Molecular Line Lists for Exoplanets and Other Atmospheres

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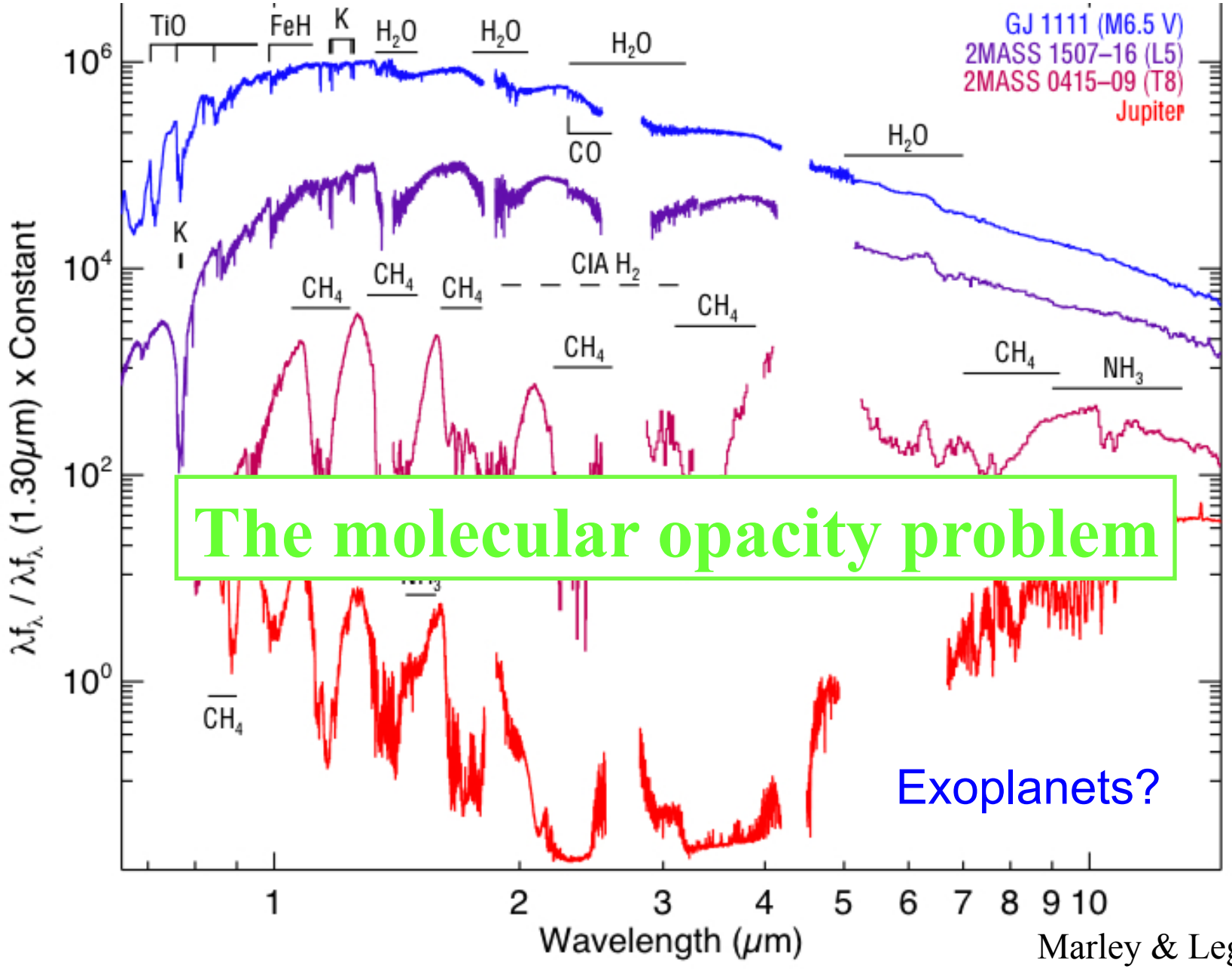
University College London

ExoMol

ICAMdata
October 2012

Artist's impression of HD189733b
C. Carreau, ESA

Cool atmospheres: dominated by molecular absorption



Marley & Leggett (2008)

Cool stars: T = 2000 – 4000 K

Thermodynamics equilibrium, 3-body chemistry

C and O combine rapidly to form CO.

M-Dwarfs: Oxygen rich, n(O) > n(C)
H_2, H_2O, TiO, ZrO, etc also grains at lower T

C-stars: Carbon rich, n(C) > n(O)
H_2, CH_4, HCN, C_3, HCCH, CS, C_2, CN, etc

S-Dwarfs: n(O) = n(C) Rare.
H_2, FeH, MgH, no polyatomics

Also (primordeal) ‘metal-free’ stars
H, H_2, He, H^-, H_3^+ only at low T

Sub-stellar objects:

CO less important

L-Dwarfs: T ~ 1500 K H_2, H_2O, CH_4 Burn D only

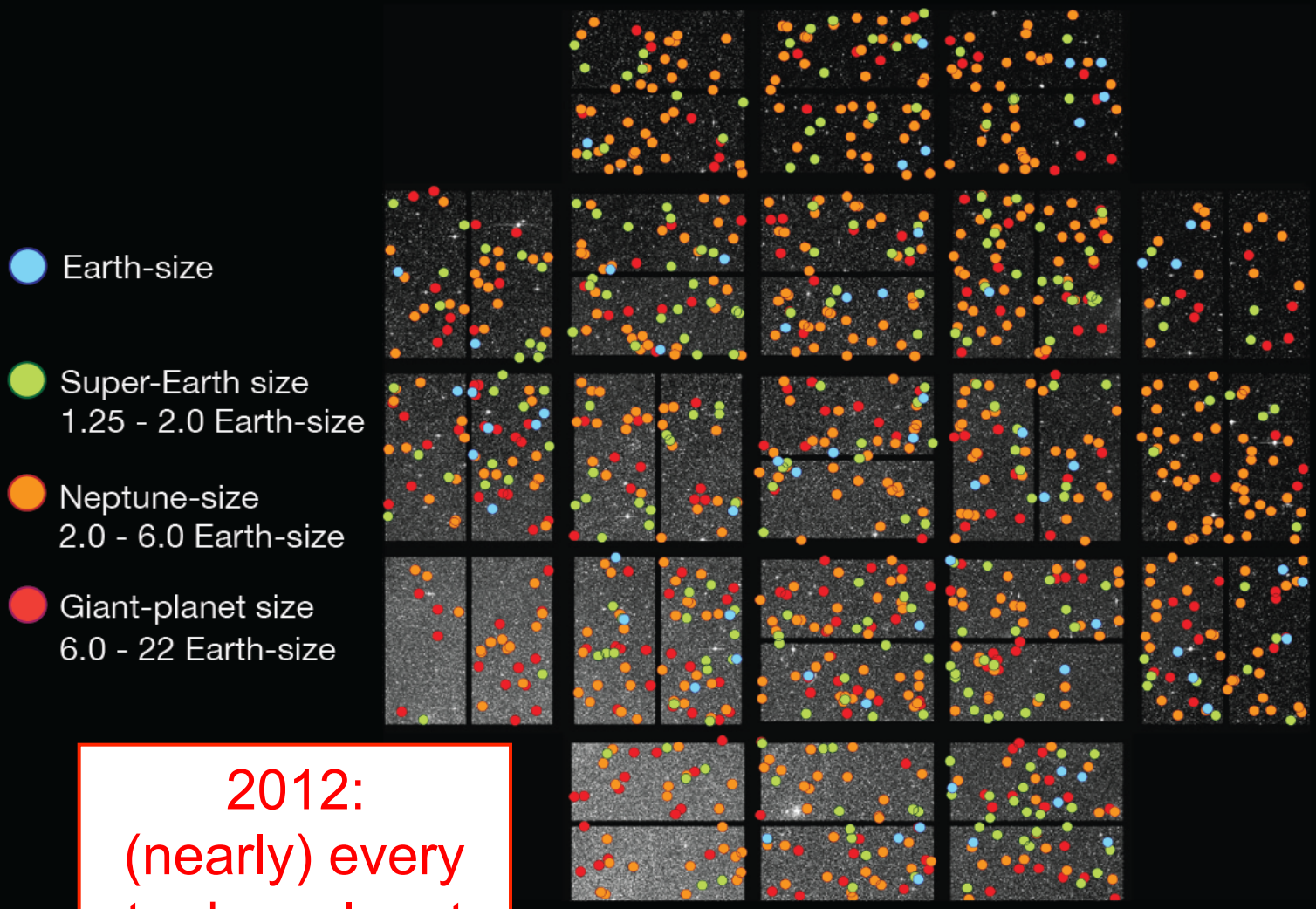
T-Dwarfs: T ~ 1000 K 'methane stars' No nuclear synthesis

Y-Dwarfs: T ~ 500 K ammonia signature

Exoplanets: hot Jupiters
super-Earths

How common are these objects?
Deuterium burning test using HDO?

