The Status of Spectroscopic Data for the ARIEL Mission

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Working group on Molecular opacity: status report

The goal of this presentation is to review the current status of the molecular data and their “TRLs” or importance for ARIEL

Acknowledgment

Science & Technology
Facilities Council

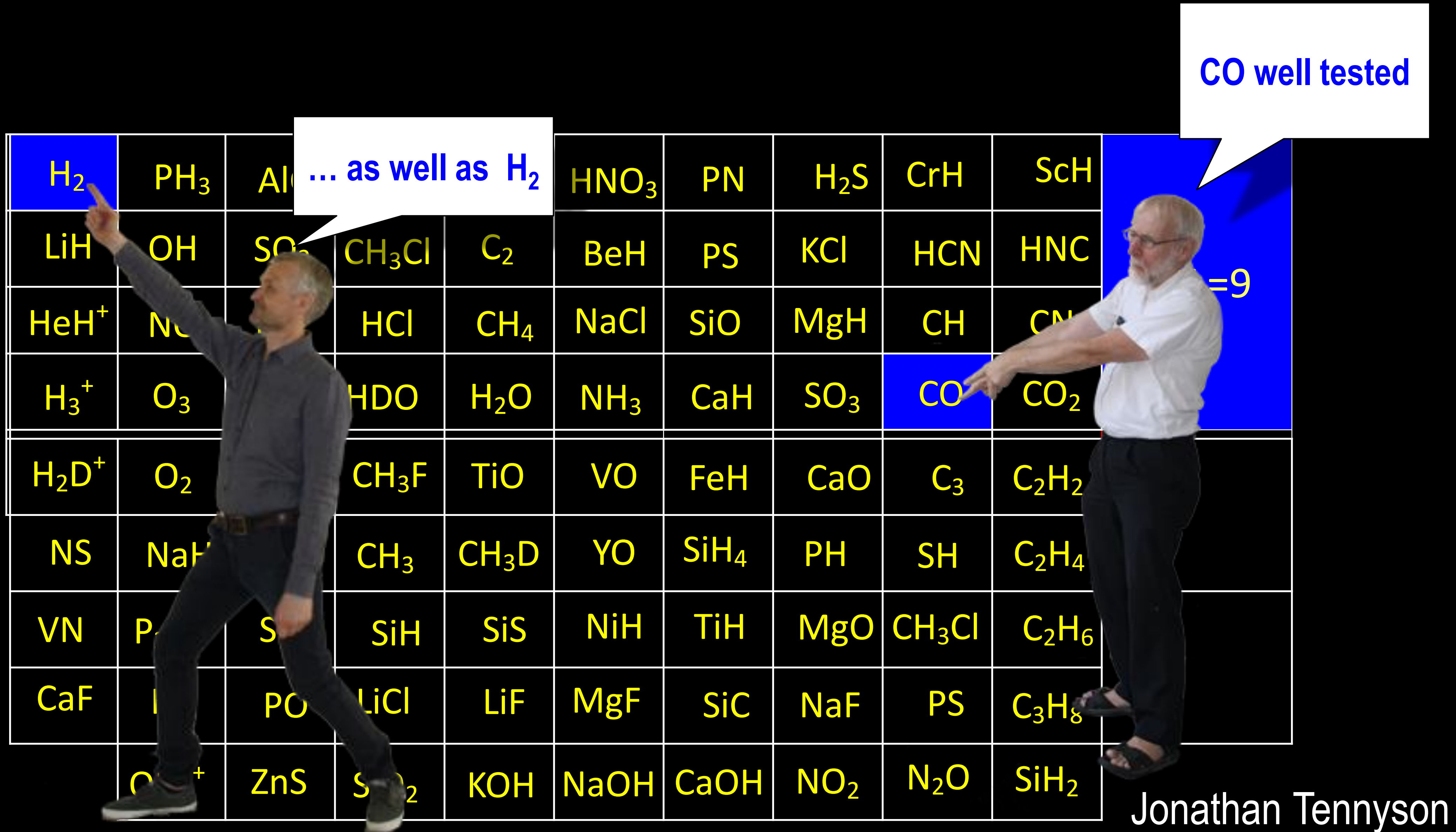
ARIEL molecules

H_2O	CO	H_3^+	NO_2	TiO
C_2H_2	CO_2	HCN	O_2	VO
C_2H_4	CrH	HDO	O_3	H_2S
C_2H_6	FeH	N_2O	PH_3	NO_2
CH_3D	H_2	NH_3	SO_2	PH_3
CH_4	H_2S	NO	TiH	

… which I am going to review

Using “TRL” as a indicator of quality and importance for ARIEL

Two species of highest rediness level
(TRL=9)

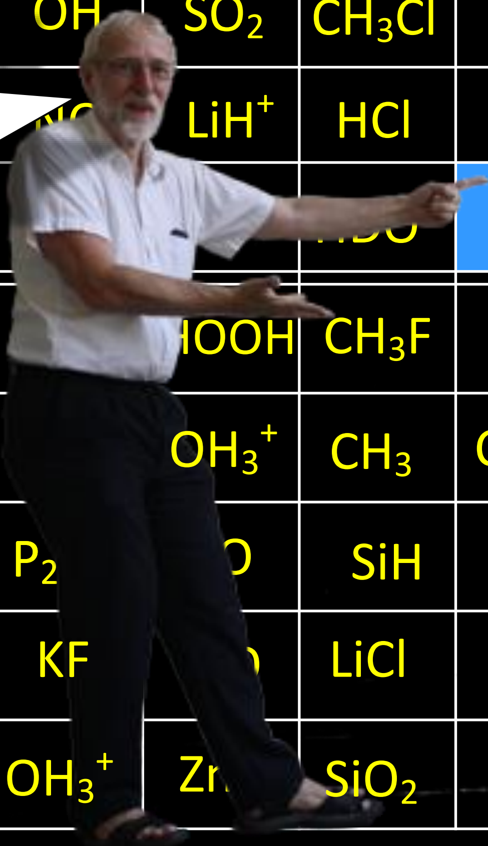


CO well tested
… as well as H2
H2 PH3 HNO3 PN H2S CrH ScH
LiH OH CH3Cl C2 BeH PS KCl HCN HNC
HeH+ HCl CH4 NaCl SiO MgH CH
H3+ O3 HDO H2O NH3 CaH SO3 CO CO2
=9
H2D+ O2 CH3F TiO VO FeH CaO C3 C2H2
NS CH3 CH3D YO SiH4 PH SH C2H4
VN SiH SiS NiH TiH MgO CH3Cl C2H6
CaF LiCl LiF MgF SiC NaF PS
ZnS KOH NaOH CaOH NO2 N2O SiH2
Jonathan Tennyson

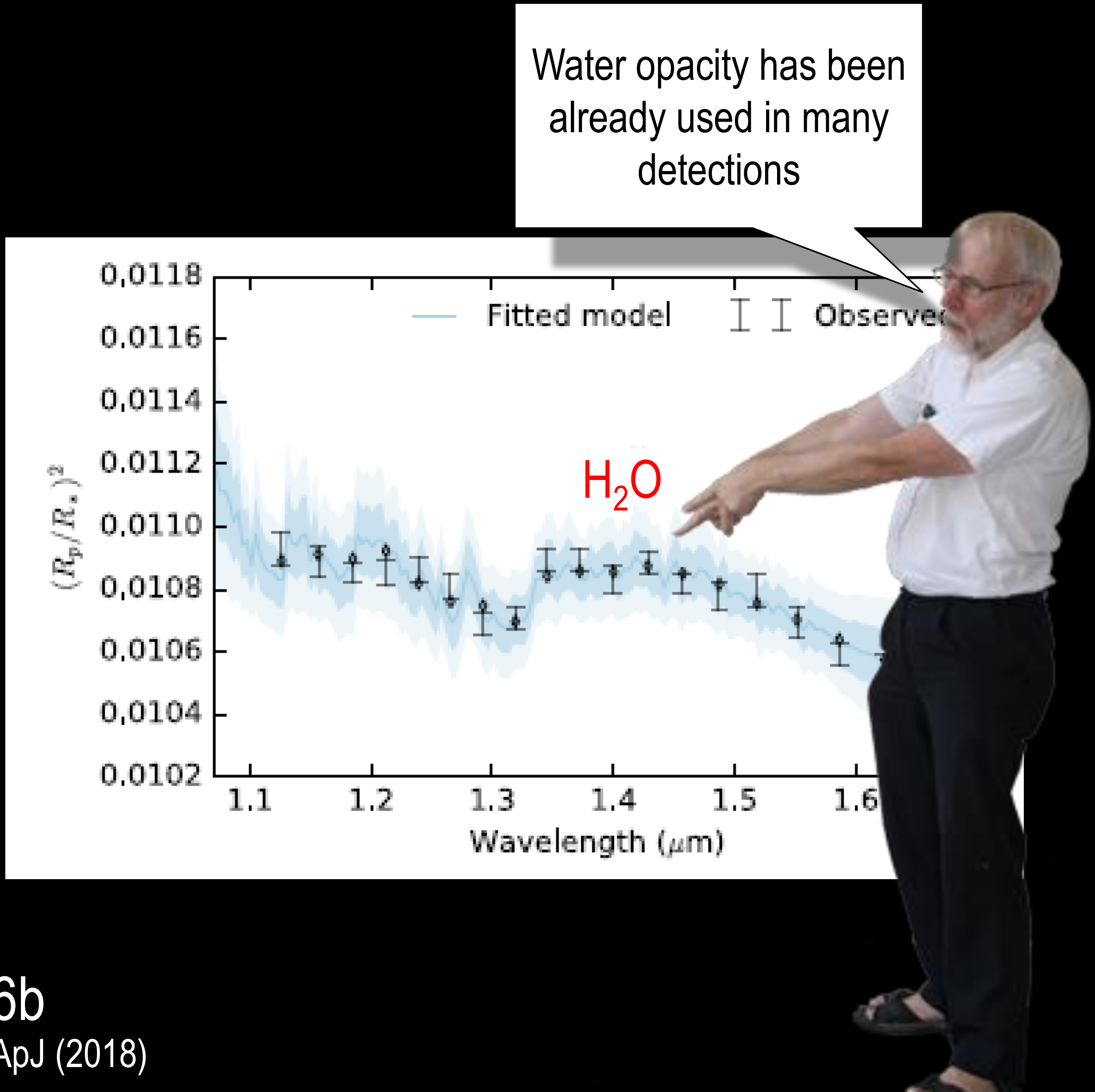
Water is an important part of the ARIEL science case with a high rediness level

