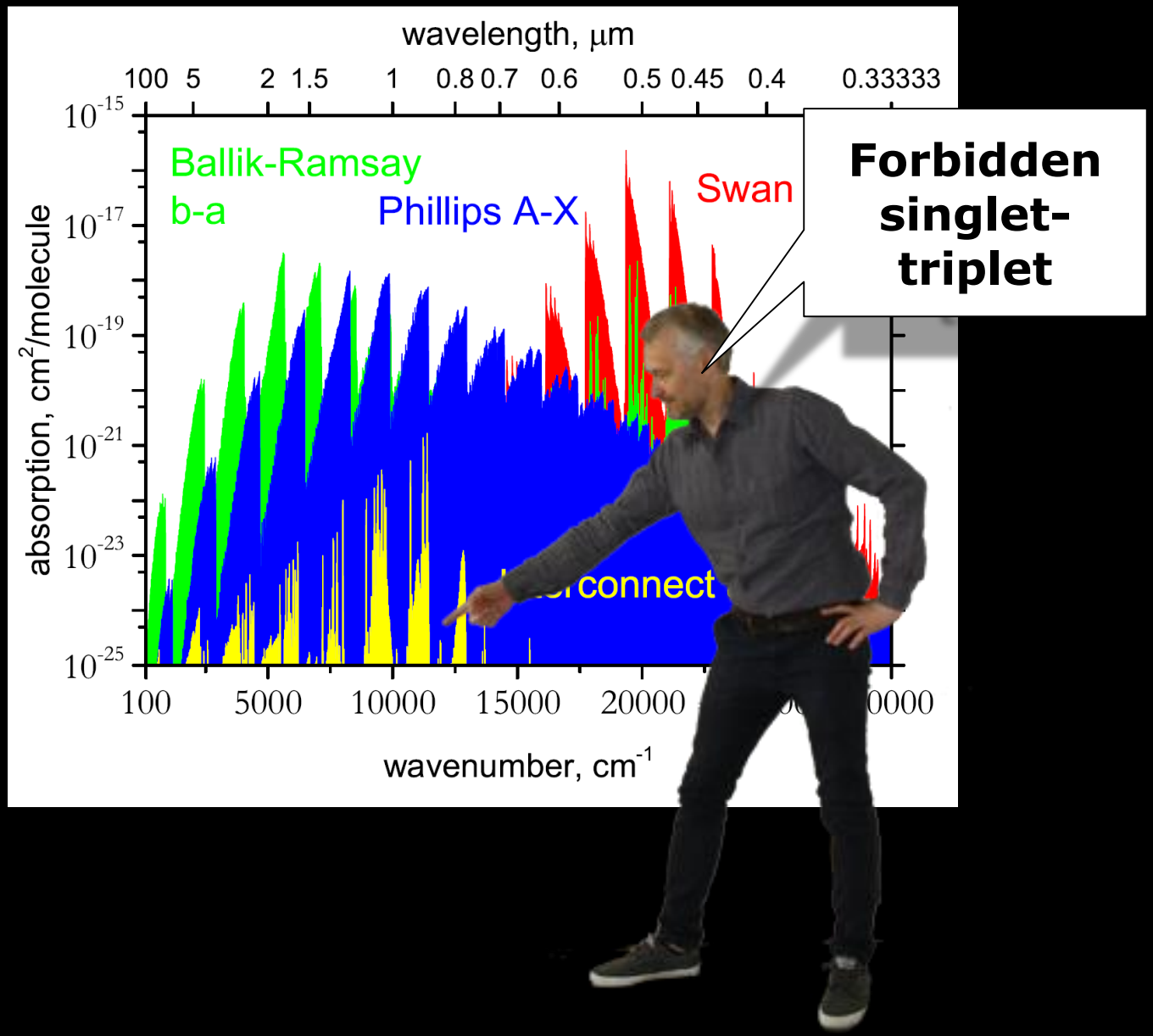


8 coupled electronic states

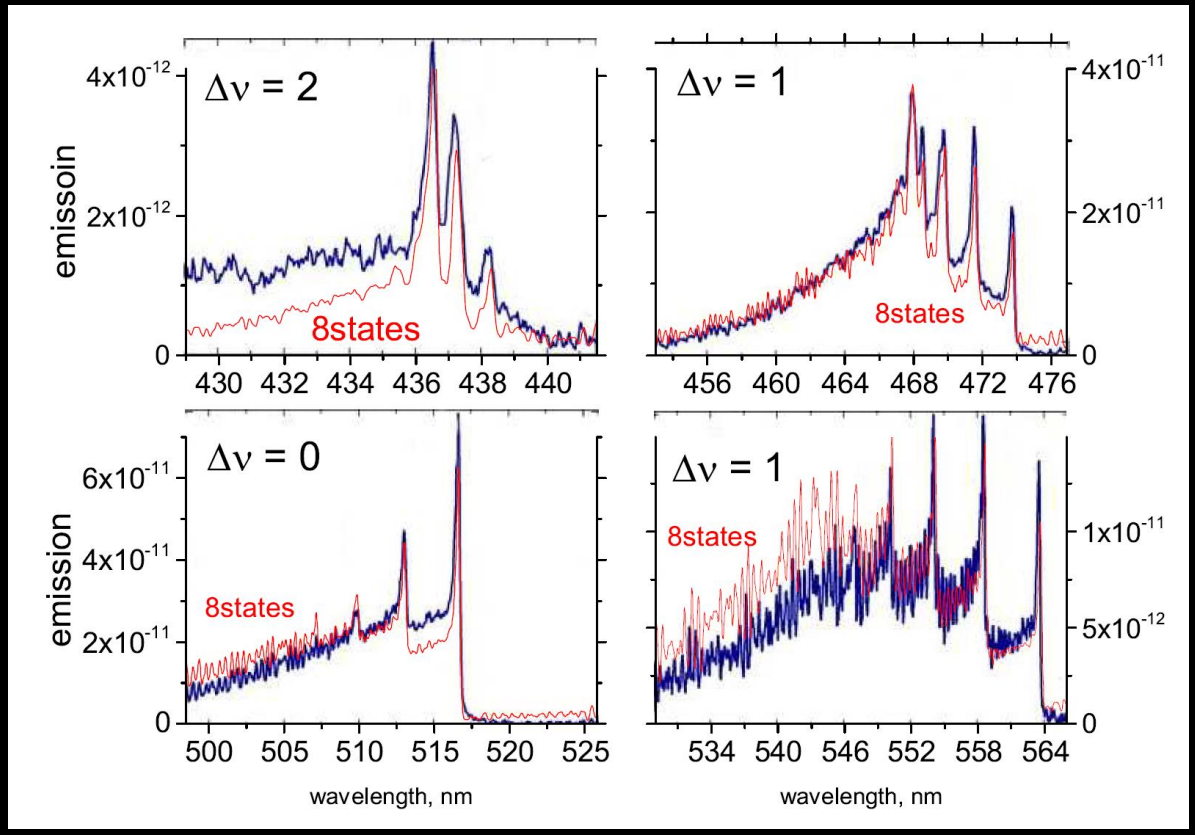

wavelength, μm
100
5
2
1.5
1
0.8
0.7
0.6
0.5
0.45
0.4
0.33333
Ballik-Ramsay
b-a
Phillips A-X
Swan d-a
Interconnect a-X
absorption, cm²/molecule
10^-15
10^-17
10^-19
10^-21
10^-23
10^-25
100
5000
10000
15000
20000
25000
30000
wavenumber, cm^-1

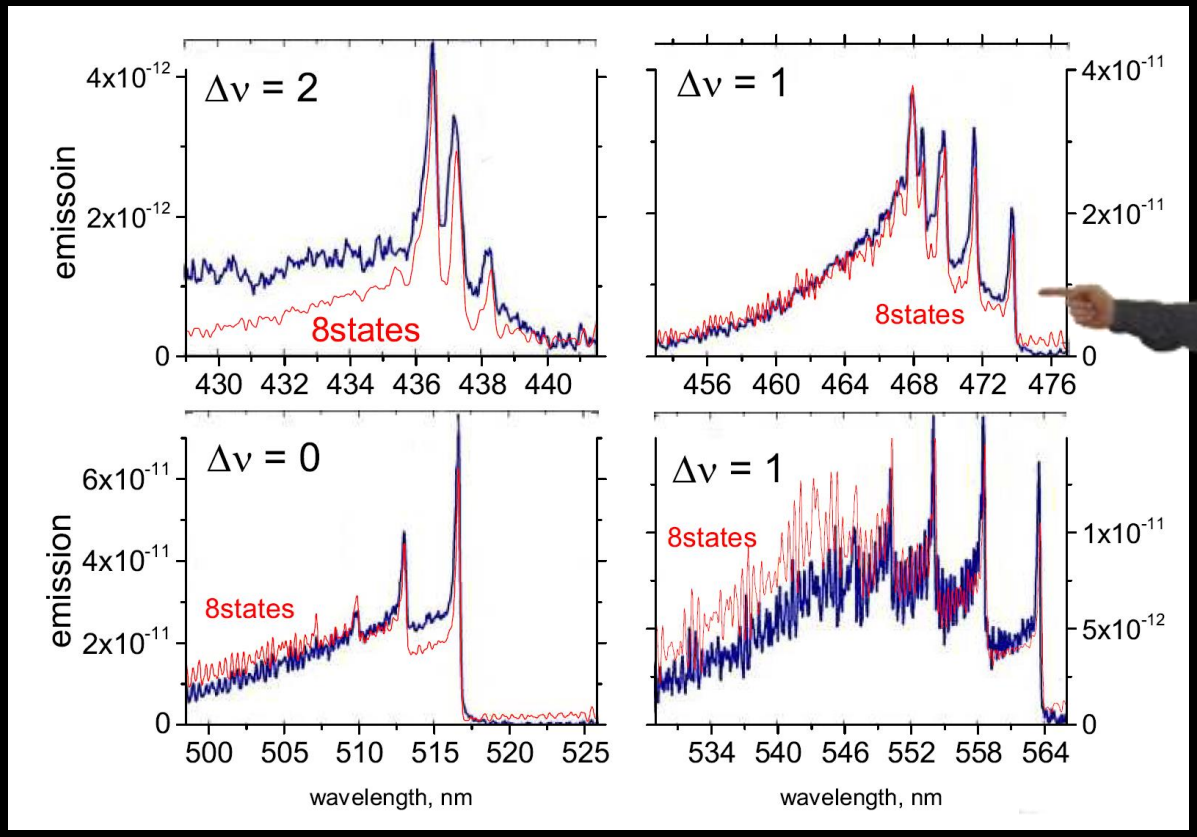


Electronic bands of C2

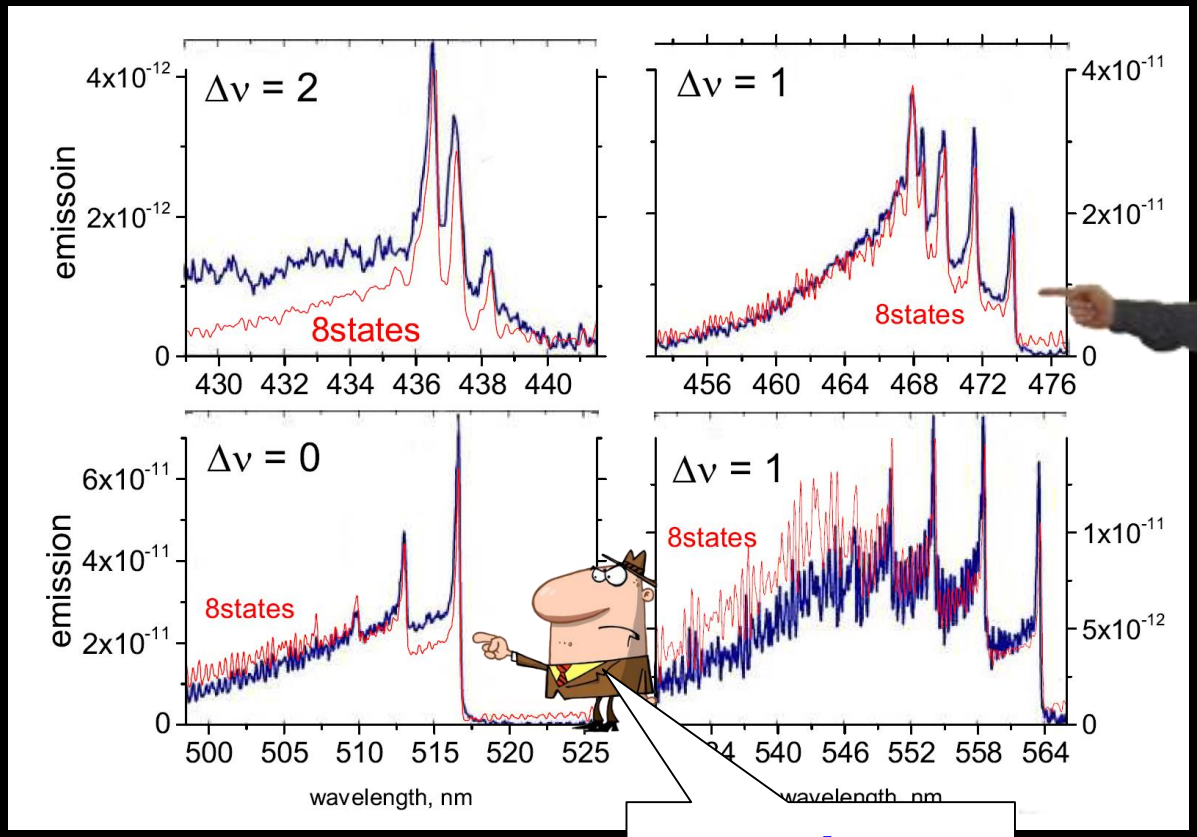

wavelength, μm
100 5 2 1.5 1 0.8 0.7 0.6 0.5 0.45 0.4 0.33333
absorption, cm²/molecule
10^-15
10^-17
10^-19
10^-21
10^-23
10^-25
Ballik-Ramsay
b-a
Phillips A-X
Swan
Forbidden singlet-triplet
100 5000 10000 15000 20000
wavenumber, cm^-1

Comparing to experimental
hot 8000 K plasma spectra


Δν = 2
8states
Δν = 1
8states
Δν = 0
8states
Δν = 1
8states
emissoin
emission
4x10-12
2x10-12
0
4x10-11
2x10-11
0
6x10-11
4x10-11
2x10-11
0
1x10-11
5x10-12
0
430 432 434 436 438 440
456 460 464 468 472 476
500 505 510 515 520 525
534 540 546 552 558 564
wavelength, nm
wavelength, nm


Δν = 2
Δν = 1
Δν = 0
Δν = 1
8states
8states
8states
8states
emissoin
emission
4x10-12
2x10-12
0
4x10-11
2x10-11
0
6x10-11
4x10-11
2x10-11
1x10-11
5x10-12
430 432 434 436 438 440
456 460 464 468 472 476
500 505 510 515 520 525
534 540 546 552 558 564
wavelength, nm
wavelength, nm


Swan band:
plasma

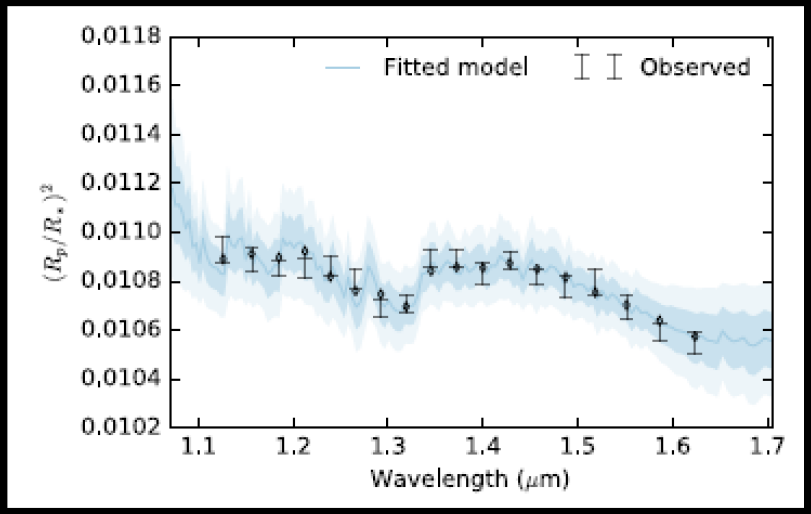


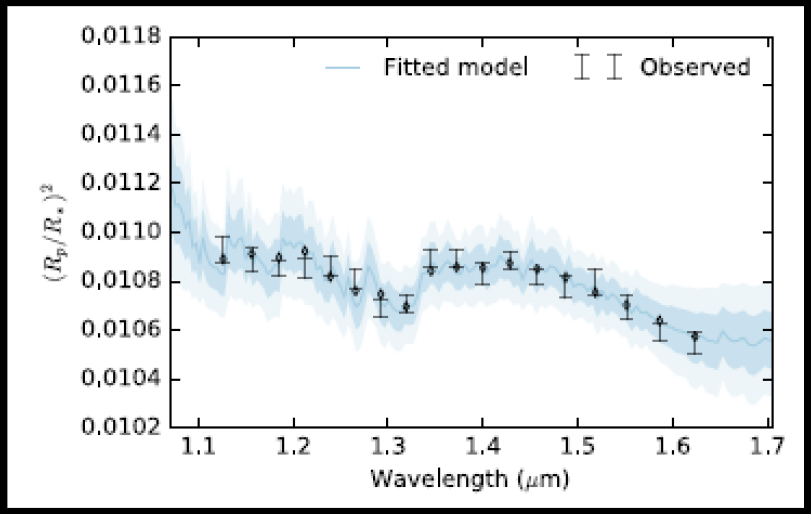
Experiment vs theory

Swan band: plasma

Swan band of C_2 is important for classification of Carbon stars

TiO/VO


Fitted model
Observed
0,0118
0.0116
0,0114
0.0112
0.0110
0,0108
0.0106
0,0104
0.0102
$(R_p/R_*)^2$
1.1
1.2
1.3
1.4
1.5
1.6
1.7
Wavelength (μm)

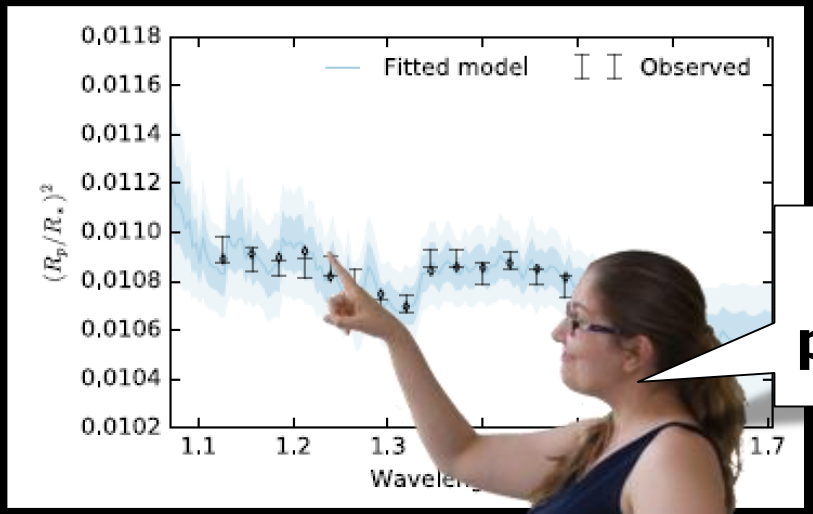


Wasp-76b

Tsiaras et al ApJ (2018)

Wasp-76b

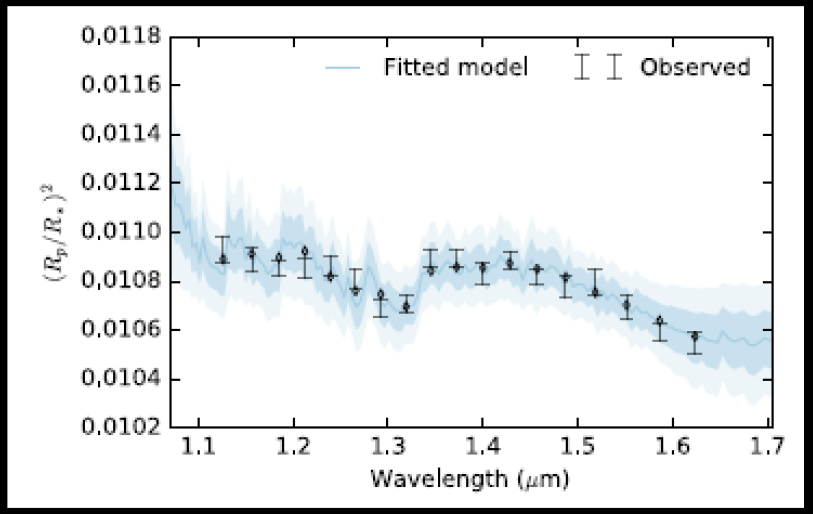
Tsiaras et al ApJ (2018)