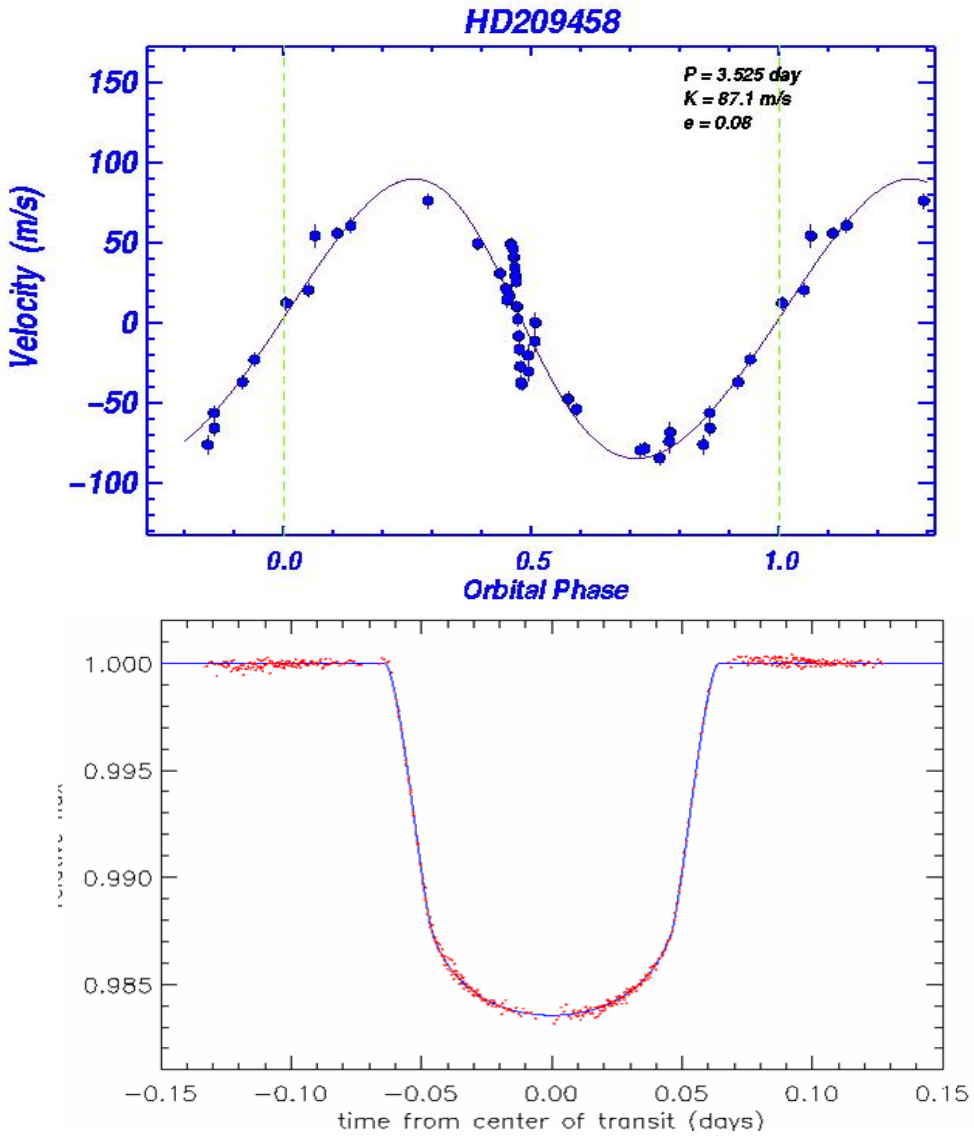
Locations of Kepler Planet Candidates



2012:
(nearly) every
star has planets

Taken from Bill Borucki's

HD 209458b



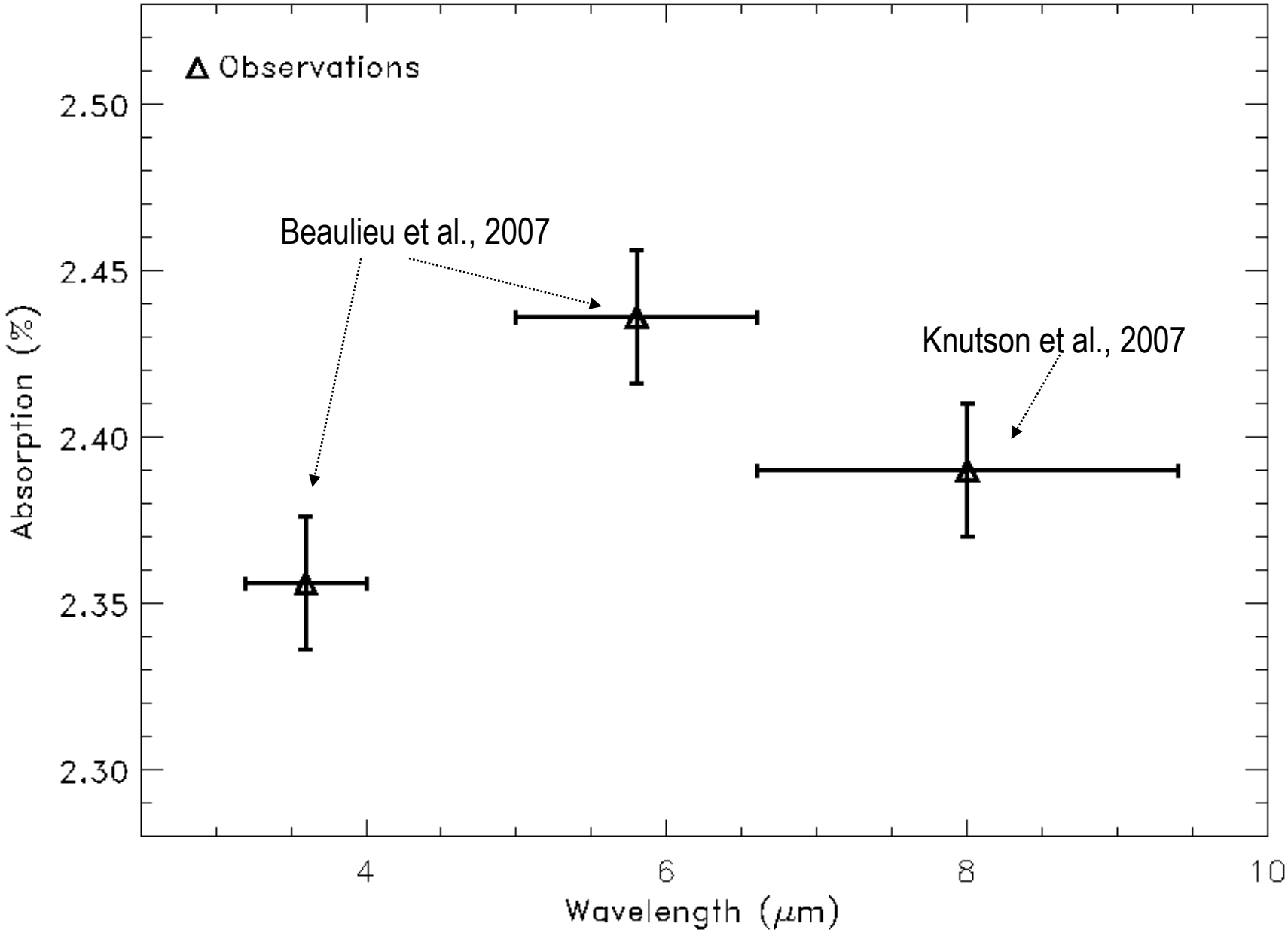
Period = 3.52 days

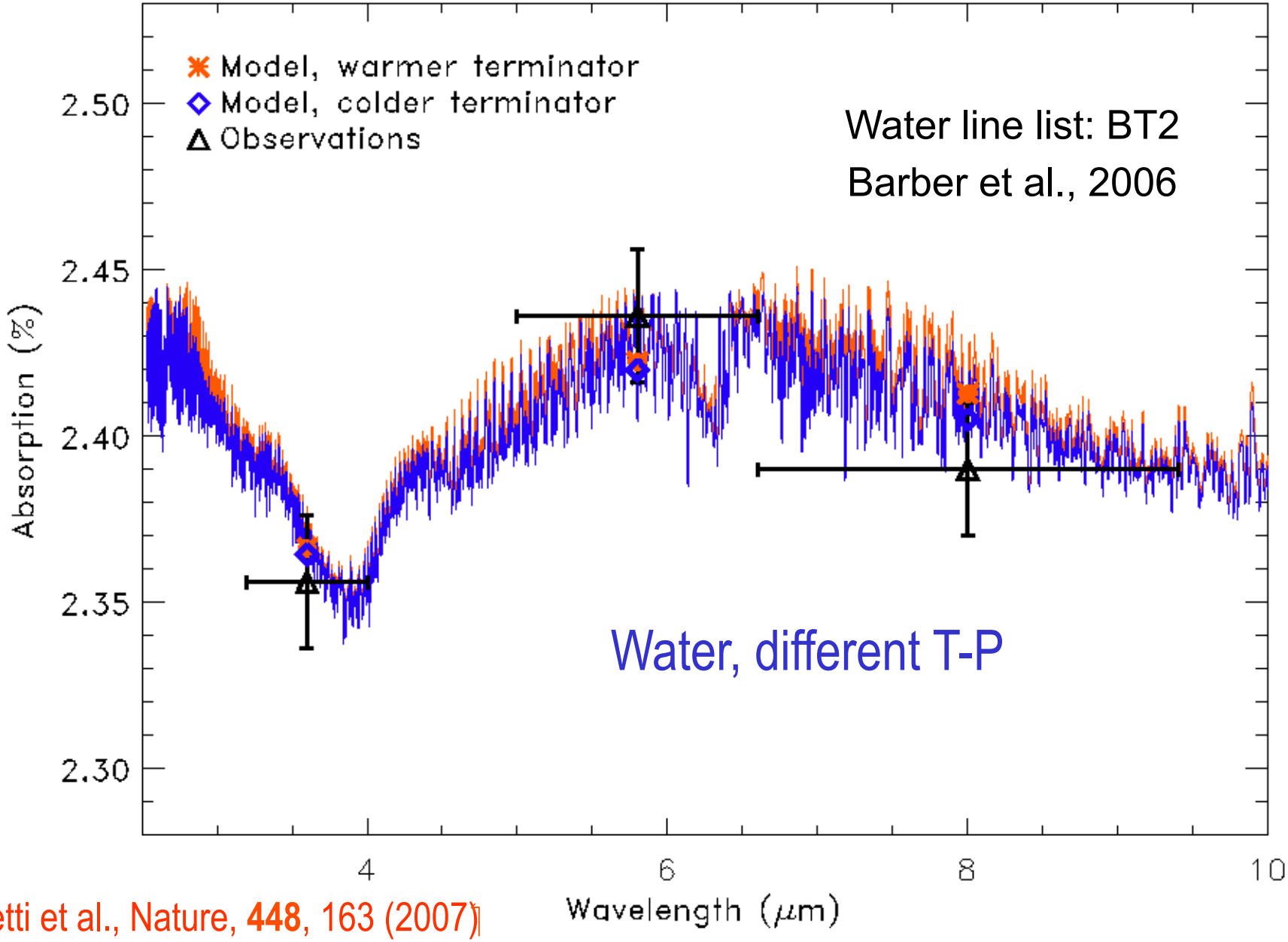
Mass = 0.69 ±0.05 $M_{Jupiter}$

Radius = 1.35 ±0.04 $R_{Jupiter}$

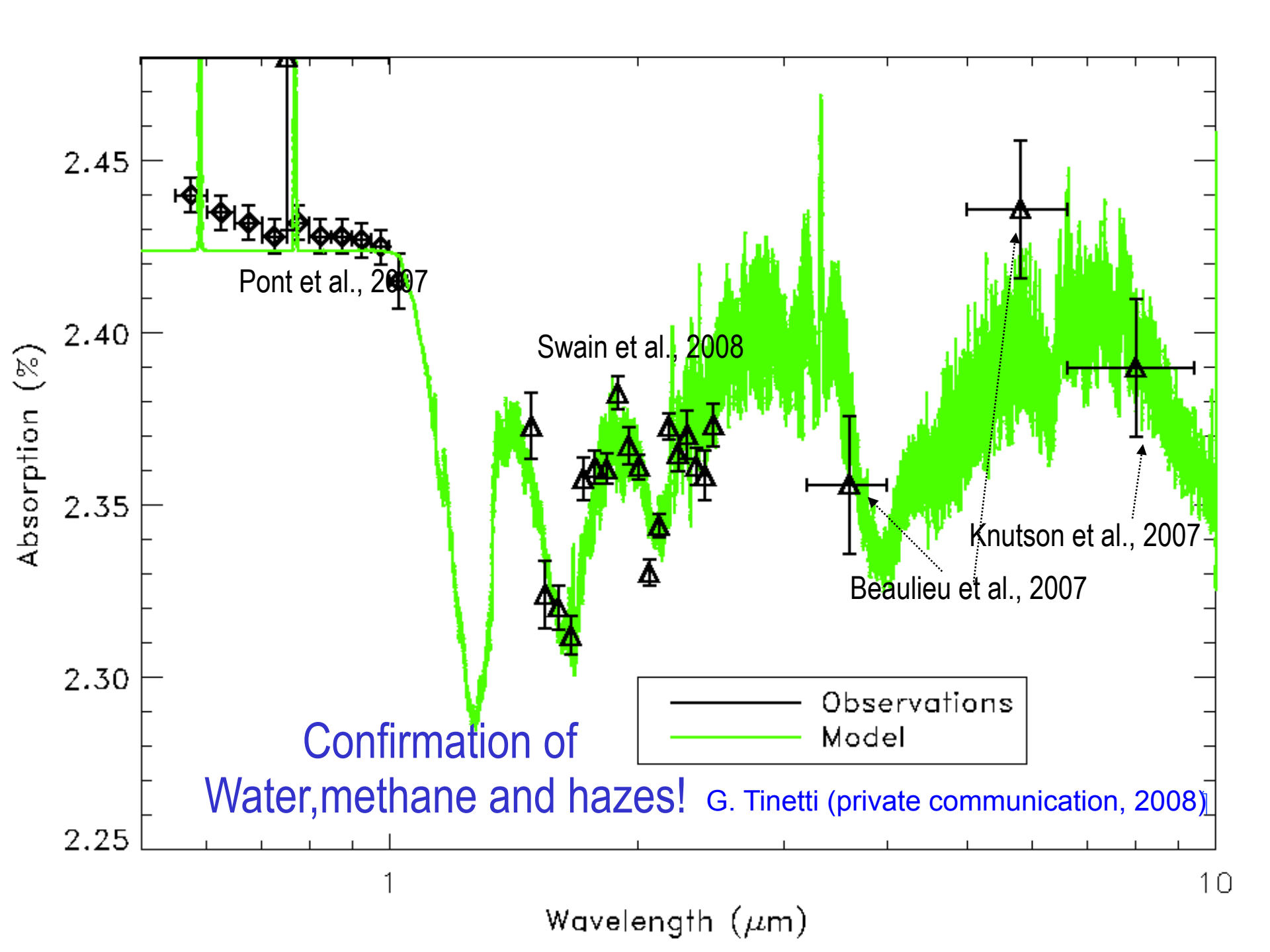
Density = 0.35 ±0.05 g/cm^3

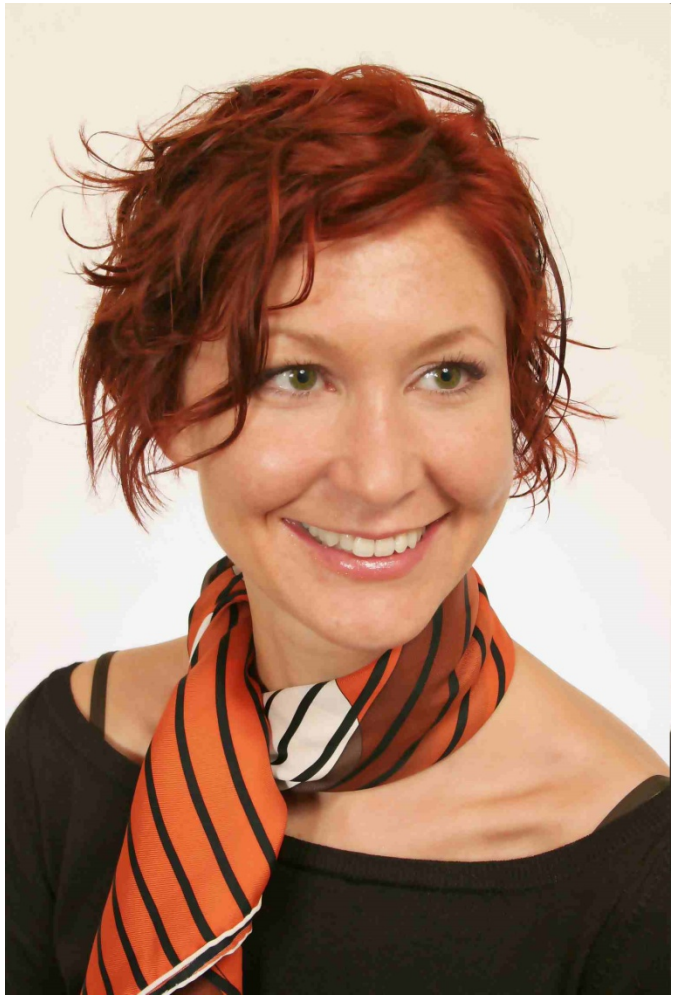
HD189733b: Primary transit with Spitzer





Tinetti et al., Nature, **448**, 163 (2007)


Absorption (%)
2.45
2.40