ExoMol

Water is almost perfect
TRL= 8



H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	TRL=8
[illegible]	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	
[illegible]	[illegible]	LiH^+	HCl	CH_4	NaCl	SiO	MgH	CH	CN	
H_3^+	[illegible]	[illegible]	[illegible]	H_2O	NH_3	CaH	SO_3	CO	CO_2	
H_2D^+	[illegible]	[illegible]	CH_3F	TiO	VO	FeH	CaO	C_3	C_2H_2	
NS	[illegible]	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
VN	P_2	[illegible]	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6	
CaF	KF	[illegible]	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8	
	OH_3^+	[illegible]	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2	



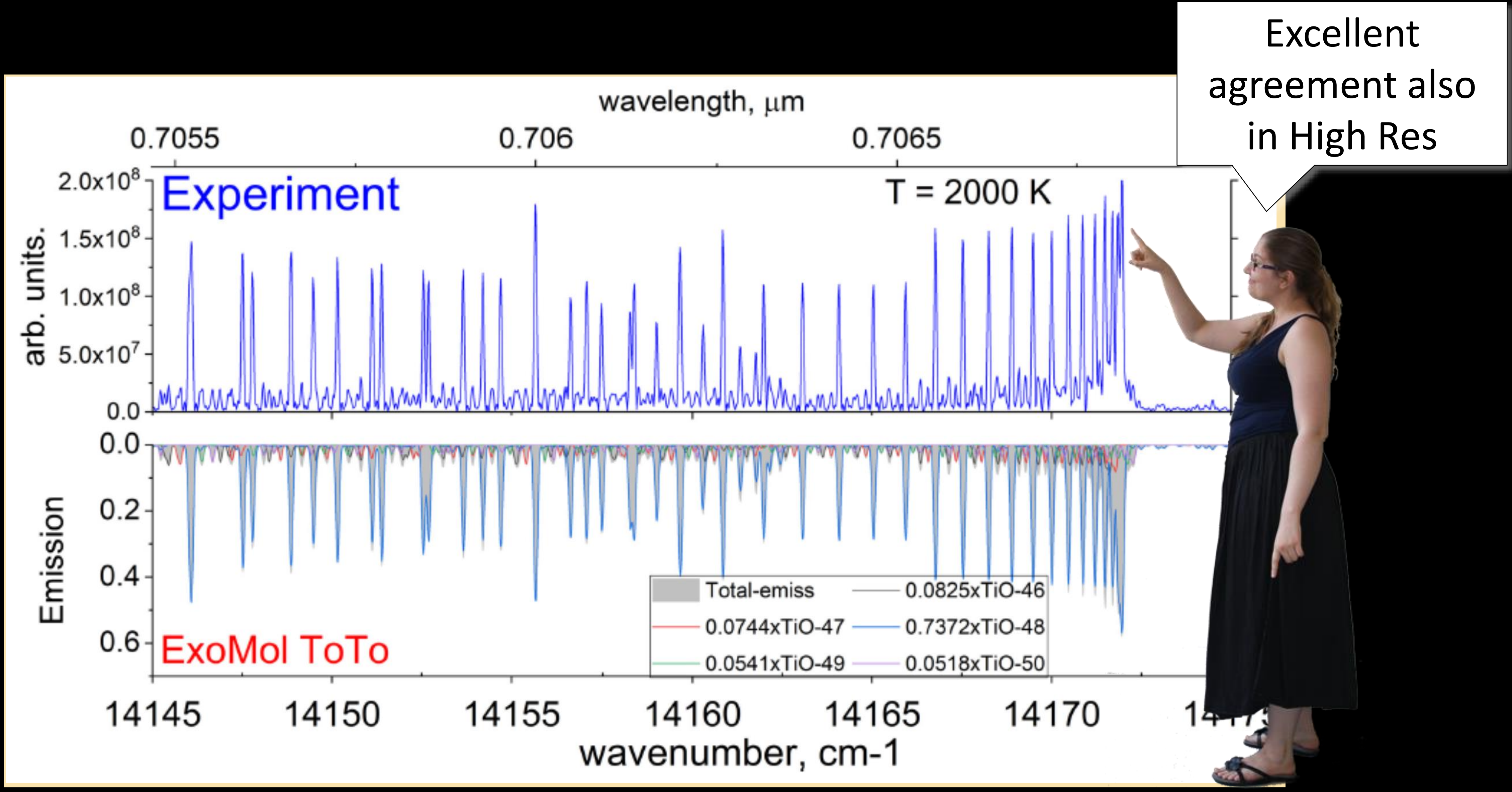
Wasp-76b

Tsiaras et al ApJ (2018)

ExoMol

H_2	PH_3	AlO	AlH	CS	HNO_3	[illegible]	H_2S	CrH	ScH	TRL=7
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	
HeH^+	NO	LiH^+	HCl	CH_4	NaCl	[illegible]	MgH	CH	CN	
H_3^+	O_3	H_2CO	HDO	H_2O	NH_3	[illegible]	SO_3	CO	CO_2	
H_2D^+	O_2	HOOH	CH_3F	TiO	VO	[illegible]	CaO	C_3	C_2H_2	
NS	NaH	OH_3^+	CH_3	CH_3D	YO	[illegible]	[illegible]	SH	C_2H_4	
VN	P_2H_2	SO	SiH	SiS	NiH	[illegible]	[illegible]	CH_3Cl	C_2H_6	
CaF	KF	PO	LiCl	LiF	MgF	[illegible]	[illegible]	PS	C_3H_8	
	OH_3^+	ZnS	SiO_2	KOH	NaOH	[illegible]	[illegible]	N_2O	SiH_2	