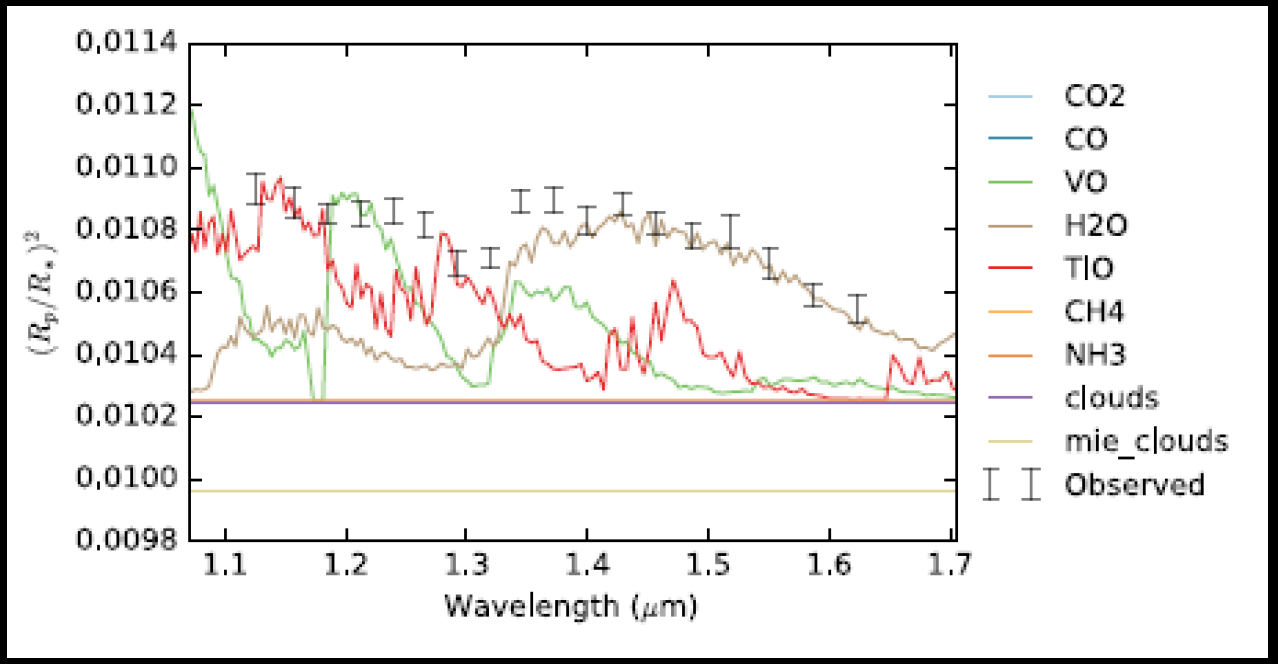


Check this part for TiO

Wasp-76b

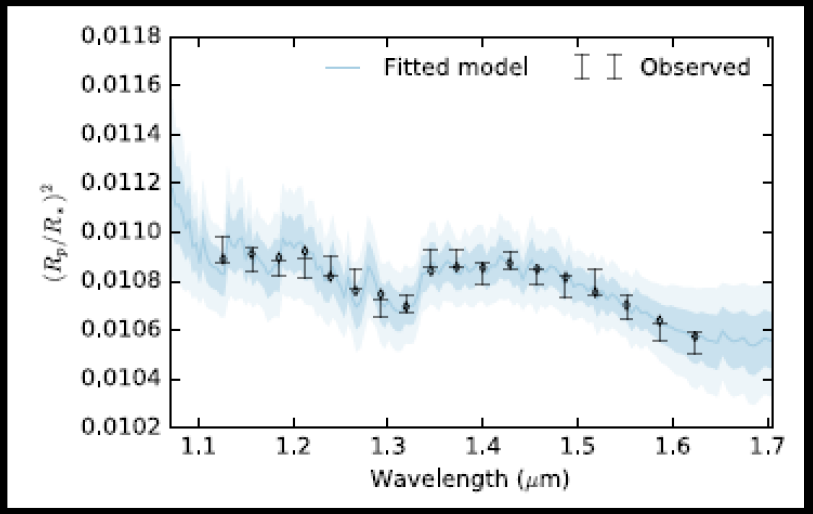
Tsiaras et al ApJ (2018)

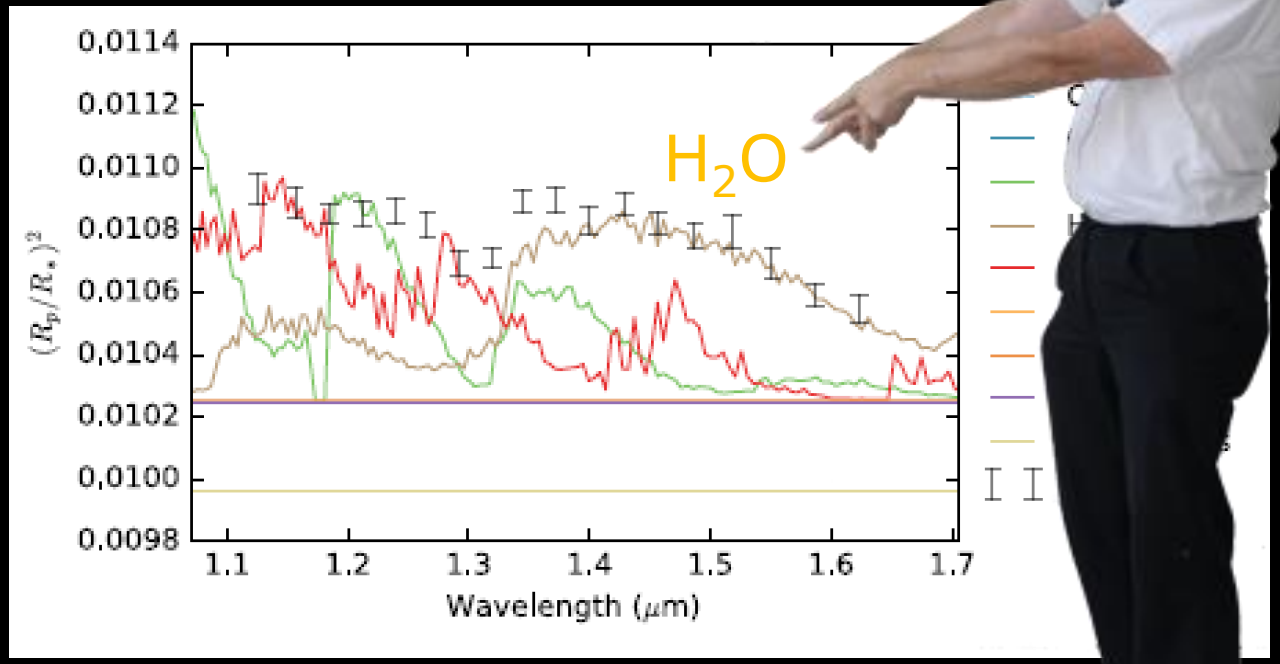




Wasp-76b

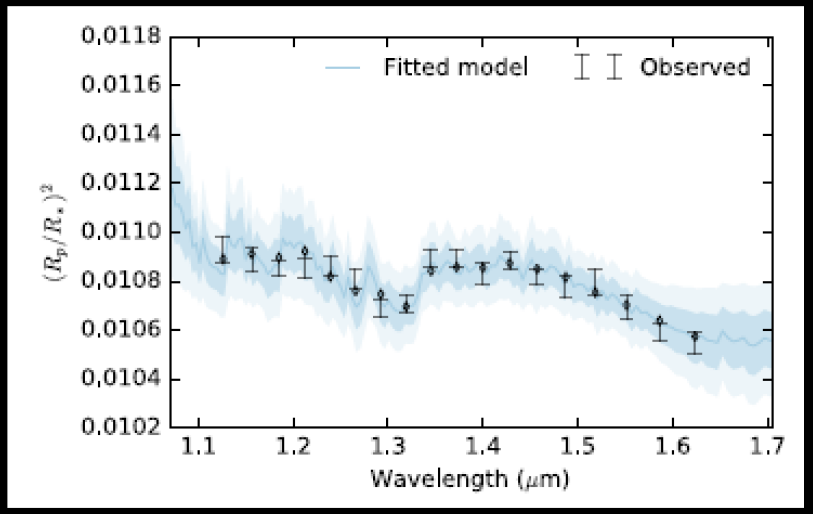
Tsiaras et al ApJ (2018)

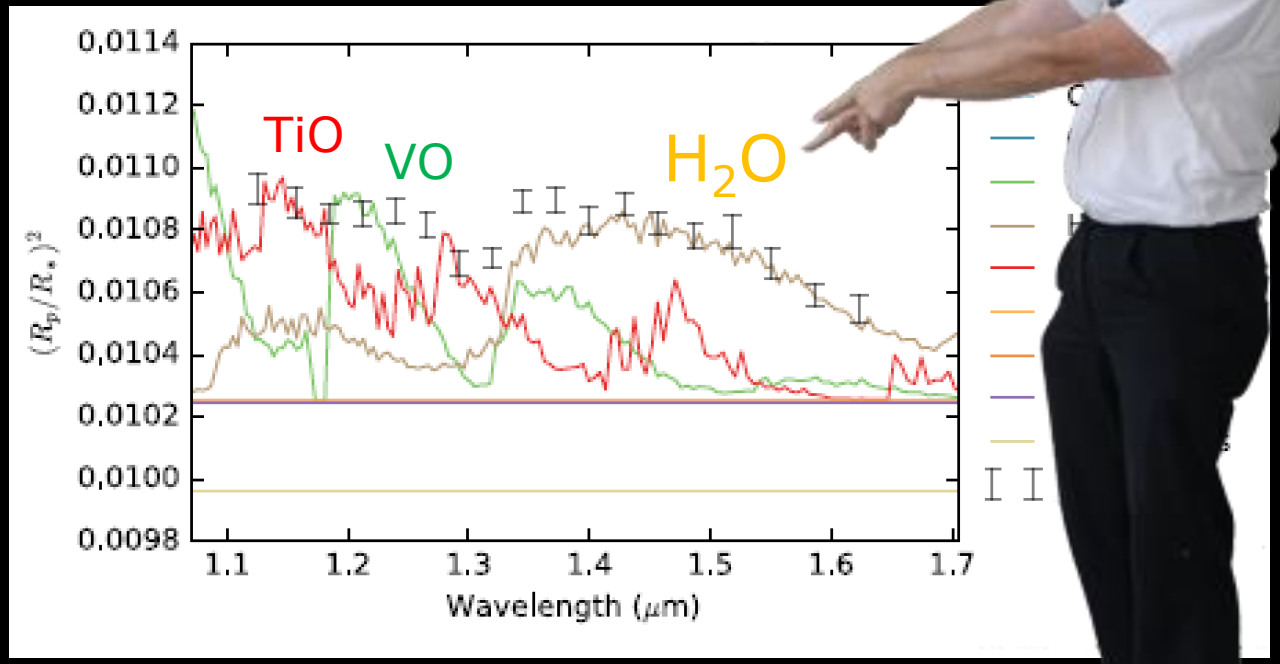




Wasp-76b

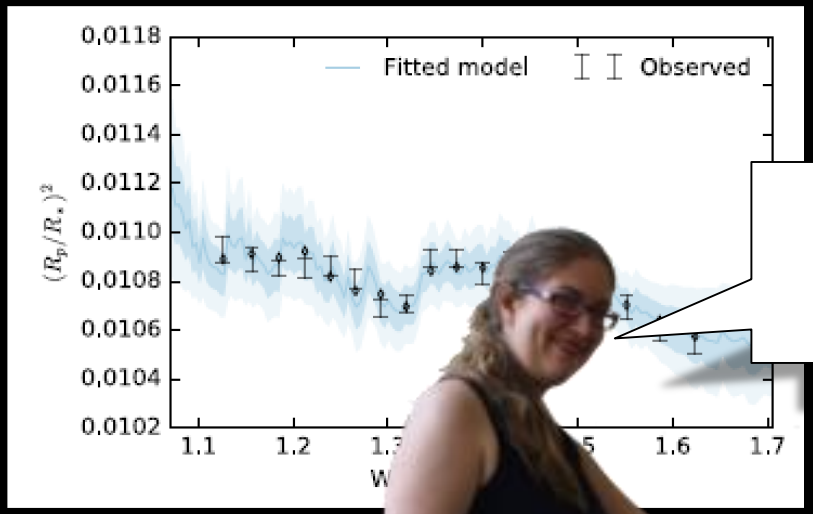
Tsiaras et al ApJ (2018)



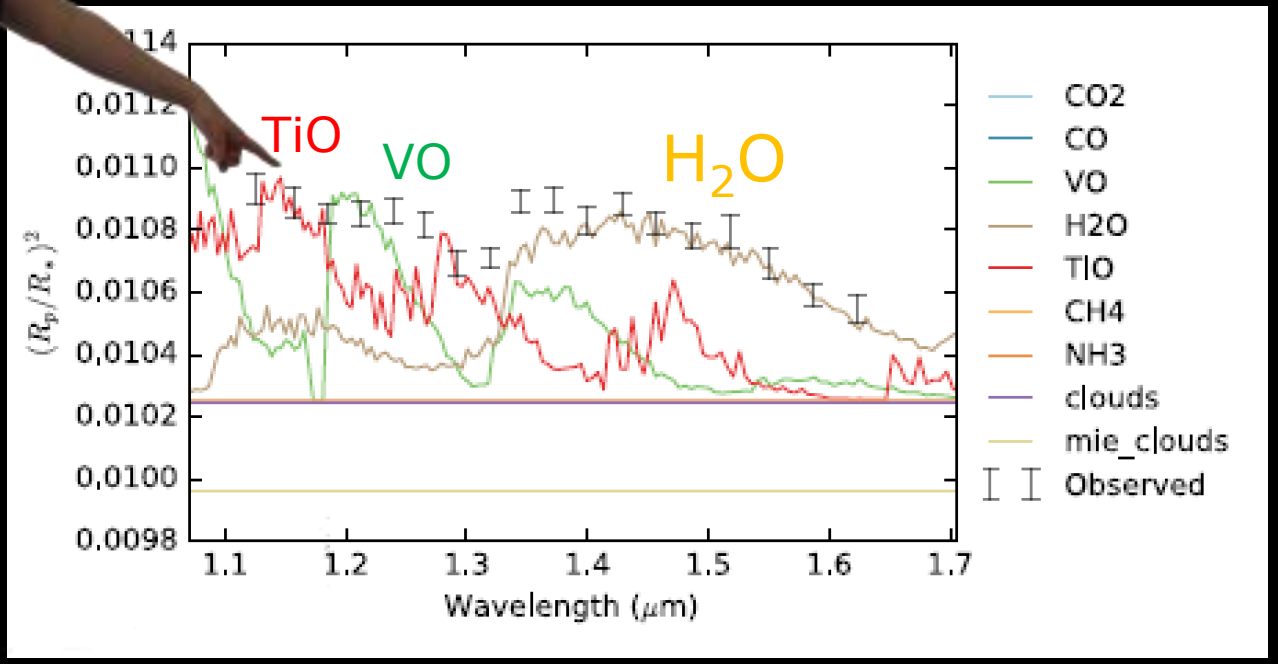


Wasp-76b

Tsiaras et al ApJ (2018)