2.35
2.30
2.25
1
10
Wavelength (μm)
Pont et al., 2007
Swain et al., 2008
Knutson et al., 2007
Beaulieu et al., 2007
Observations
Model
Confirmation of
Water,methane and hazes!
G. Tinetti (private communication, 2008)



Giovanna Tinetti, UCL

So far discovered:

Water	H_2O
Methane	CH_4
Carbon dioxide	CO_2
Carbon monoxide	CO

HCCH / HCN degeneracy

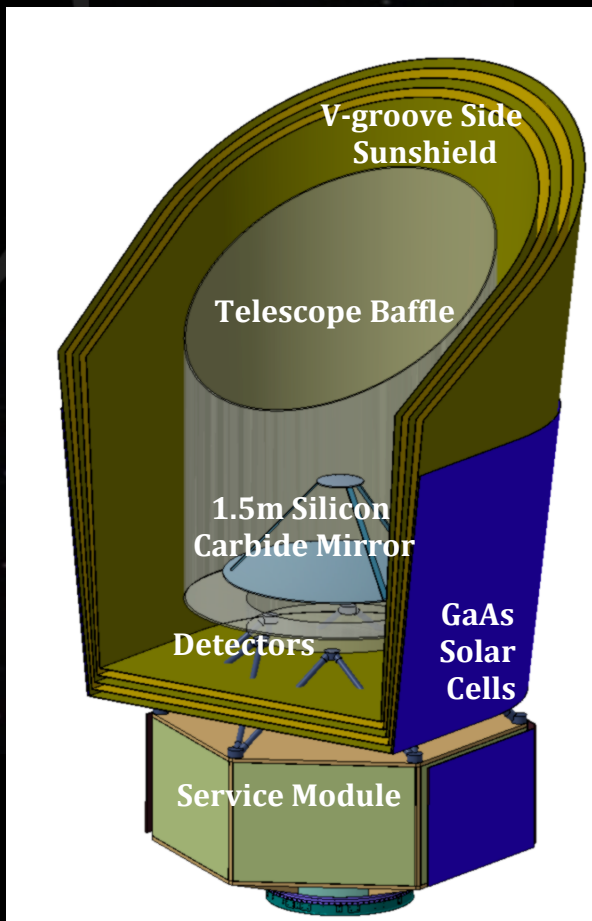
On HD189733b
with more to come

HD189733b too hot for life

Exoplanet Characterisation Observatory

ESA M3 candidate mission
PI Giovanna Tinetti (UCL)
launch 2024?