Laura McKemmish

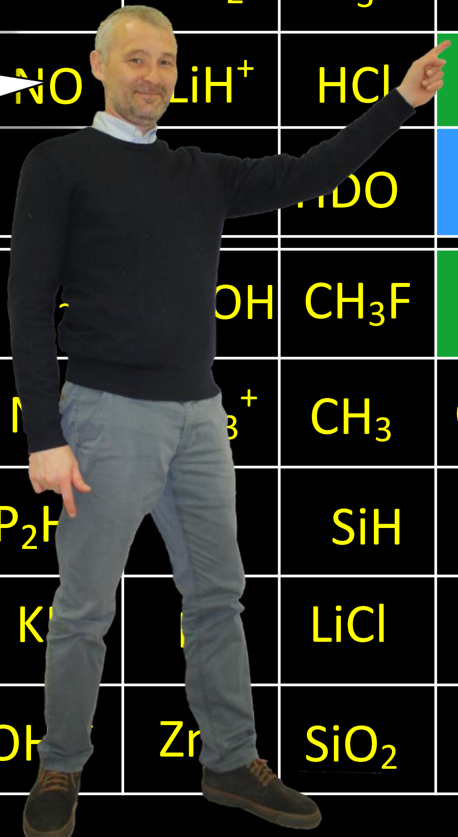


Laura McKemmish

ExoMol

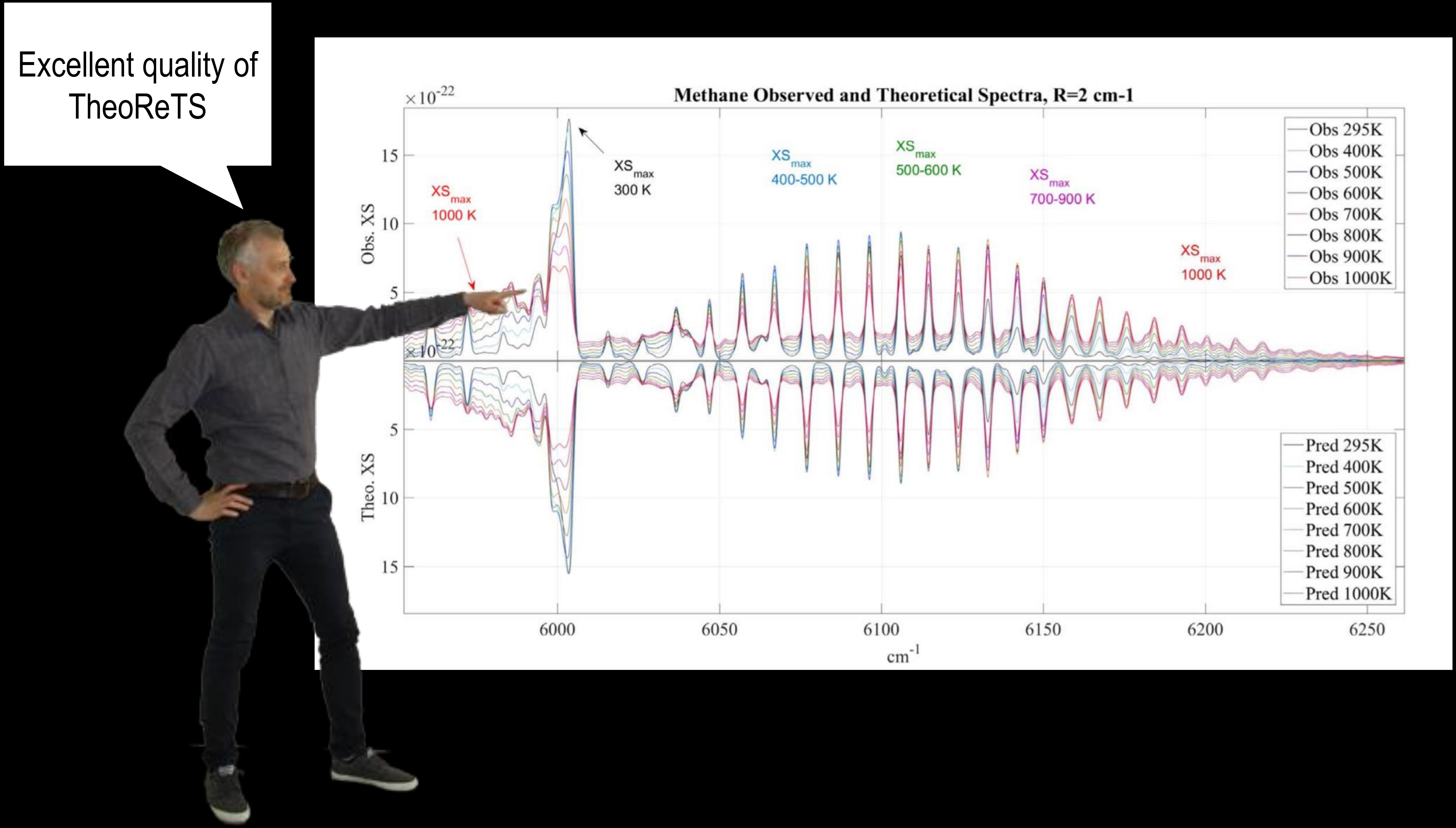
As well as CH_4

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	TRL=7
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	
[illegible]	NO	LiH^+	HCl	CH_4	NaCl	SiO	MgH	CH	CN	
H_3^+	[illegible]	[illegible]	[illegible]DO	H_2O	NH_3	CaH	SO_3	CO	CO_2	
H_2D^+	[illegible]	[illegible]OH	CH_3F	TiO	VO	FeH	CaO	C_3	C_2H_2	
NS	N[illegible]	[illegible]$_3^+$	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
VN	P_2H[illegible]	[illegible]	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6	
CaF	K[illegible]	[illegible]	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8	
	OH[illegible]	Zr[illegible]	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2	



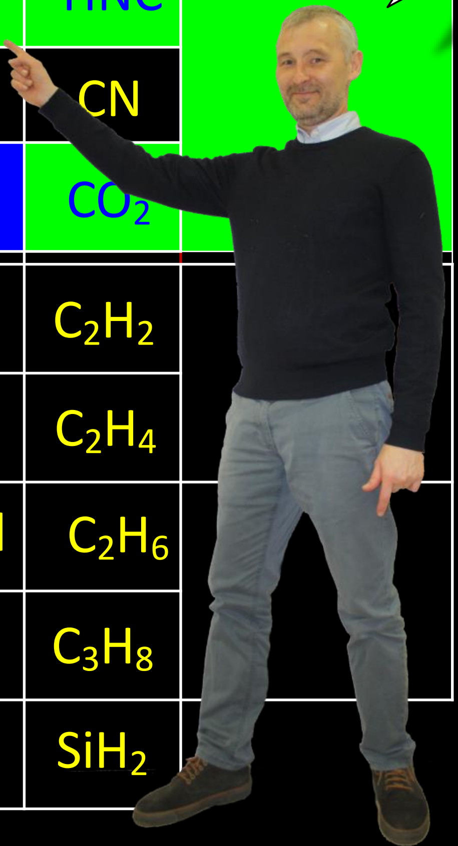
The Methane data has proved
to be of a good quality

… not only from ExoMol


Excellent quality of TheoReTS
Methane Observed and Theoretical Spectra, R=2 cm-1
×10^-22
Obs. XS
Theo. XS
XSmax 1000 K
XSmax 300 K
XSmax 400-500 K
XSmax 500-600 K
XSmax 700-900 K
XSmax 1000 K
Obs 295K
Obs 400K
Obs 500K
Obs 600K
Obs 700K
Obs 800K
Obs 900K
Obs 1000K
Pred 295K
Pred 400K
Pred 500K
Pred 600K
Pred 700K
Pred 800K
Pred 900K
Pred 1000K
6000
6050
6100
6150
6200
6250
cm-1

ExoMol

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC
HeH^+	NO	LiH^+	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
NS	NaH	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4
VN	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2