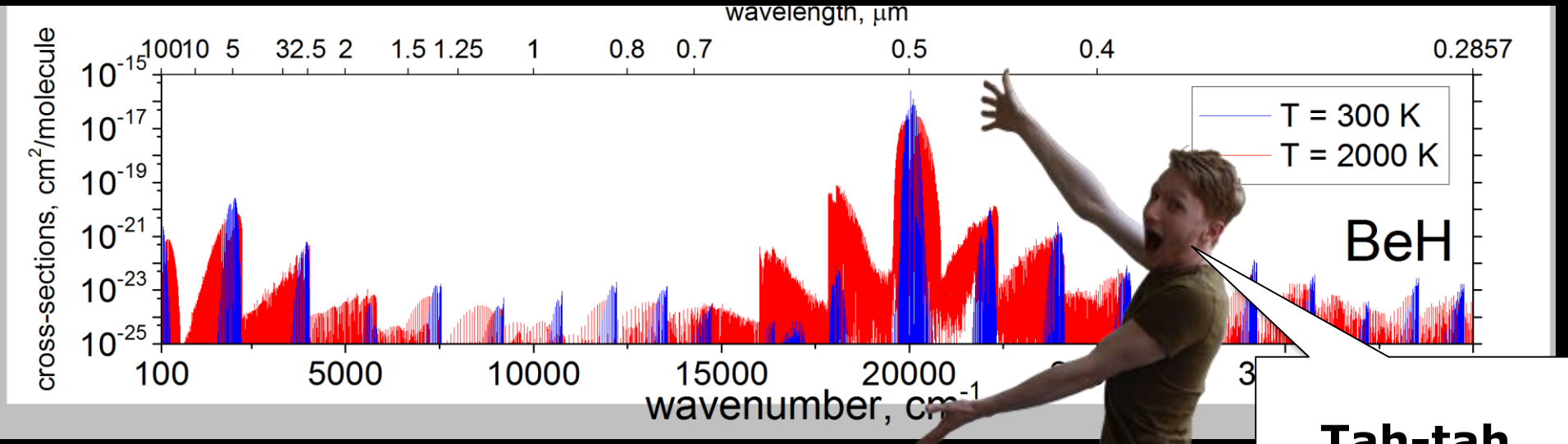


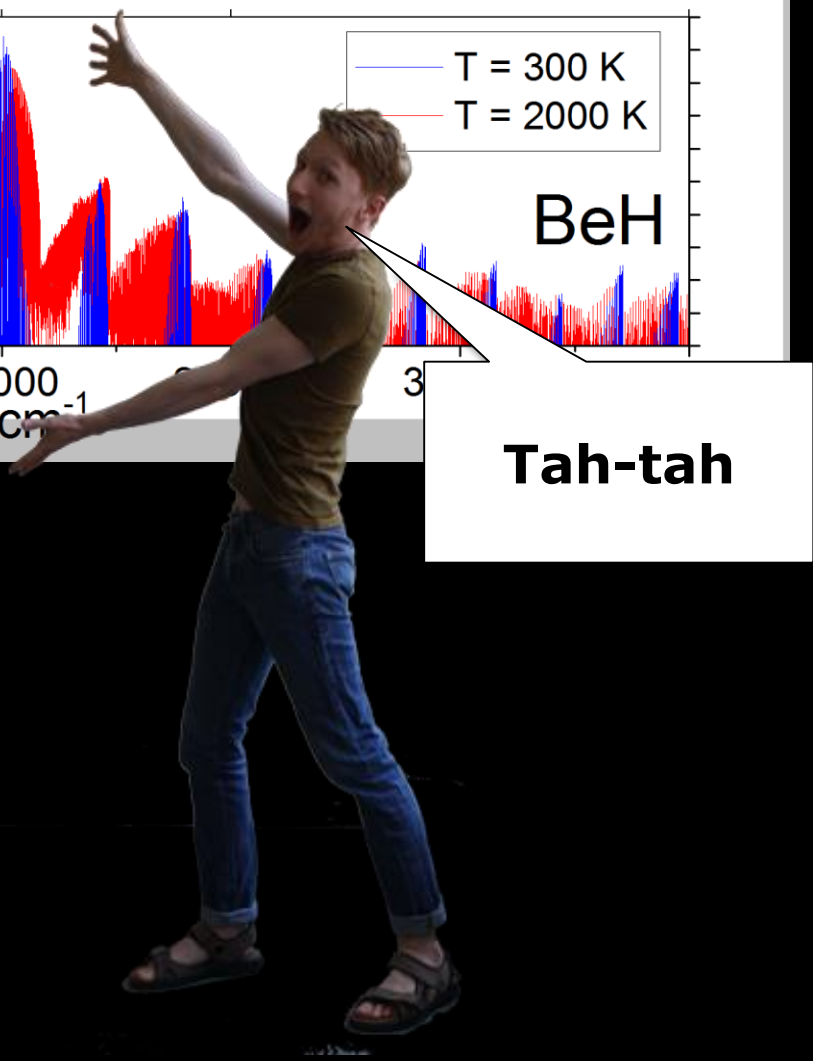
Almost ready



BeH line list

Amazing BeH spectrum for JET plasma applications

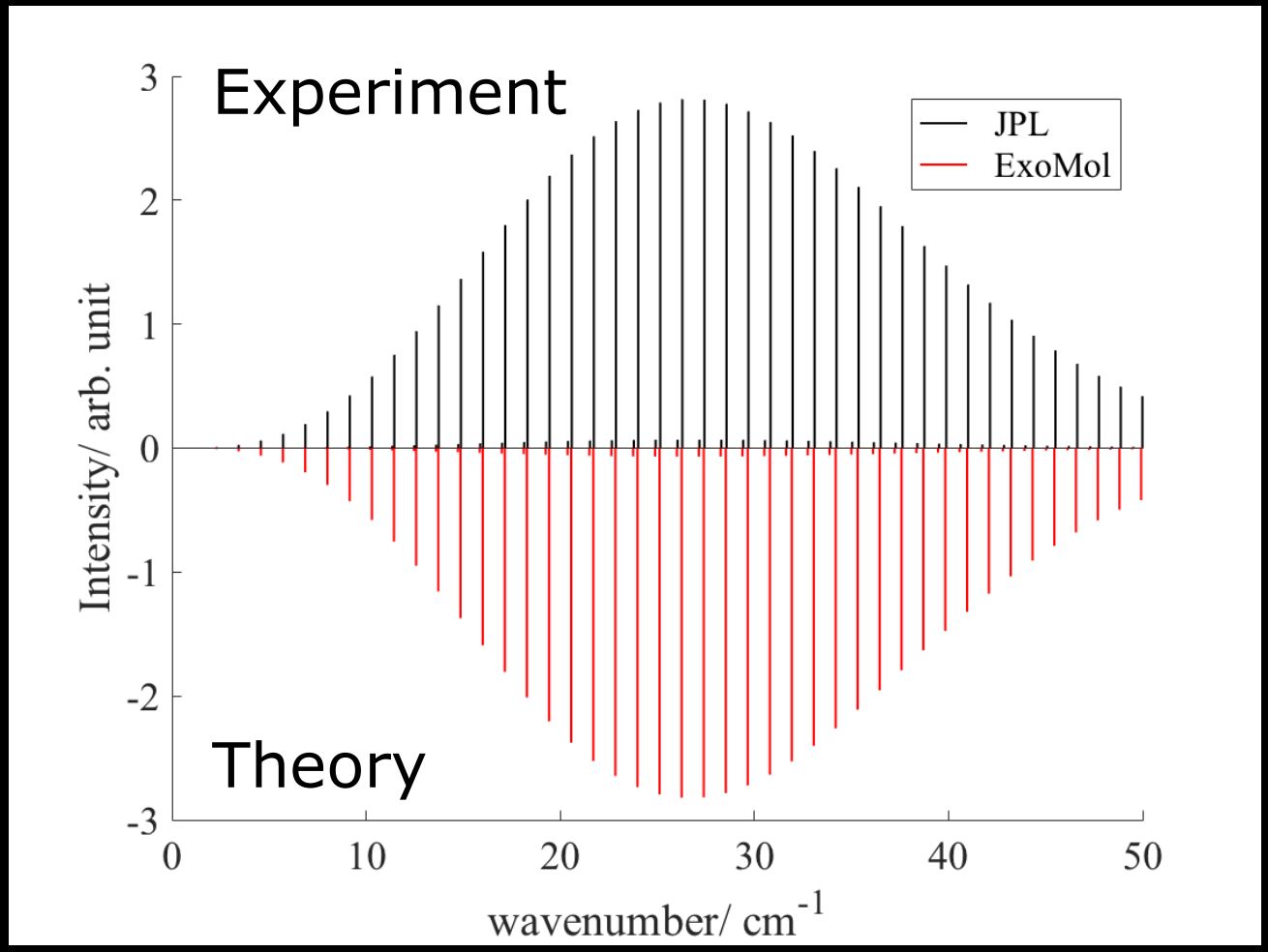


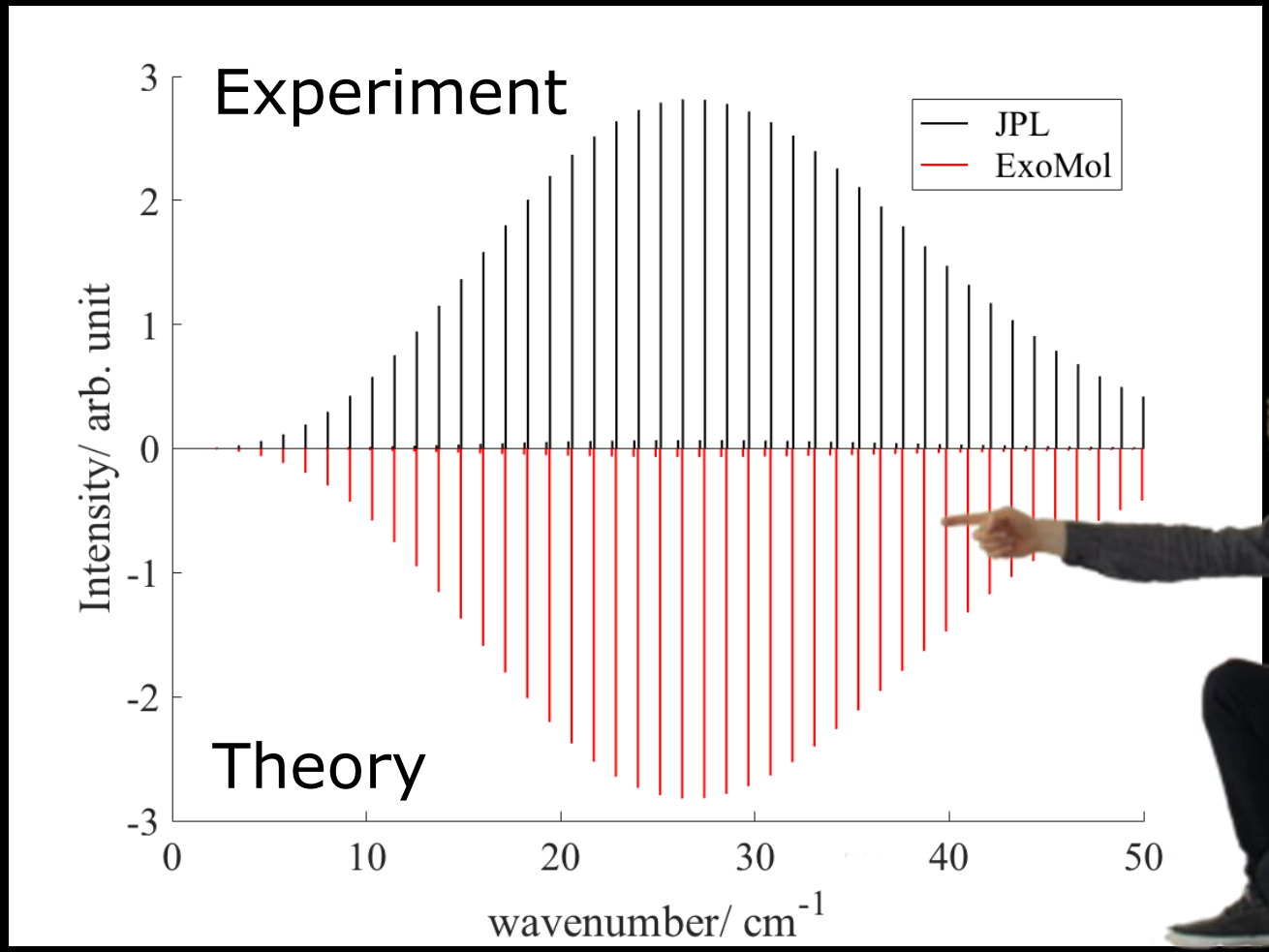


Amazing BeH spectrum for JET plasma applications

Refinement of our pure theoretical model to experiment is always mandatory

How accurate are we?


Experiment
Theory
JPL
ExoMol
Intensity/ arb. unit
wavenumber/ cm-1
3
2
1
0
-1
-2
-3
0
10
20
30
40
50

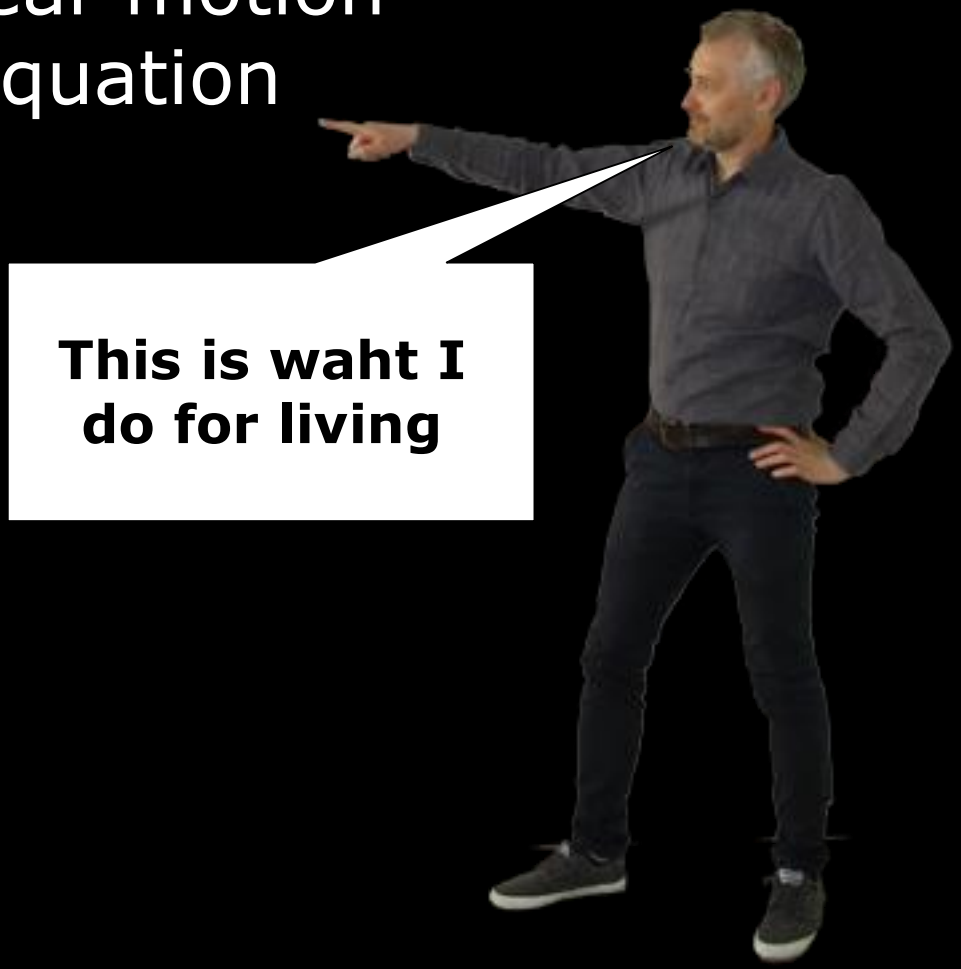


MgO: Only after refinement

Method

Solving the nuclear motion Schrödinger equation

Solving the nuclear motion Schrödinger equation



Diatomics: Duo

Diatomics: Duo

Diatomics:
Duo

Polyatomics:
TROVE

Diatomics:
Duo

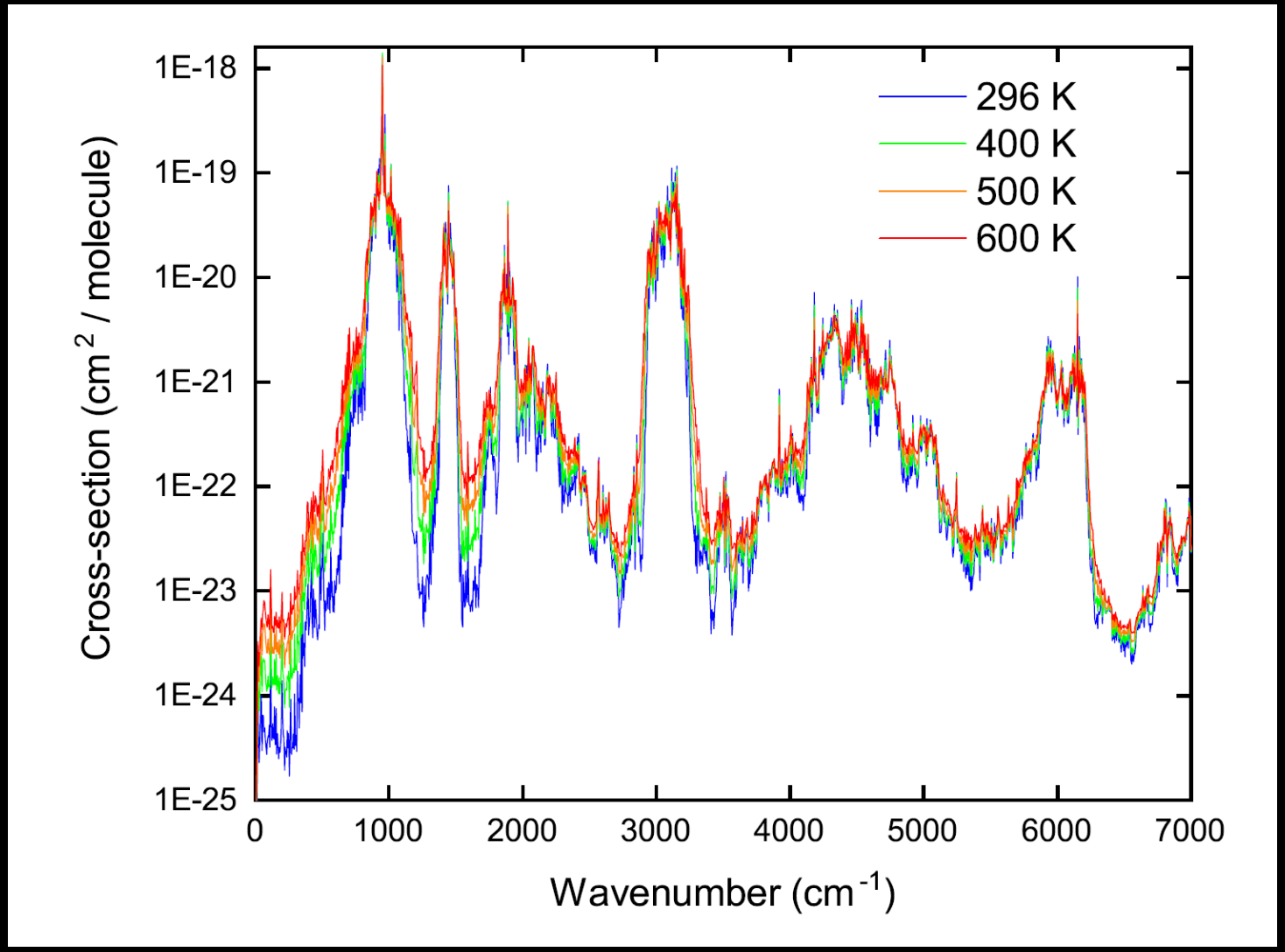
Polyatomics:
TROVE

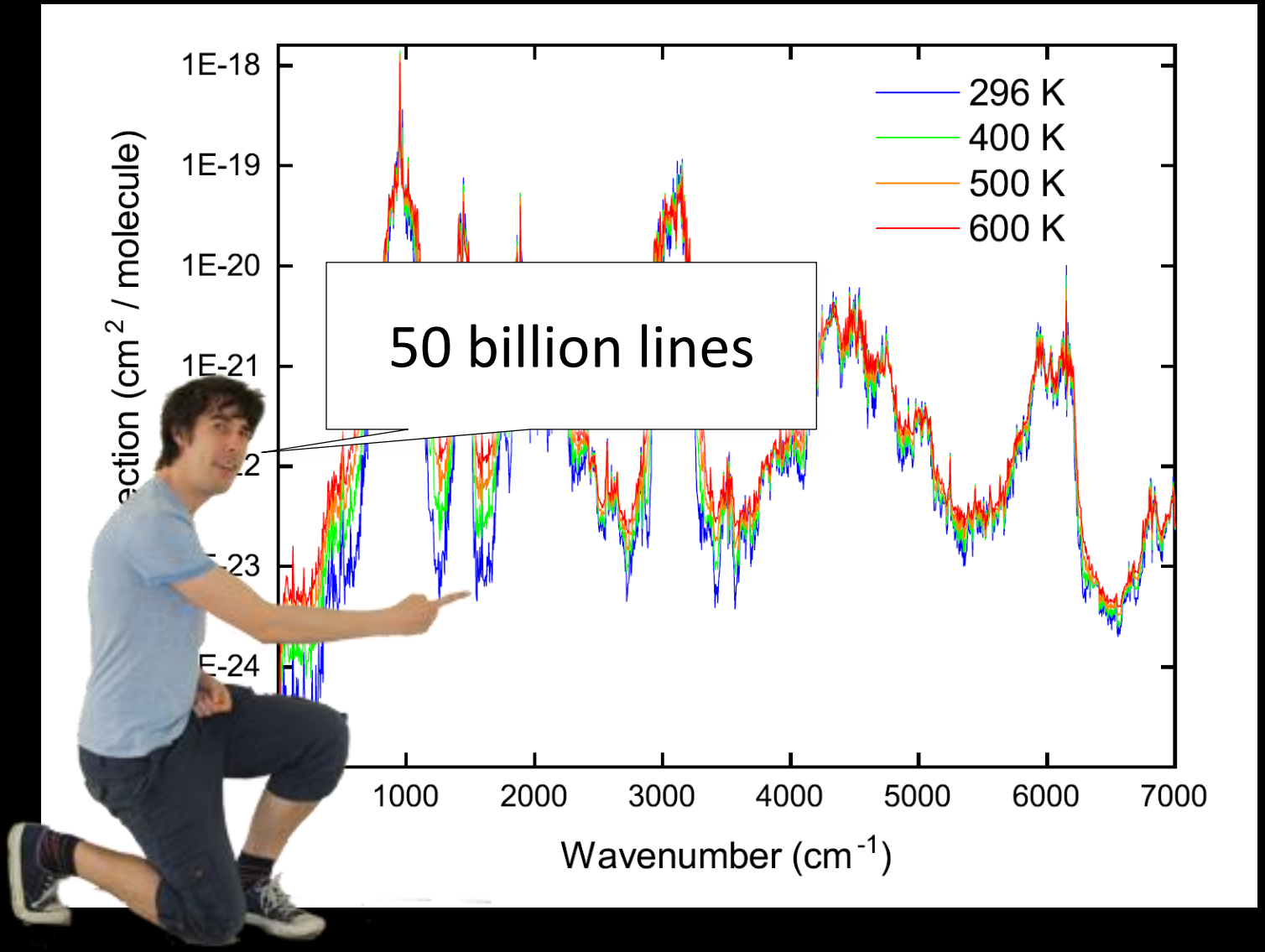
Ingredients and calculation steps are essentially the same as for diatomics