0.4 - 16 μm R ~ 300



ExoMol list of molecules

Molecular line lists for exoplanet & other atmospheres

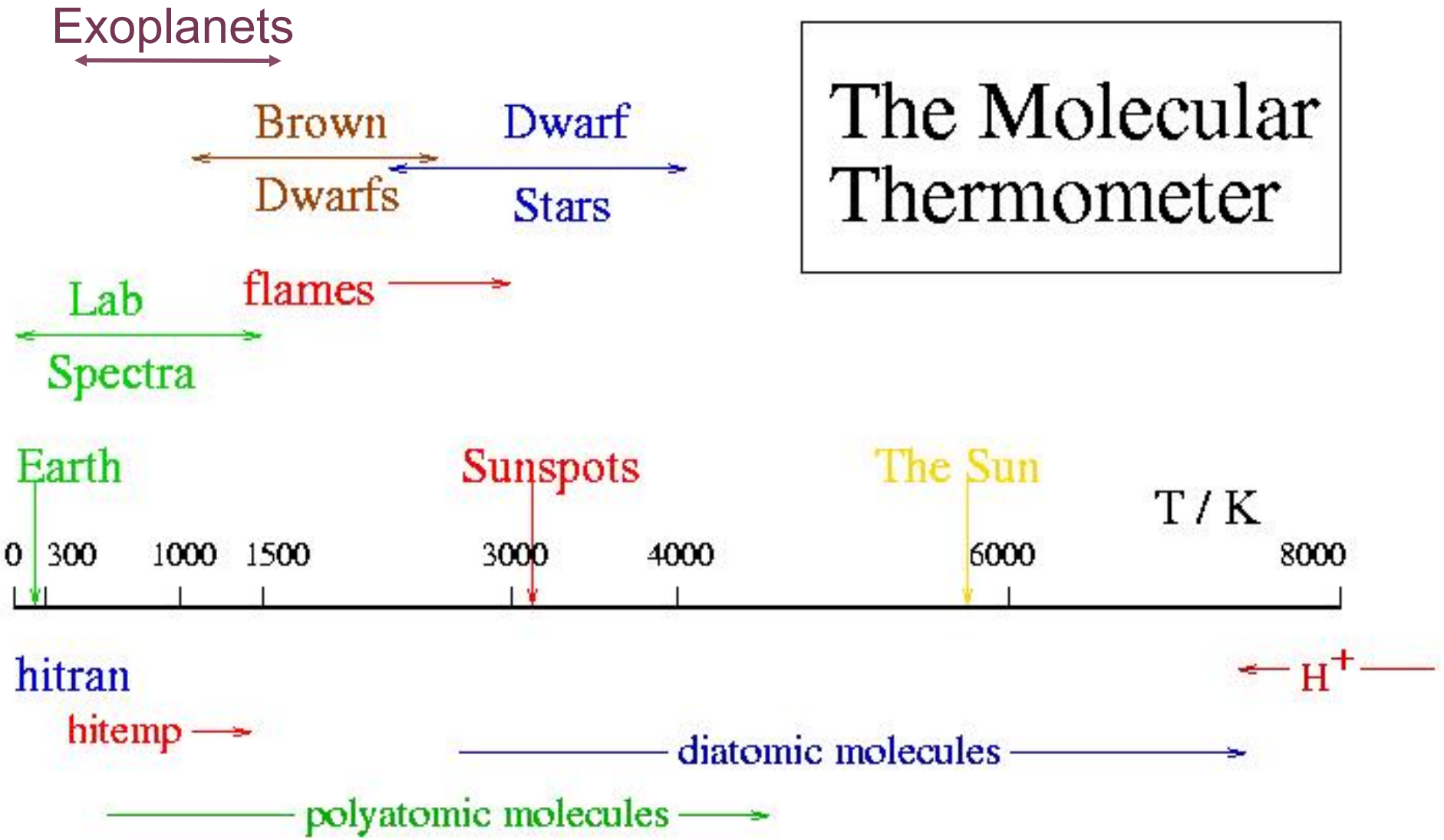
	Primordial (Metal-poor)	Terrestrial Planets (Oxidising)	Giant-Planets & Cool Stars (Reducing atmospheres)
Already available	H_2, LiH **HeH^+, H_3^+** **H_2D^+**	OH, CO_2, O_3, NO **H_2O, HDO, NH_3**	H_2, CN, CH, CO, **CO_2**, TiO **HCN/HNC, H_2O, NH_3,**
ExoMol		**O_2, CH_4, SO_2, SO_3 HOOH, H_2CO, HNO_3**	**CH_4, PH_3, C_2, C_3, HCCH, H_2S, C_2H_6, C_3H_8, VO, O_2, AlO, MgO,** **CrH, MgH, FeH, CaH, AlH, SiH, TiH, NiH, BeH, YO** **NaH, HF, HCl**

Available from elsewhere
Already calculated at UCL
Will be calculated during the ExoMol project

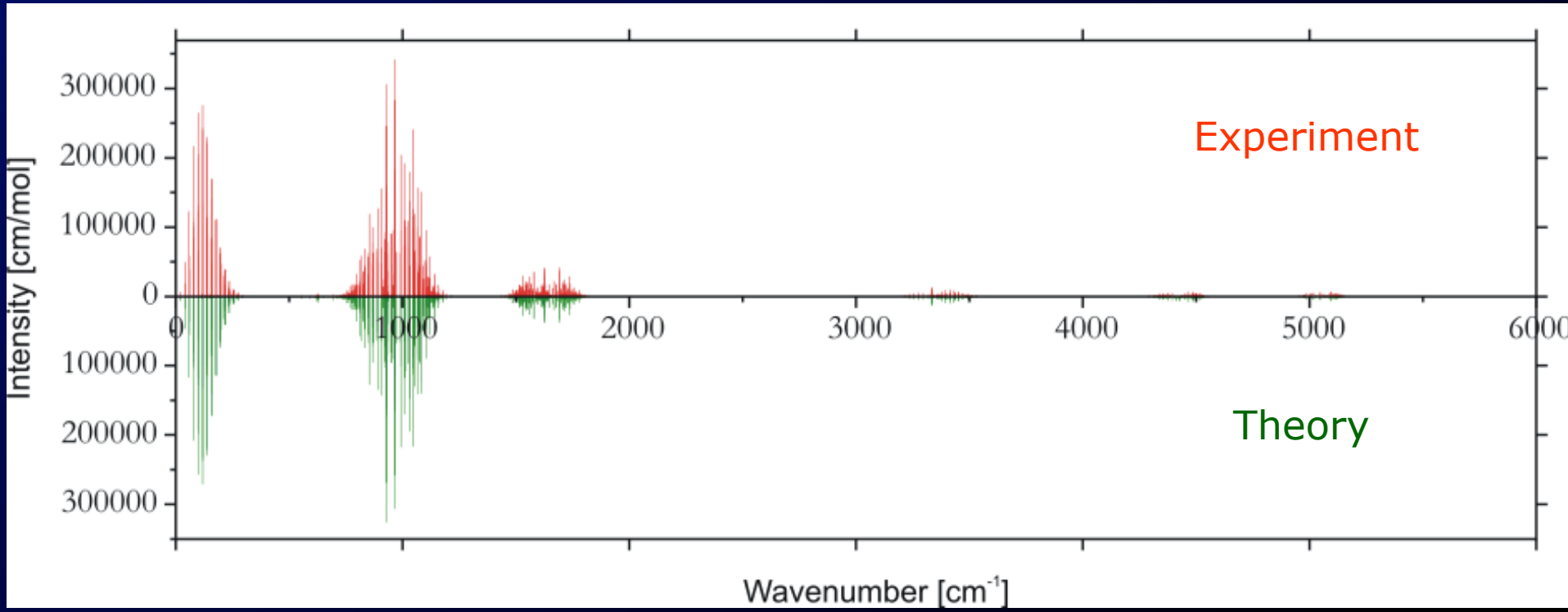
www.exomol.com

Full details:
J. Tennyson and S.N. Yurchenko, Mon. Not. Roy. Astron. Soc., 425, 21 (2012)

Why theory, not experiment?


Exoplanets
Brown Dwarfs
Dwarf Stars
The Molecular Thermometer
Lab Spectra
flames
Earth
Sunspots
The Sun
T / K
0
300
1000
1500
3000
4000
6000
8000
hitran
hitemp
H+
diatomic molecules
polyatomic molecules