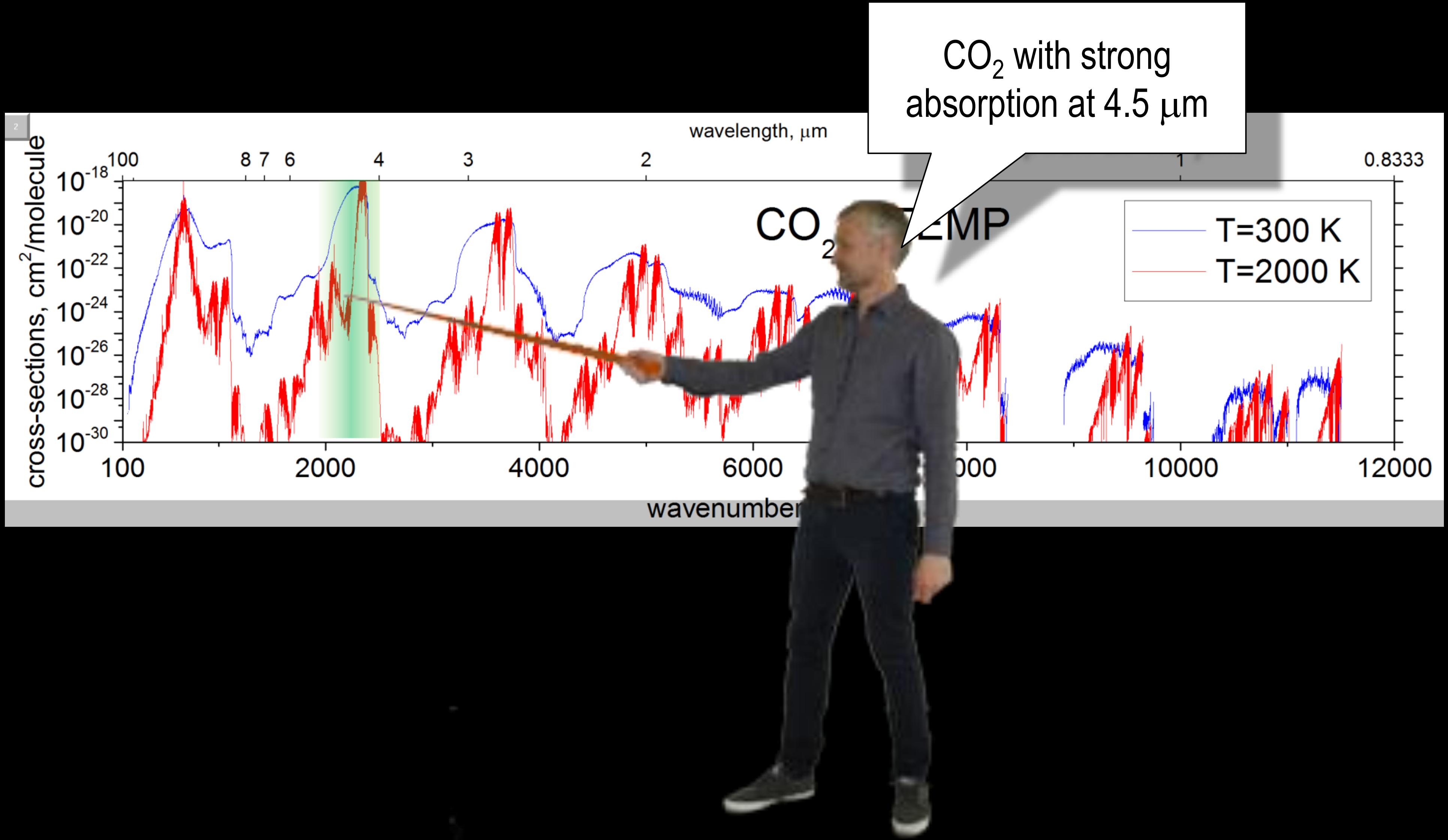


HCN, SO_2, O_2, O_3, NO, H_3^+ etc

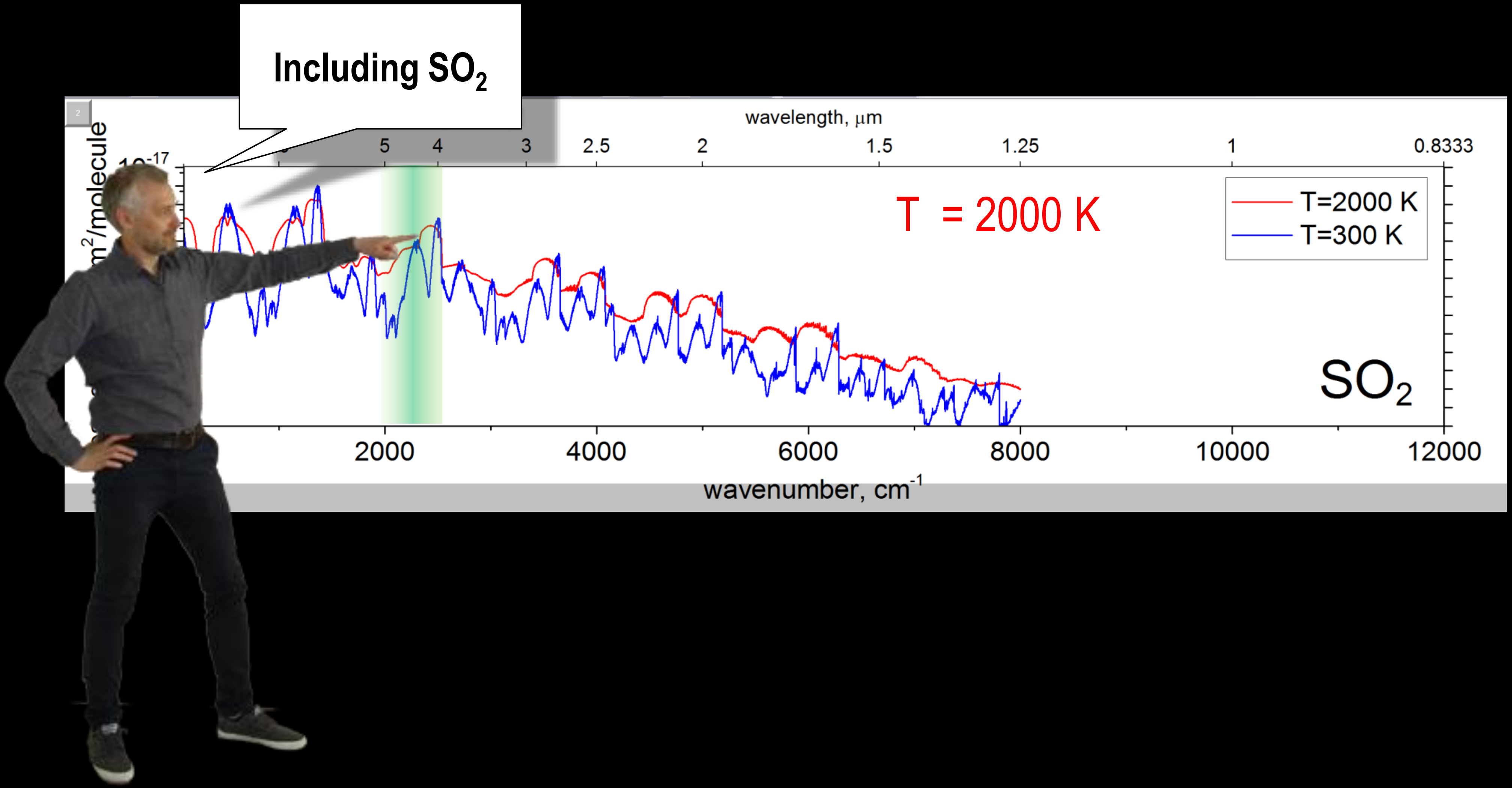
Wilf Somogyi

Including oxygen, currently taken from HITRAN

Including CO_2

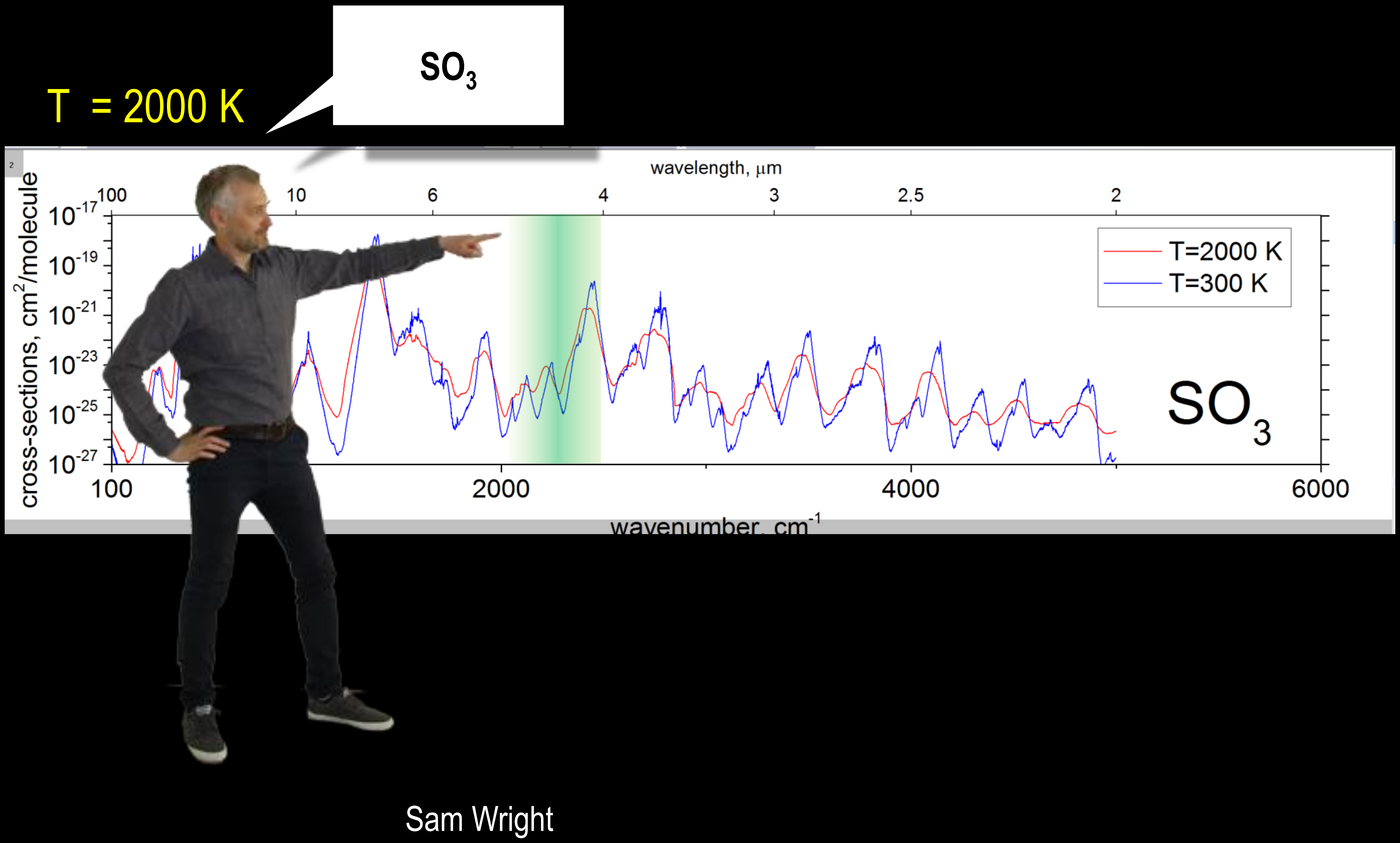


CO_2 with strong absorption at 4.5 μm
wavelength, μm
100
8 7 6
4
3
2
1
0.8333
cross-sections, cm^2/molecule
10^{-18}
10^{-20}
10^{-22}
10^{-24}
10^{-26}
10^{-28}
10^{-30}
T=300 K
T=2000 K
100
2000
4000
6000
10000
12000



