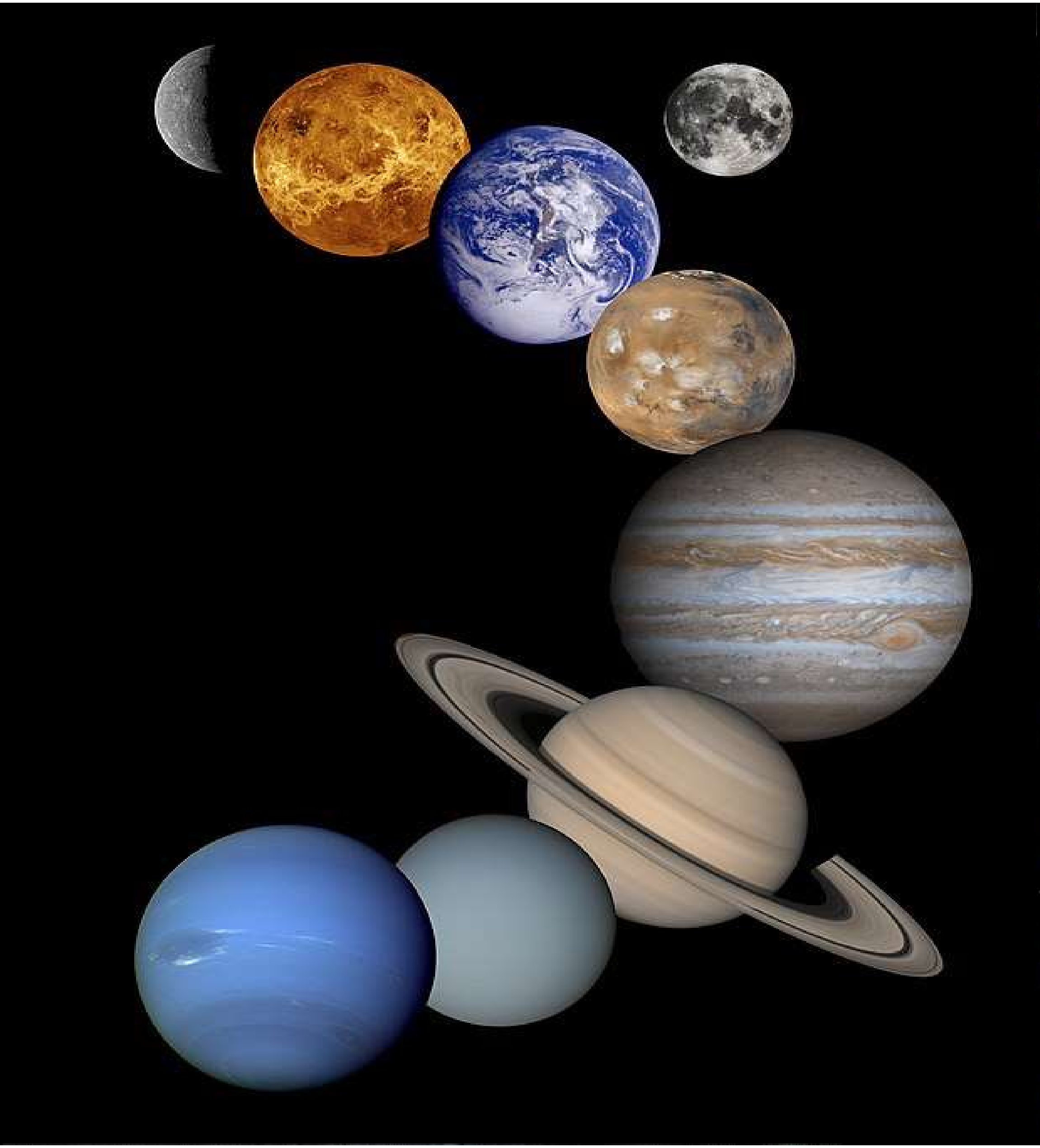
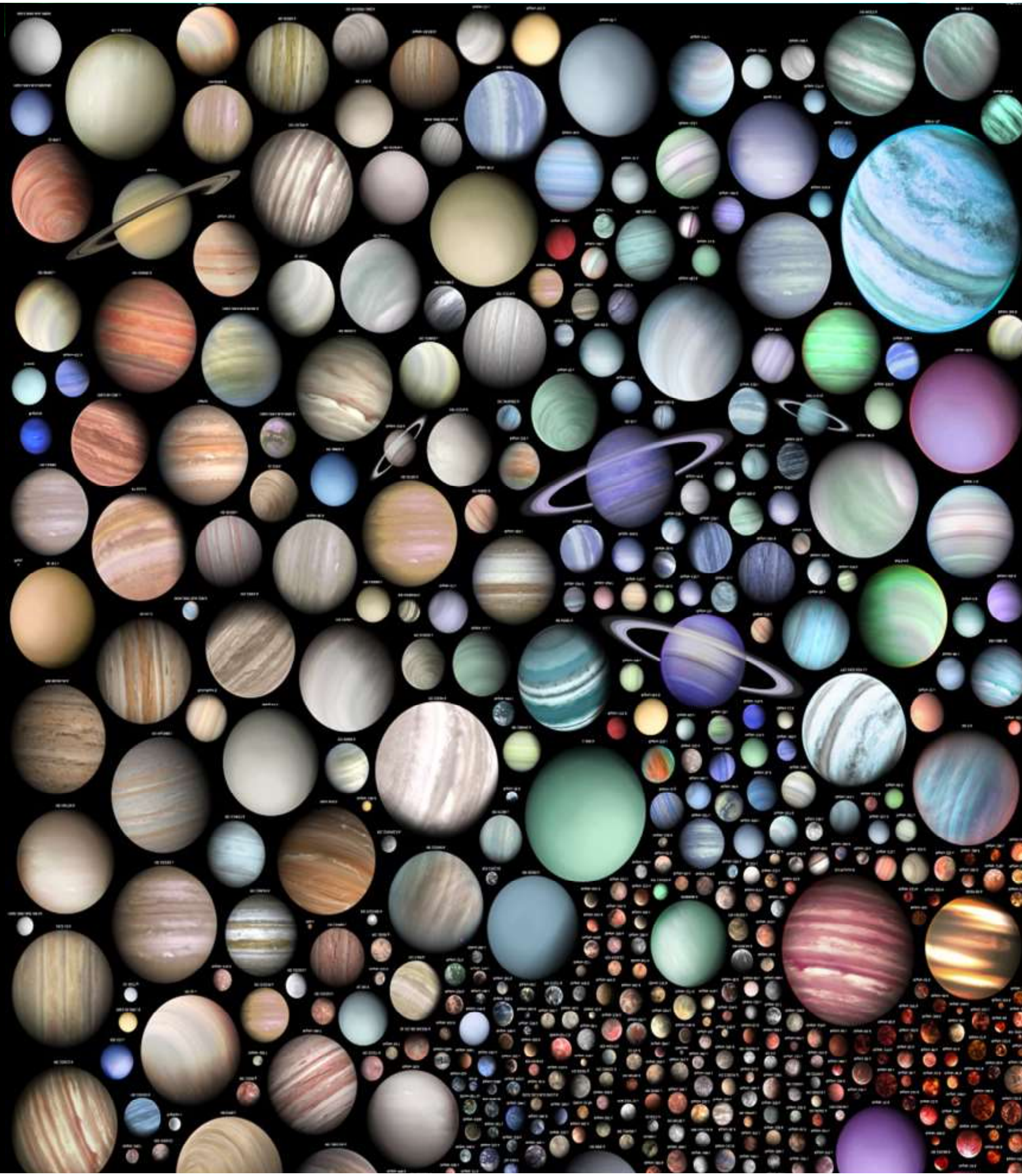
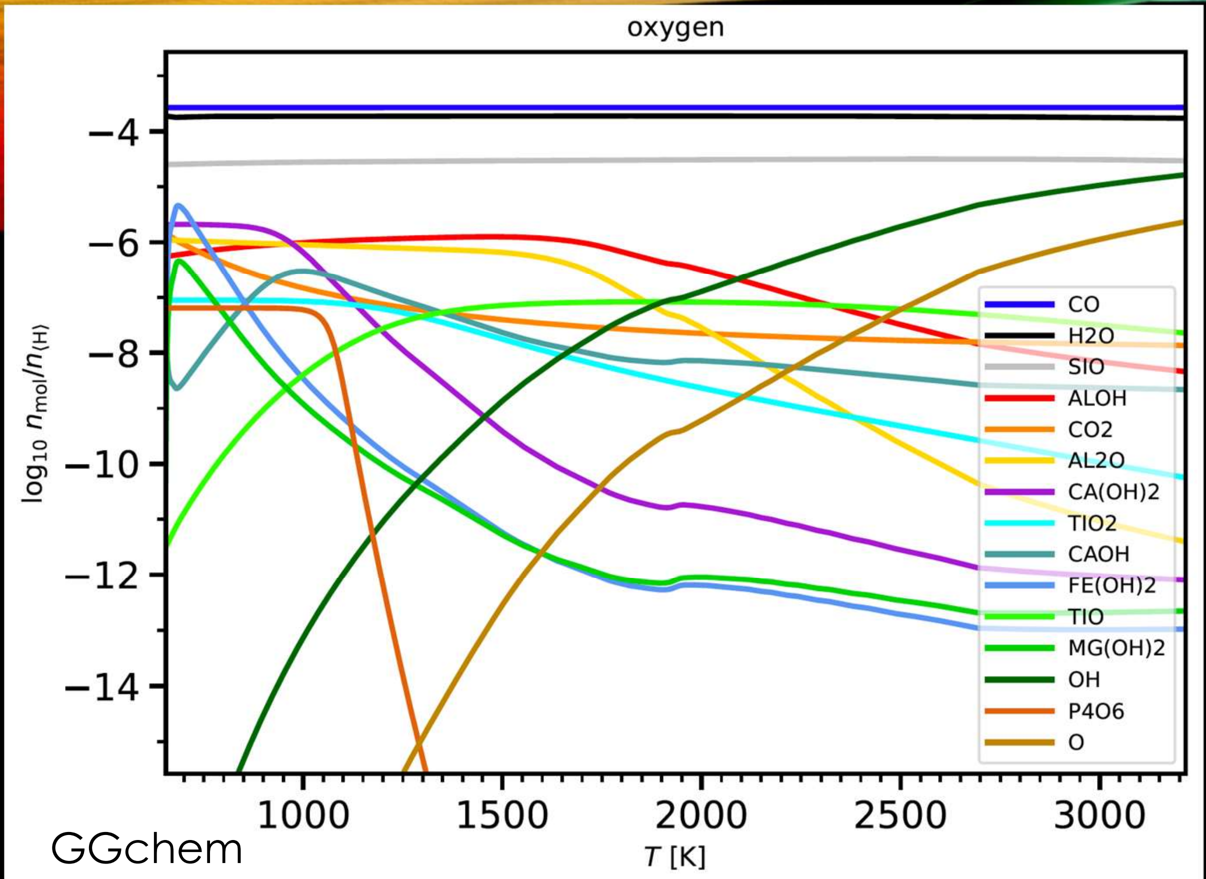
USING A VARIETY OF MOLECULES IN EXOPLANET ATMOSPHERE RETRIEVALS

Katy Chubb, SRON Netherlands Institute for Space Research / St Andrews University







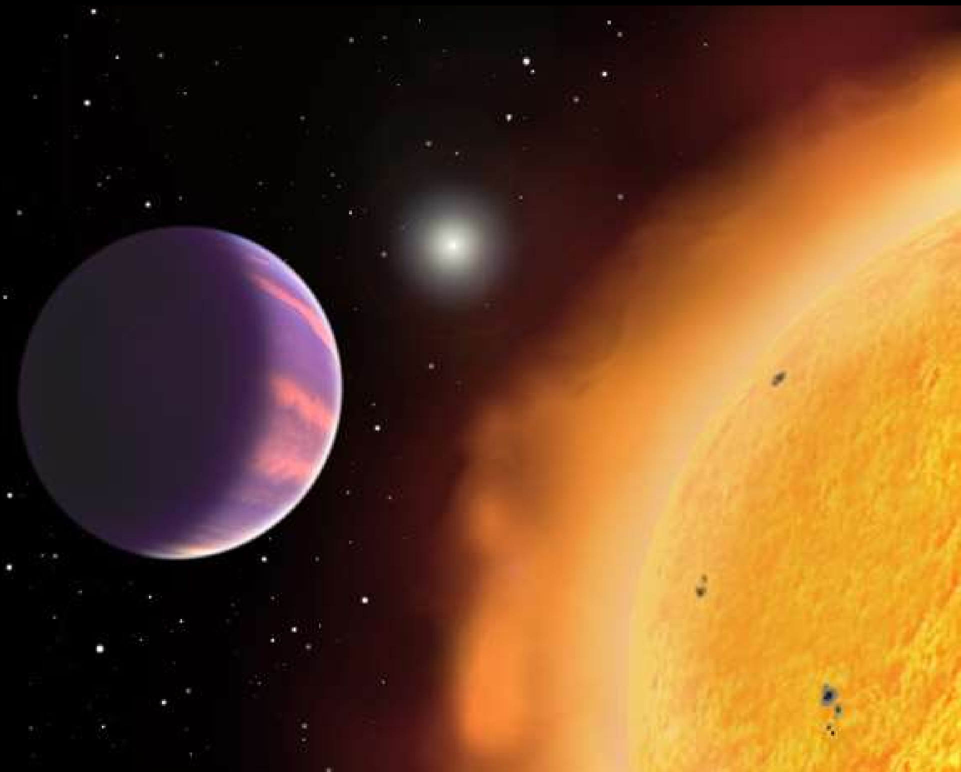
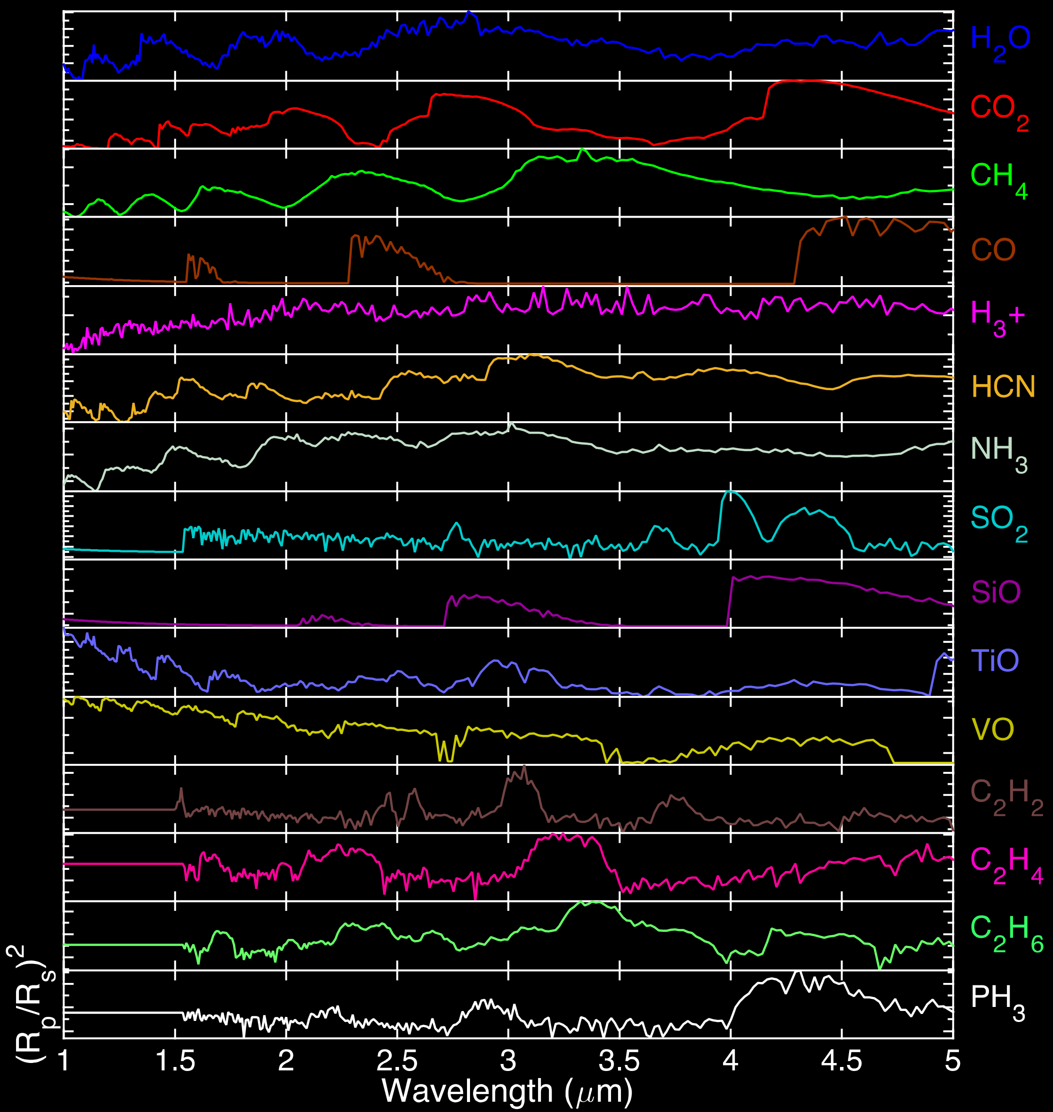