Absorption (T=300K) spectrum of NH_3: Accuracy



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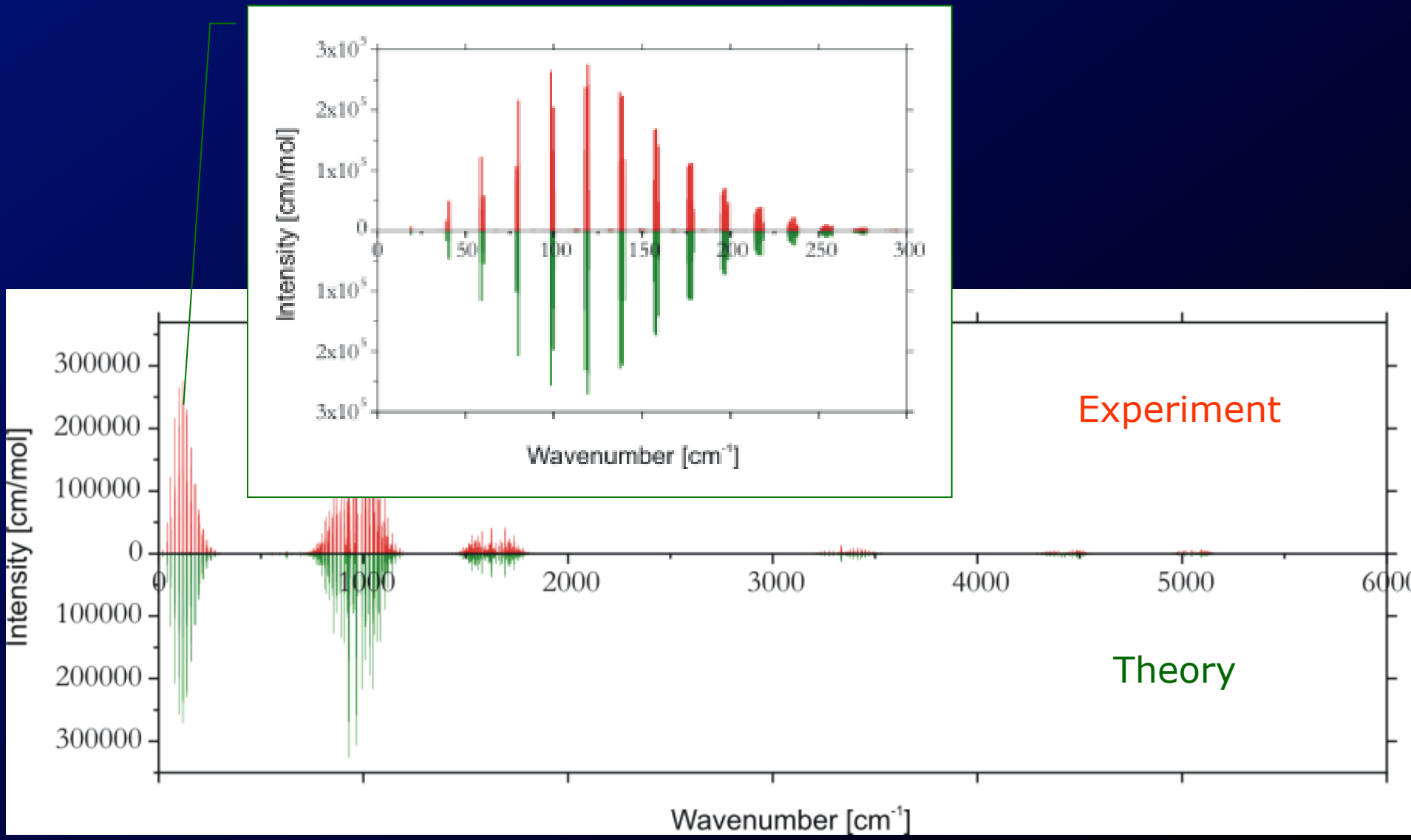
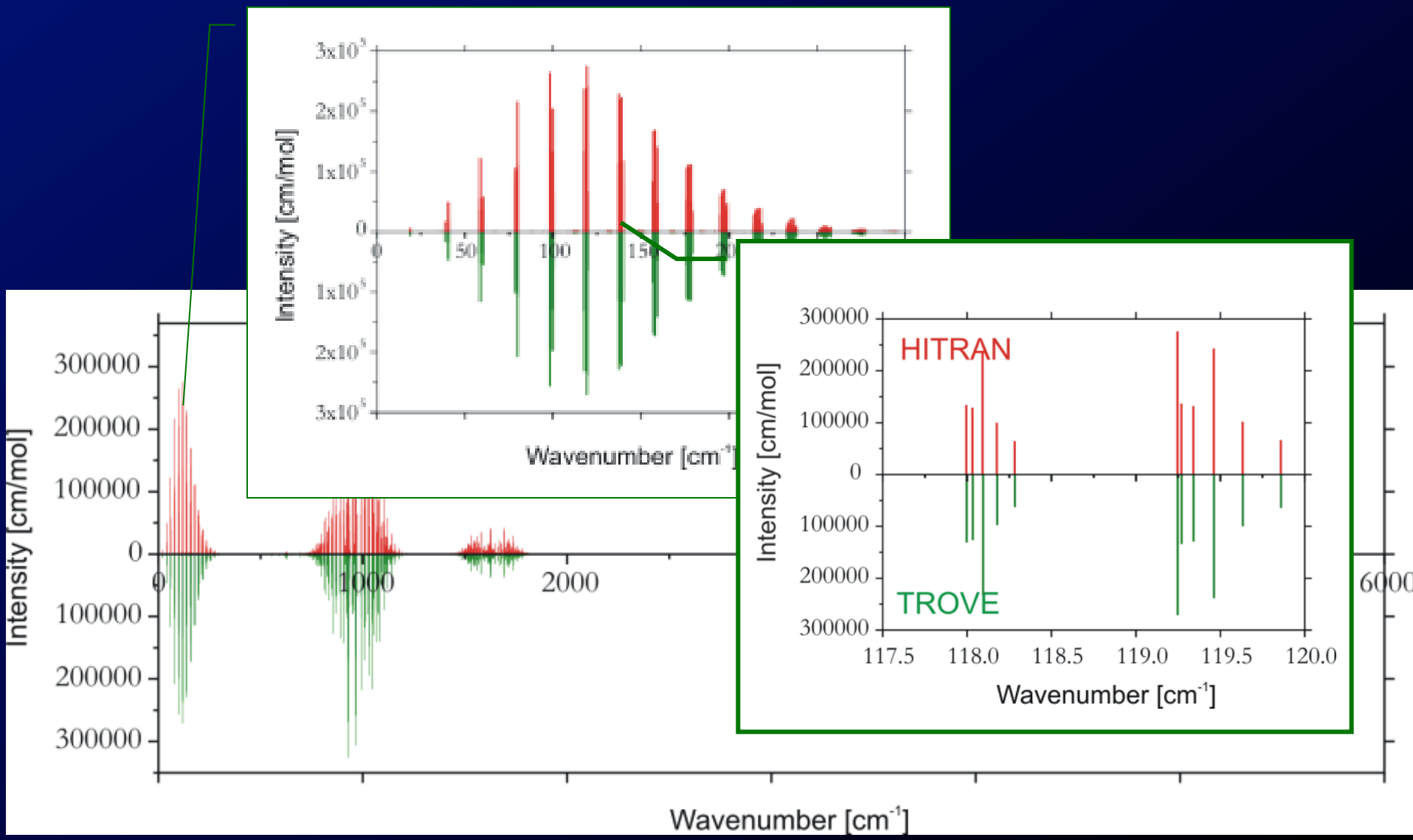
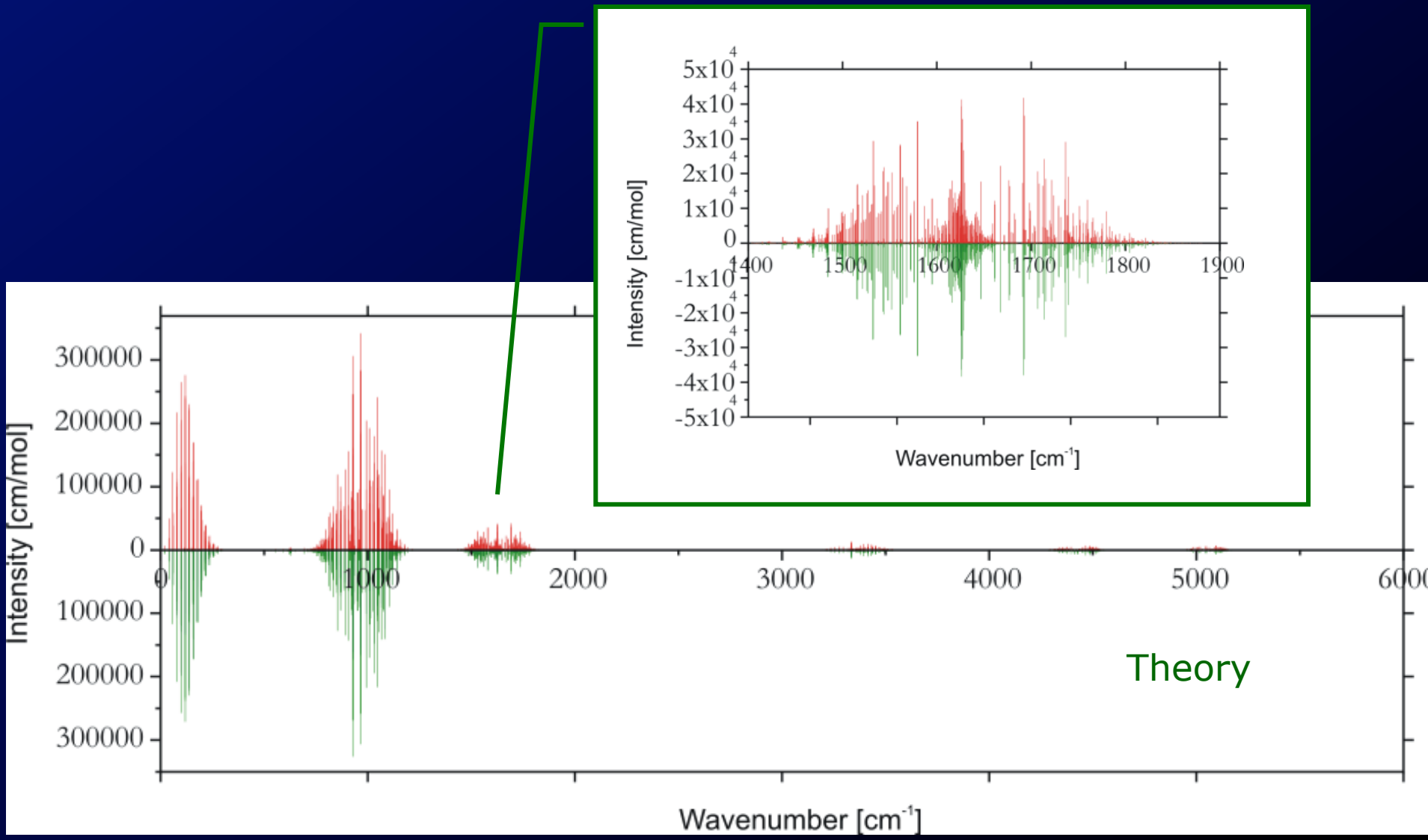


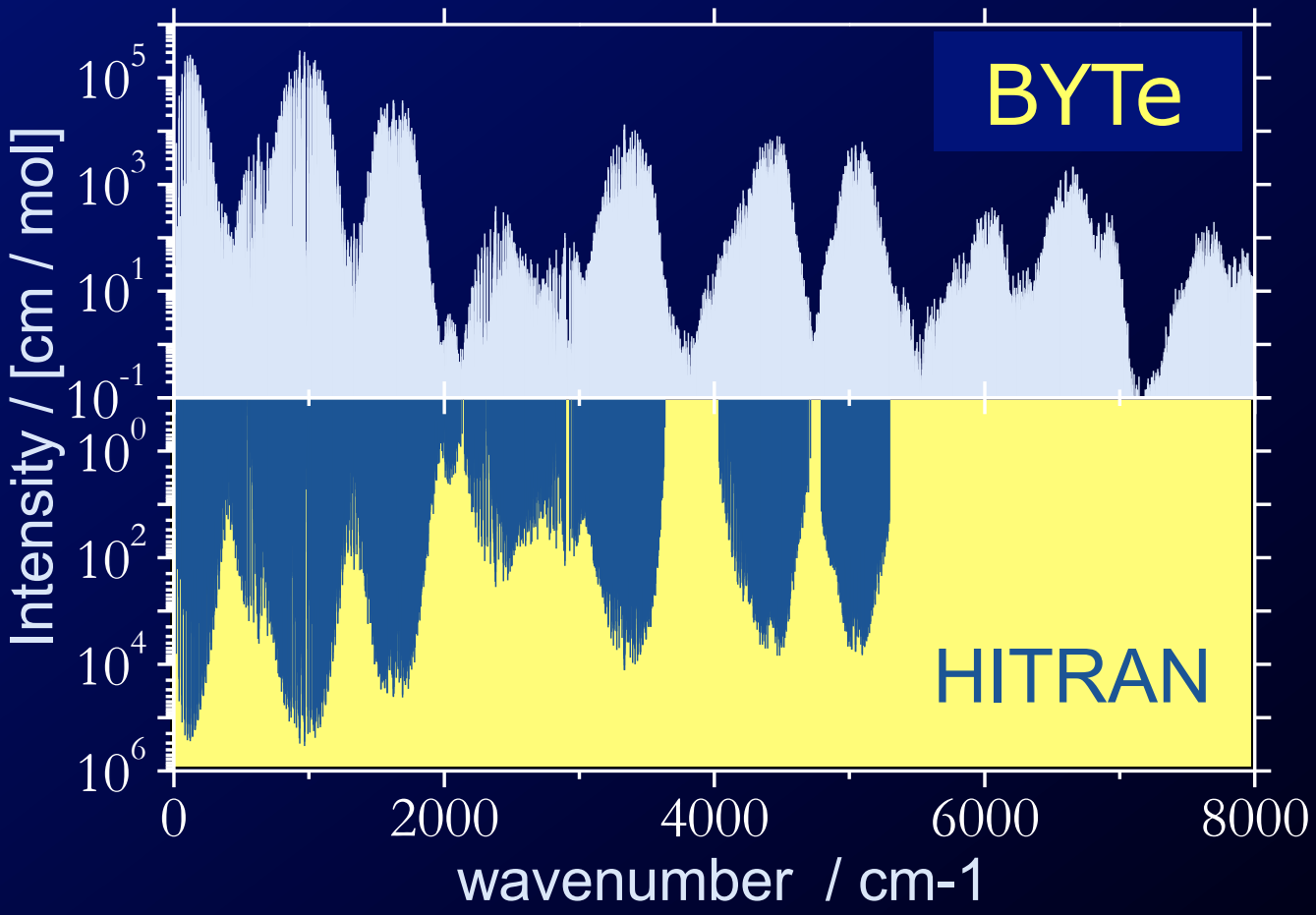
Absorption (T=300K) spectrum of NH_3: Accuracy