Barry Mant

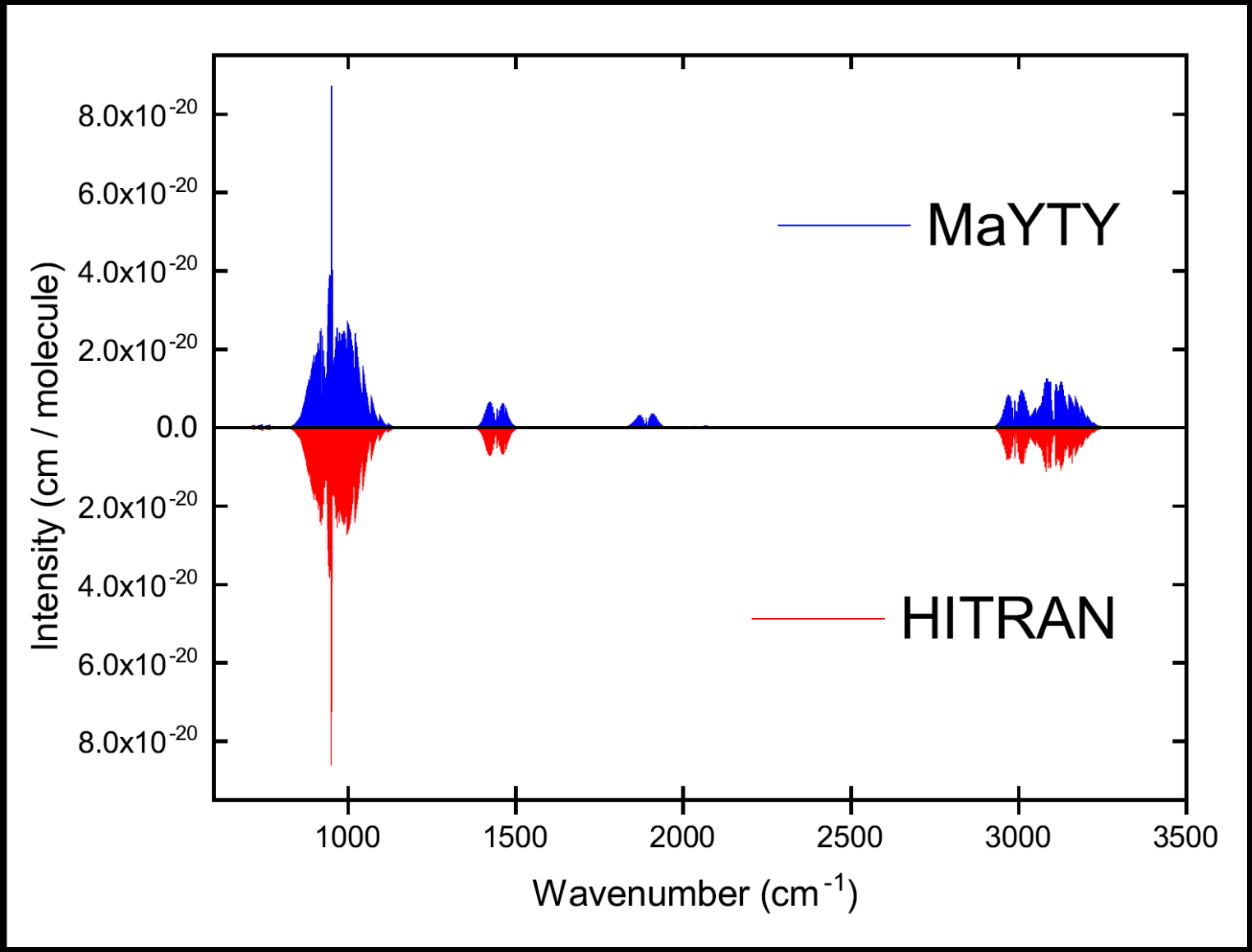
Ethylene:
new ExoMol ~~song~~ line list

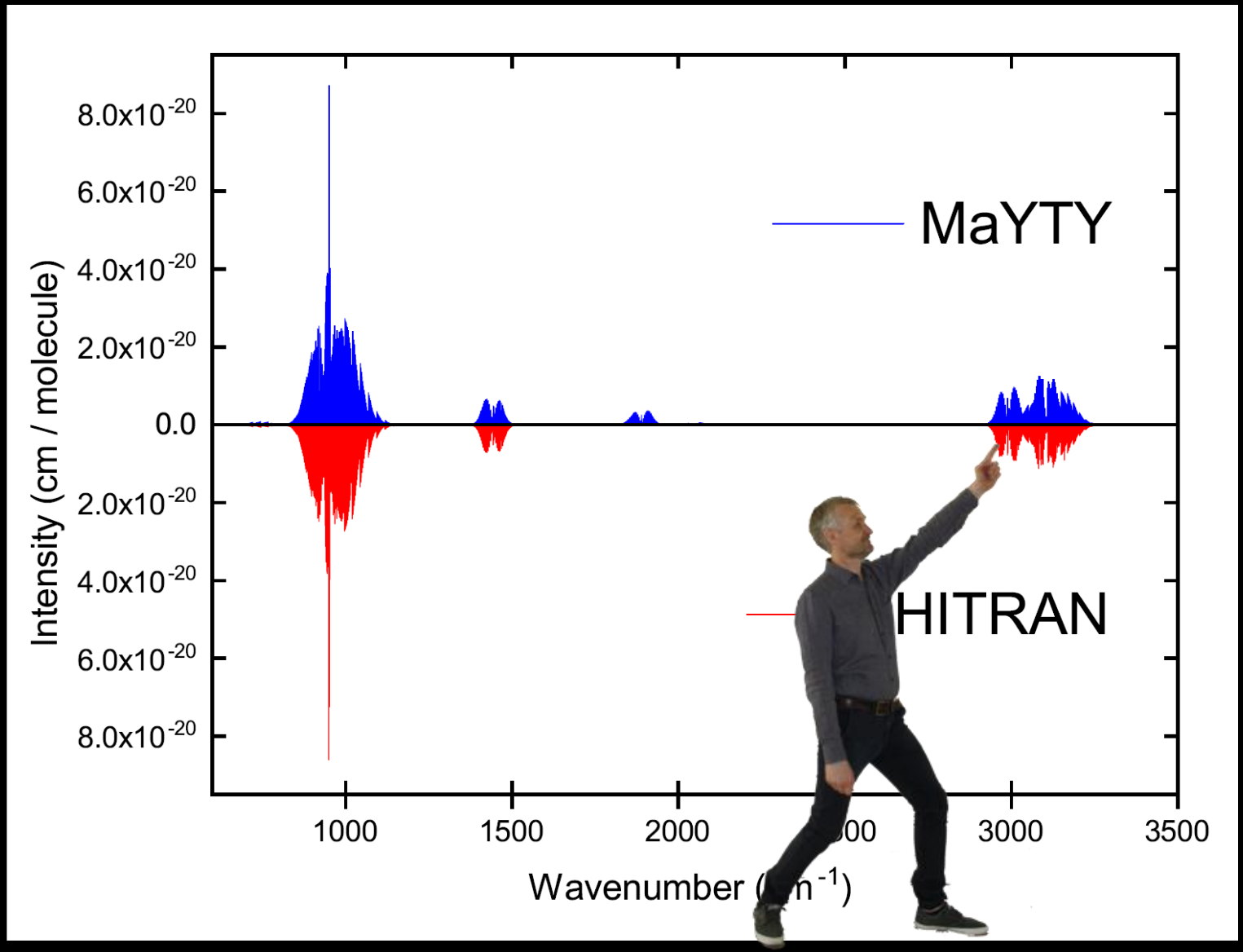
Barry Mant

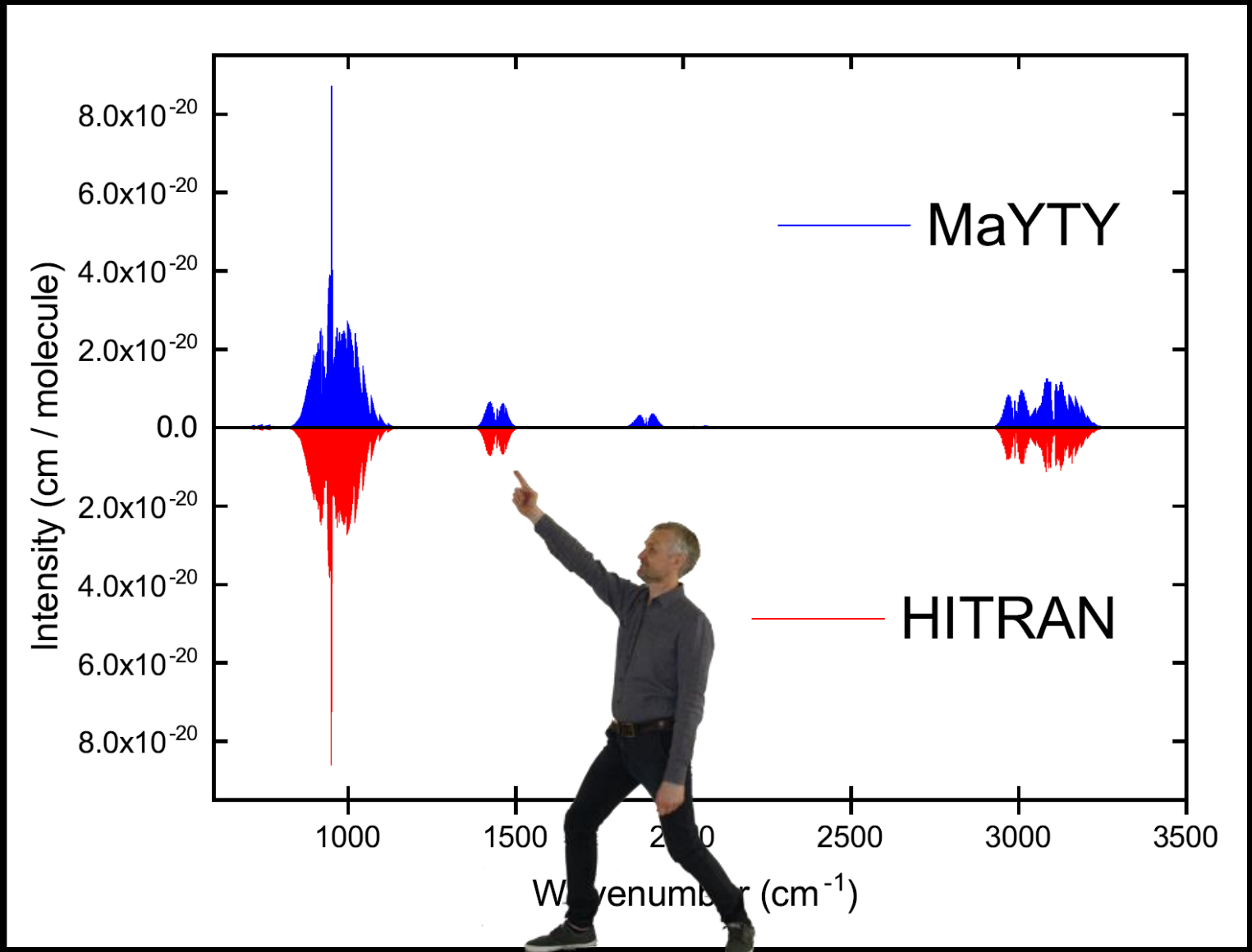

Cross-section (cm^2 / molecule)
1E-18
1E-19
1E-20
1E-21
1E-22
1E-23
1E-24
1E-25
0
1000
2000
3000
4000
5000
6000
7000
Wavenumber (cm^{-1})
296 K
400 K
500 K
600 K

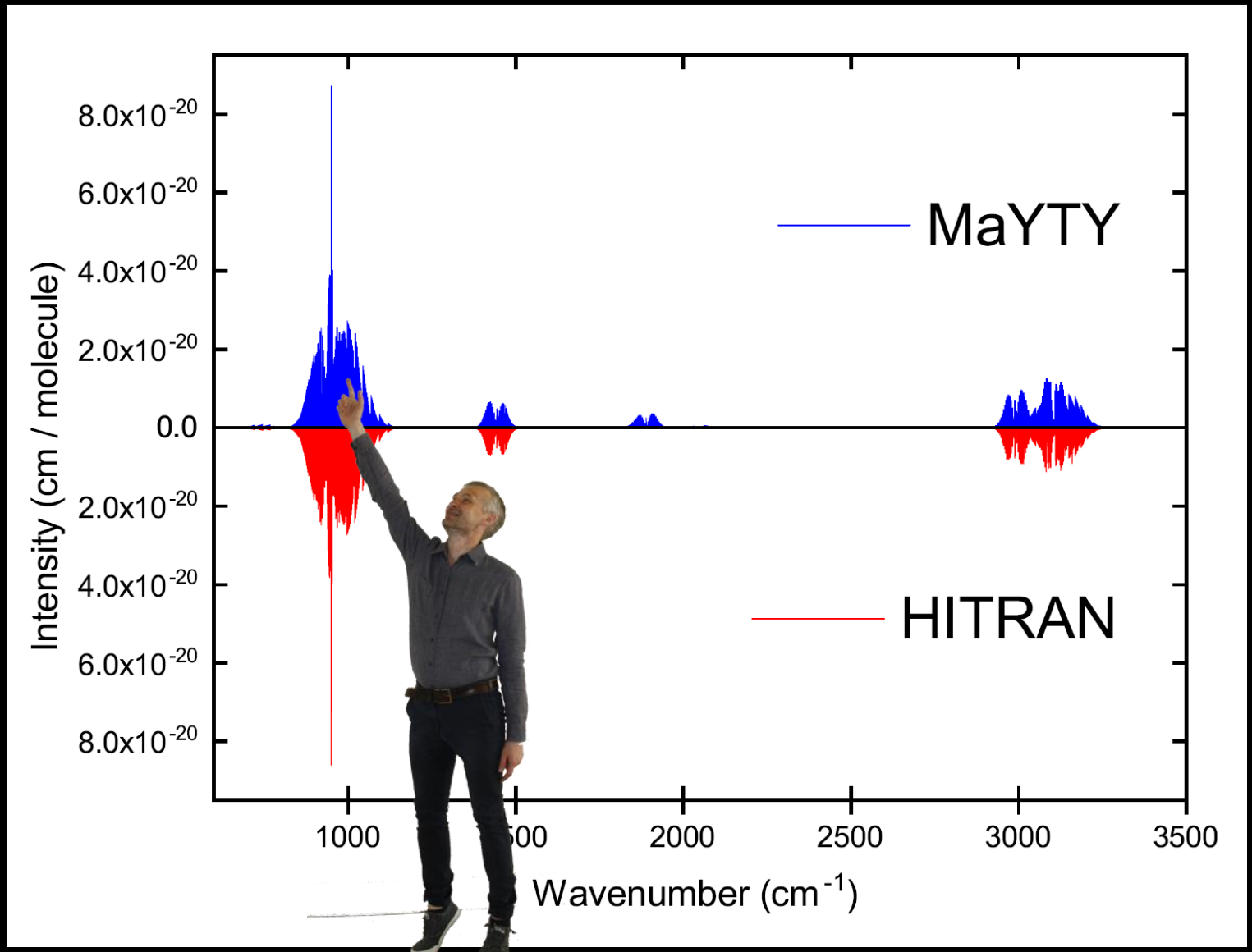

1E-18
1E-19
1E-20
1E-21
296 K
400 K
500 K
600 K
50 billion lines
1000
2000
3000
4000
5000
6000
7000
Wavenumber (cm-1)

3 band model:
Vibrational spectrum of C_2H_4

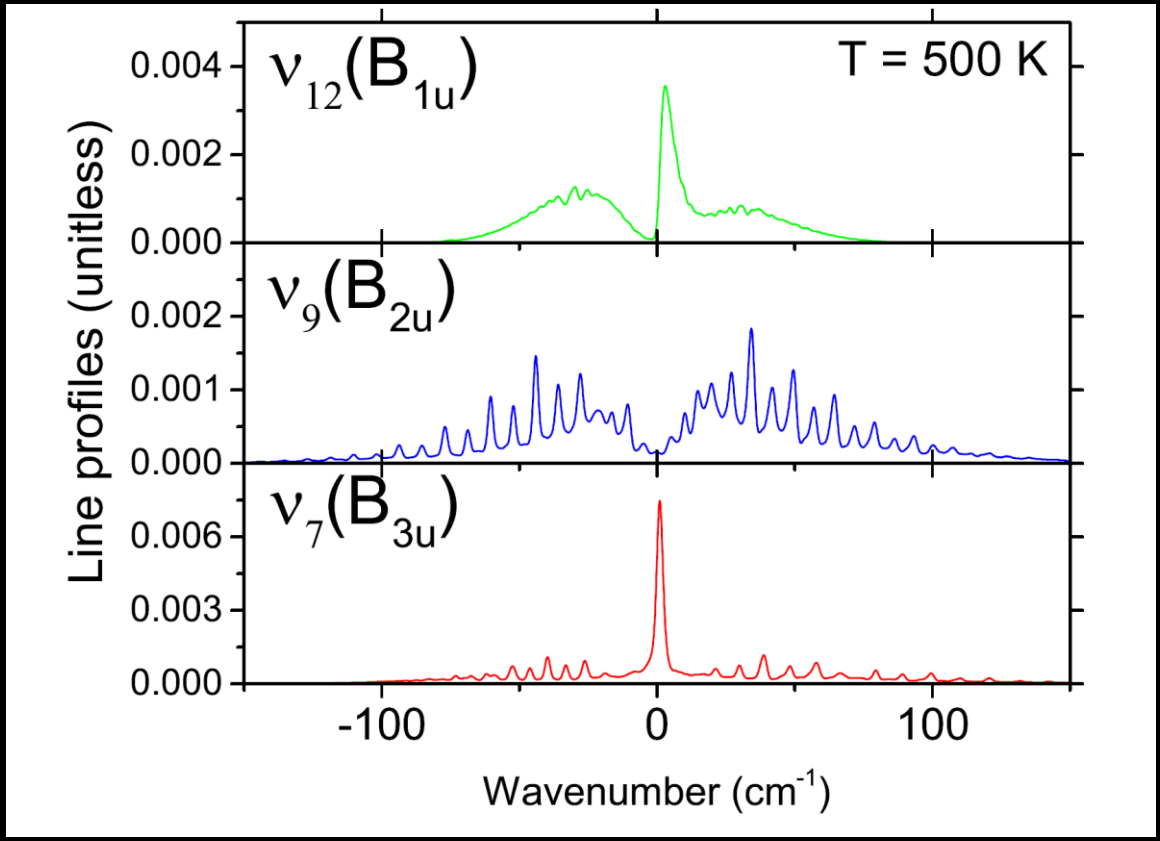

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)

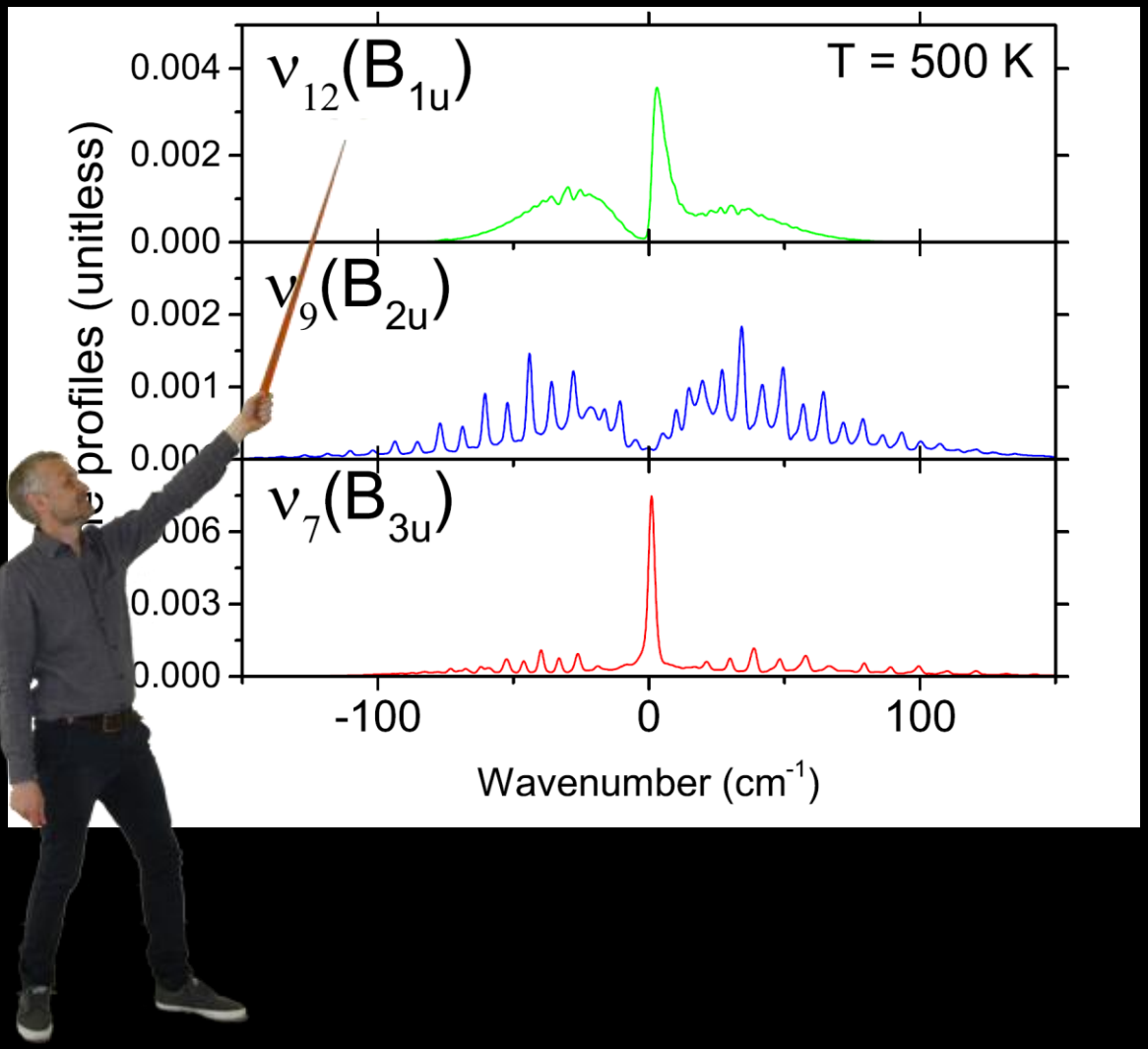

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)