Image: David A. Aguilar, Harvard-Smithsonian Center for Astrophysics


H2O
CO2
CH4
CO
H3+
HCN
NH3
SO2
SiO
TiO
VO
C2H2
C2H4
C2H6
PH3
(Rp/Rs)2
1 1.5 2 2.5 3 3.5 4 4.5 5
Wavelength (μm)

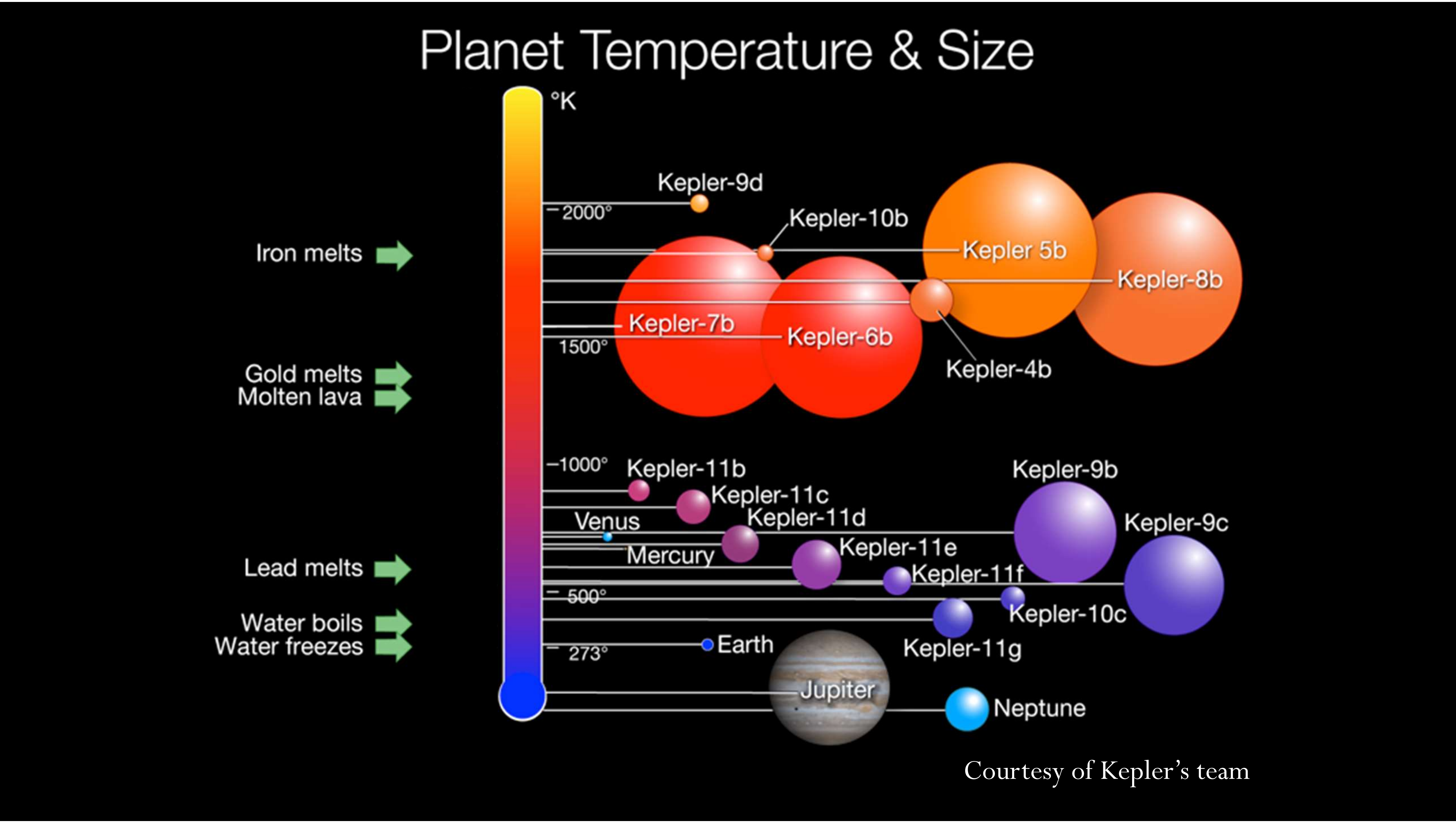
- How do we know what these molecular spectra look like?
- What are some of the challenges associated with finding out?
- How do we use these in our exoplanet retrieval models
- Differences between data for low and high resolution observations

Laboratory

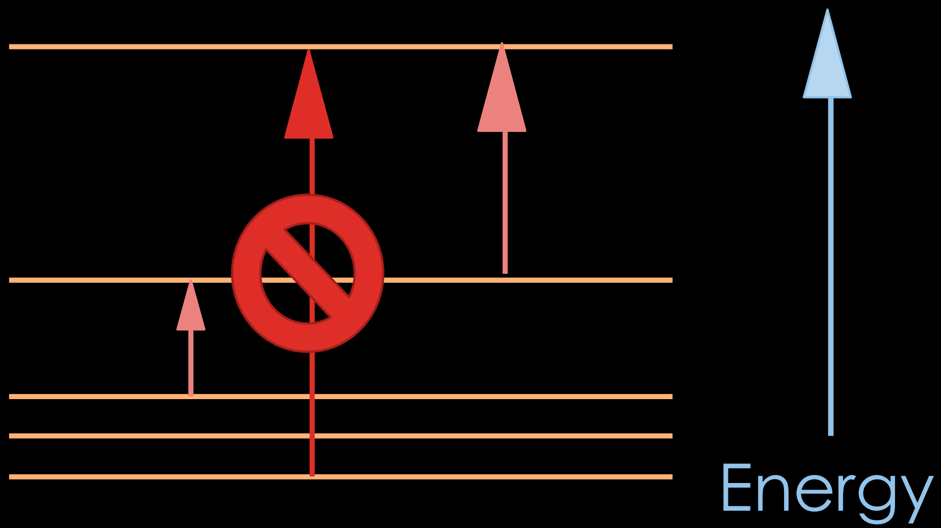
molecular spectra
observations

=

typically valid only at the temperature & pressure of measurement


Planet Temperature & Size
°K
2000°
1500°
1000°
500°
273°
Iron melts
Gold melts
Molten lava
Lead melts
Water boils
Water freezes
Kepler-9d
Kepler-10b
Kepler 5b
Kepler-8b
Kepler-7b
Kepler-6b
Kepler-4b
Kepler-11b
Kepler-11c
Kepler-11d
Kepler-11e
Kepler-11f
Kepler-11g
Kepler-9b
Kepler-9c
Kepler-10c
Venus
Mercury
Earth
Jupiter
Neptune
Courtesy of Kepler's team

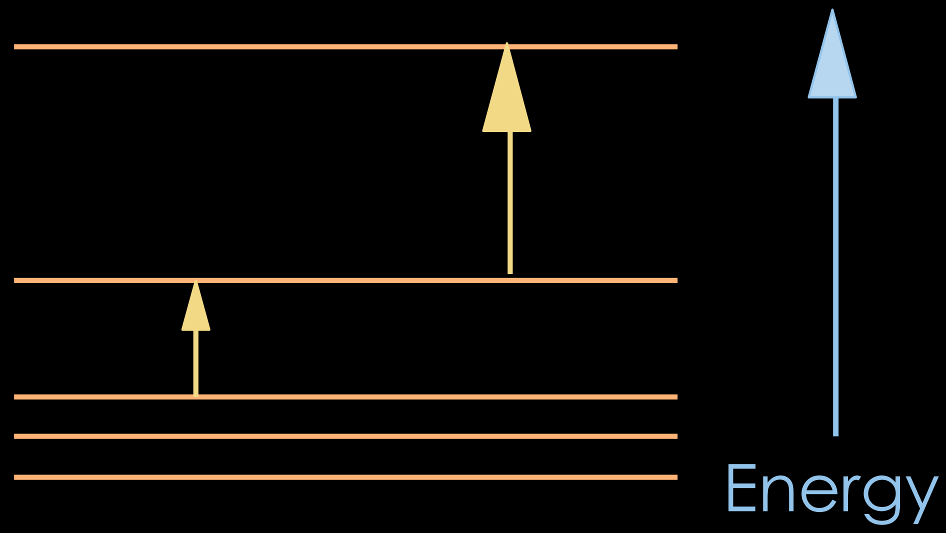
Theoretical quantum methods:



Energy levels (typically millions)

Allowed transitions (millions – billions)

Theoretical quantum methods:



Energy levels (typically millions)
Allowed transitions (millions – billions)
Einstein-A coeffs (Probability of transitions)

THEORETICAL DATA: VALID UP TO HIGH TEMPERATURES

ExoMol

PETER BERNATH

atmospheric science | molecular astronomy | Laser & FTS

Home | Curriculum Vitae | Research | MoLLIST | Publications | Contact | Robert J. LeRoy Programs

MoLLIST (Molecular Line Lists, Intensities and Spectra)

MoLLIST: Molecular Line Lists, Intensities and Spectra (2020)

TheoReTS

HITRANonline

Home | Data Access

HITEMP

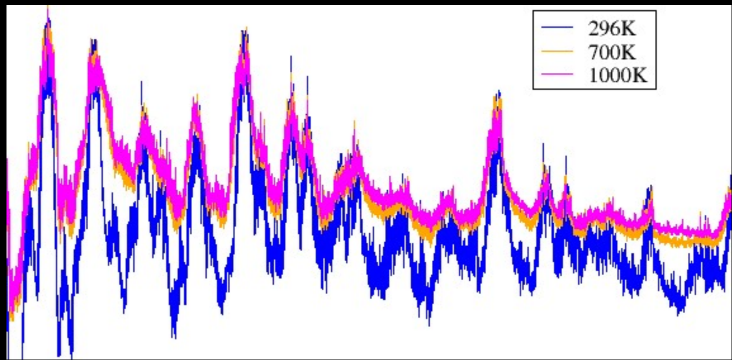
Line list:

1	0.000000	1	0	0	0	0	0	0	A1
2	1594.746306	1	0	0	0	0	1	0	A1
3	3151.629850	1	0	0	0	0	2	0	A1
4	3657.053255	1	0	0	0	1	0	0	A1
5	4666.790461	1	0	0	0	0	3	0	A1
6	5234.975555	1	0	0	0	1	1	0	A1
7	6134.015008	1	0	0	0	0	4	0	A1
8	6775.093508	1	0	0	0	1	2	0	A1
9	7201.539855	1	0	0	0	2	0	0	A1
10	7445.056211	1	0	0	0	0	0	2	A1
11	7542.372492	1	0	0	0	0	5	0	A1
12	8273.975695	1	0	0	0	1	3	0	A1
13	8761.581581	1	0	0	0	2	1	0	A1
14	8869.950054	1	0	0	0	0	6	0	A1
15	9000.136035	1	0	0	0	0	1	2	A1
16	9724.195645	1	0	0	0	1	4	0	A1