Absorption (T=300K) spectrum of NH_3: Accuracy

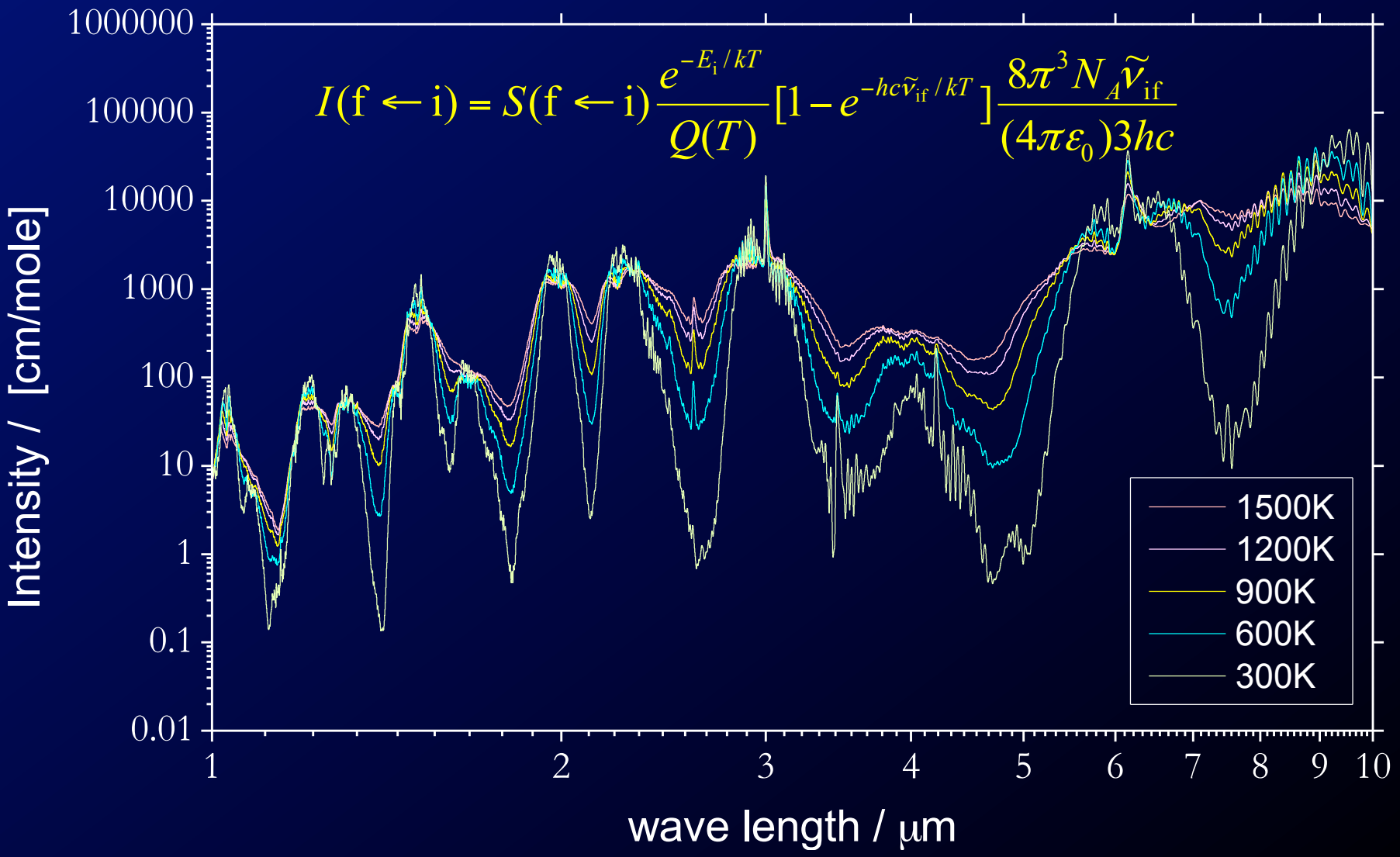


Completeness: Absorption of ammonia (T=300 K)

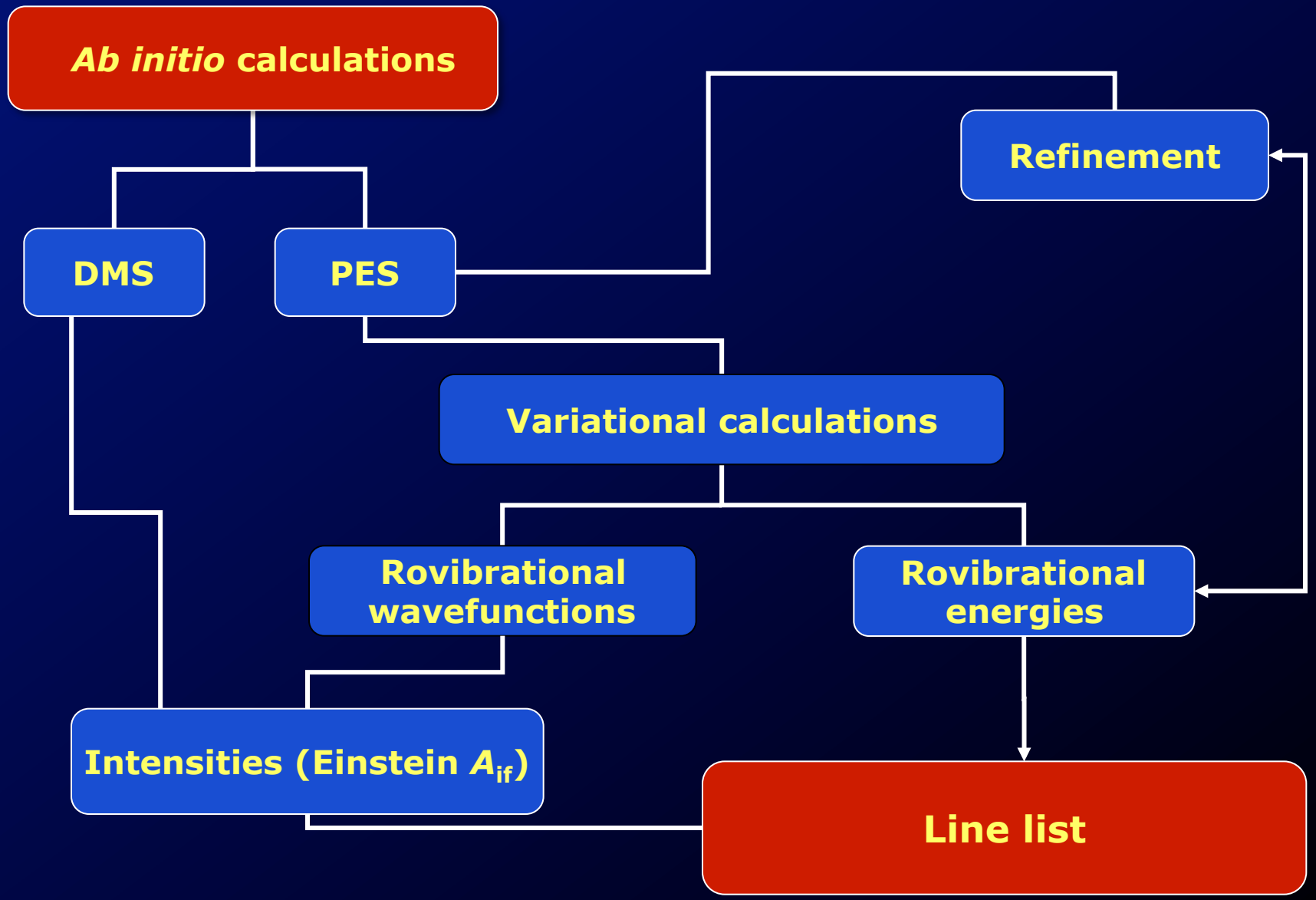


Less than 30,000 NH_3 lines known experimentally:
BYTe contains 1.1 billion lines, about 40,000 times as many!