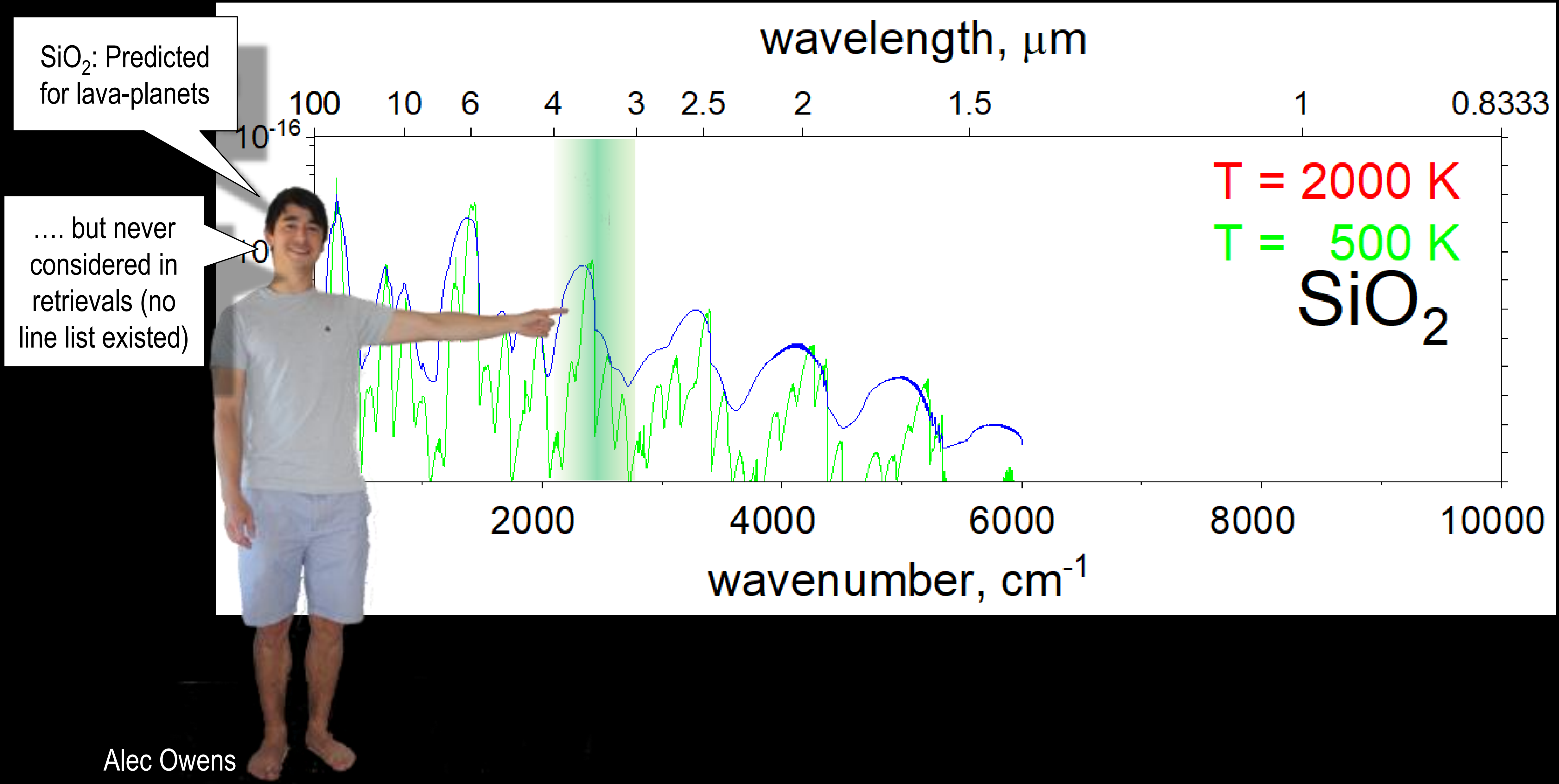
Clara Sousa Silva

… and SO_3



T = 2000 K
SO_3
wavelength, µm
100
10
6
4
3
2.5
2
10^{-17}
10^{-19}
10^{-21}
10^{-23}
10^{-25}
10^{-27}
cross-sections, cm^2/molecule
T=2000 K
T=300 K
SO_3
100
2000
4000
6000
wavenumber, cm^{-1}
Sam Wright

… and some other molecules you have not heard of before



SiO2: Predicted for lava-planets
…. but never considered in retrievals (no line list existed)
wavelength, µm
100
10
6
4
3
2.5
2
1.5
1
0.8333
10-16
T = 2000 K
T = 500 K
SiO2
2000
4000
6000
8000
10000
wavenumber, cm-1
Alec Owens

ExoMol

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC
HeH^+	NO	LiH^+	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
NS	NaH	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4
VN	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2

TRL=5

Next level of rediness

Including PH_3, CN, VO, H_2S

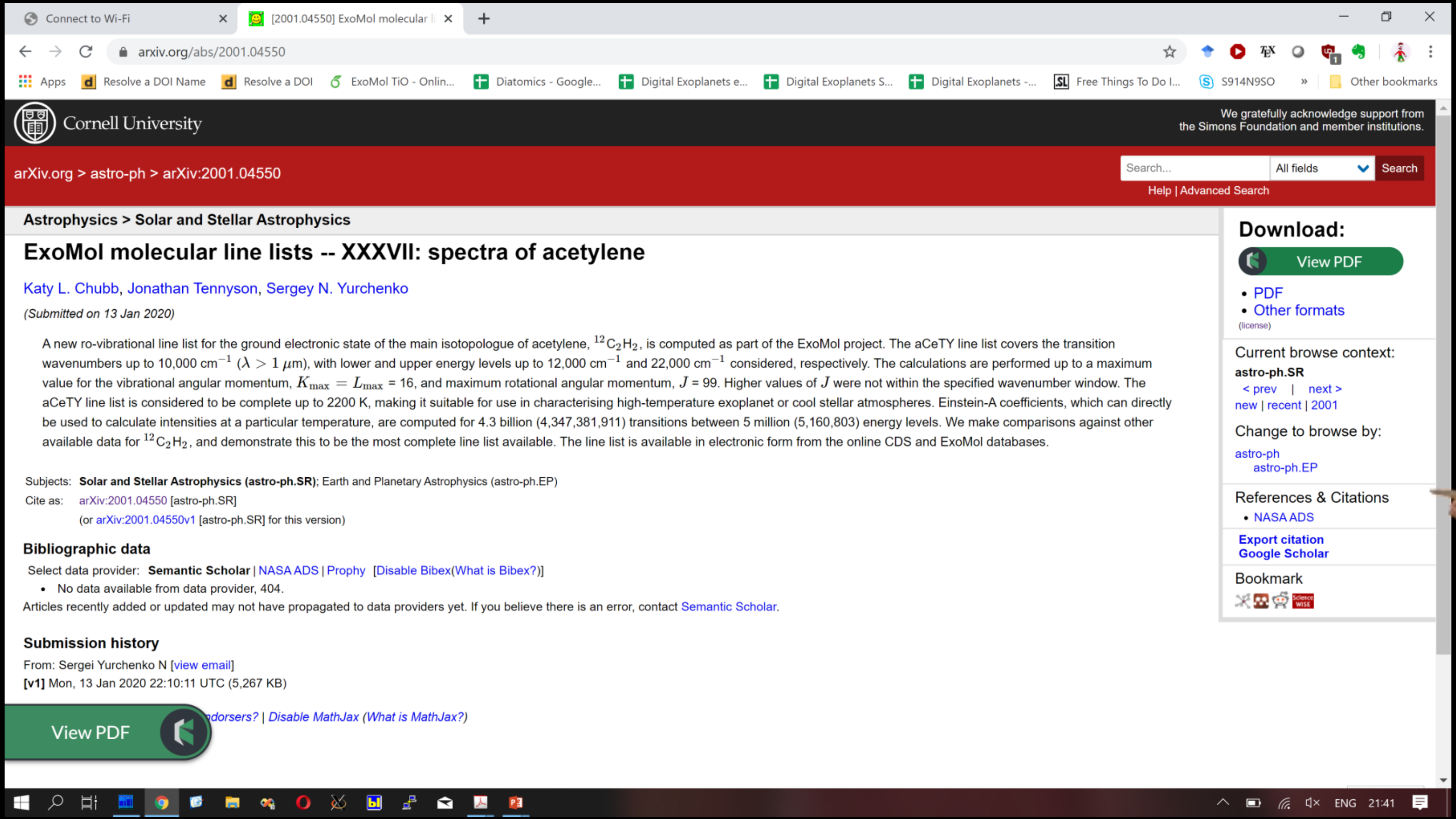
ExoMol

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC
HeH^+	NO	LiH^+	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
NS	NaH	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4
VN	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2

Next level of rediness include hydrocarbons

TRL=4

… with acetylene with a
new line list from ExoMol


[2001.04550] ExoMol molecular l

arxiv.org/abs/2001.04550

Cornell University

We gratefully acknowledge support from the Simons Foundation and member institutions.

arXiv.org > astro-ph > arXiv:2001.04550

Astrophysics > Solar and Stellar Astrophysics

ExoMol molecular line lists -- XXXVII: spectra of acetylene

Katy L. Chubb, Jonathan Tennyson, Sergey N. Yurchenko

(Submitted on 13 Jan 2020)

A new ro-vibrational line list for the ground electronic state of the main isotopologue of acetylene, $^{12}C_2H_2$, is computed as part of the ExoMol project. The aCeTY line list covers the transition wavenumbers up to 10,000 cm^{-1} ($\lambda > 1$ μm), with lower and upper energy levels up to 12,000 cm^{-1} and 22,000 cm^{-1} considered, respectively. The calculations are performed up to a maximum value for the vibrational angular momentum, $K_{max} = L_{max}$ = 16, and maximum rotational angular momentum, J = 99. Higher values of J were not within the specified wavenumber window. The aCeTY line list is considered to be complete up to 2200 K, making it suitable for use in characterising high-temperature exoplanet or cool stellar atmospheres. Einstein-A coefficients, which can directly be used to calculate intensities at a particular temperature, are computed for 4.3 billion (4,347,381,911) transitions between 5 million (5,160,803) energy levels. We make comparisons against other available data for $^{12}C_2H_2$, and demonstrate this to be the most complete line list available. The line list is available in electronic form from the online CDS and ExoMol databases.