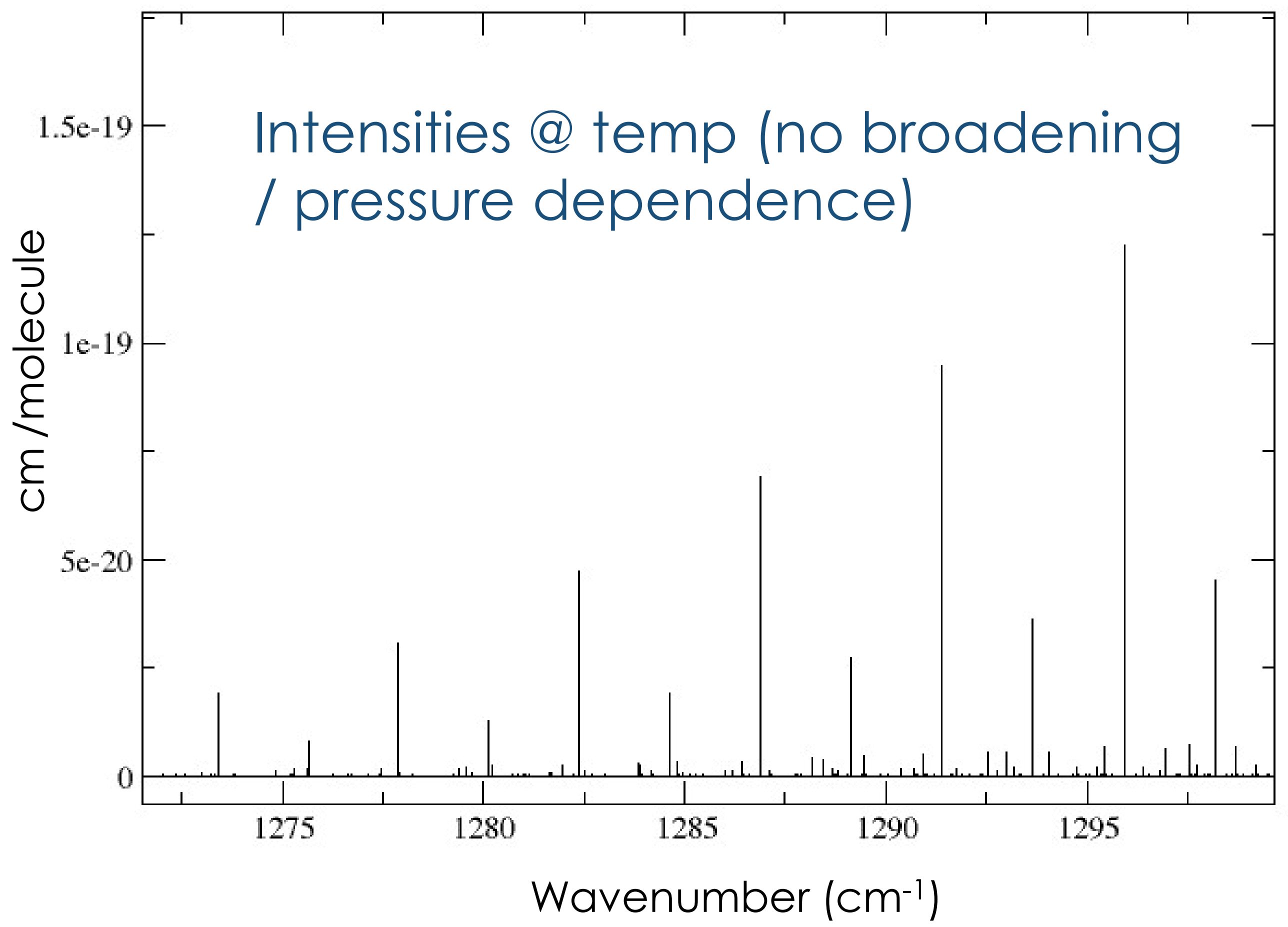
60303	1	2.49323641E-01	1941.016206
60304	1	9.41024052E-01	1958.409110
60305	1	1.74883981E+00	2179.706146
60306	1	6.53131226E-03	2567.657191
60307	1	1.78850008E-02	2706.875827
60308	1	3.21961708E-04	2768.881548
60309	1	7.53501237E-02	3212.444279
60310	1	1.64101339E-02	3228.043358
60311	1	2.49827621E+01	3278.384461
60312	1	5.37295273E+00	3294.955008
60313	1	1.56573889E-01	3387.151052
60314	1	7.40913751E-02	3394.615642
60315	1	1.11121145E-03	3417.184240
60316	1	8.12508441E-05	3617.496491
60317	1	3.98761139E-01	3877.194074

List of energy levels, transitions, A-coeffs

Cross-sections:



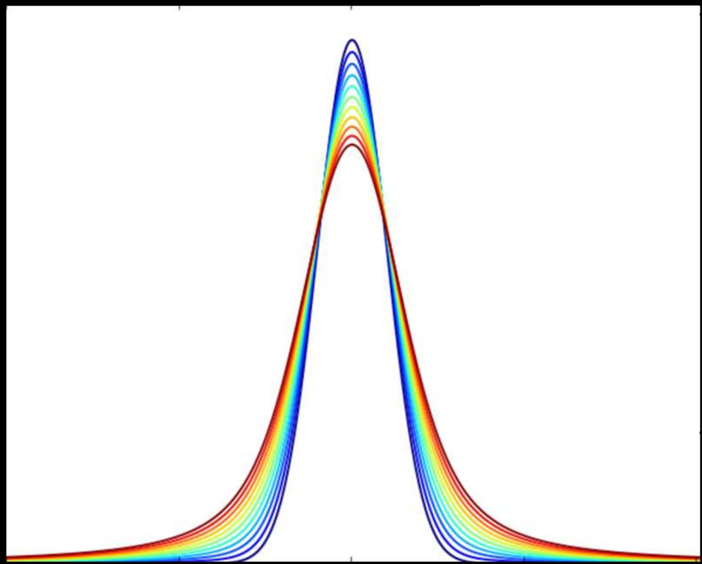
Pressure and temperature dependent spectra (line positions from energy level transitions + line strengths from A-coeffs)



Intensities @ temp (no broadening / pressure dependence)
cm /molecule
1.5e-19
1e-19
5e-20
0
1275
1280
1285
1290
1295
Wavenumber (cm-1)

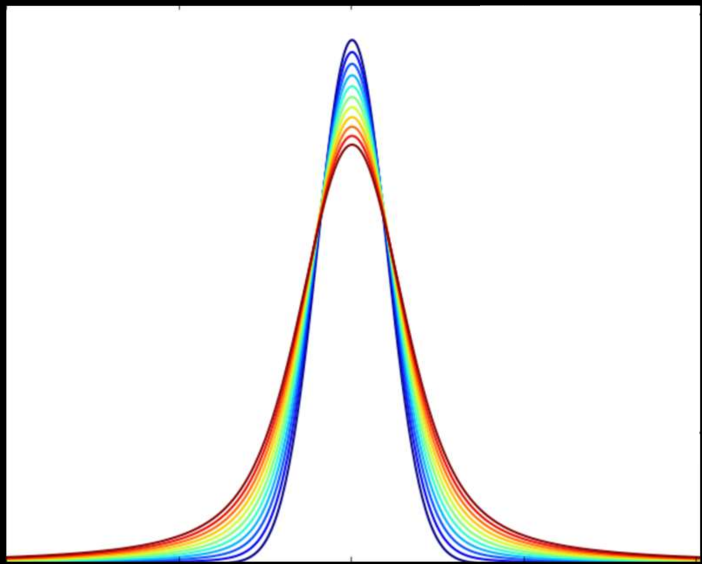
LINE BROADENING:

- Natural broadening (Pauli exclusion principle)
- Temperature broadening (due to molecules moving away and towards us – slight blue and red shift to either side)
- Pressure broadening (due to other atoms and molecules colliding with the molecule as it absorbs)



LINE BROADENING:

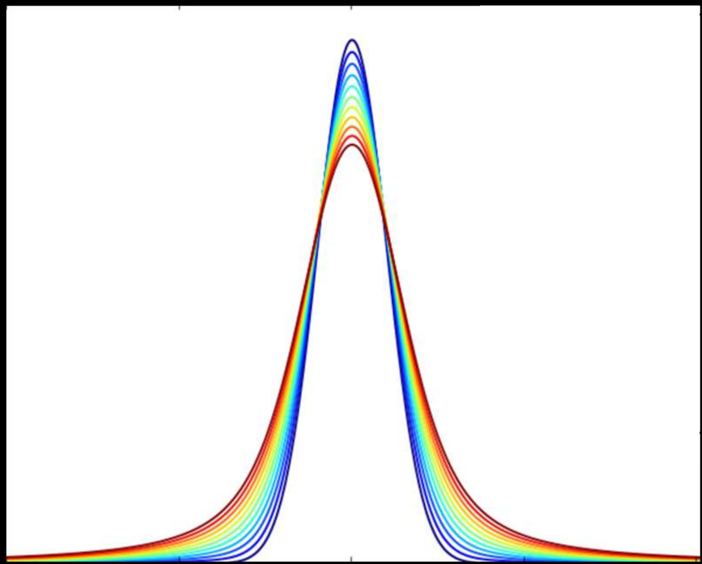
- Temperature broadening (due to molecules moving away and towards us – slight blue and red shift to either side)
- Pressure broadening (due to other atoms and molecules colliding with the molecule as it absorbs)

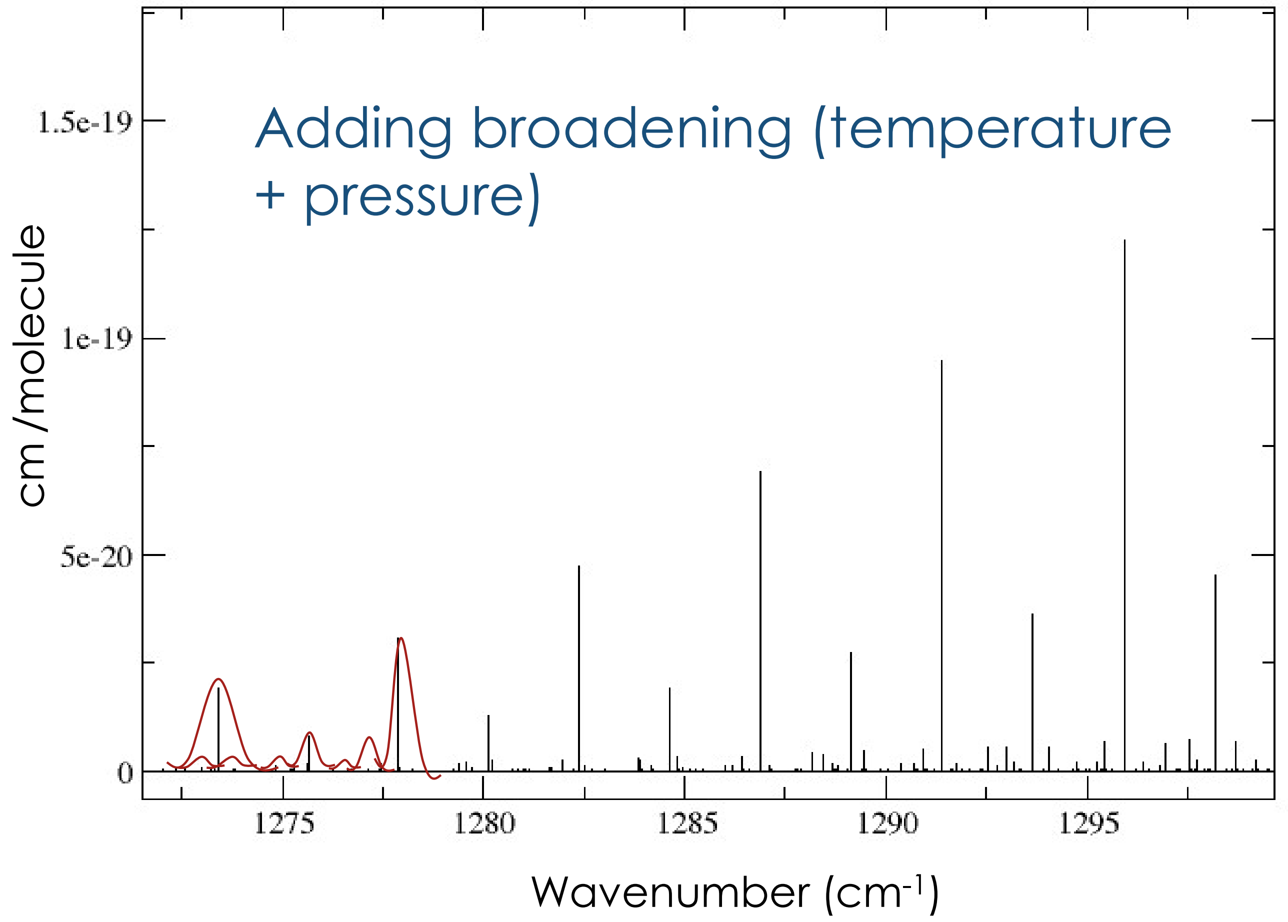


LINE BROADENING:

H2/He broadening for "hot Jupiter" exoplanets

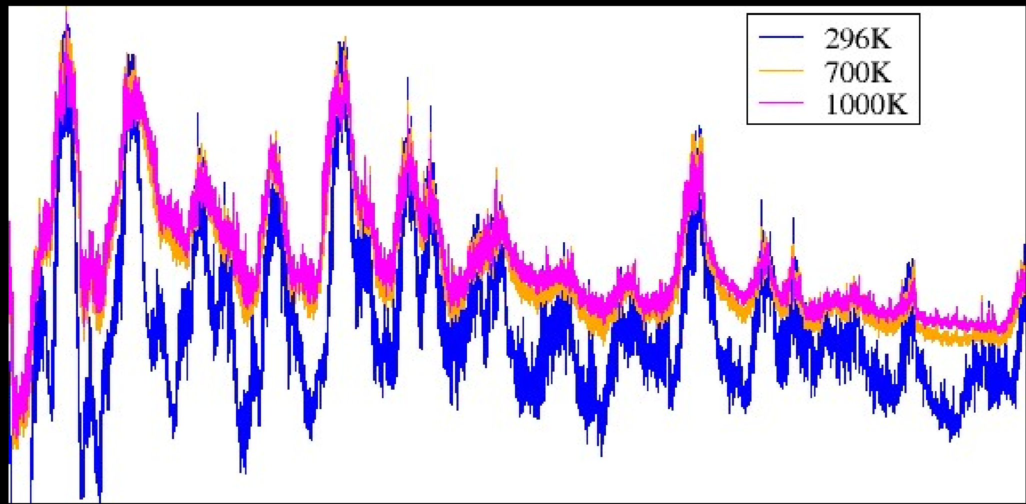
- Pressure broadening (due to other atoms and molecules colliding with the molecule as it absorbs)




Adding broadening (temperature
+ pressure)
1.5e-19
1e-19
5e-20
0
cm /molecule
1275
1280
1285
1290
1295
Wavenumber (cm-1)

ExoCross

Software to compute spectra (@ particular temp/pressure) from linelist (temp/pressure independent)



exocross.readthedocs.io

ExoMolOP

Database of opacities (cross-sections and k-tables) for characterizing exoplanet atmospheres tailored for four atmospheric retrieval codes

ARCiS – ARtful modelling Code for exoplanet Science

NEMESIS

petitradtrans.readthedocs.io

taurex3-public.readthedocs.io

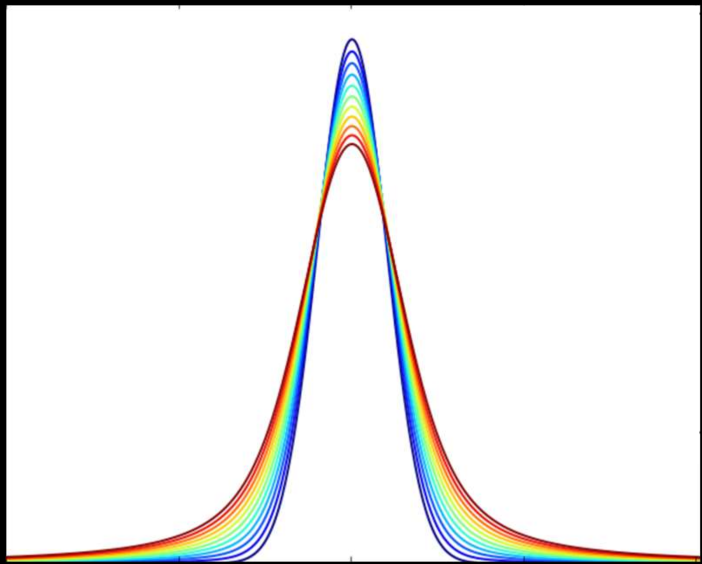
TauREx 3.0

petit RADTRANS

ExoMolOP

Database of opacities (cross-sections and k-tables) for characterizing exoplanet atmospheres tailored for four atmospheric retrieval codes