Absorption spectra of $^{14}NH_3$: Temperature effect



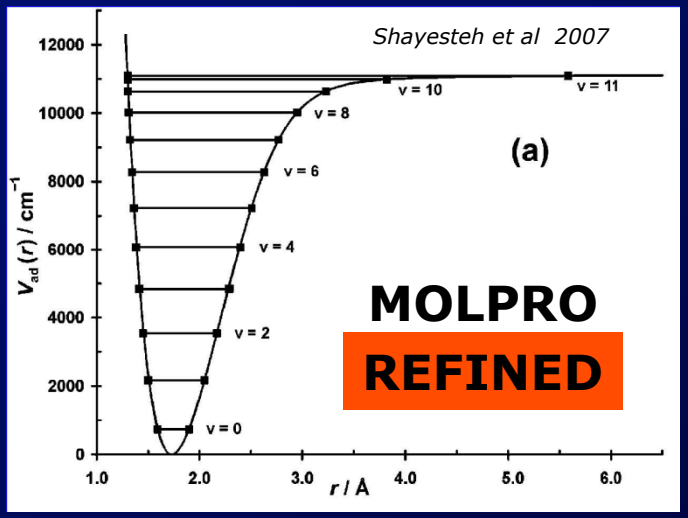
Method: Spectrum from the “first-principles”



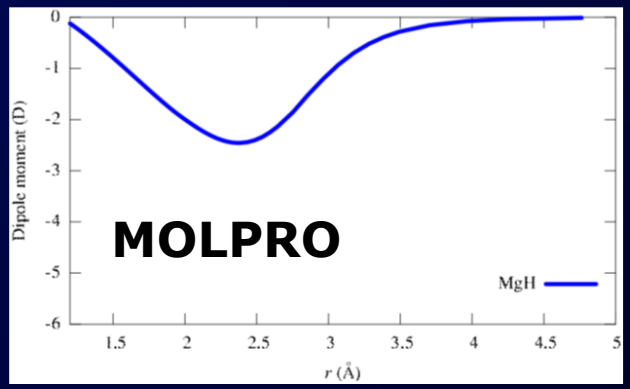
Ab initio: solve for motion of electrons

Line list: MgH

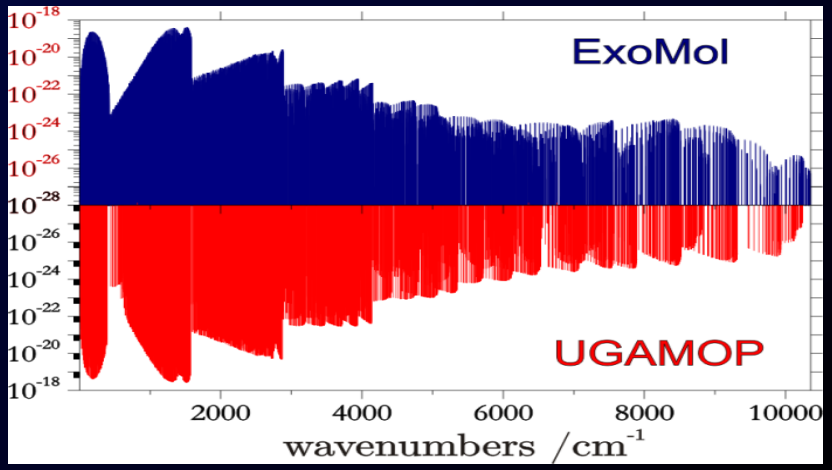
Potential energy curve



Dipole moment curve



Line list: 6690 lines, N_{max}=60



Solve for the motion of the nuclei

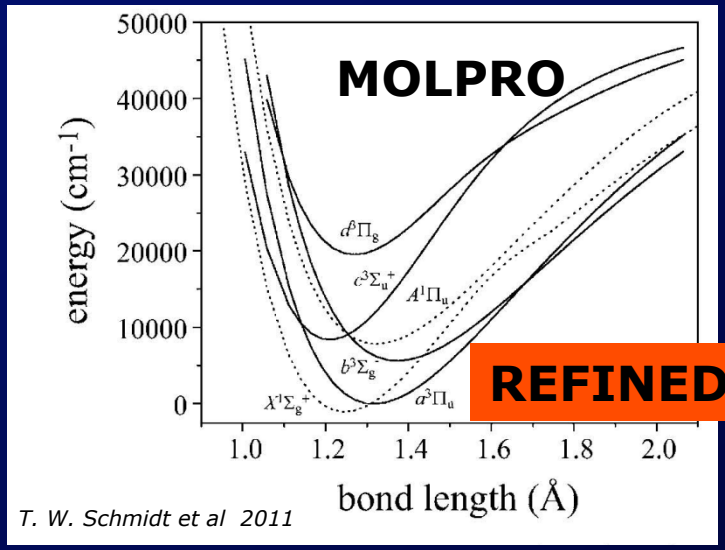
LEVEL 8.0
R. Le Roy,
Waterloo, Canada

B Yadin et al, MNRAS 425, 34 (2012)

Line list (in progress): C_2

Istvan Szabo

Potential energy

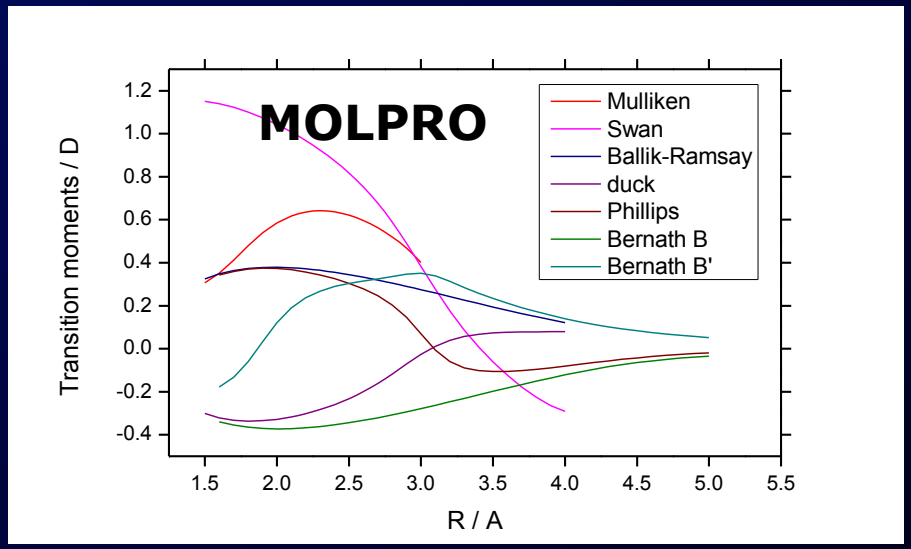


REFINED

T. W. Schmidt et al 2011

Dipole moment

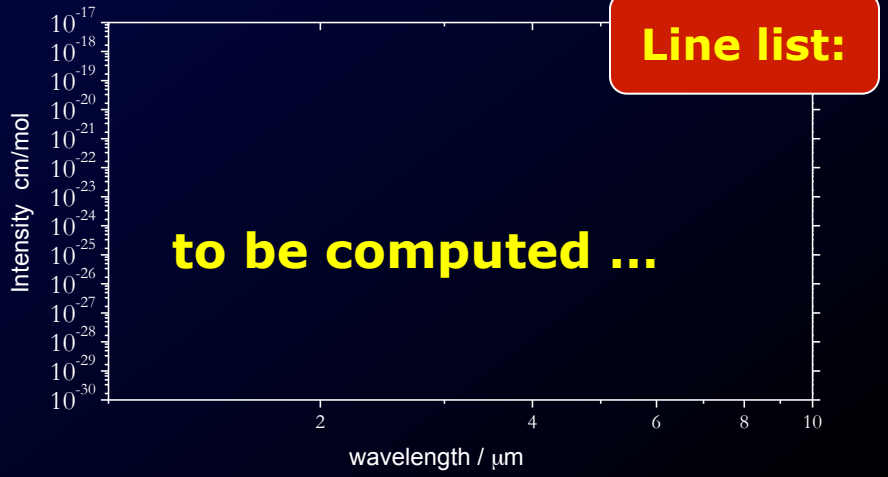
Timothy W. Scmidt
George B. Bacskay
University of Sydney



Solve for the motion of the nuclei

New program *duo*
Sergei Yurchenko

Line list:



to be computed …

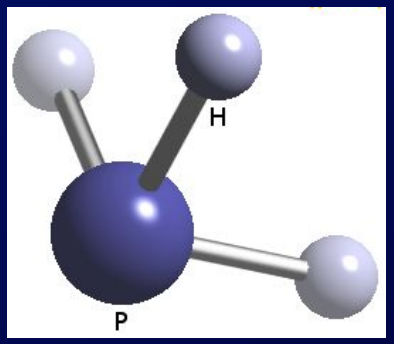
300 K line list, Clara Sousa-Silva

PH_3

Potential energy

Ab initio PES
[CCSD(T)/aug-cc-pV(Q+d)Z]
R. I. Ovsyannikov et al.
J. Chem. Phys 129, 044309 (2008).

Refined using lab spectra



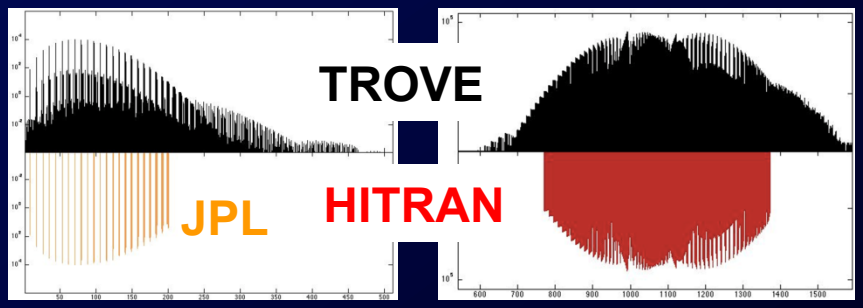
First principles Predictions of tunnelling being investigated

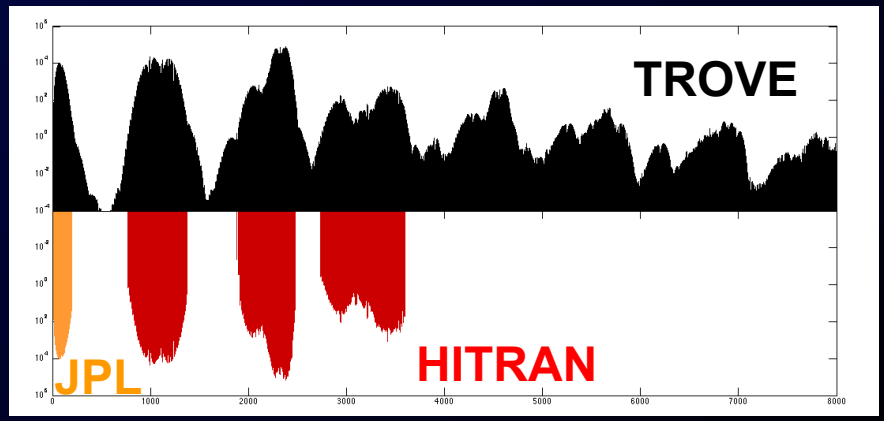
Dipole moment

Ab initio:
CCSD(T)/aug-cc-pVTZ
S.N. Yurchenko et al.
J. Mol. Spectrosc 239, 71 (2006).