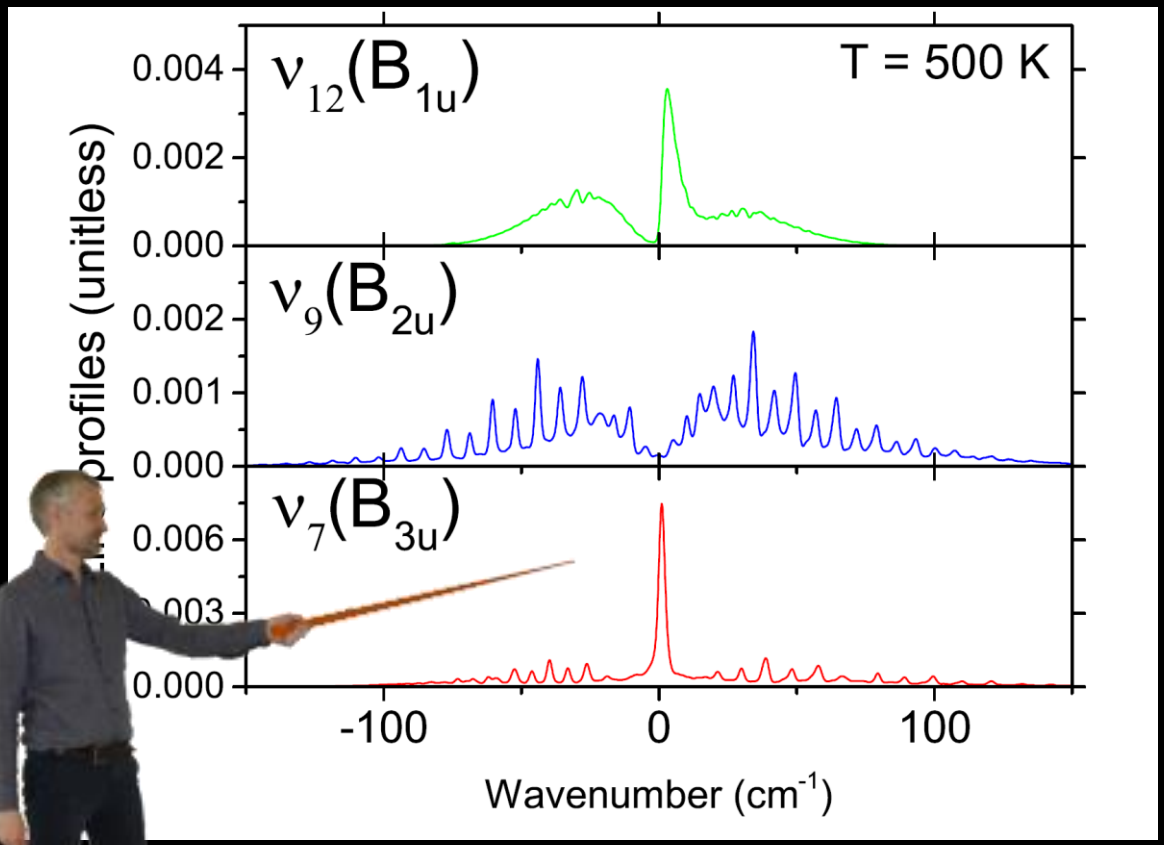

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2500
3000
3500
(cm-1)


8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
2000
2500
3000
3500
Wavenumber (cm-1)

Extract their shapes


ν12(B1u)
T = 500 K
ν9(B2u)
ν7(B3u)
Line profiles (unitless)
0.004
0.002
0.000
0.002
0.001
0.000
0.006
0.003
0.000
-100
0
100
Wavenumber (cm-1)


ν12(B1u)
T = 500 K
ν9(B2u)
ν7(B3u)
0.004
0.002
0.000
0.002
0.001
0.00
006
0.003
0.000
-100
0
100
Wavenumber (cm-1)
profiles (unitless)


ν12(B1u)
T = 500 K
ν9(B2u)
ν7(B3u)
0.004
0.002
0.000
0.002
0.001
0.000
0.006
0.000
-100
0
100
Wavenumber (cm-1)