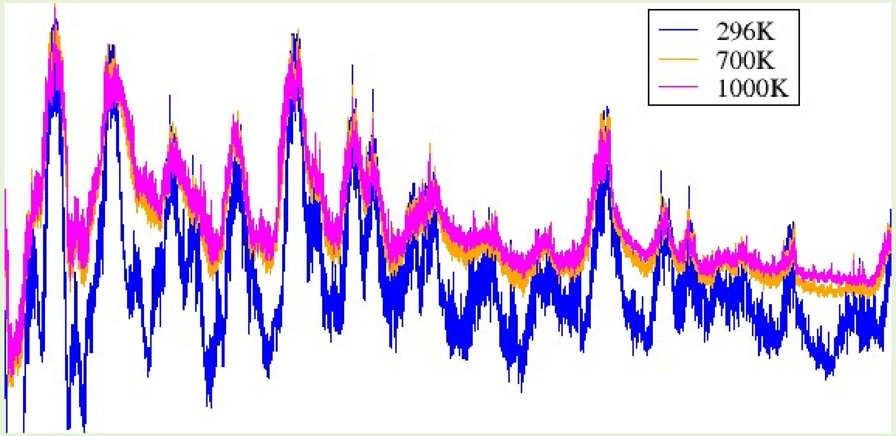
H2/He broadening for "hot Jupiter" exoplanets: new cross-sections required for other planets



PRESSURE TEMPERATURE GRID

27 temperatures

22 pressures

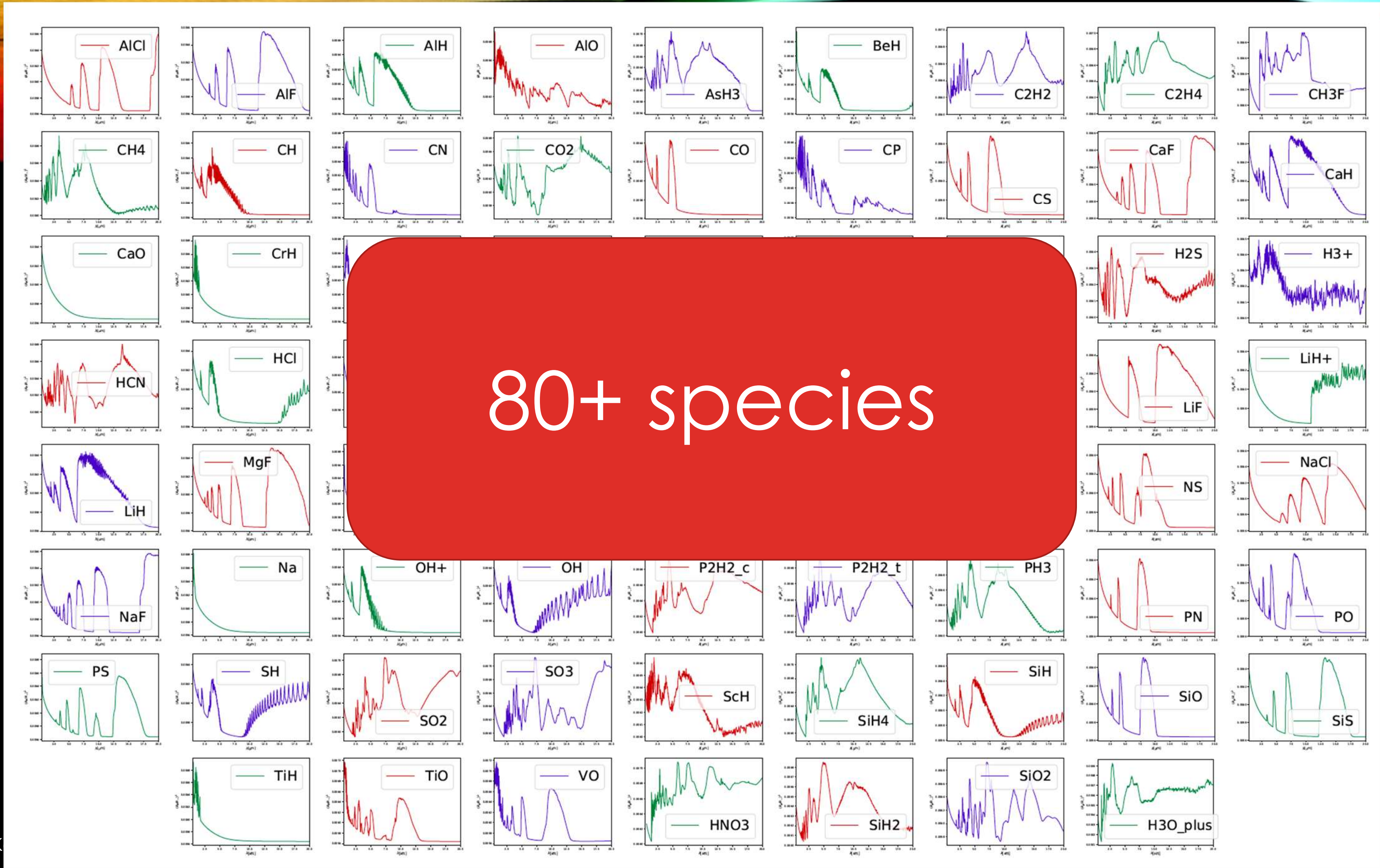


594 T/P points / species

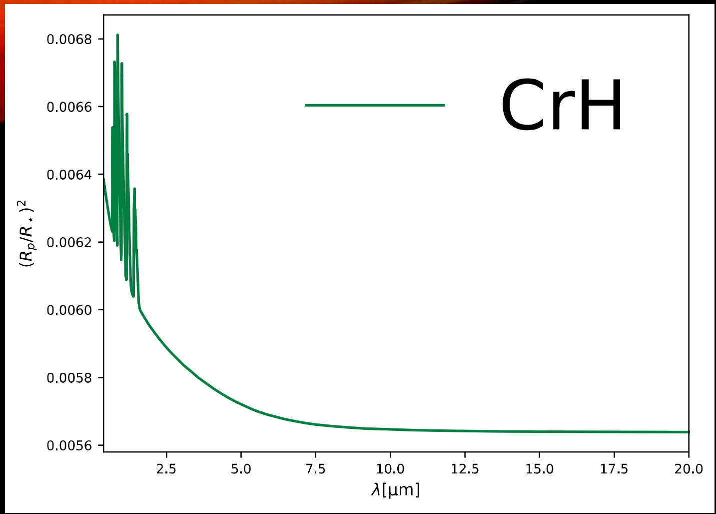
From 1E-5 - 100 bar

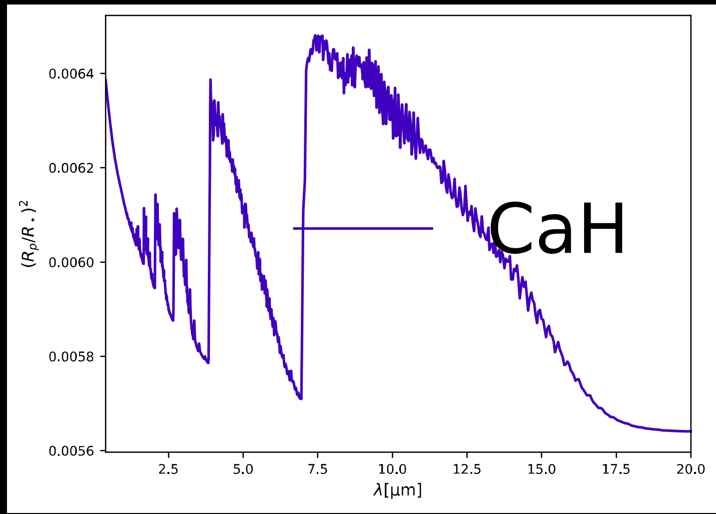
And

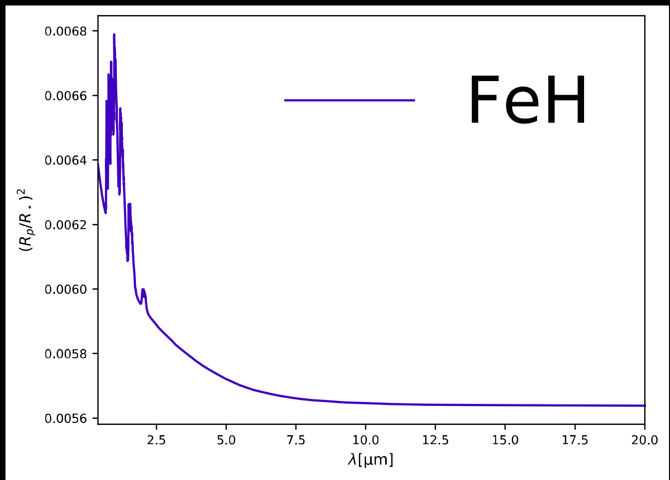
From 100K – 3400K

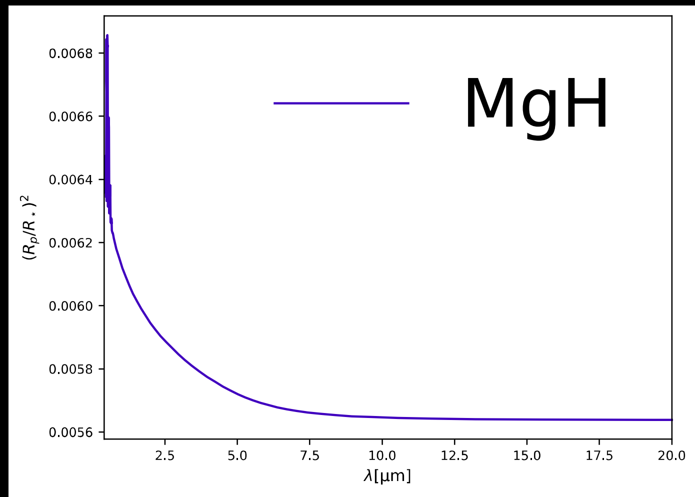


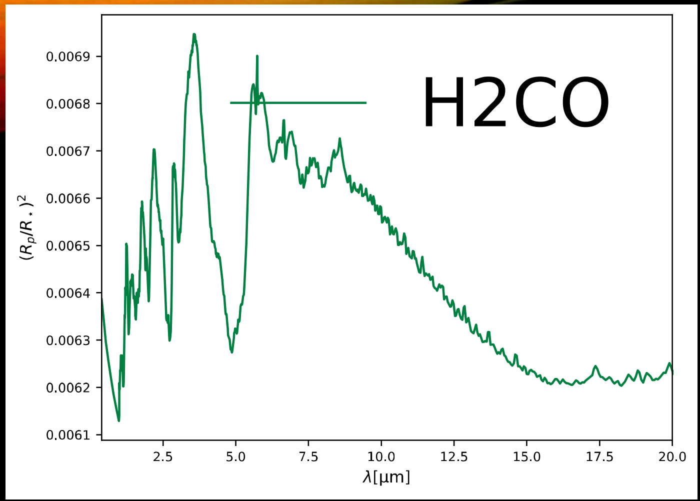
AlCl
AlF
AlH
AlO
AsH3
BeH
C2H2
C2H4
CH3F
CH4
CH
CN
CO2
CO
CP
CS
CaF
CaH
CaO
CrH
H2S
H3+
HCN
HCl
LiF
LiH+
LiH
MgF
NS
NaCl
80+ species
NaF
Na
OH+
OH
P2H2_c
P2H2_t
PH3
PN
PO
PS
SH
SO2
SO3
ScH
SiH4
SiH
SiO
SiS
TiH
TiO
VO
HNO3
SiH2
SiO2
H3O_plus

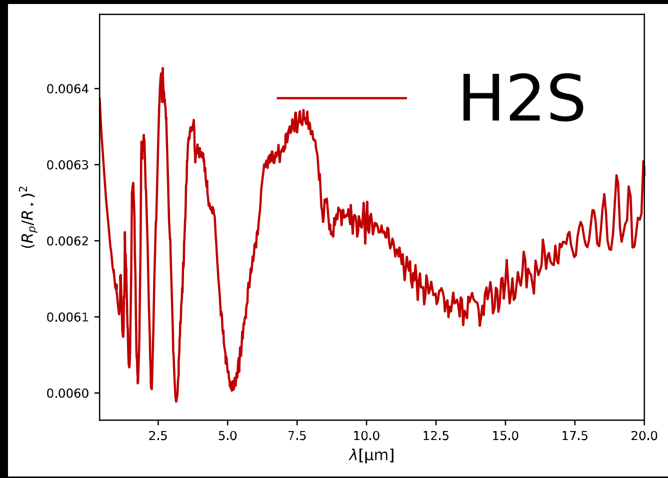

CrH
0.0068
0.0066
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[μm]

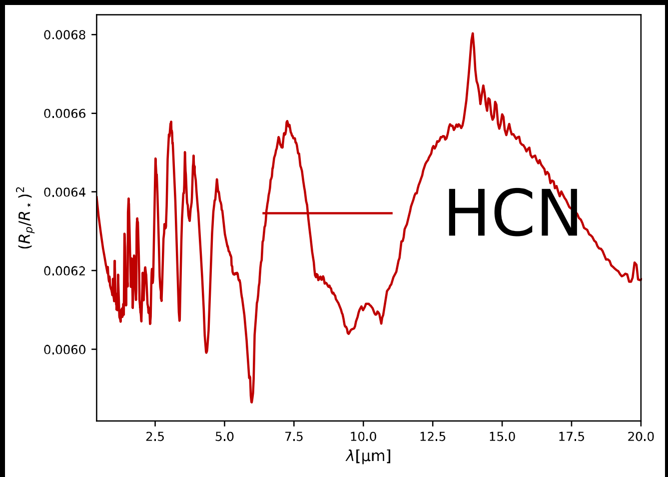

CaH
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[μm]

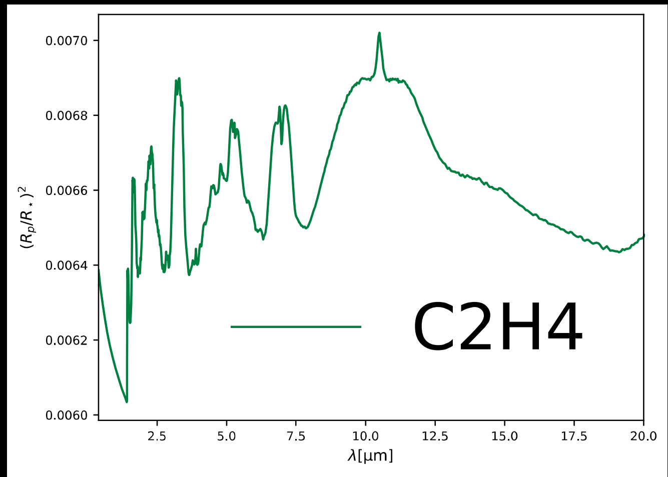

FeH
0.0068
0.0066
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[μm]