Subjects: **Solar and Stellar Astrophysics (astro-ph.SR)**; Earth and Planetary Astrophysics (astro-ph.EP)
Cite as: arXiv:2001.04550 [astro-ph.SR]
(or arXiv:2001.04550v1 [astro-ph.SR] for this version)

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Katy Chubb

And ExoMol

exomol.com/data/molecules/C2H2/12C2-1H2/aCeTY/

- **By Molecule**
- By Data Type
- Bibliography

The aCeTY dataset for $^{12}C_2{}^1H_2$

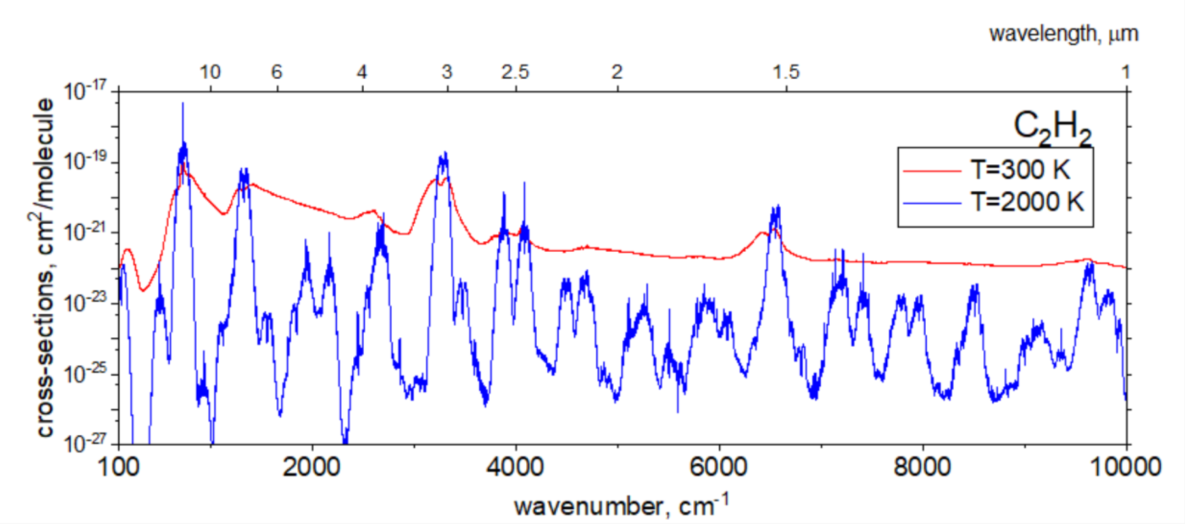
Definitions file

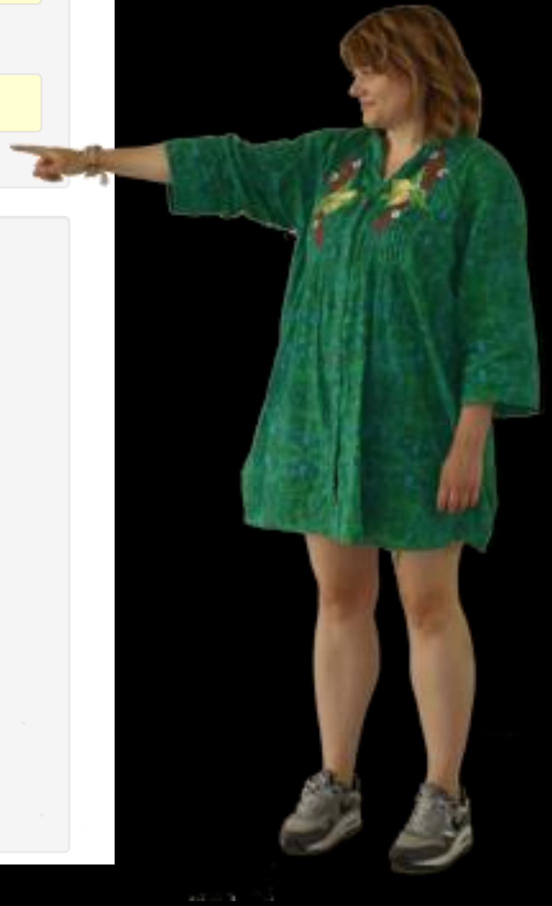
12C2-1H2__aCeTY.def

Spectroscopic Model

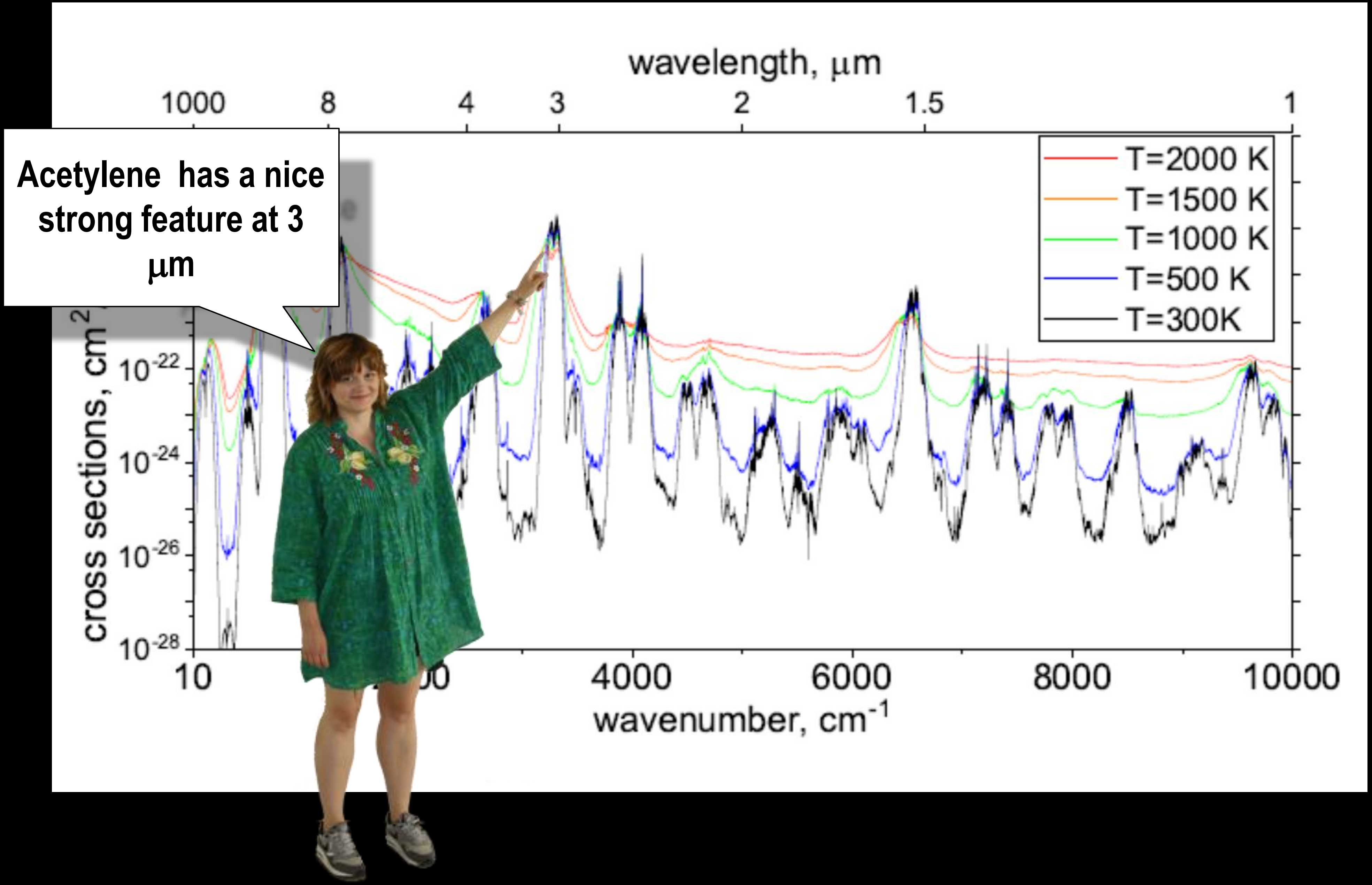
12C2-1H2__aCeTY.model

Spectrum overview

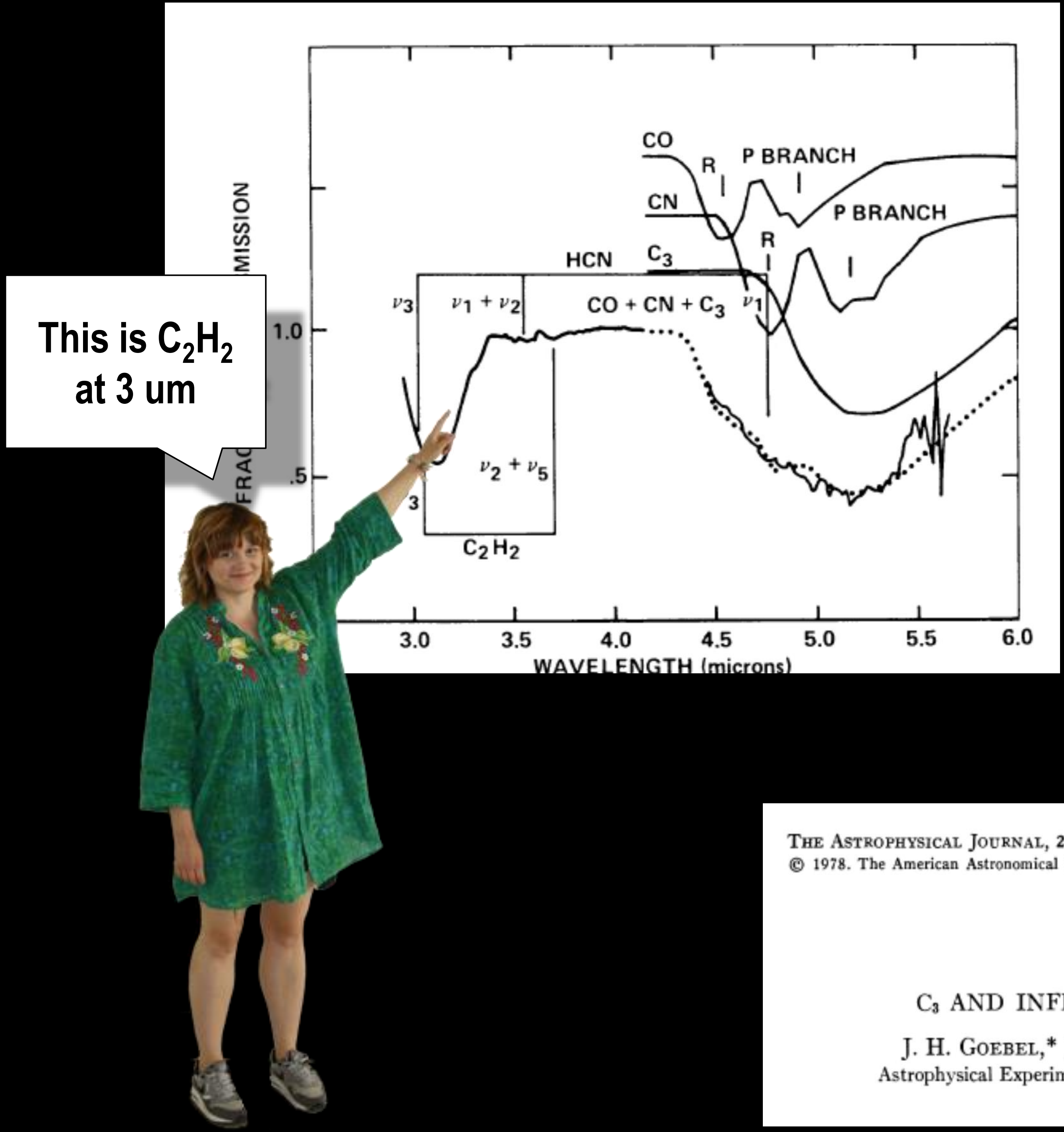




Acetylene spectrum


Acetylene has a nice strong feature at 3 μm
wavelength, μm
1000 8 4 3 2 1.5 1
T=2000 K
T=1500 K
T=1000 K
T=500 K
T=300K
cross sections, cm²
10⁻²²
10⁻²⁴
10⁻²⁶
10⁻²⁸
10 4000 6000 8000 10000
wavenumber, cm⁻¹