… and apply to all other bands

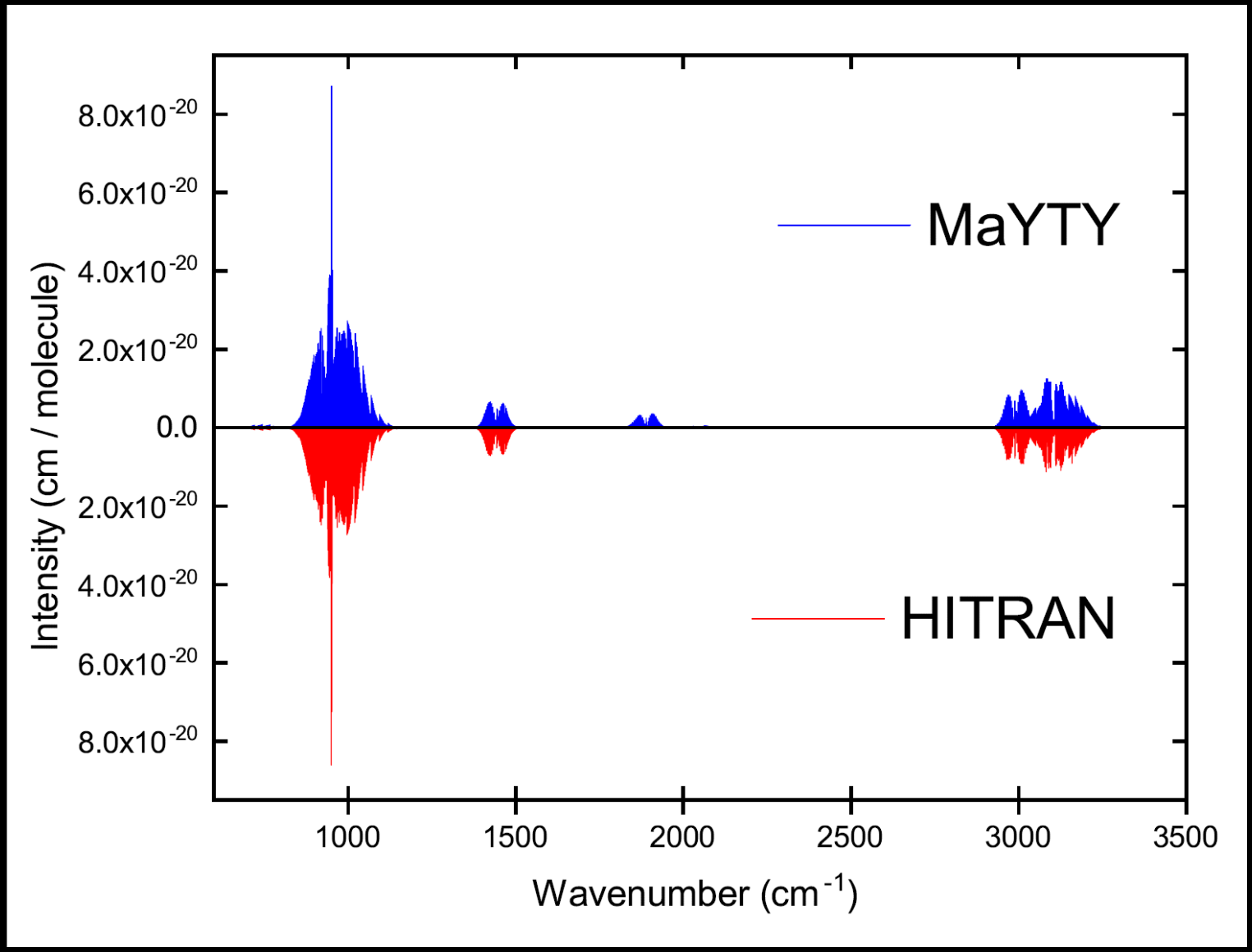
… and apply to all other bands

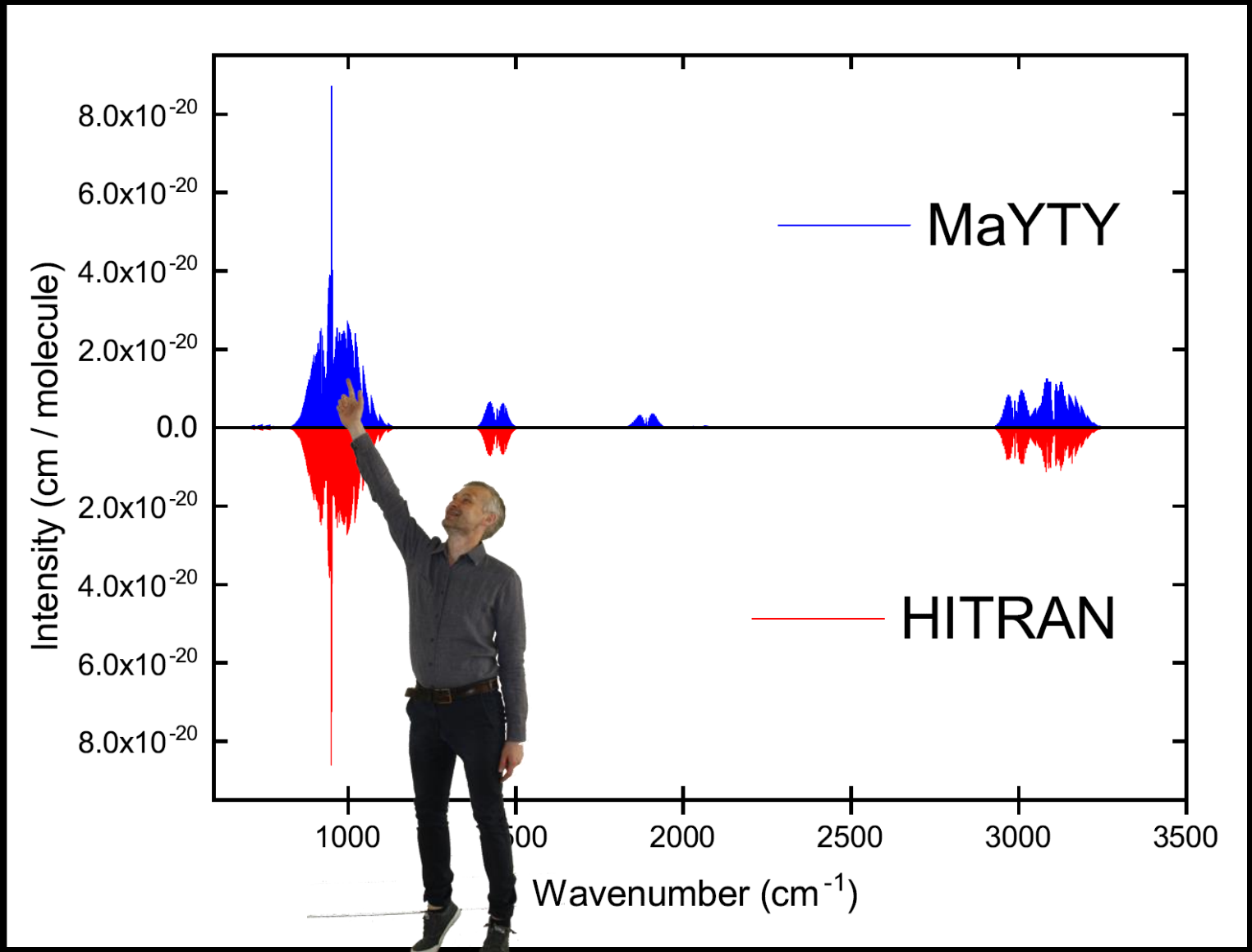
Low cost vibrational
band intensities

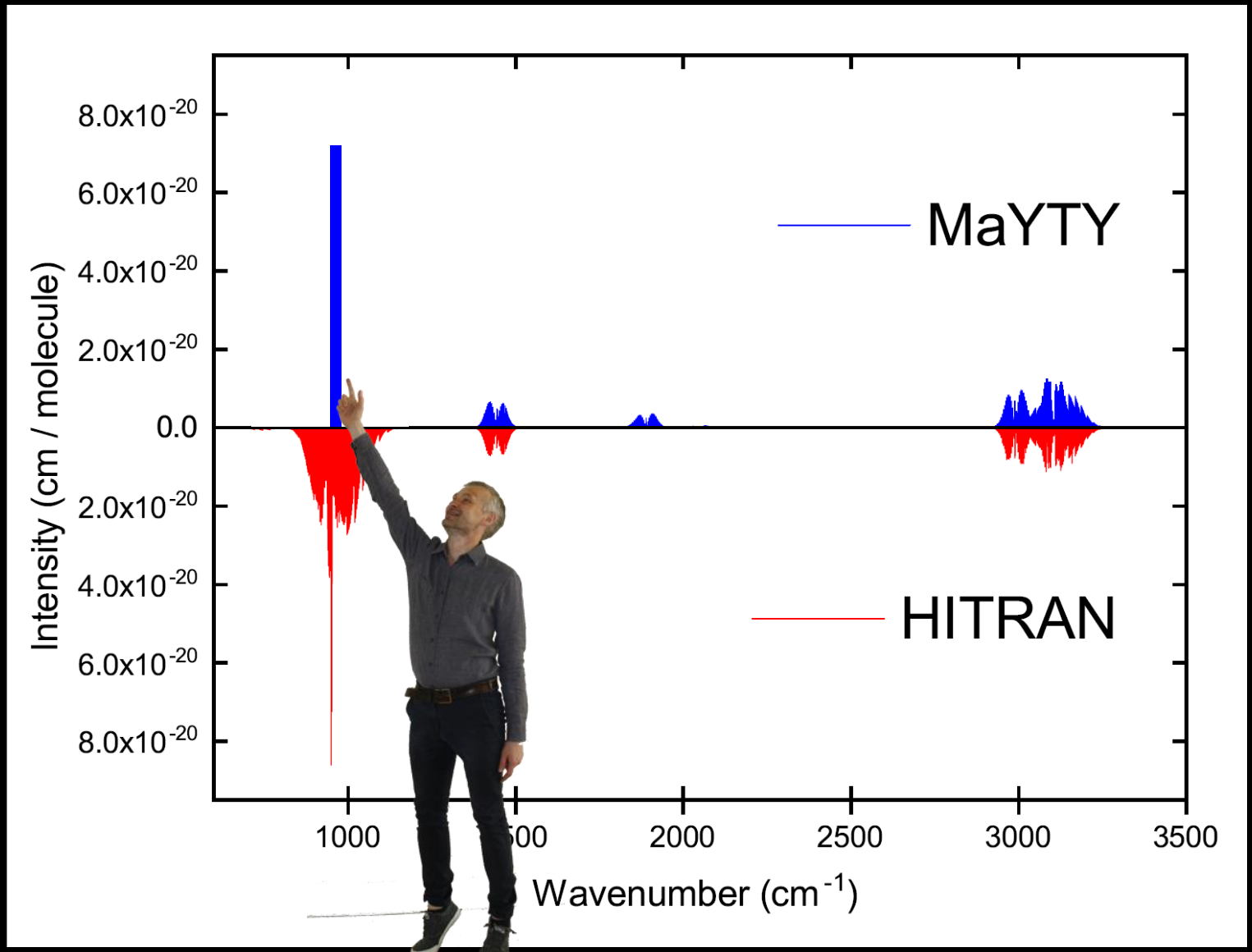
Cheating on variational calculations

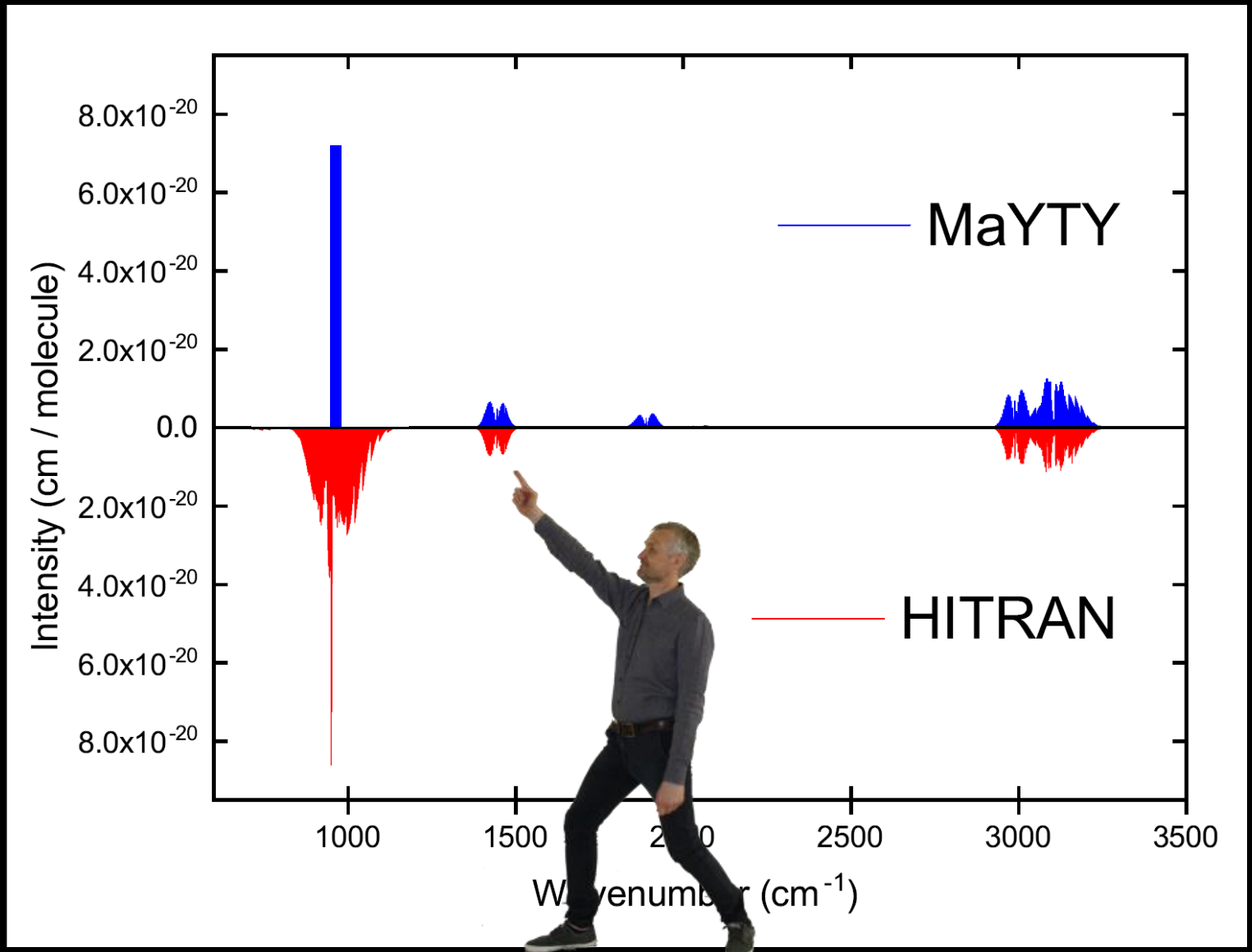
… and apply to all other bands

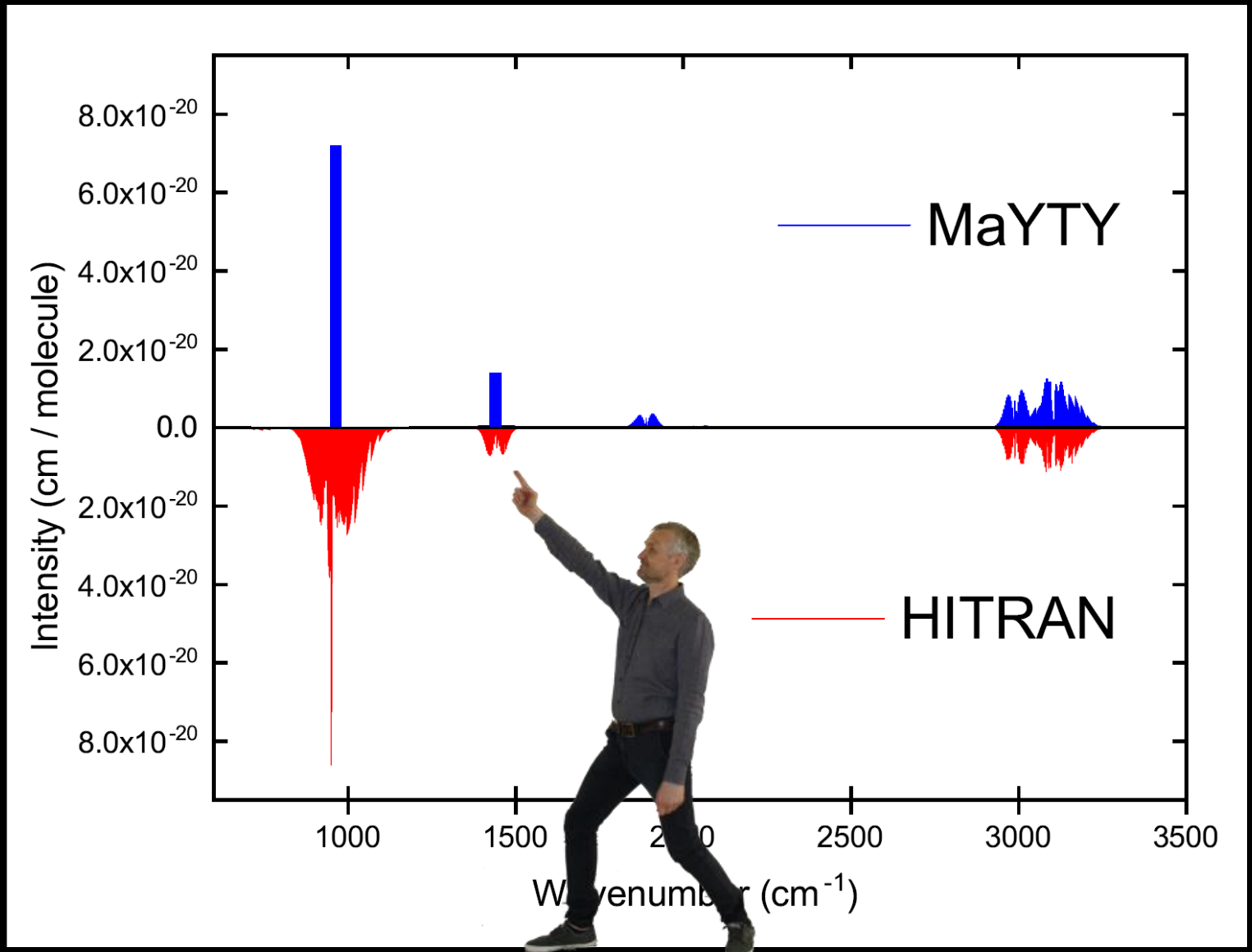
Low cost vibrational band intensities

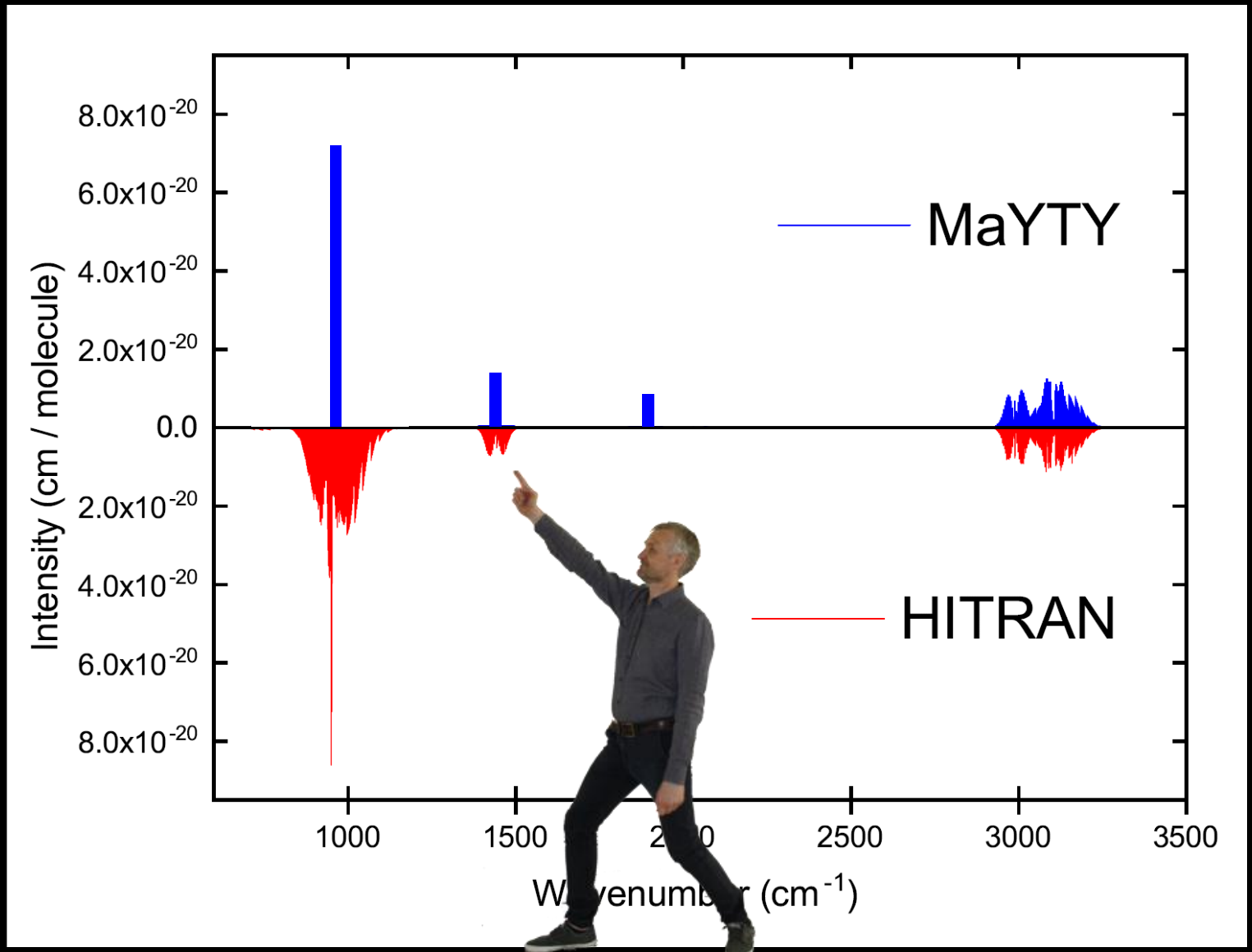

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)

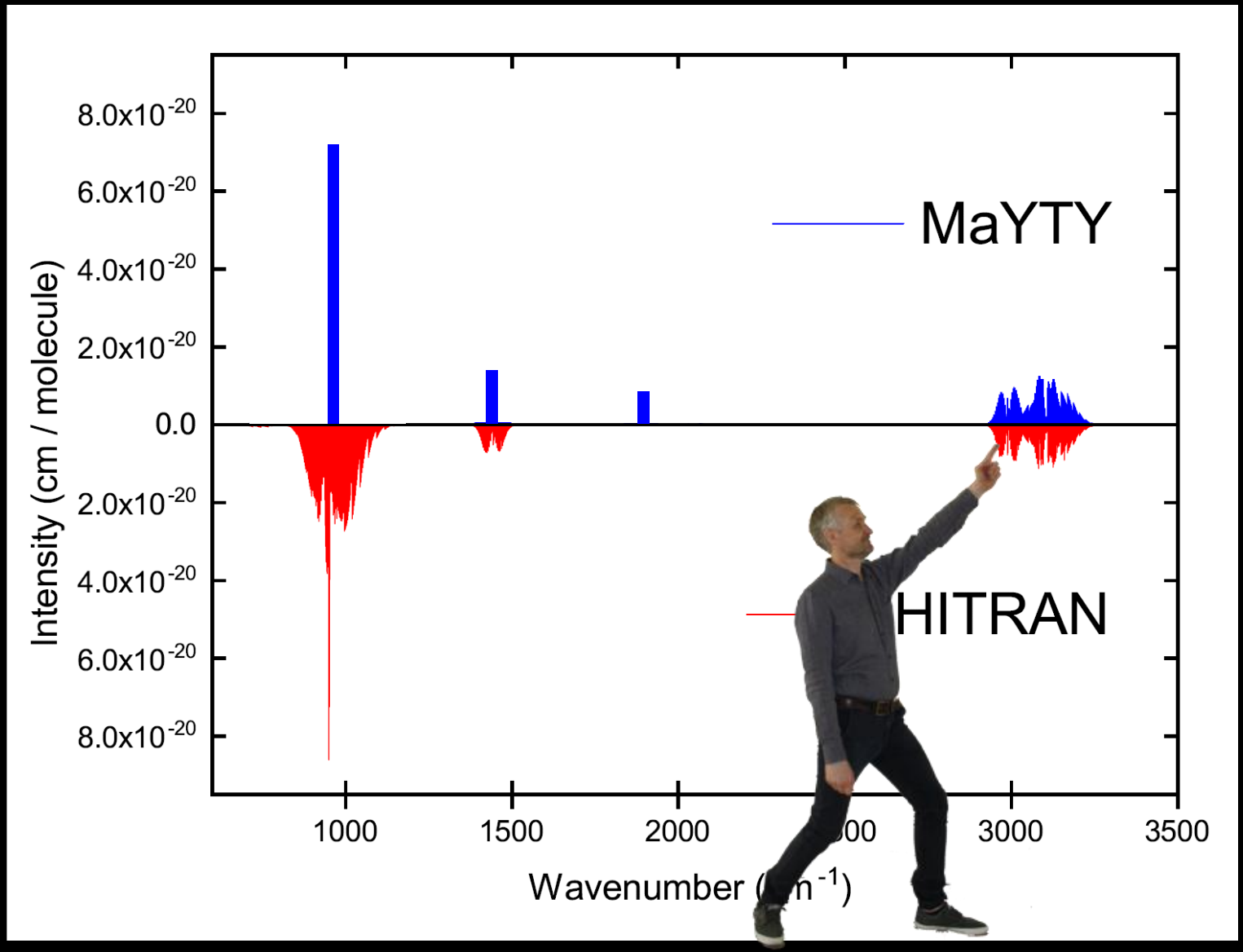

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
2000
2500
3000
3500
Wavenumber (cm-1)

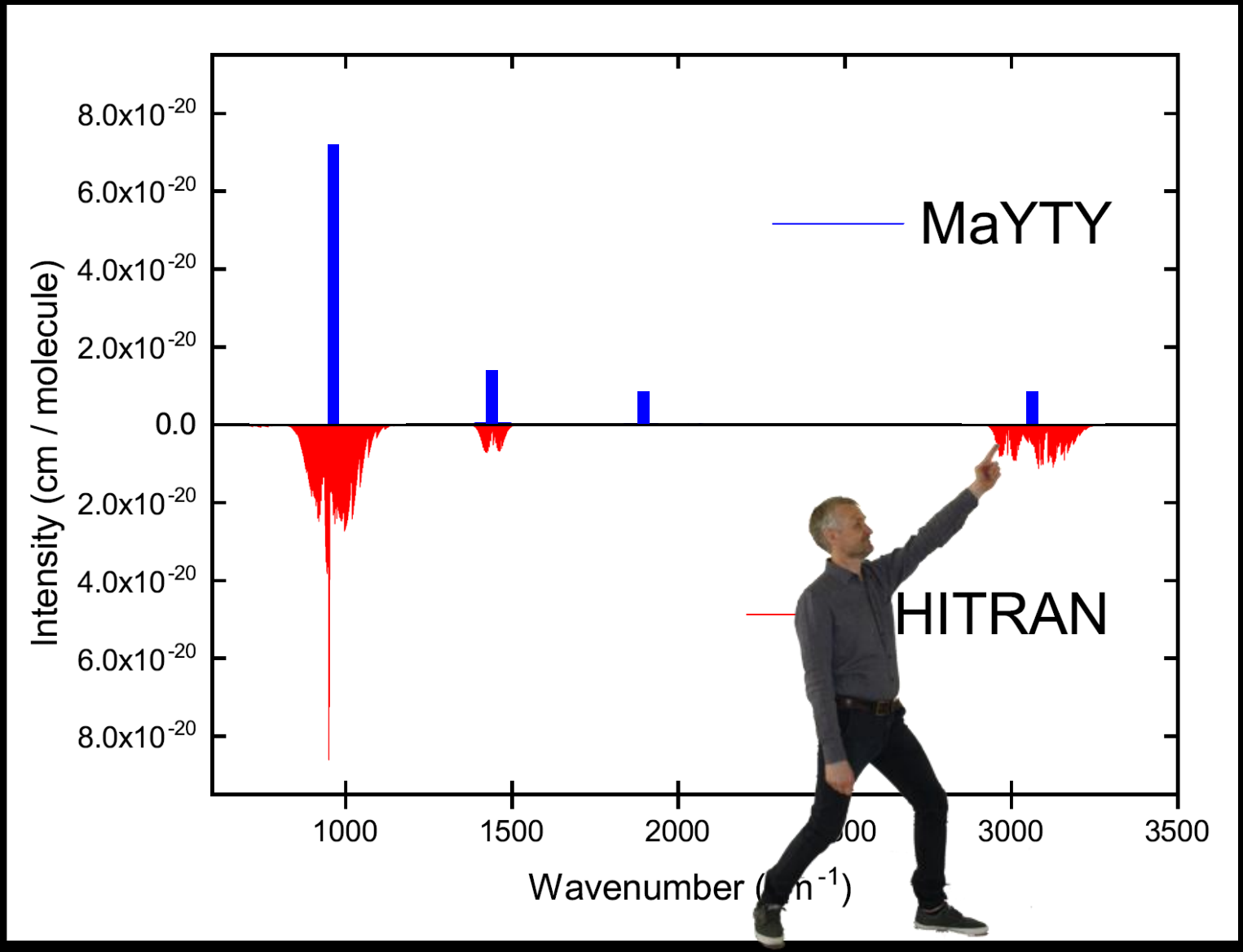

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
2000
2500
3000
3500
Wavenumber (cm-1)


8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2500
3000
3500
(cm-1)


8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2500
3000
3500
(cm-1)


8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2500
3000
3500
(cm-1)