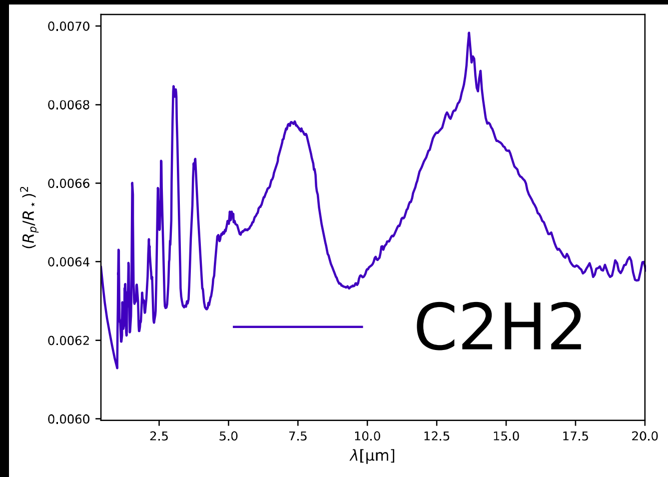

MgH
0.0068
0.0066
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[μm]











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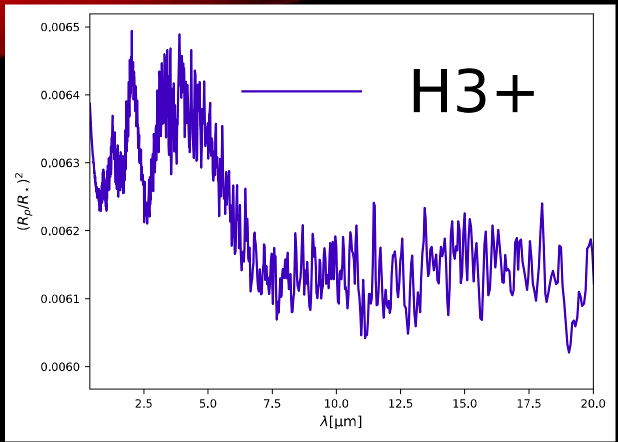
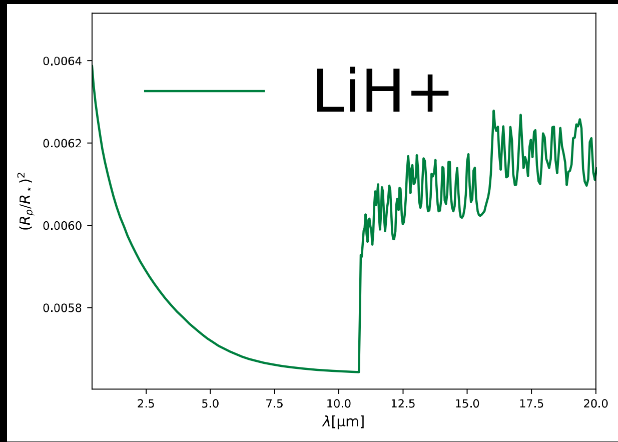
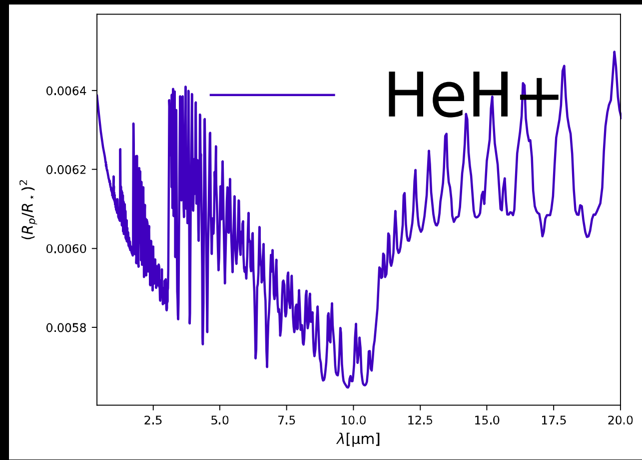
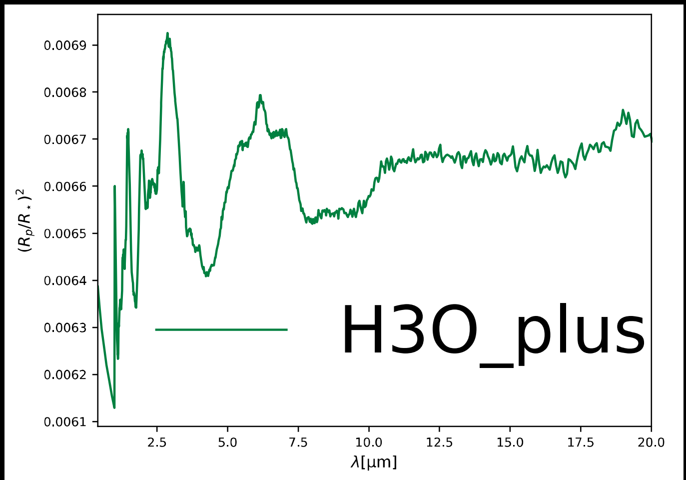
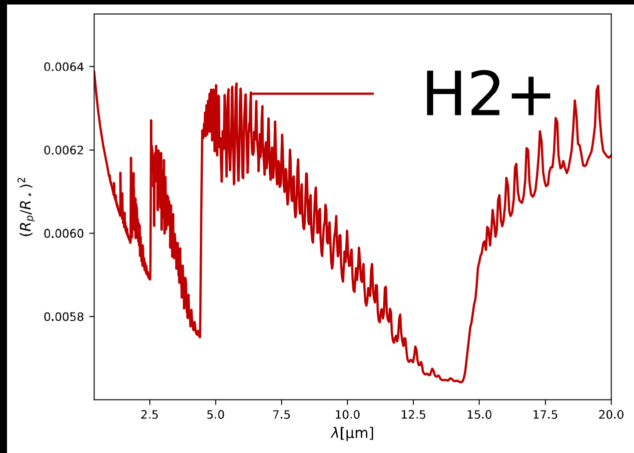
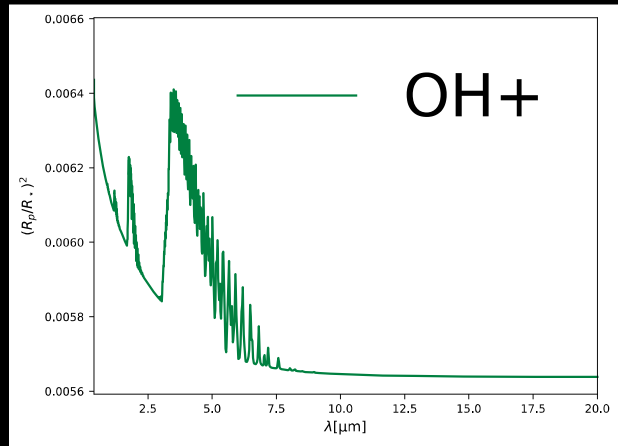




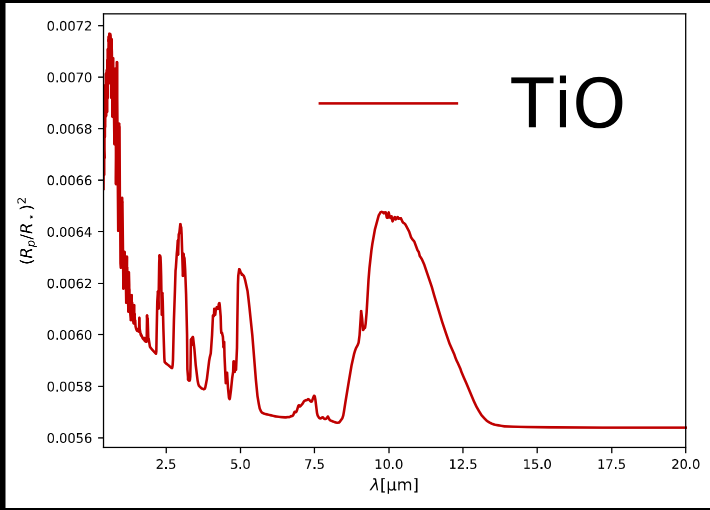


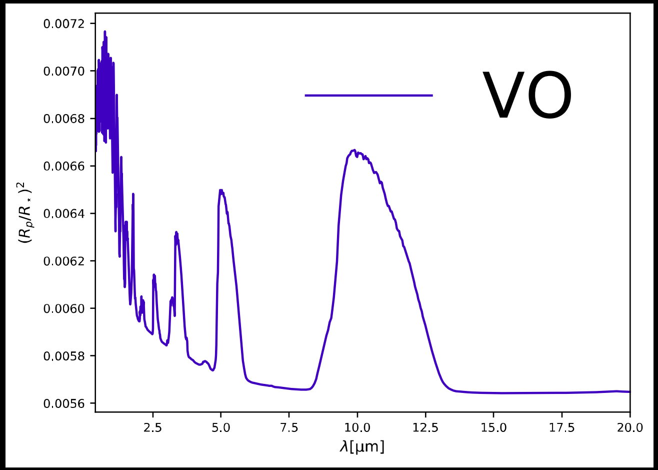


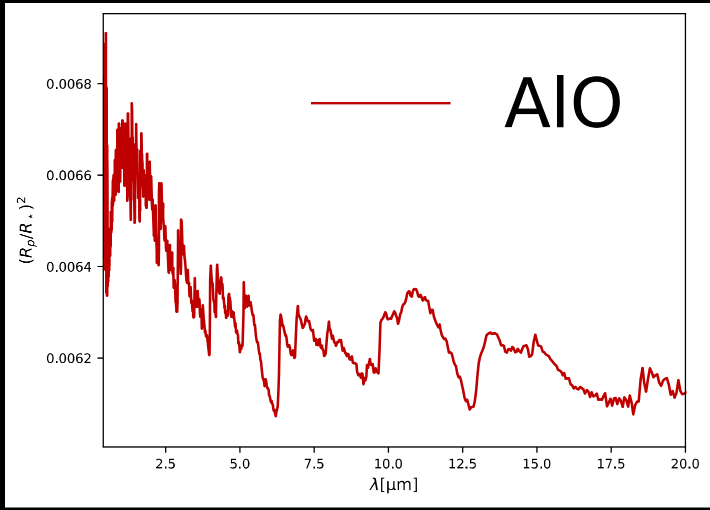




Katy Chubb, SRON

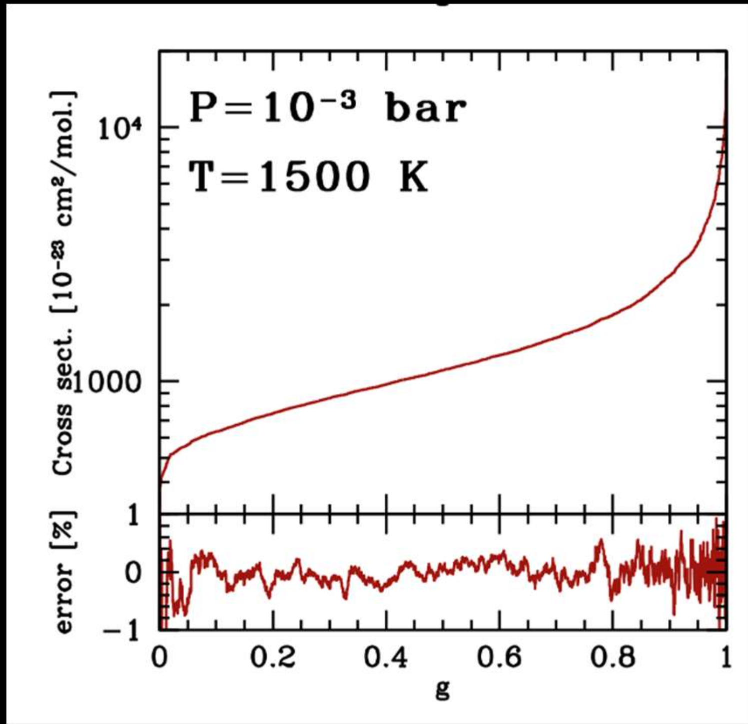

TiO
0.0072
0.0070
0.0068
0.0066
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[µm]


VO
0.0072
0.0070
0.0068
0.0066
0.0064
0.0062
0.0060
0.0058
0.0056
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[µm]


AlO
0.0068
0.0066
0.0064
0.0062
$(R_p/R_*)^2$
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
λ[µm]

CORRELATED-K TABLES

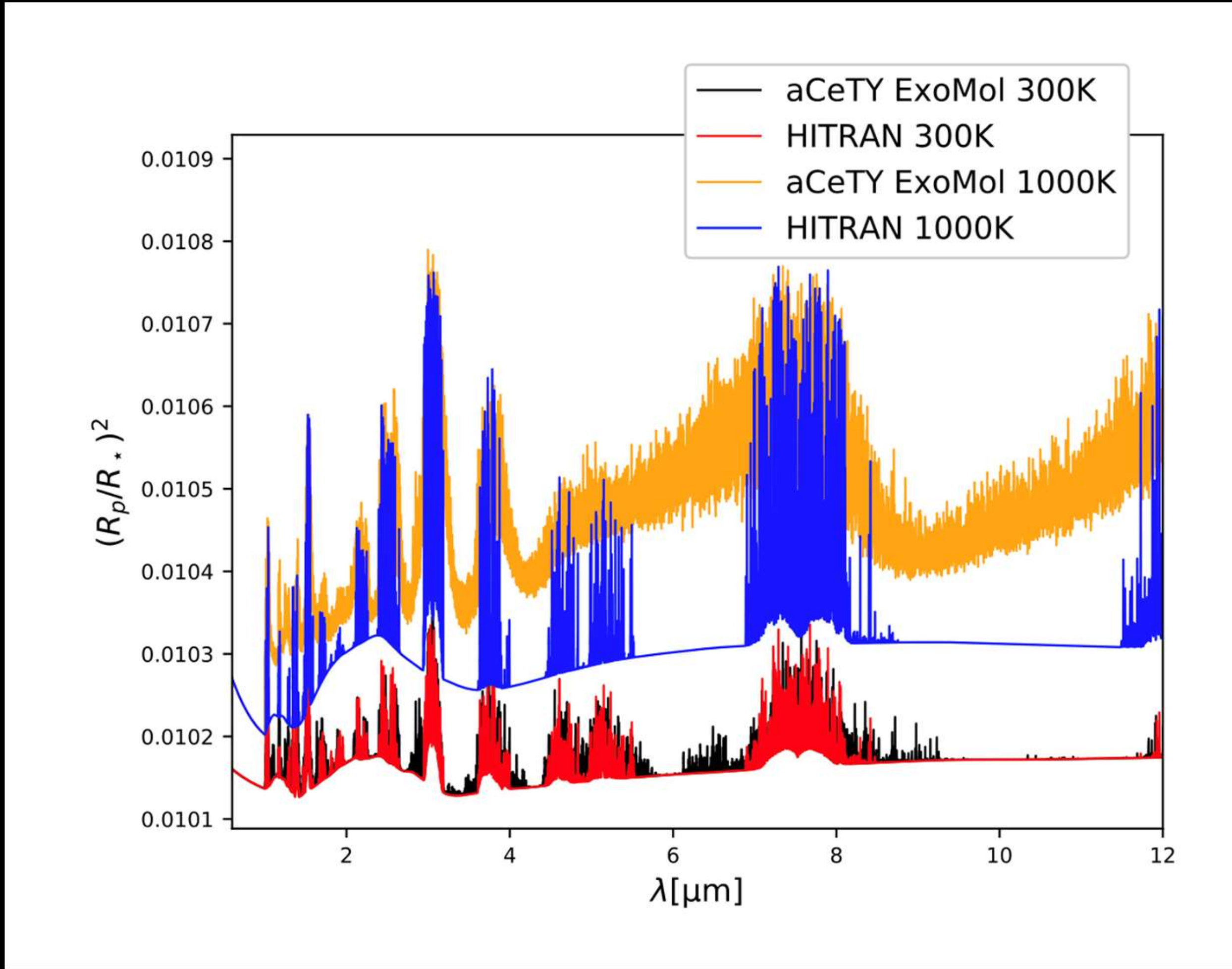
- Cumulative opacity function
- Lower resolution required than for sampled cross-sections