C_2H_2 is known to be present in carbon stars



The Astrophysical Journal, 222: L129–L132, 1978 June 15

C_3 AND INFRARED SPECTROPHOTOMETRY OF Y CANUM VENATICORUM

J. H. Goebel,* J. D. Bregman,* D. W. Strecker,† F. C. Witteborn, and E. F. Erickson
Astrophysical Experiments Branch, Space Science Division, NASA Ames Research Center, Moffett Field, California
Received 1977 August 8; accepted 1978 March 14

ExoMol

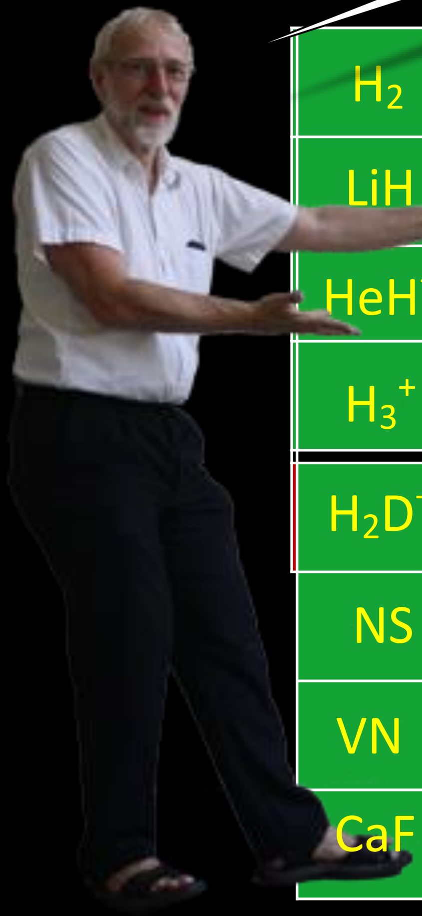
H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	ExoMol
HeH^+	NO	LiH^+	HCl	CH_4	NaCl	SiO	MgH	CH	CN	
H_3^+	O_3	H_2CO	HDO	H_2O	NH_3	CaH	SO_3	CO	CO_2	
H_2D^+	O_2	HOOH	CH_3F	TiO	VO	FeH	CaO	C_3	C_2H_2	
NS	NaH	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
VN	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6	
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8	
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	NO_2	N_2O	SiH_2	