8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)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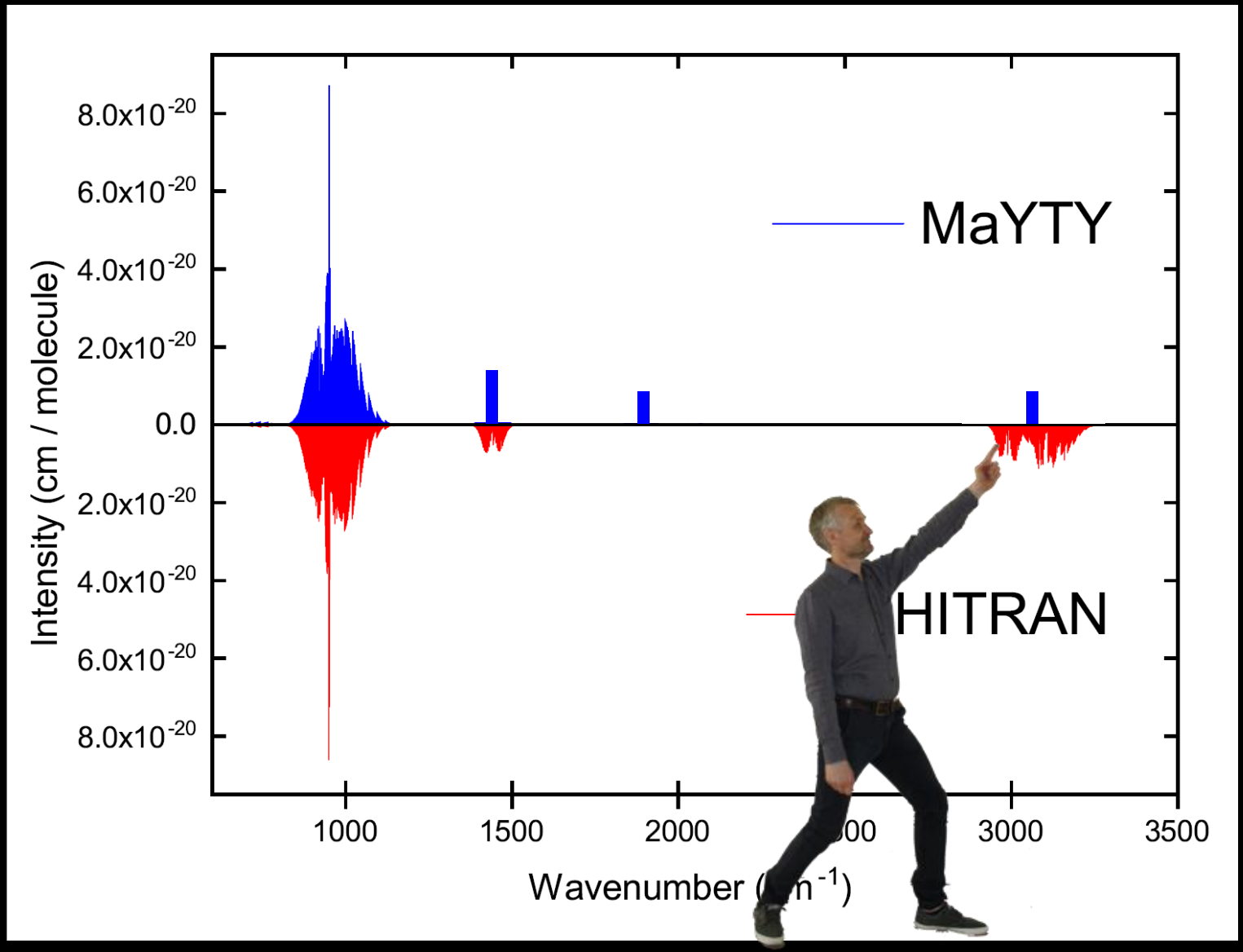
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)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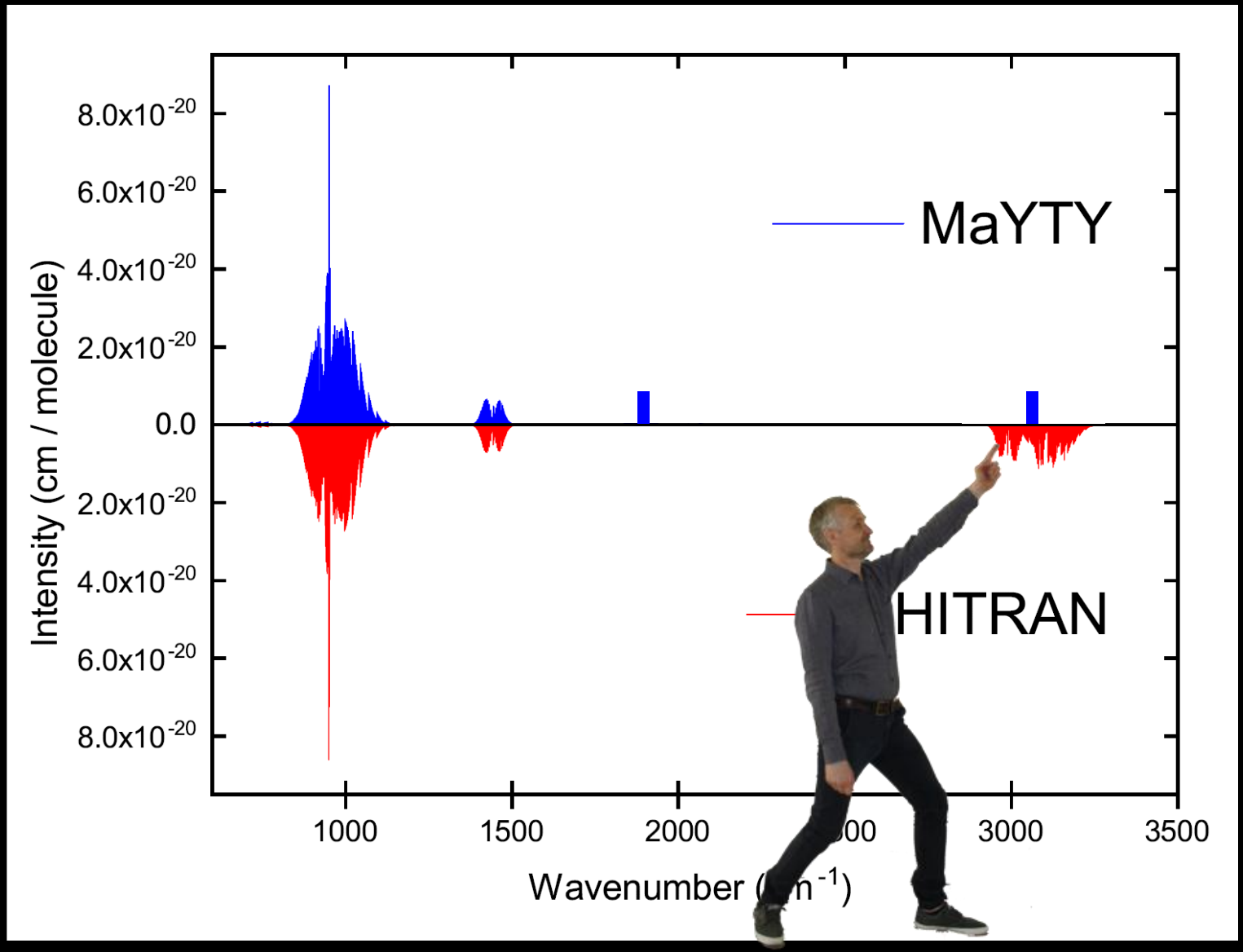
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)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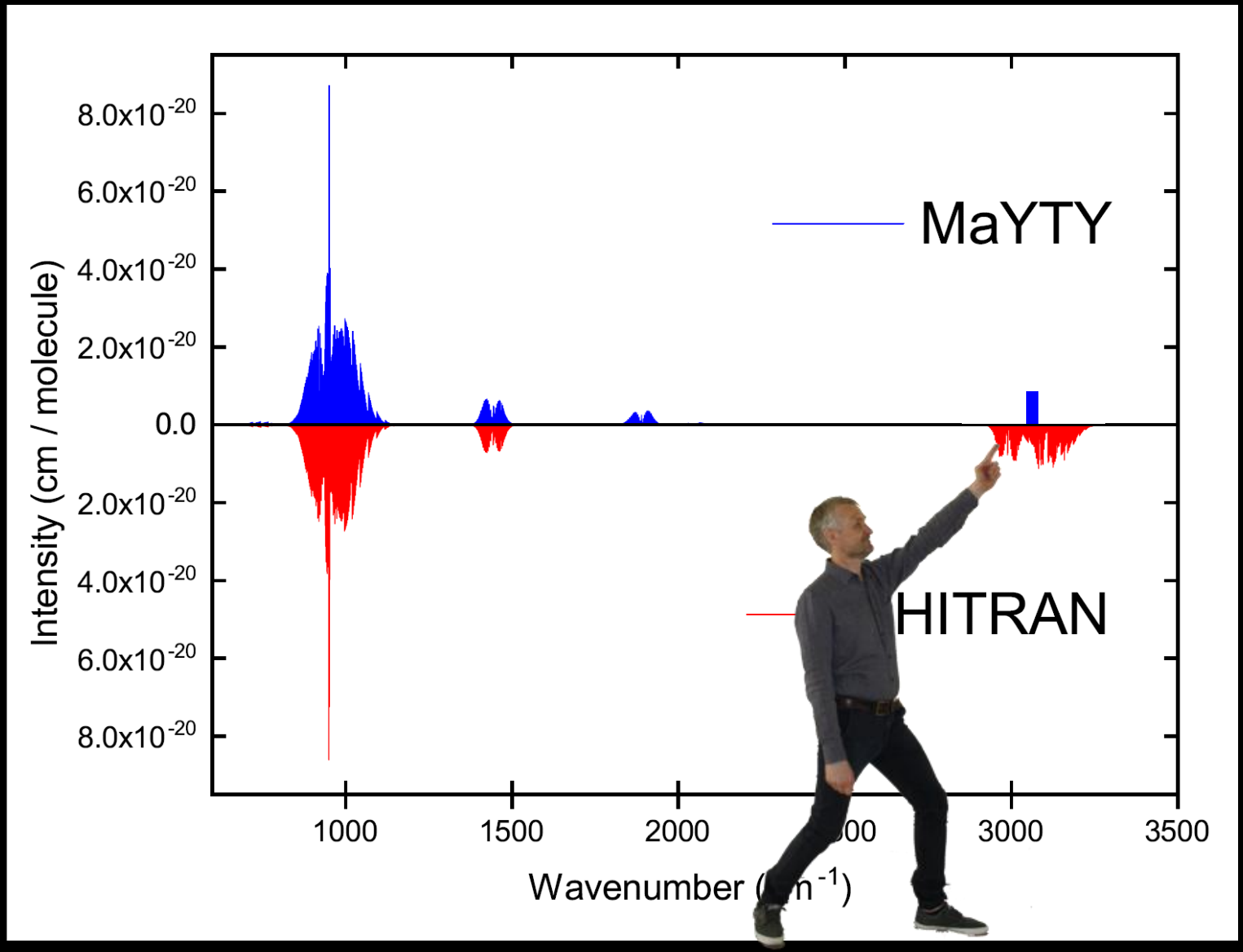
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)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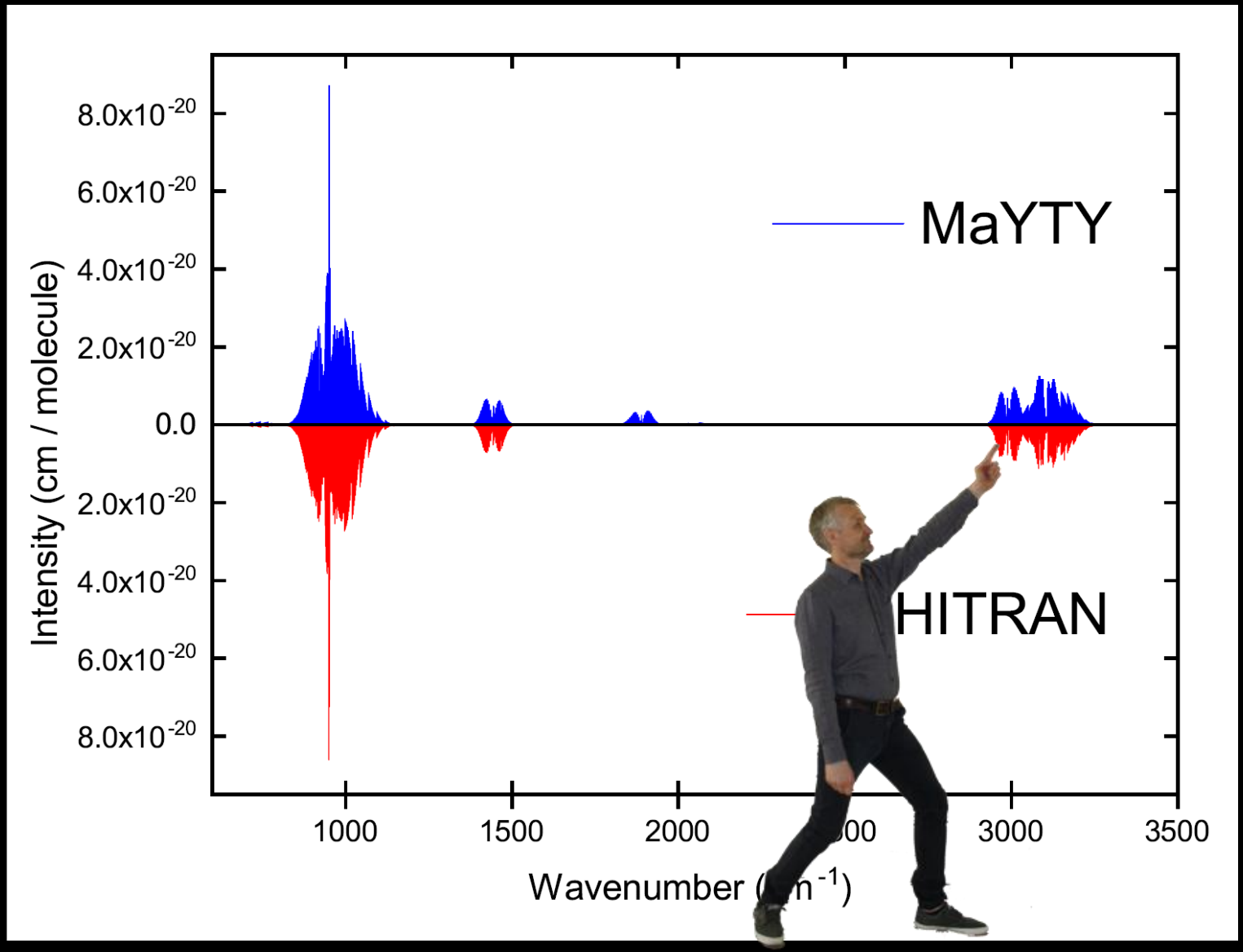
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)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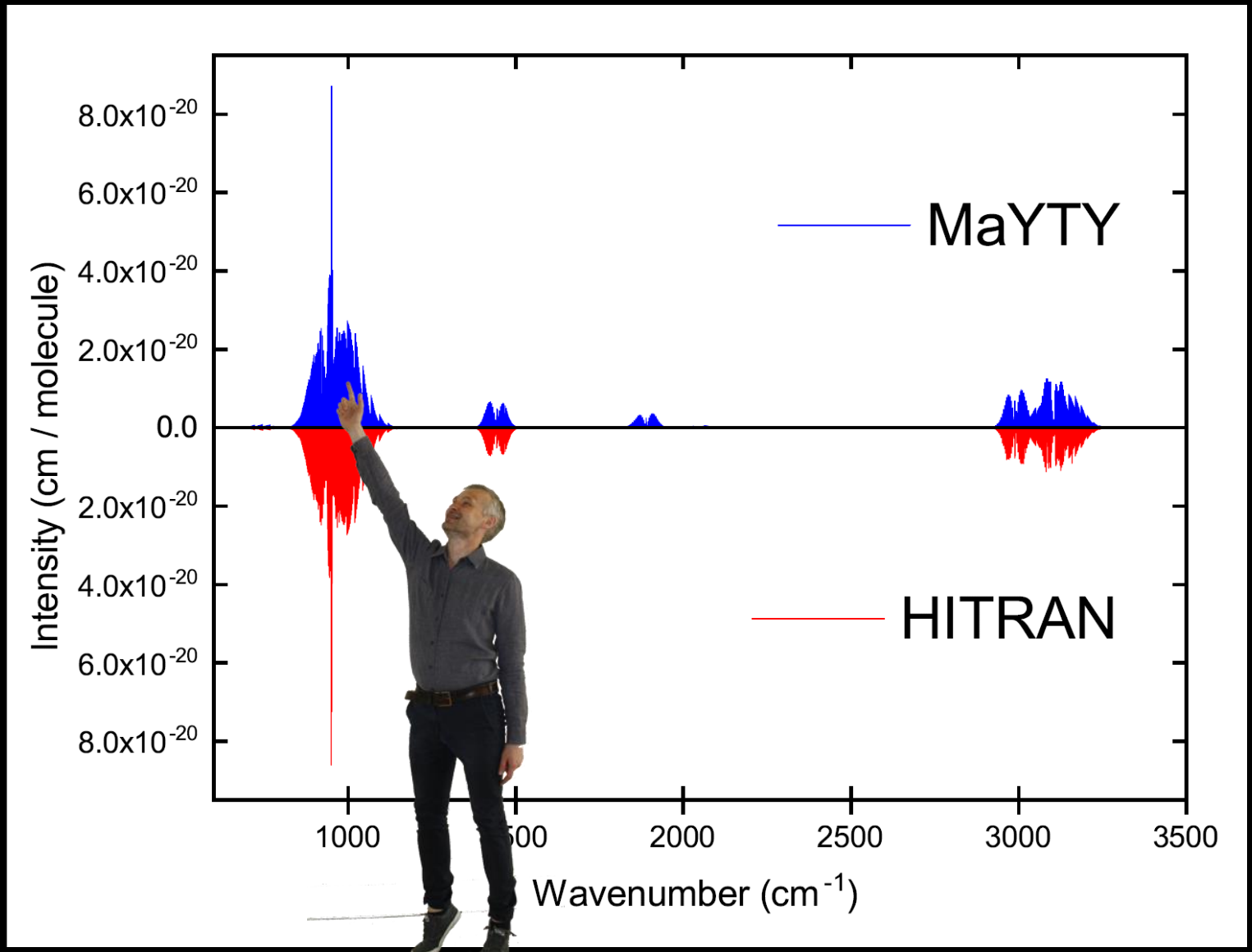
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2000
3000
3500
Wavenumber (cm-1)