From Min 2018

arXiv:1710.01997

C_2H_2 AT DIFFERENT TEMPERATURES



aCeTY ExoMol = theory

HITRAN = room-temp laboratory data

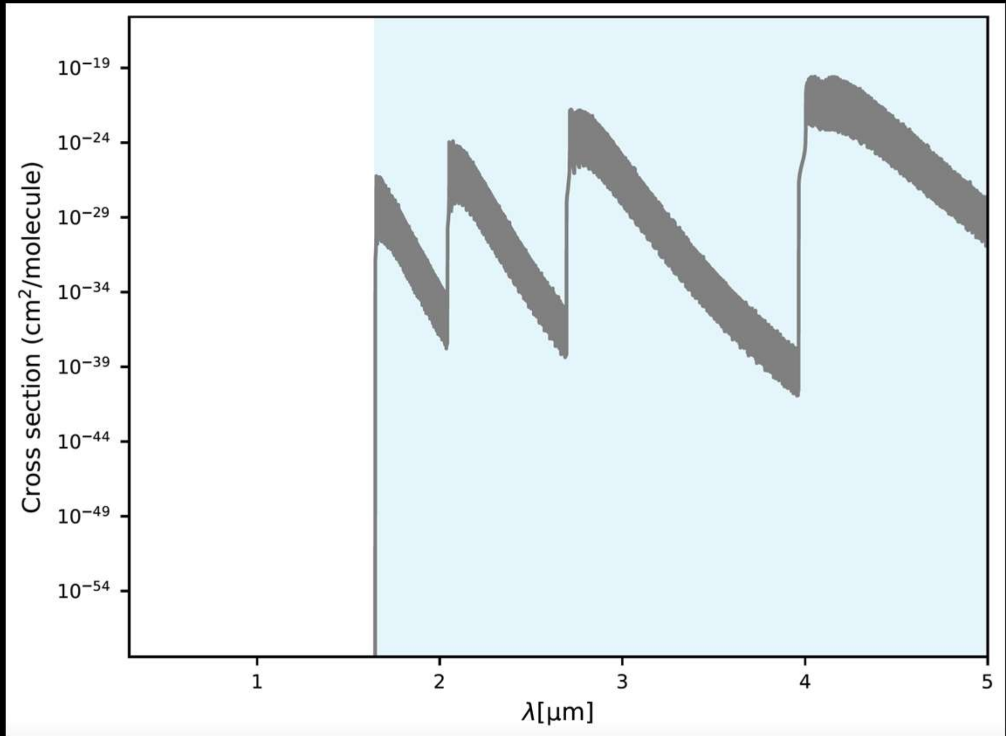
Chubb et al. 2020

arXiv:2001.04550

Katy Chubb, SRON

WARNING: WAVELENGTH

Species	Line list	Ref	E_l (cm^{-1})	E_u (cm^{-1})	λ_l (μm)	λ_u (μm)
SiO	ExoMol EBJT	Barton et al. (2013)	100	6049	1.65	100



Katy Chubb, SRON

arXiv:2009.00687

HITRAN

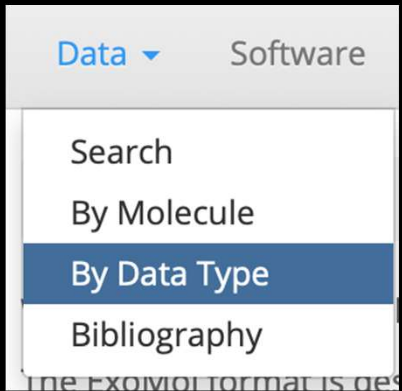
Laboratory data: largely room-temp

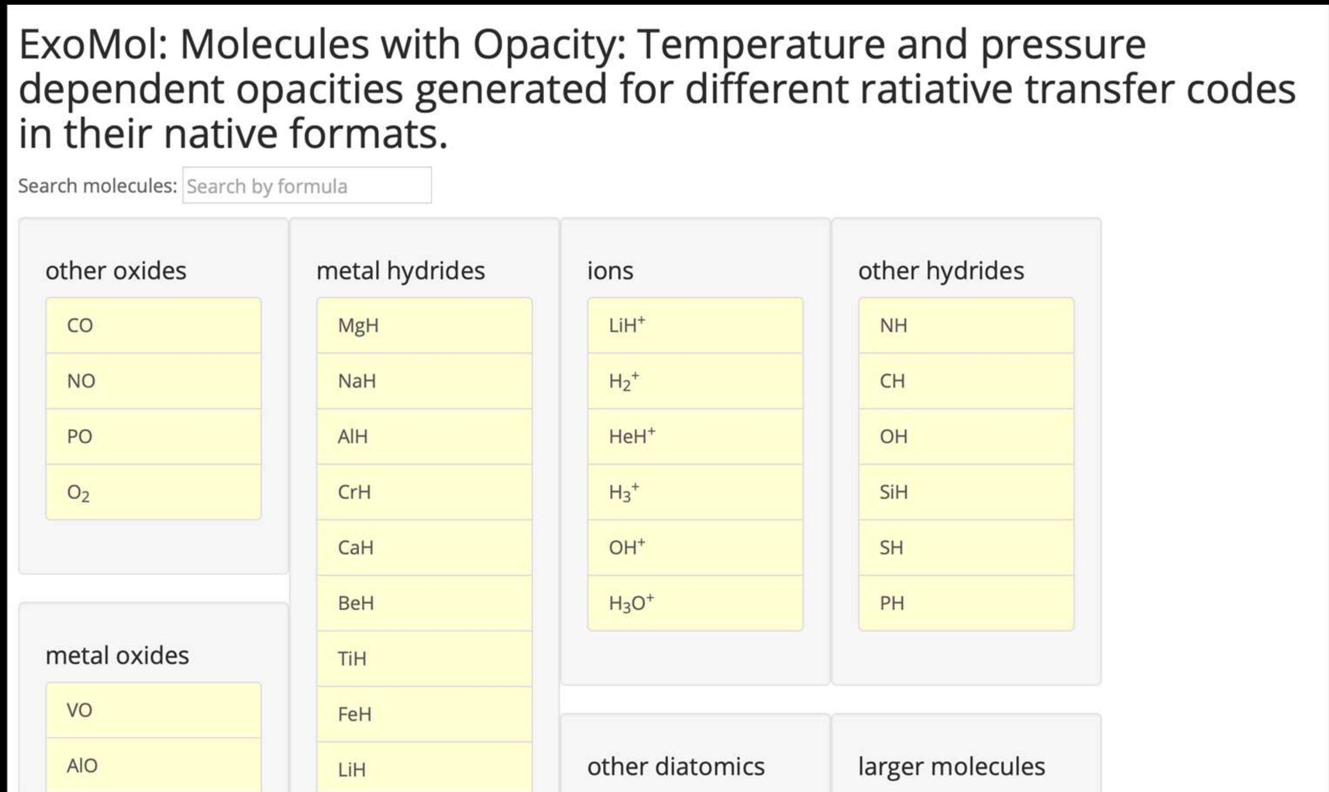
ExoMol

Theoretical data: typically valid up to high temps (check each species)

EXOMOLOP: DOWNLOAD FROM WWW.EXOMOL.COM

www.exomol.com/data/data-types/opacity/





CoYuTe: opacity

Hot Temperature line list for (14N)(1H)3, 0-20000 cm-1.

Please cite all line lists!

14N-1H3__CoYuTe.R1000_0.3-50mu.ktable.NEMESIS.kta
NEMESIS k-tables at R= 1000 (0.3-50mu) in NEMESIS-kta format: CoYuTe (14N)(1H)3 line list.

14N-1H3__CoYuTe.R15000_0.3-50mu.xsec.TauREx.h5
TauREx cross sections at R= 15000 (0.3-50mu) in HDF5 format: CoYuTe (14N)(1H)3 line list.

14N-1H3__CoYuTe.R1000_0.3-50mu.ktable.ARCiS.fits.gz
ARCiS k-tables at R= 1000 (0.3-50mu) in fits format (gzipped): CoYuTe (14N)(1H)3 line list.

14N-1H3__CoYuTe.R1000_0.3-50mu.ktable.petitRADTRANS.h5
petitRADTRANS k-tables at R= 1000 (0.3-50mu) in HDF5 format: CoYuTe (14N)(1H)3 line list.

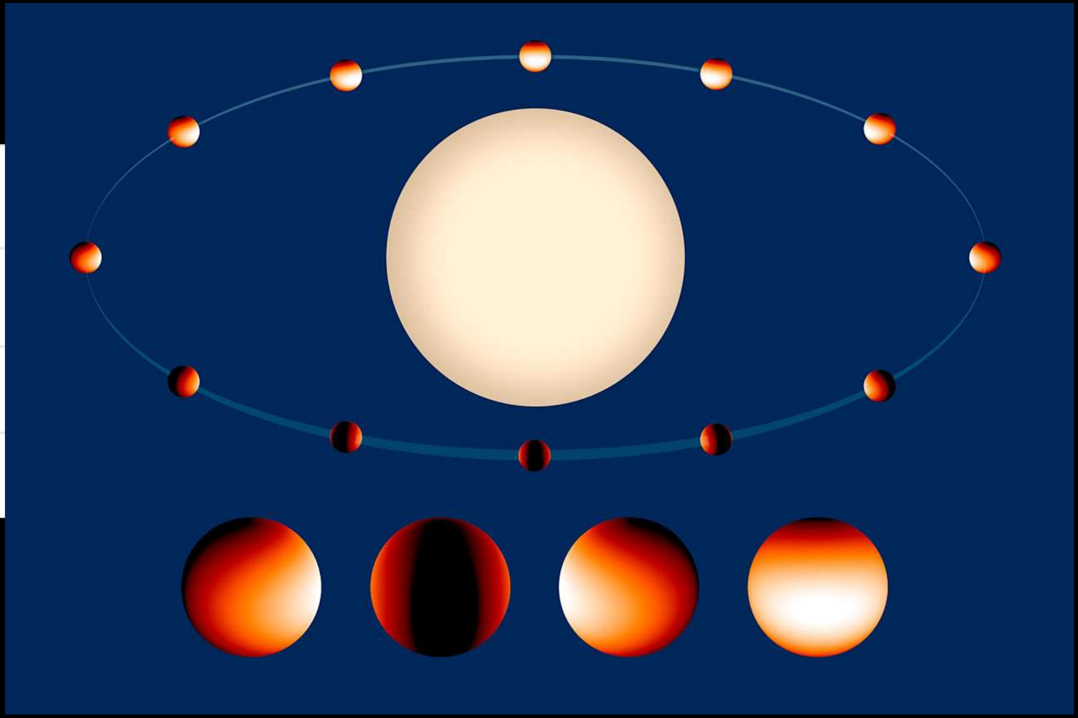
References

1. Coles, P. A., Yurchenko, S. N., Tennyson, J., "ExoMol molecular line lists – XXXV. A rotation-vibration line list for hot ammonia", *Monthly Notices of the Royal Astronomical Society* **490**, 4638-4647 (2019). [link to article][19CoYuTe.NH3]
2. Chubb, K.L., Rocchetto, M., Yurchenko, S.N., Min, M., Waldmann, I., Barstow, J.K., Molliere, P., Al-Refaie, A.F, Phillips, M.W., Tennyson, J., "The ExoMolOP Database: Cross-sections and k-tables for Molecules of Interest in High-Temperature Exoplanet Atmospheres", *Astronomy and Astrophysics* **Accepted** (2020).