Most of the molecular data for ARIEL is from ExoMol

More than 80 molecules and 240 isotopologues

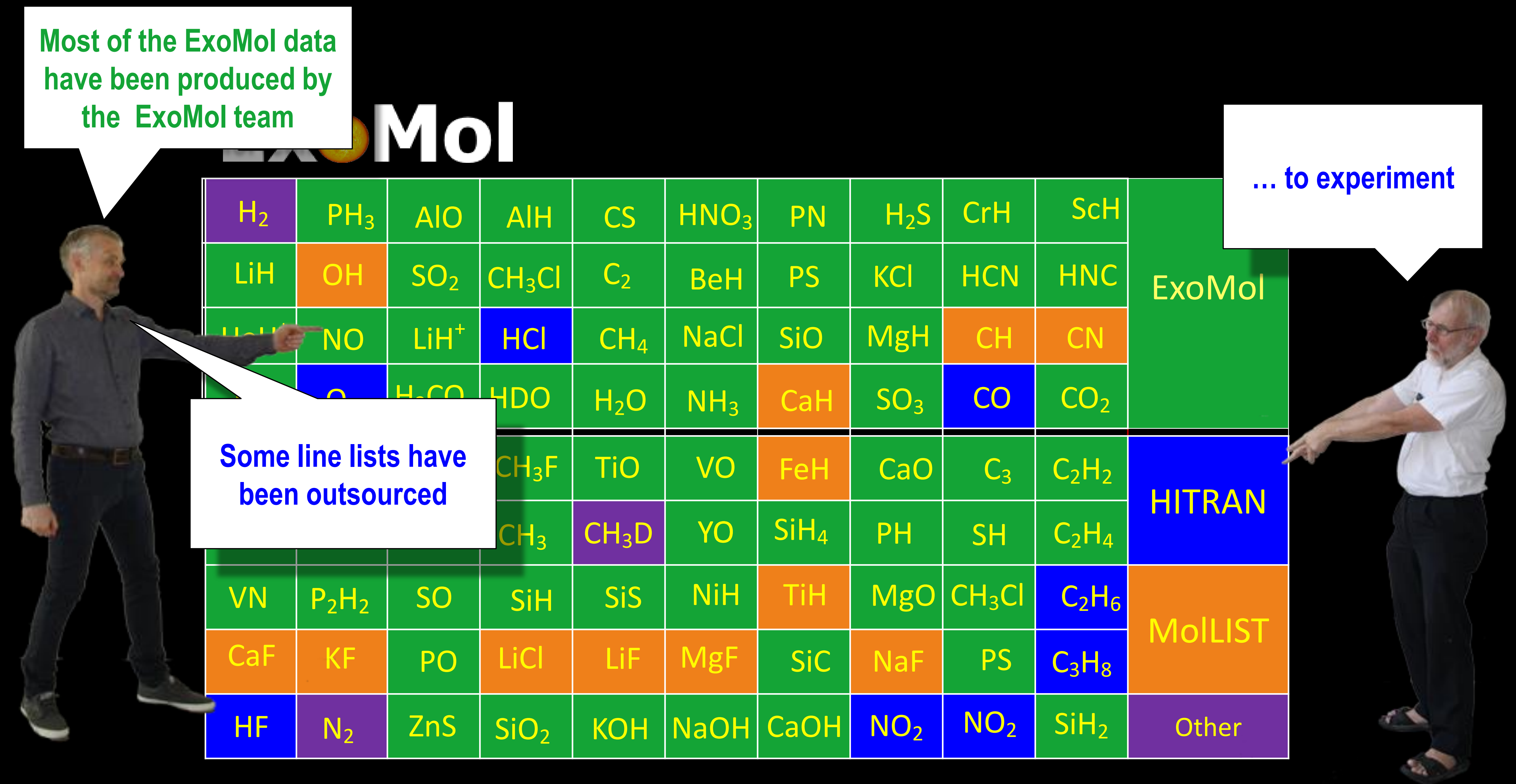
Red: difficult or in progress

ExoMol



H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	2020
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	
HeH^+	NO	LiH^+	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	
NS	NaH	OH_3^+	CH_3	CH_3D	YO	SiH_4				
VN	P_2H_2	SO	SiH	SiS	NiH	TiH			6	To-Do
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8	
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	PO_2	N_2	iH_2	

Hot Super-Earth molecules


Most of the ExoMol data have been produced by the ExoMol team
ExoMol
… to experiment
Some line lists have been outsourced
H2
PH3
AlO
AlH
CS
HNO3
PN
H2S
CrH
ScH
LiH
OH
SO2
CH3Cl
C2
BeH
PS
KCl
HCN
HNC
NO
LiH+
HCl
CH4
NaCl
SiO
MgH
CH
CN
HDO
H2O
NH3
CaH
SO3
CO
CO2
CH3F
TiO
VO
FeH
CaO
C3
C2H2
CH3
CH3D
YO
SiH4
PH
SH
C2H4
VN
P2H2
SO
SiH
SiS
NiH
TiH
MgO
CH3Cl
C2H6
CaF
KF
PO
LiCl
LiF
MgF
SiC
NaF
PS
C3H8
HF
N2
ZnS
SiO2
KOH
NaOH
CaOH
NO2
NO2
SiH2
ExoMol
HITRAN
MolLIST
Other

The line list database
contains >1 trillion lines

ARIEL opacity database

R=15,000

In form of cross-sections

and k-tables

Temperature and Pressure grids
had to be standardized

Temperatures (K)	100	200	300	400	500	600
	700	800	900	1000	1100	1200
	1300	1400	1500	1600	1700	1800
	1900	2000	2200	2400	2600	2800
	3000	3200	3400			

Pressures (bar)	1×10^{-5}	2.1544×10^{-5}	4.6416×10^{-5}
	1×10^{-4}	2.1544×10^{-4}	4.6416×10^{-4}
	1×10^{-3}	2.1544×10^{-3}	4.6416×10^{-3}
	1×10^{-2}	2.1544×10^{-2}	4.6416×10^{-2}
	1×10^{-1}	2.1544×10^{-1}	4.6416×10^{-1}
	1	2.1544	4.6416
	10	21.544	46.416
	100		

Different groups use different formats for opacities

Formats for retrieval codes were considered:

ARCiS, TauREx, NEMESIS, petitRADTRANS

TauREX3 (London) uses cross-sections in the HDF5 format

Because hdf5 is faster to load than e.g. pickle

Ahmed Al-Refaie

NEMESIS (Oxford):
K-tables (R=1000)
binary format

ARCiS (Utrecht):

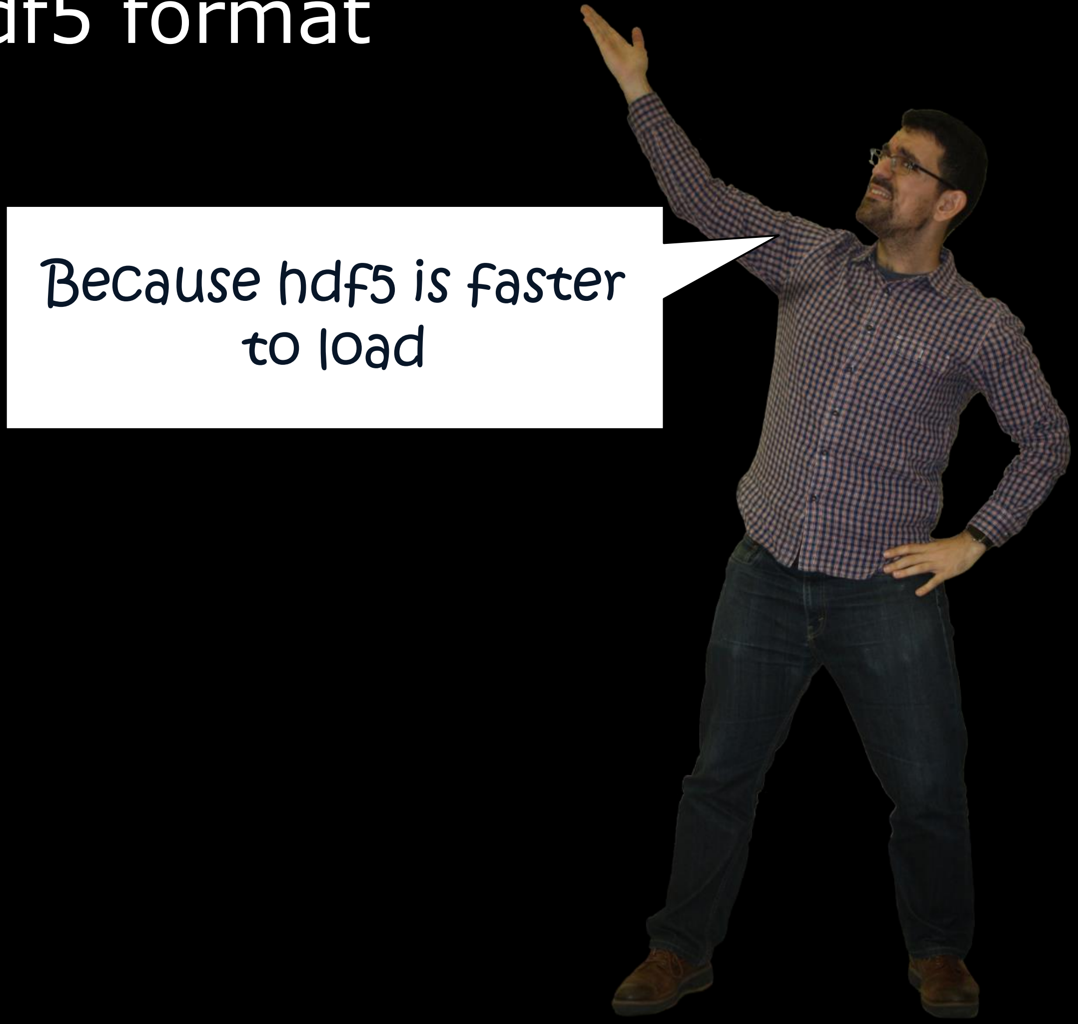
K-tables (R=1000)

.fits format

petitRADTRANS (Paul Molliere)

K-tables (R=1000)

hdf5 format



Volume of the data:

ExoMol line lists contains > trillion lines
in ~20 Tb

TauREx3
Cross-sections: 348MB

NEMESIS:
K-tables 232MB
binary

ARCiS:
K-tables 89MB
.fits

petitRADTRANS:
K-tables 371MB
hdf5

… just contact us

We are prepared to extend to other formats

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All data will be open access

ARIEL opacities

ARIEL opacities

For all 80+ species

H_2	PH_3	AlO	AlH	CS	HNO_3	PN	H_2S	CrH	ScH	ARIEL: tauREX NEMESIS ARCiS petitRADTRANS
LiH	OH	SO_2	CH_3Cl	C_2	BeH	PS	KCl	HCN	HNC	
HeH^+	NO	LiH^+	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	
[illegible]	[illegible]	HOOH	CH_3F	TiO	VO	FeH	CaO	C_3	C_2H_2	Other
[illegible]	[illegible]	OH_3^+	CH_3	CH_3D	YO	SiH_4	PH	SH	C_2H_4	
VN	P_2H_2	SO	SiH	SiS	NiH	TiH	MgO	CH_3Cl	C_2H_6	ExoMol
CaF	KF	PO	LiCl	LiF	MgF	SiC	NaF	PS	C_3H_8	
	OH_3^+	ZnS	SiO_2	KOH	NaOH	CaOH	NO_2	NO_2	SiH_2	

… let us know if something is missing

For 4 retrieval codes, contact us about your format