8.0x10-20
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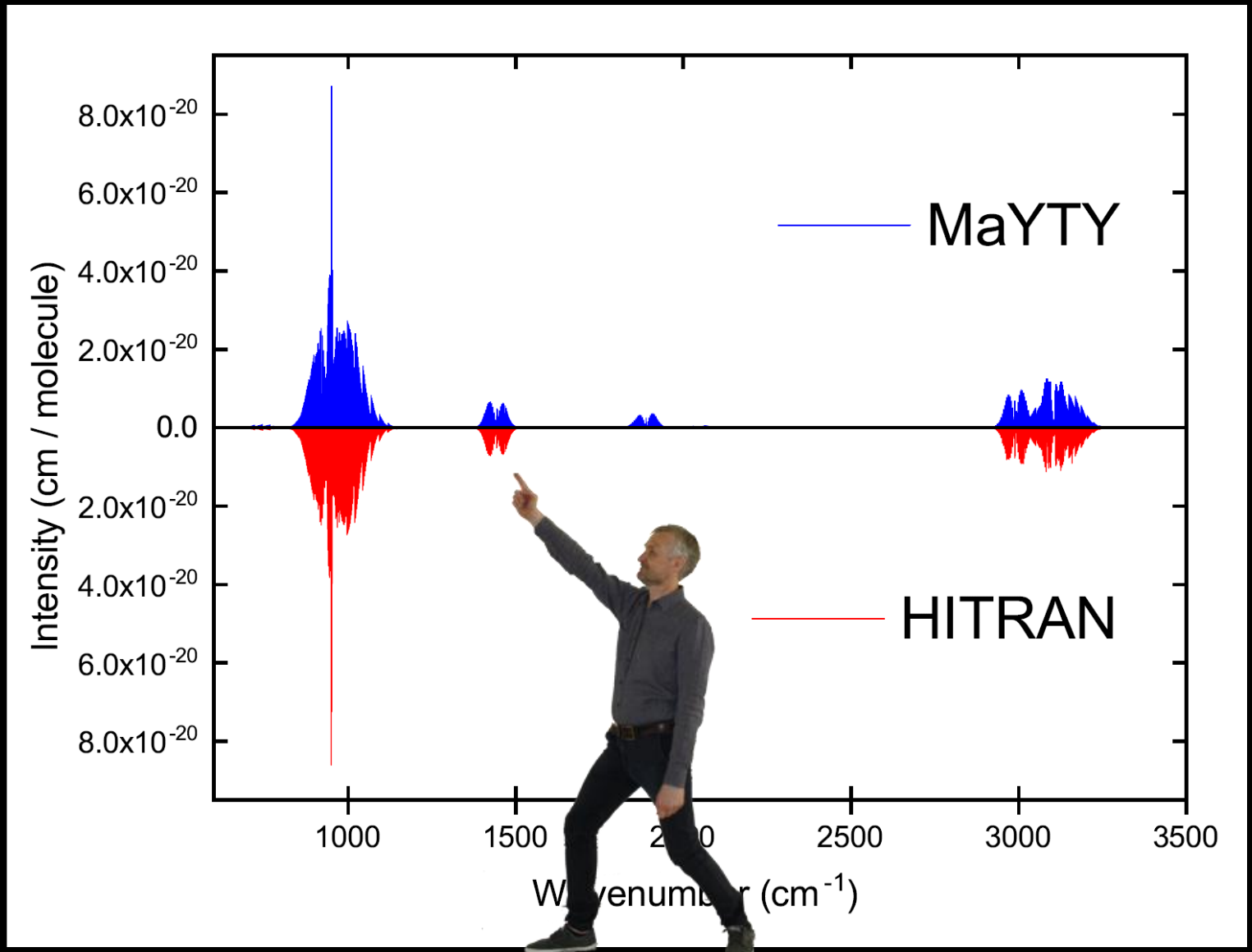
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
2000
2500
3000
3500
Wavenumber (cm-1)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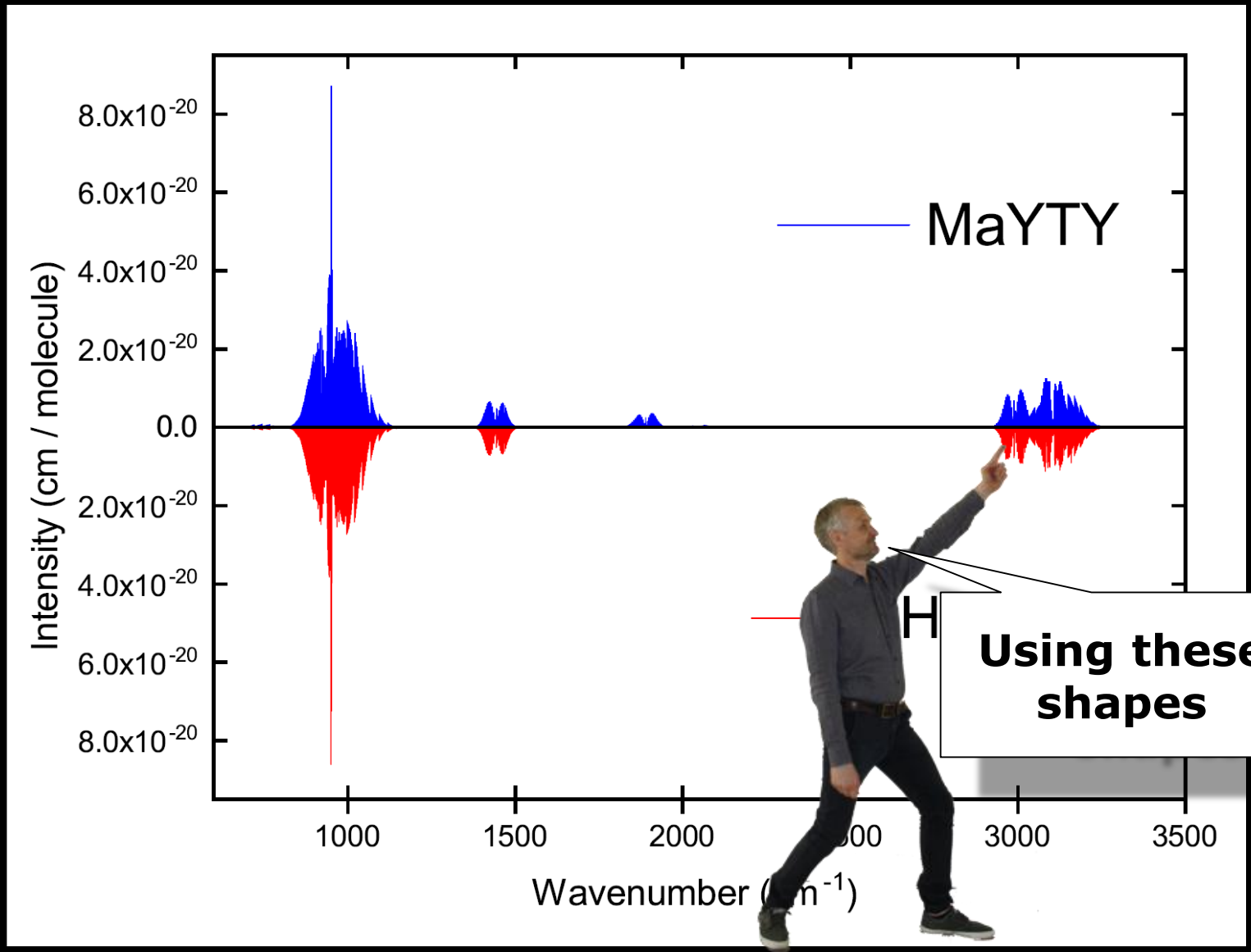
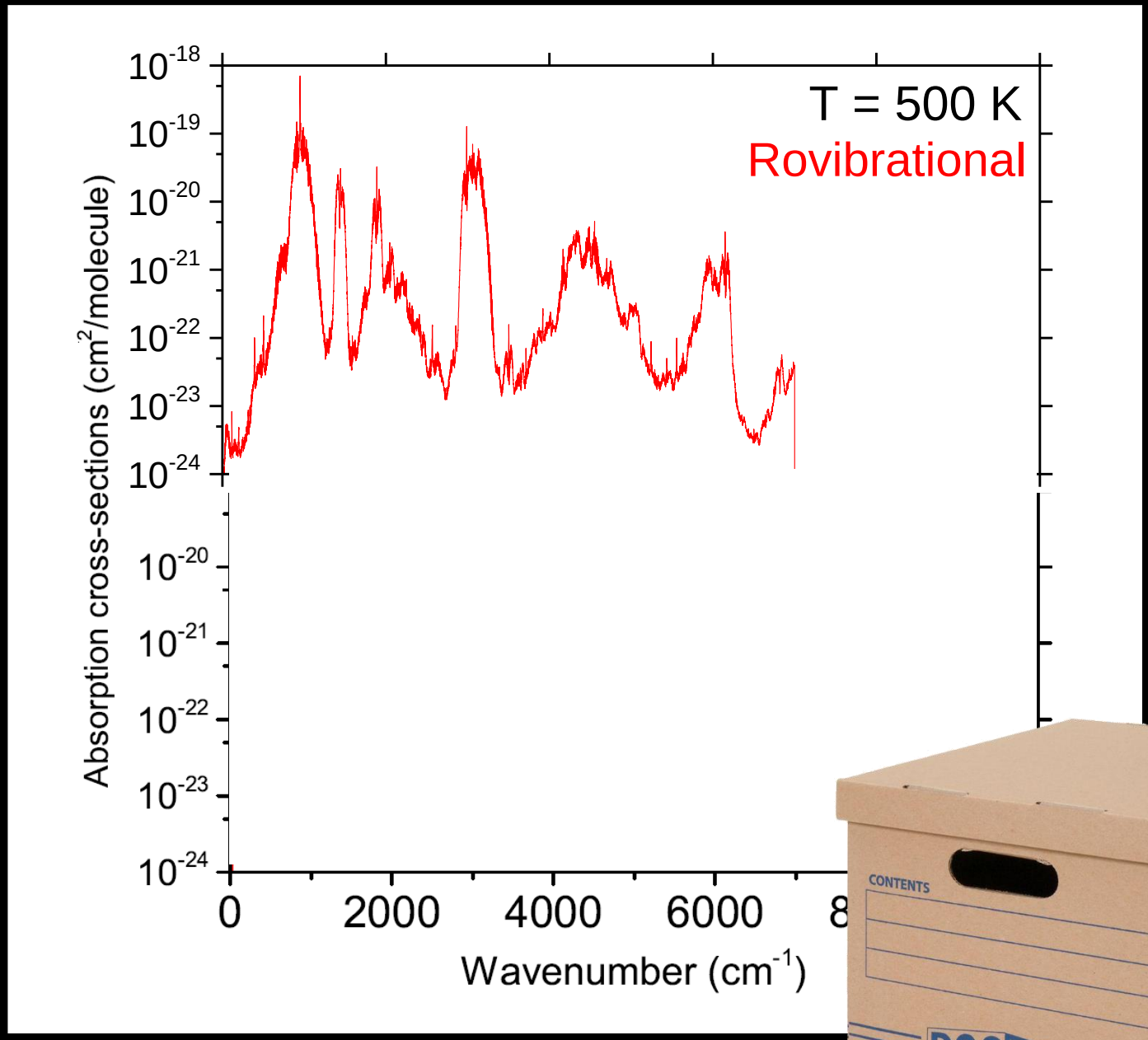
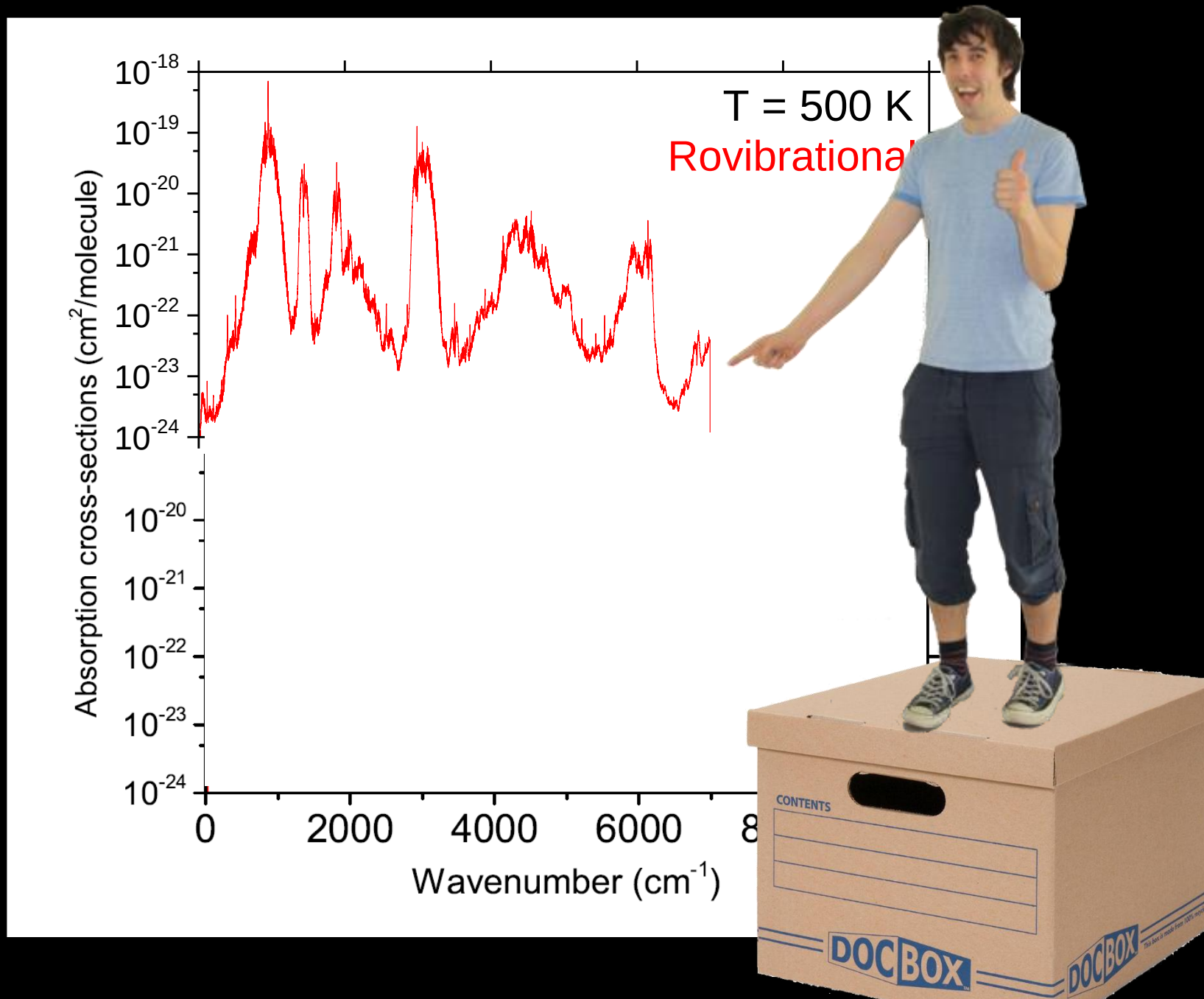
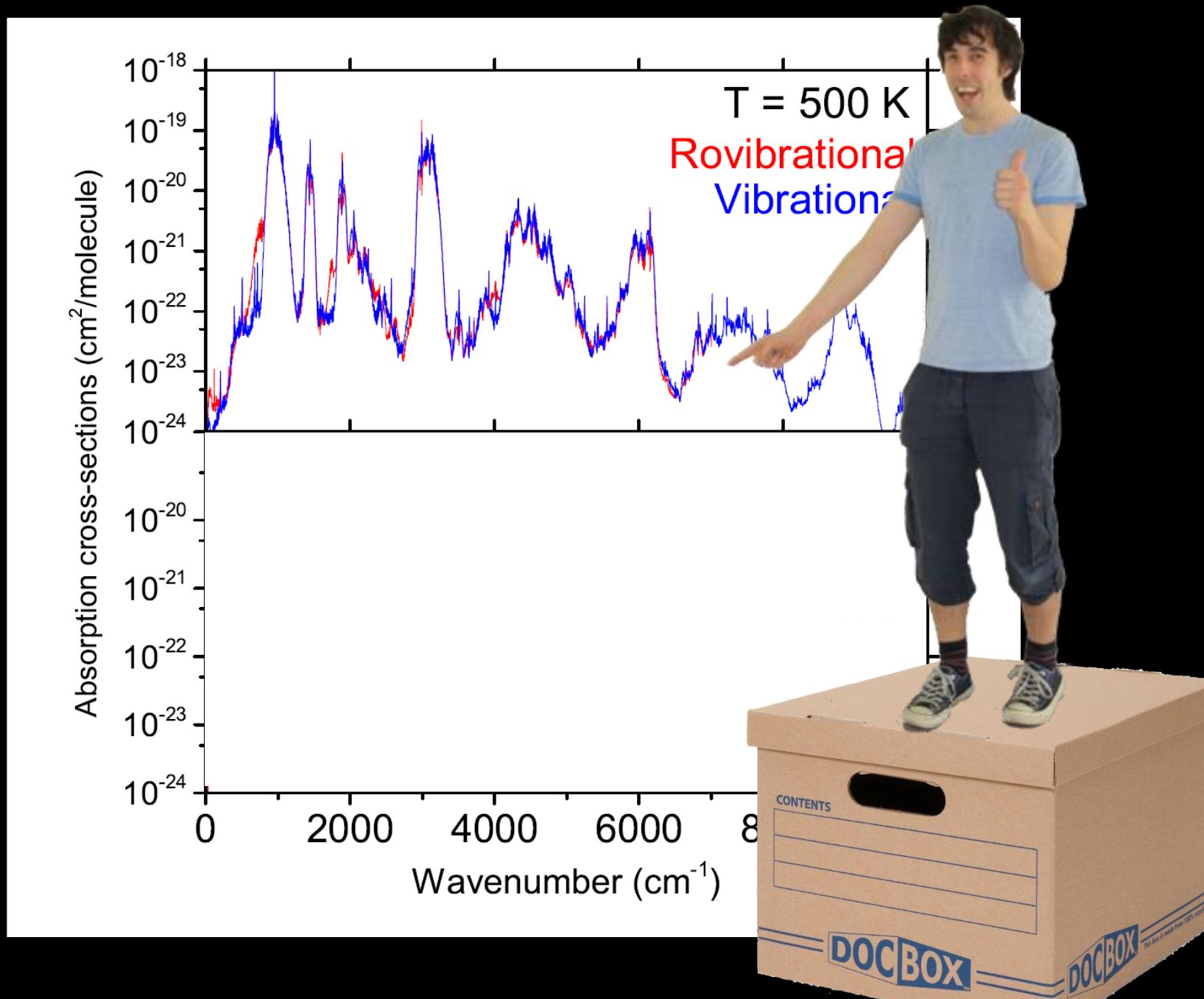
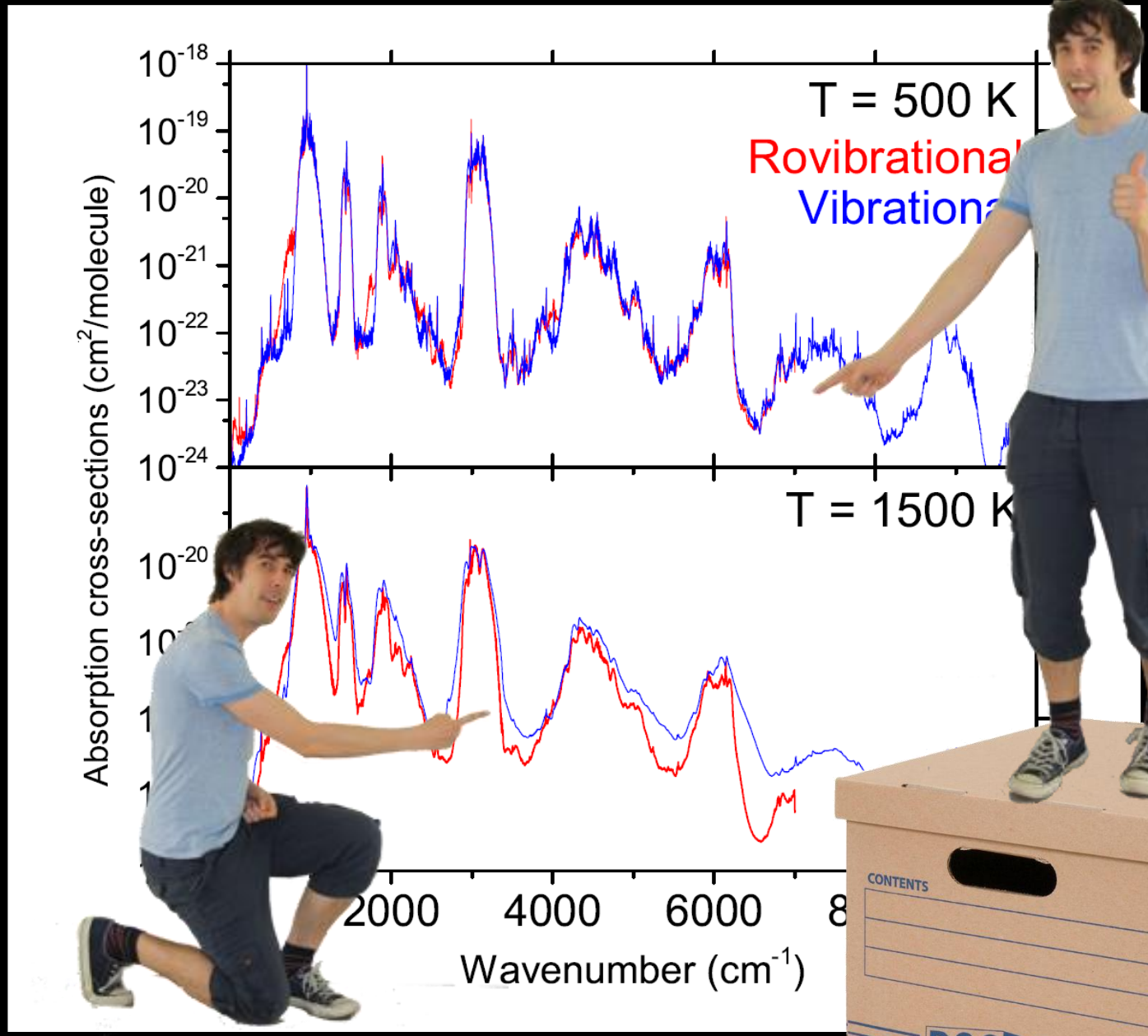
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
HITRAN
1000
1500
2500
3000
3500
(cm-1)

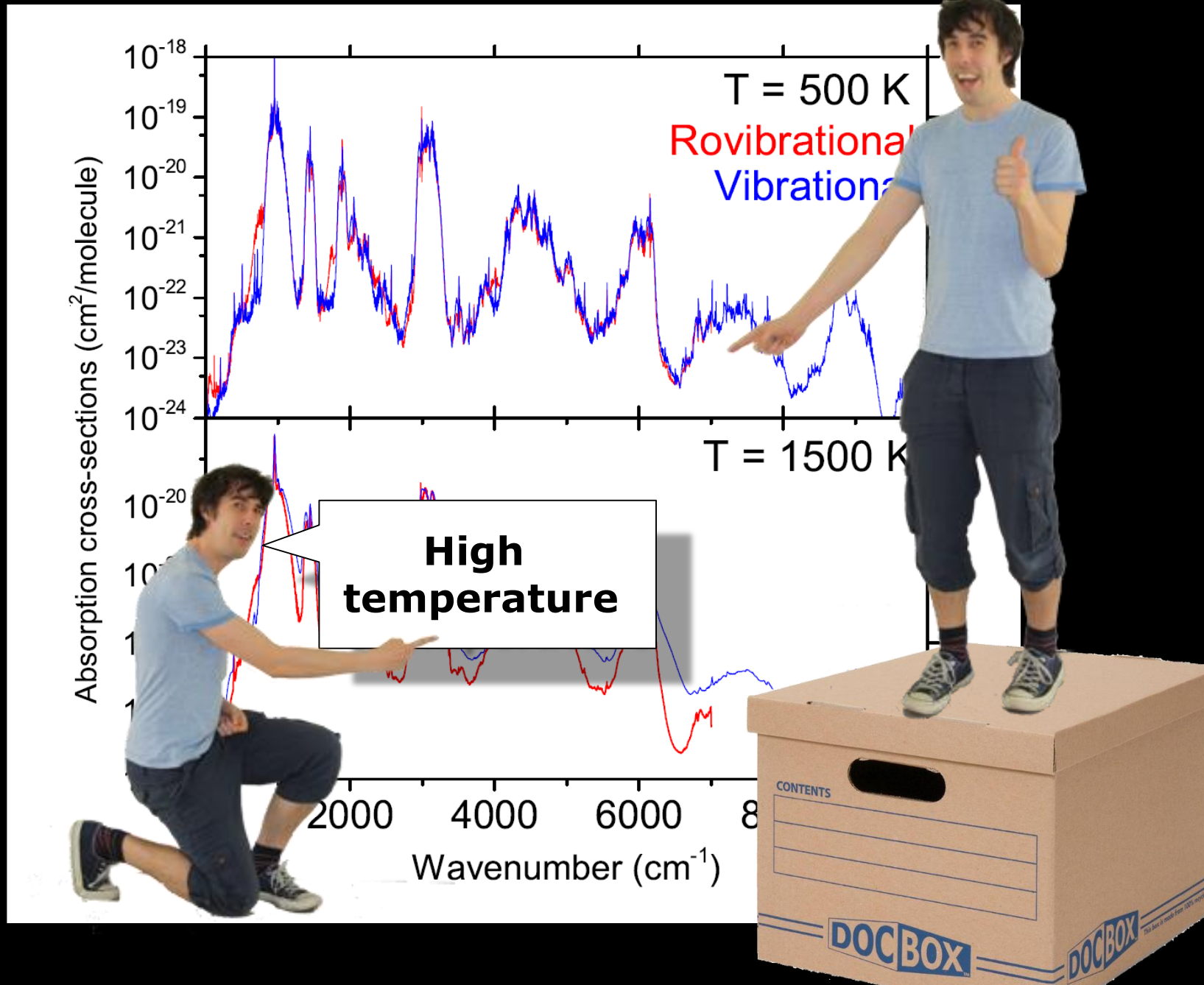

8.0x10-20
6.0x10-20
4.0x10-20
2.0x10-20
0.0
2.0x10-20
4.0x10-20
6.0x10-20
8.0x10-20
Intensity (cm / molecule)
MaYTY
1000
1500
2000
3000
3500
Wavenumber (cm-1)
Using these shapes

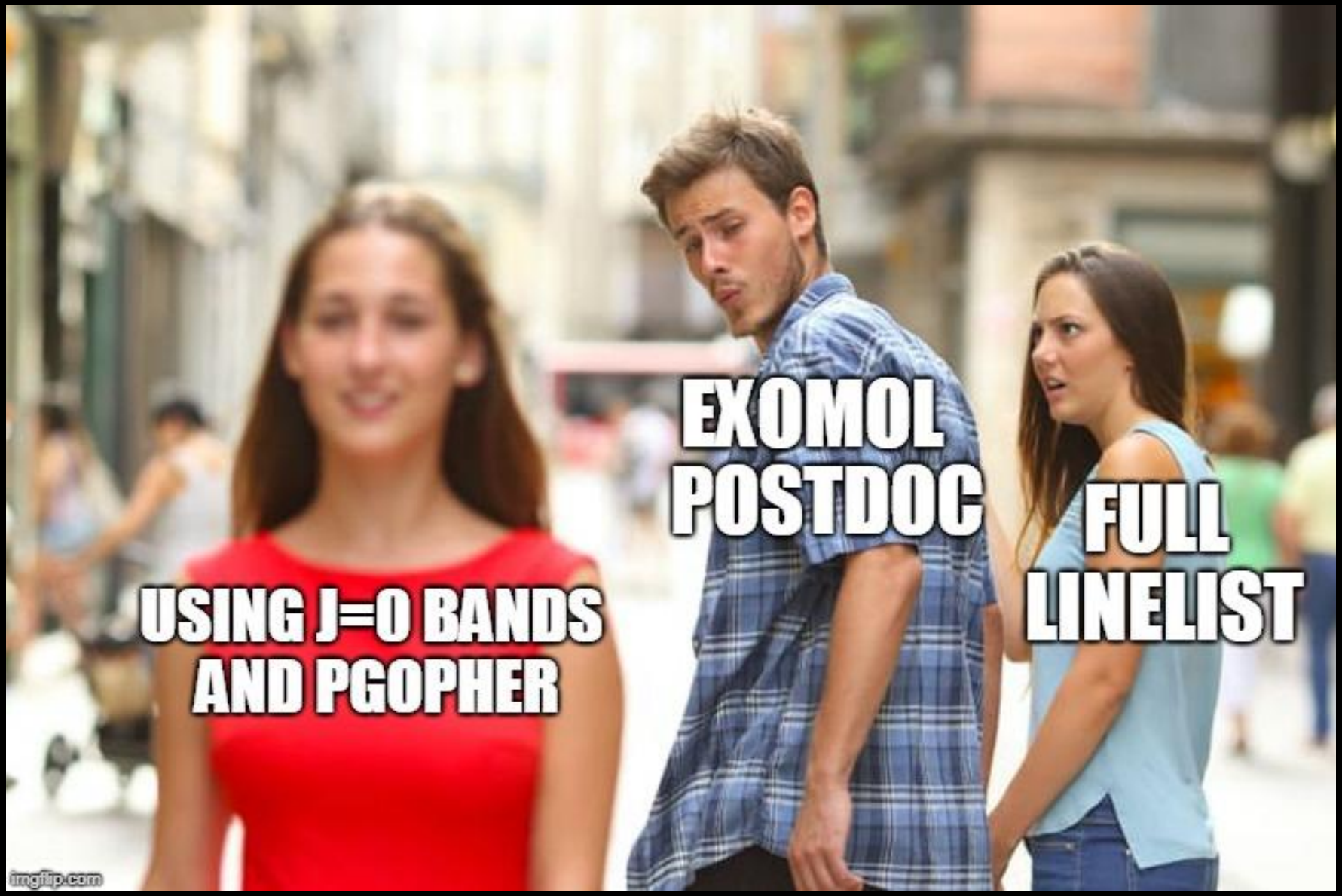

T = 500 K
Rovibrational
Absorption cross-sections (cm²/molecule)
10-18
10-19
10-20
10-21
10-22
10-23
10-24
10-20
10-21
10-22
10-23
10-24
0
2000
4000
6000
Wavenumber (cm-1)
CONTENTS
DOCBOX
DOCBOX


T = 500 K
Rovibrational
Absorption cross-sections (cm²/molecule)
10-18
10-19
10-20
10-21
10-22
10-23
10-24
10-20
10-21
10-22
10-23
10-24
0
2000
4000
6000
Wavenumber (cm-1)
CONTENTS
DOCBOX
DOCBOX


T = 500 K
Rovibrational
Vibrationa
Absorption cross-sections (cm²/molecule)
10^-18
10^-19
10^-20
10^-21
10^-22
10^-23
10^-24
10^-20
10^-21
10^-22
10^-23
10^-24
0
2000
4000
6000
Wavenumber (cm^-1)
CONTENTS
DOCBOX
DOCBOX


T = 500 K
Rovibrational
Vibrational
T = 1500 K
Absorption cross-sections (cm²/molecule)
10^-18
10^-19
10^-20
10^-21
10^-22
10^-23
10^-24
10^-20
2000
4000
6000
Wavenumber (cm^-1)
CONTENTS
DOCBOX
DOCBOX


T = 500 K
Rovibrational
Vibrational
T = 1500 K
High temperature
Absorption cross-sections (cm²/molecule)
Wavenumber (cm⁻¹)
CONTENTS
DOCBOX


EXOMOL
POSTDOC
USING J=0 BANDS
AND PGOPHER
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LINELIST
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Conclusions and take-home messages

Huge thank you for coming