RE-ANALYSIS OF ARCHIVE HST WFC3 DATA: WASP43B

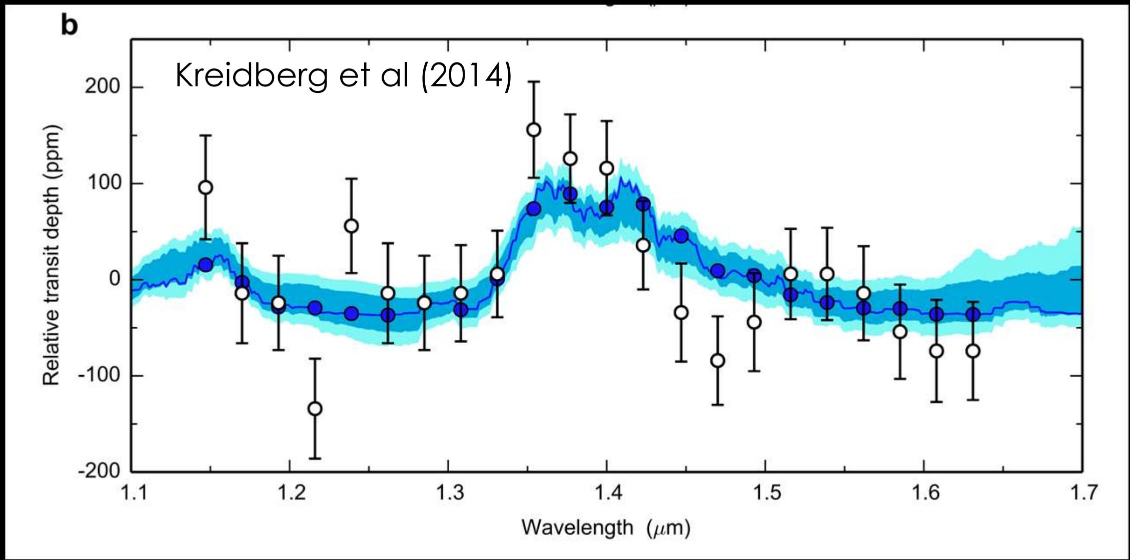
TauREx 3.0

Radius	1.036 ($_{-0.019}^{+0.019}$) R_J
Mass*sin(i)	2.034 ($_{-0.052}^{+0.052}$) M_J
Semi-Major Axis	0.01526 (± 0.00018) AU
Orbital Period	0.81347753 (± 7e-07) day



arXiv:2004.13679 Chubb et al., 2020

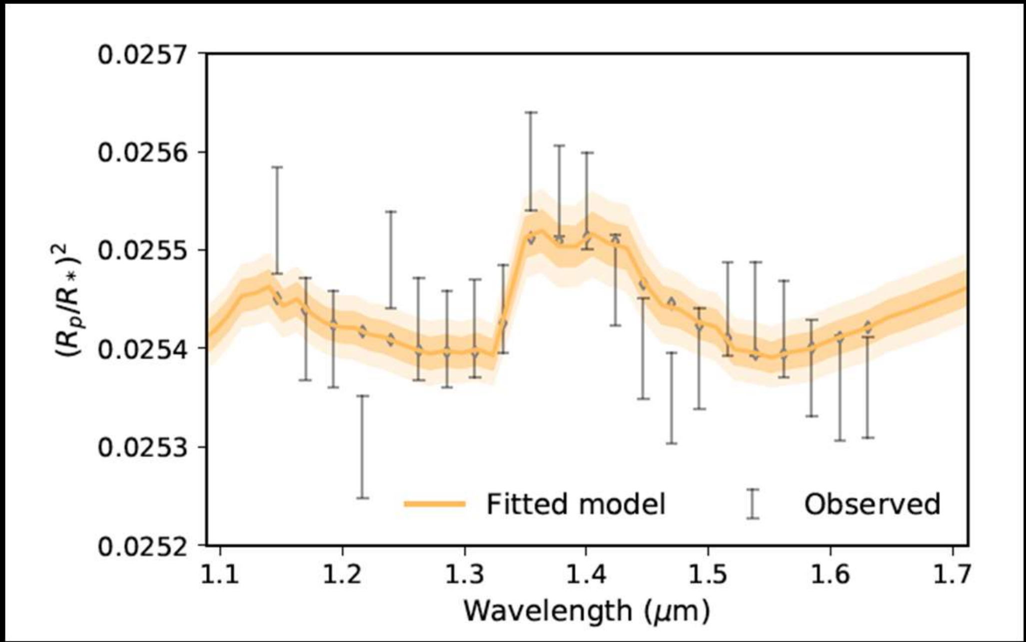
RE-ANALYSIS OF ARCHIVE HST WFC3 DATA: WASP43B



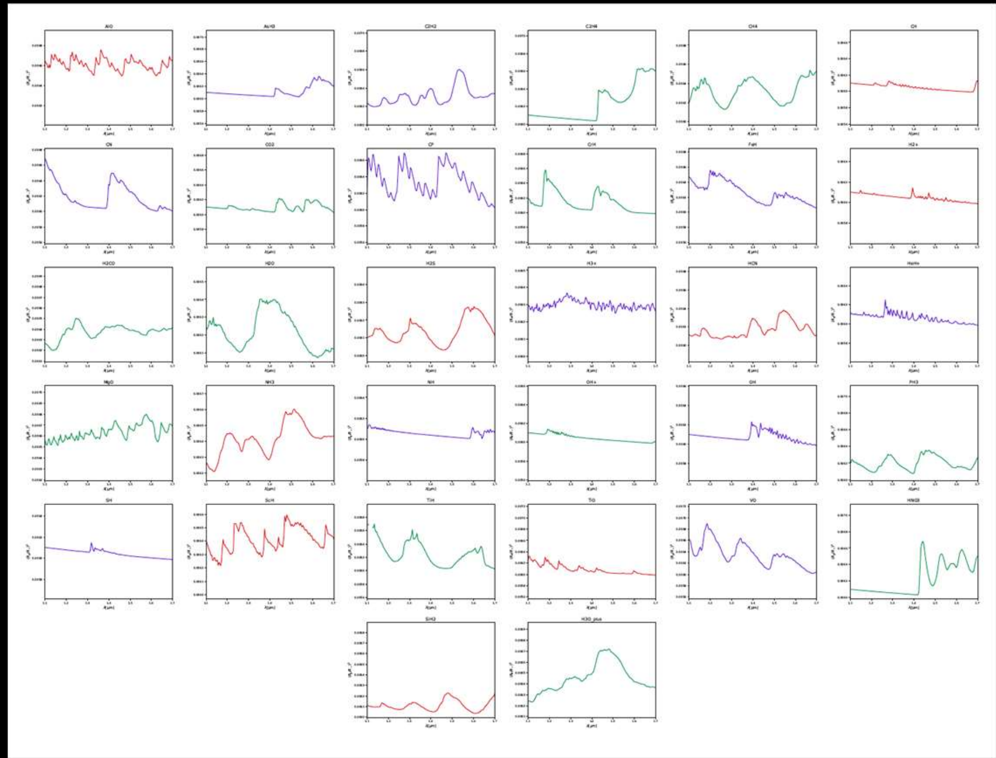
arXiv:2004.13679 Chubb et al., 2020

RE-ANALYSIS OF ARCHIVE HST WFC3 DATA: WASP43B

TauREx 3.0



H2O only

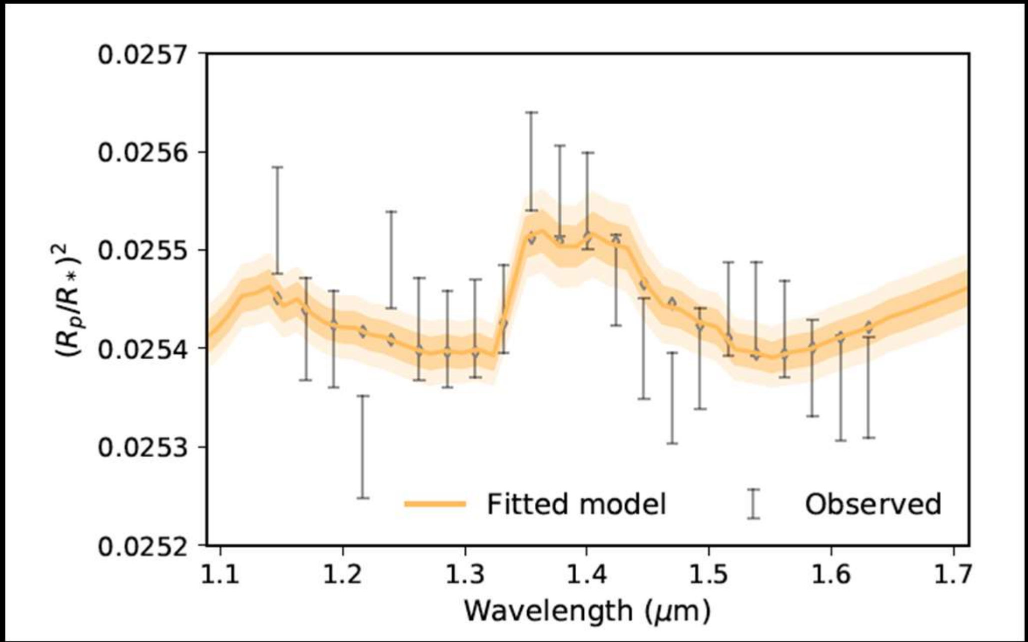


Katy Chubb, SRON

arXiv:2004.13679 Chubb et al., 2020

RE-ANALYSIS OF ARCHIVE HST WFC3 DATA: WASP43B

TauREx 3.0



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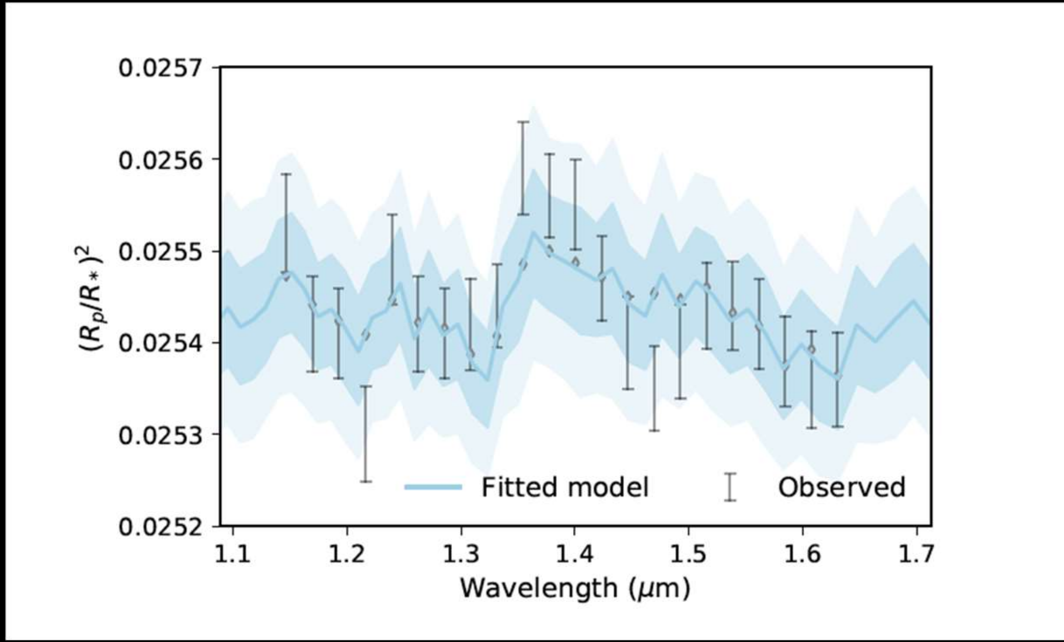


AlO + H2O

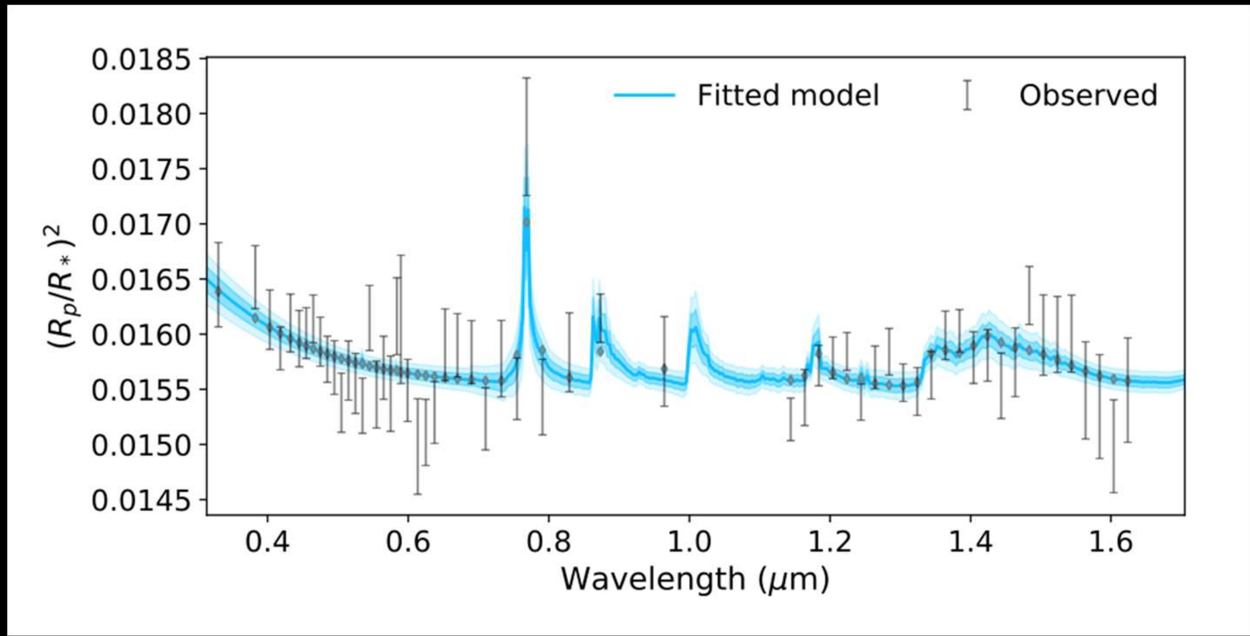
Katy Chubb, SRON

arXiv:2004.13679 Chubb et al., 2020

TauREx 3.0

EVIDENCE FOR CrH IN WASP31b

Molecule	Wavelength range
AlH	0.37–100μm
AlO	0.29–100μm
C_2H_2	1.00–100μm
C_2H_4	1.41–100μm
CaH	0.45–100μm
CH_4	0.83–100μm
CN	0.23–100μm
CO	0.45–100μm
CO_2	1.04–100μm
CP	0.67–100μm
CrH	0.67–100μm
FeH	0.67–100μm
H_2CO	0.99–100μm
H_2O	0.24–100μm
HCN	0.56–100μm
K	0.29–100μm
MgH	0.34–100μm
MgO	0.27–100μm
Na	0.24–100μm
NH_3	0.43–100μm
OH	0.23–100μm
ScH	0.63–100μm
TiH	0.42–100μm
TiO	0.33–100μm
VO	0.29–100μm



Braam et al., 2020

arXiv:2011.10558

High resolution spectroscopy

VLT. Image credit: ESO

Requires very accurate spectral data

HIGHER ACCURACY

HITRAN

EXPERIMENT
(room-temp)

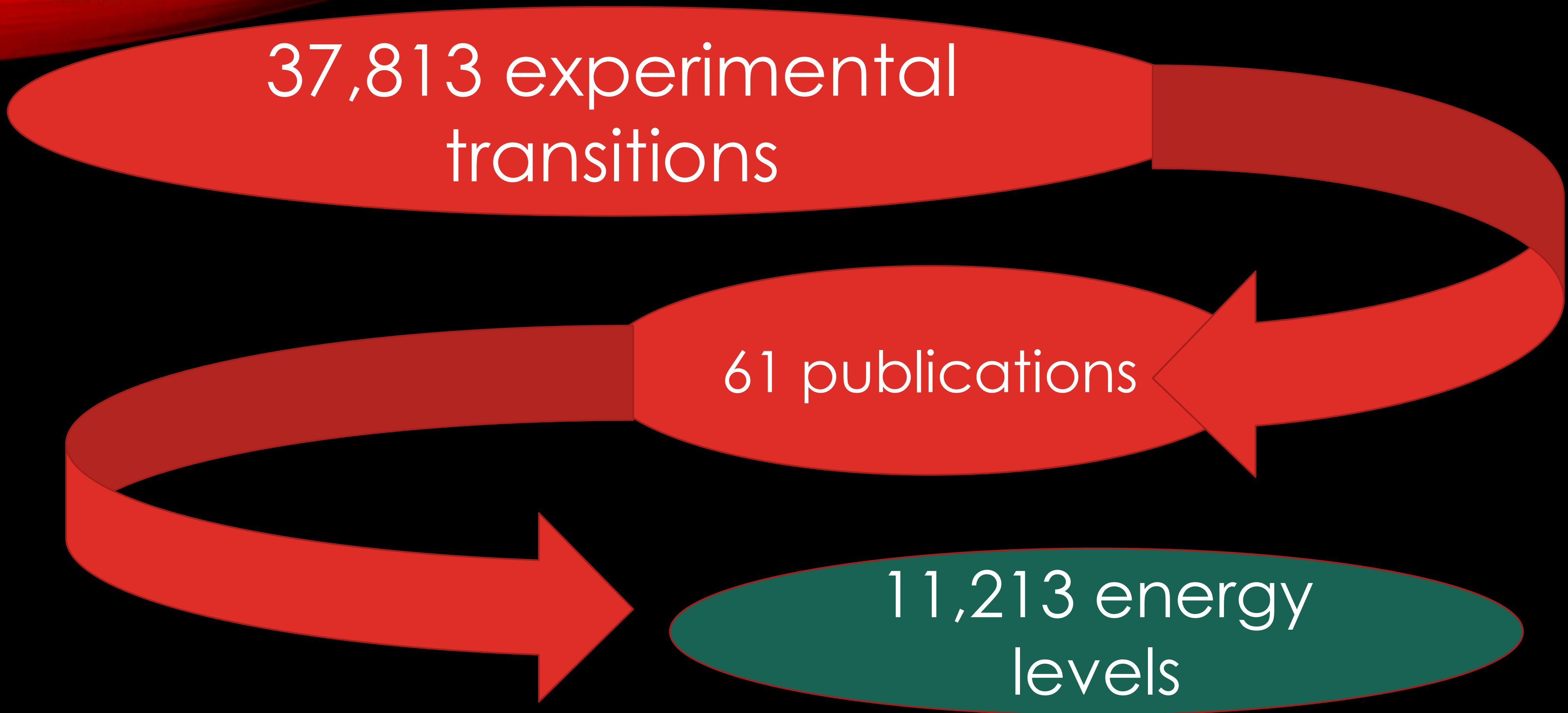
ExoMol

THEORY
(high temp)

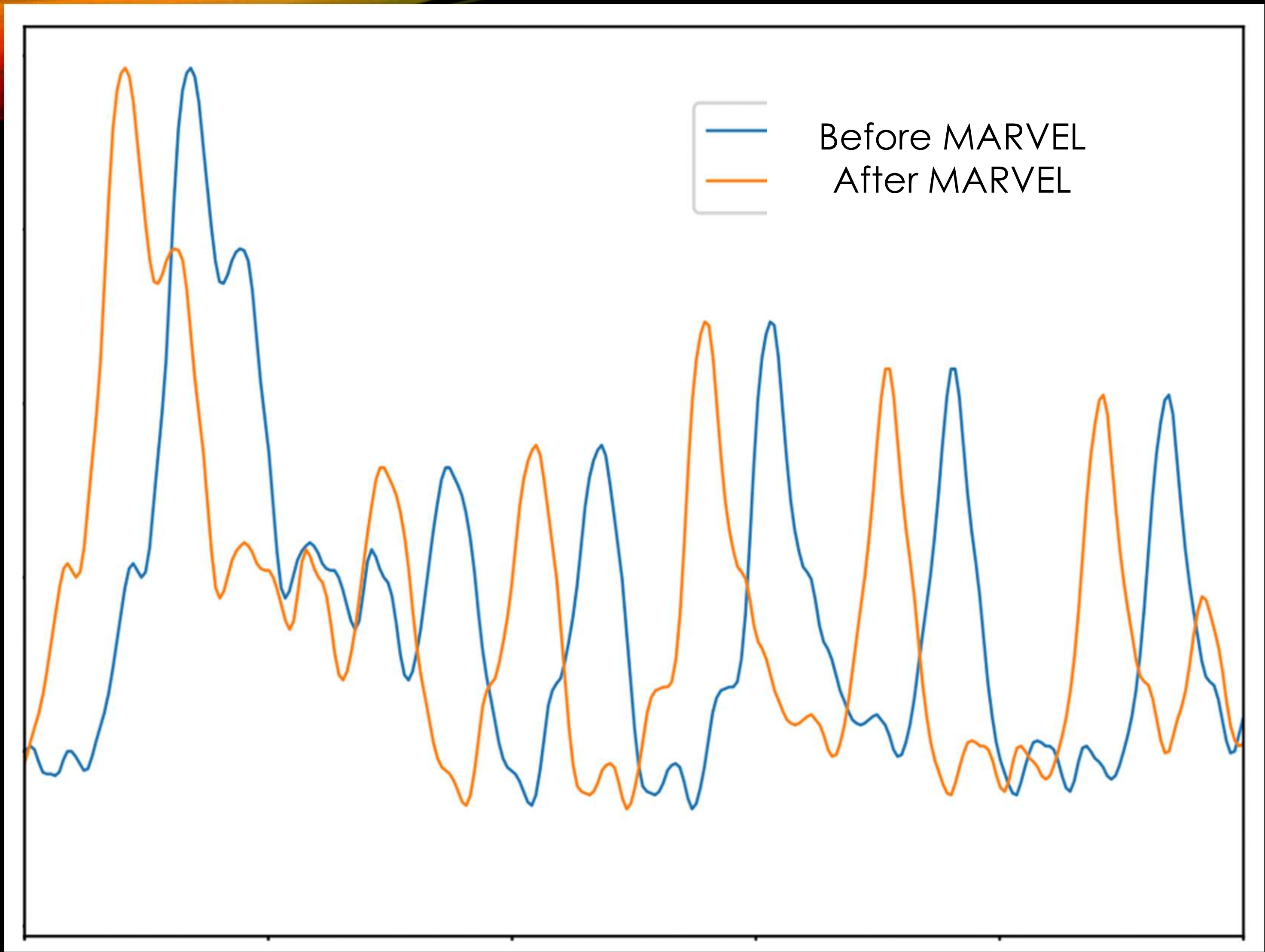
MARVEL

(Measured Active Rotational-Vibrational Energy Levels)

$$H-C\equiv C-H$$



37,813 experimental transitions
61 publications
11,213 energy levels


Before MARVEL
After MARVEL

Original Research By Young Twinkle Students

Twinkle

TWINKLE

A MISSION TO UNRAVEL THE STORY OF PLANETS IN OUR GALAXY

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

MARVEL analysis of the measured high-resolution rovibrational spectra of C_2H_2

Katy L. Chubb[a,*], Megan Joseph[b], Jack Franklin[b], Naail Choudhury[b], Tibor Furtenbacher[c], Attila G. Császár[c], Glenda Gaspard[b], Patari Oguoko[b], Adam Kelly[b], Sergei N. Yurchenko[a], Jonathan Tennyson[a,*], Clara Sousa-Silva[d,a,b]

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Article

Five carbon- and nitrogen-bearing species in a hot giant planet's atmosphere

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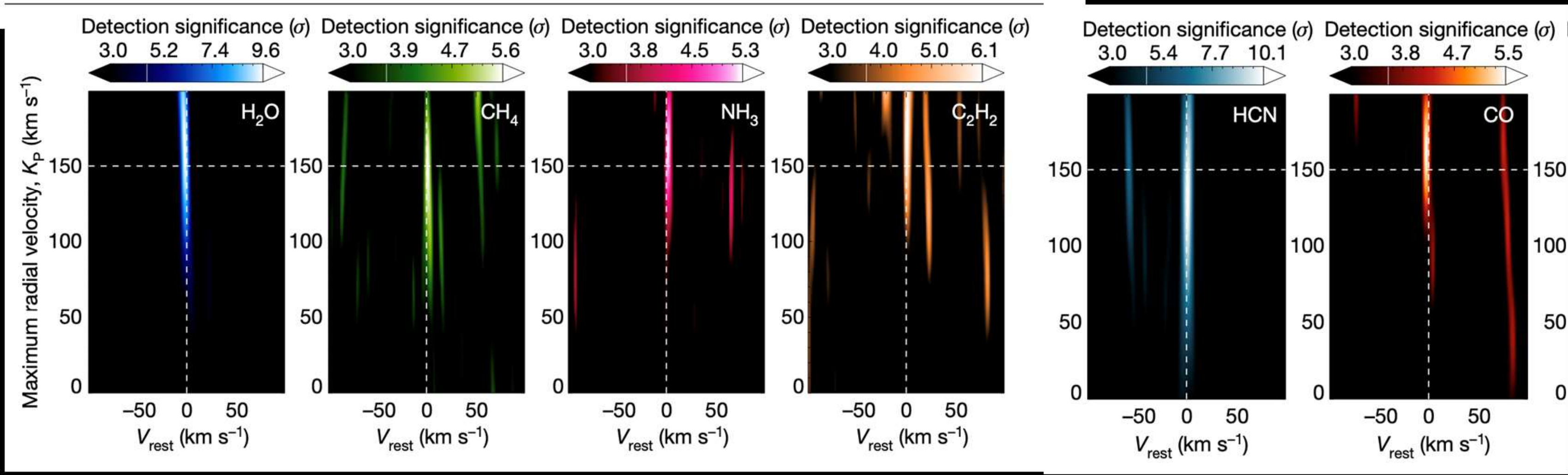
Check for updates

Paolo Giacobbe[1]✉, Matteo Brogi[1,2,3], Siddharth Gandhi[2,3], Patricio E. Cubillos[4], Aldo S. Bonomo[1], Alessandro Sozzetti[1], Luca Fossati[4], Gloria Guilluy[1,5], Ilaria Carleo[6], Monica Rainer[7], Avet Harutyunyan[8], Francesco Borsa[9], Lorenzo Pino[7,10], Valerio Nascimbeni[11], Serena Benatti[12], Katia Biazzo[13], Andrea Bignamini[14], Katy L. Chubb[15], Riccardo Claudi[16], Rosario Cosentino[8], Elvira Covino[17], Mario Damasso[1], Silvano Desidera[16], Aldo F. M. Fiorenzano[8], Adriano Ghedina[8], Antonino F. Lanza[18], Giuseppe Leto[18], Antonio Maggio[12], Luca Malavolta[11], Jesus Maldonado[12], Giuseppina Micela[12], Emilio Molinari[19], Isabella Pagano[18], Marco Pedani[8], Giampaolo Piotto[11], Ennio Poretti[8], Gaetano Scandariato[18], Sergei N. Yurchenko[20], Daniela Fantinel[16], Alberto Galli[7], Marcello Lodi[12], Nicoletta Sanna[7] & Andrea Tozzi[7]



ExoMolOP: low-res only
High-res: only some line lists suitable (some xsecs available from e.g. Gandhi et al. 2020)

Molecular cross-sections for high-resolution spectroscopy of super-Earths, warm Neptunes, and hot Jupiters

Siddharth Gandhi ✉, Matteo Brogi, Sergei N Yurchenko, Jonathan Tennyson, Phillip A Coles, Rebecca K Webb, Jayne L Birkby, Gloria Guilluy, George A Hawker, Nikku Madhusudhan ... Show more

Monthly Notices of the Royal Astronomical Society, Volume 495, Issue 1, June 2020, Pages 224–237, https://doi.org/10.1093/mnras/staa981
Published: 23 April 2020 **Article history ▾**

SUMMARY

- How do we know what these molecular spectra look like?

Combination of laboratory experiments and theoretical quantum methods

- What are some of the challenges associated with finding out?

Both lab and theory is challenging at high temps. Computing a line list for one species can take years, particularly for molecules with more atoms/electrons

- How do we use these in our exoplanet retrieval models

Low-res: Databases such as ExoMolOP (codes: petitRADTRANS, ARCiS, TauREX, NEMESIS)

High-res: only some line lists suitable (some xsecs available from e.g. Gandhi et al. 2020)

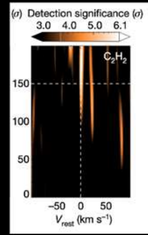
- Differences between low and high resolution data

Completeness most important for low-res but accuracy most important for high-res
(Please check a line list is suitable for high-res before using it!)

3 MAIN RETRIEVAL INGREDIENTS

ARtful modelling Code for exoplanet Science ARCiS

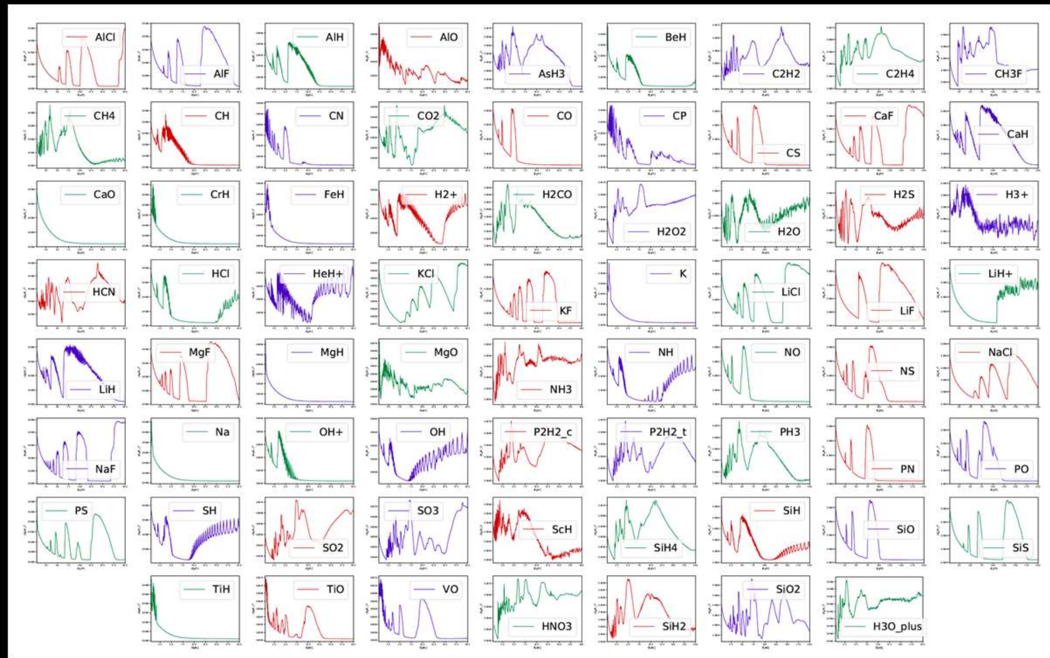
TauREx 3.0



NEMESIS

petit RADTRANS

VLT. Image credit: ESO



THANK YOU FOR LISTENING

katy@sron.nl / workshop slack (Katy Chubb)

www.exomol.com/data/data-types/opacity/

arXiv:2009.00687

The ExoMolOP Database: Cross-sections and k-tables for Molecules of Interest in High-Temperature Exoplanet Atmospheres

Katy L. Chubb[1,2★], Marco Rocchetto[2], Sergei N. Yurchenko[2], Michiel Min[1], Ingo Waldmann[2], Joanna K. Barstow[2], Paul Mollière[3], Ahmed F. Al-Refaie[2], Mark W. Phillips[4], and Jonathan Tennyson[2]