Solve for the motion of the nuclei

TROVE: Yurchenko, Thiel, Jensen





T=300 K ~ 14 M transitons
Hot: will be > billion

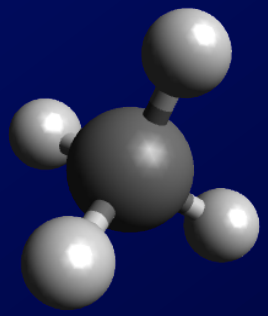
Ab initio: solve for motion of electrons

CH_4

Potential energy

9D surface
130 000
geometries

MOLPRO
CCSD(T)-f12/QZ



Ab initio
10 electrons
Ground
electronic state

Dipole moment

Three 9D surfaces
130 000
geometries

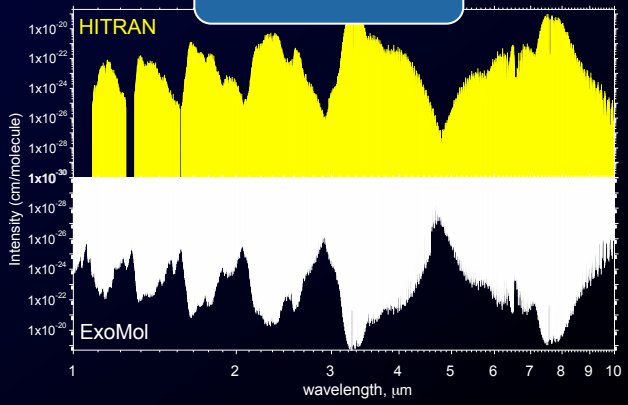
MOLPRO
CCSD(T)-f12/QZ

Solve for the motion of the nuclei

TROVE
Yurchenko, Thiel, Jensen

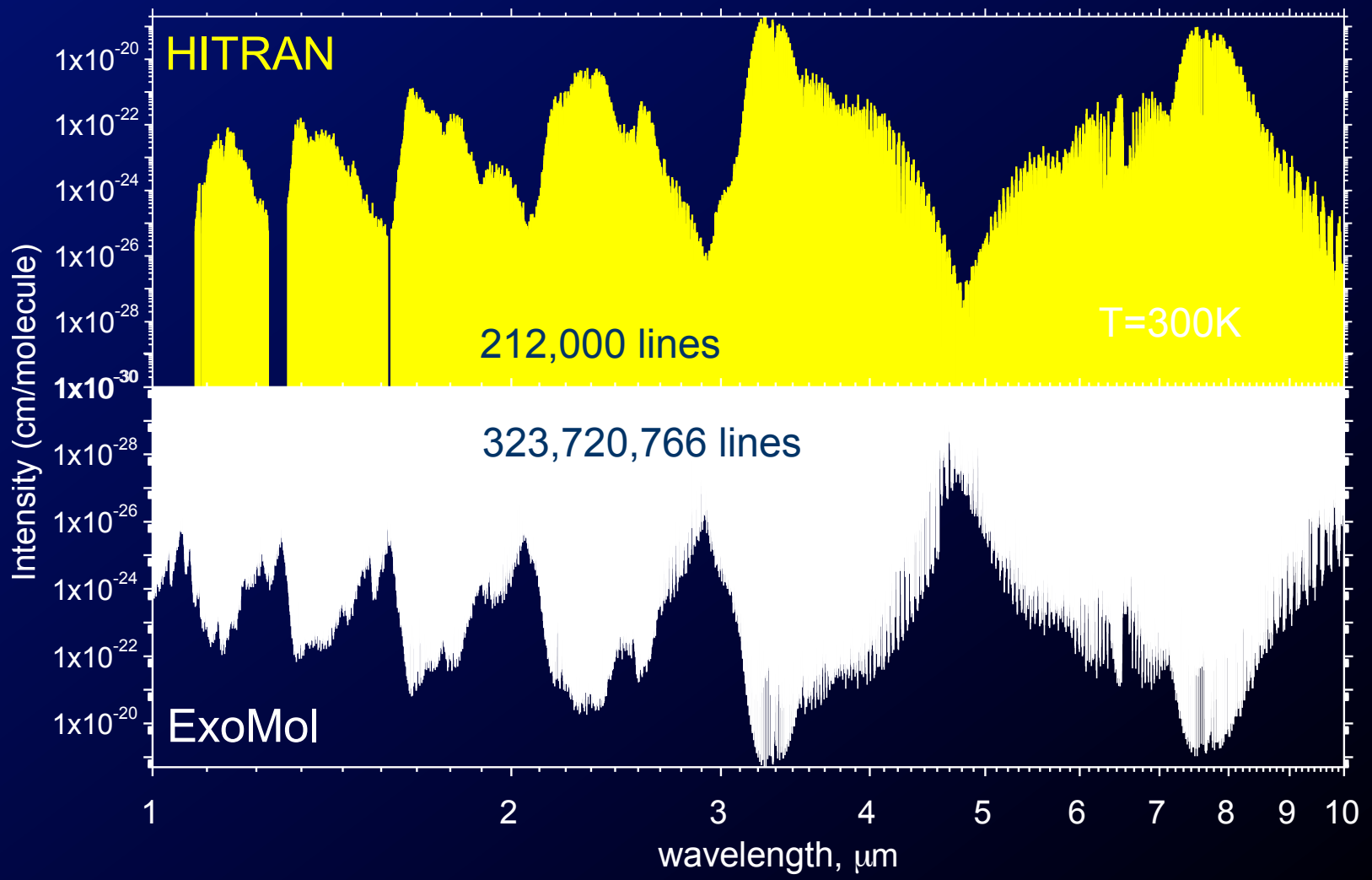
Sergei Yurchenko

Line list:



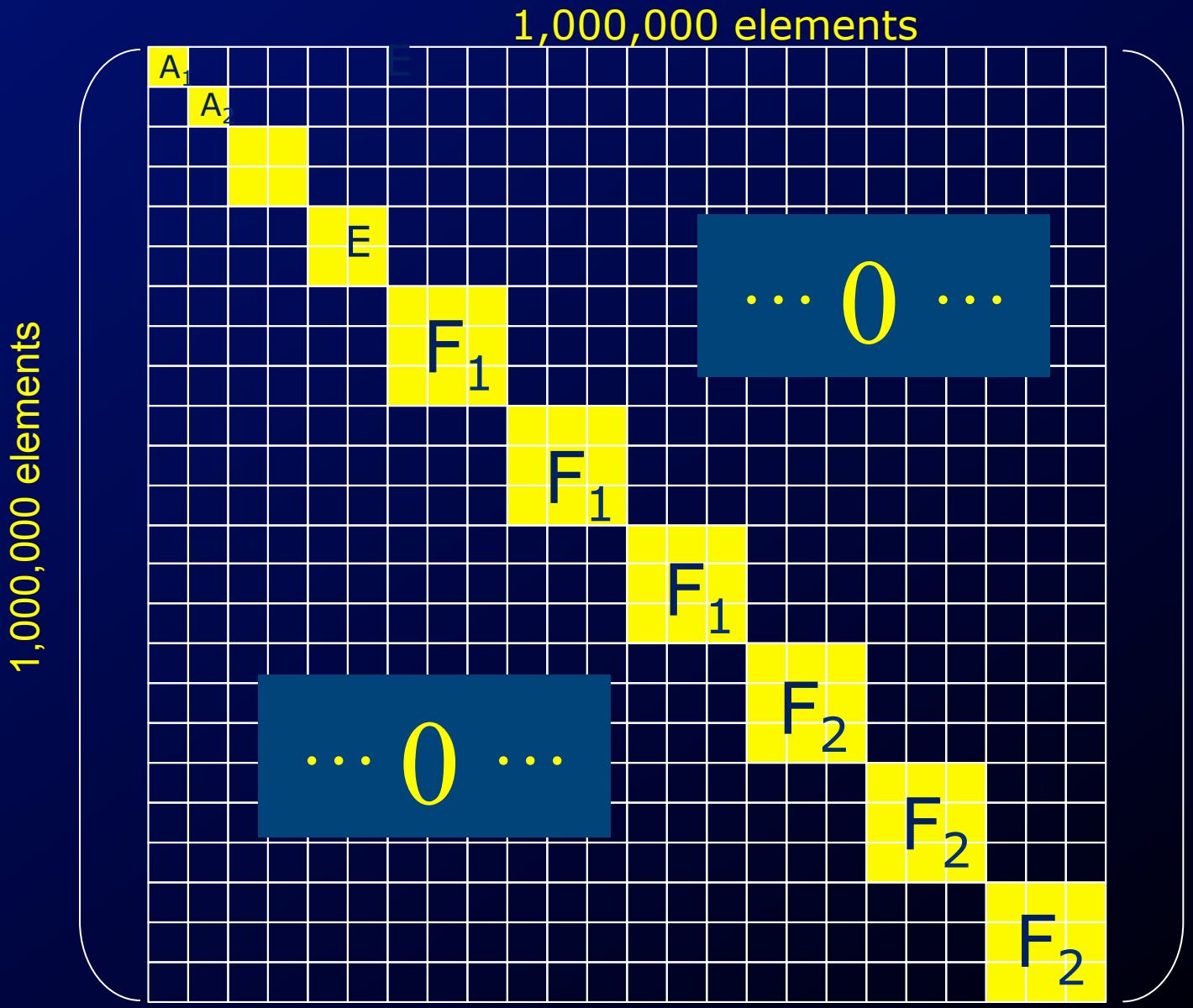
Billions of transitions

Line list for warm Methane (T>600 K, J≤34) : line positions, Einstein coefficients, lower state energies, quantum numbers



CH_4: Matrix diagonalization (Symmetry representation)

$T_d(M)$



CH_4: Matrix diagonalization (Symmetry representation)

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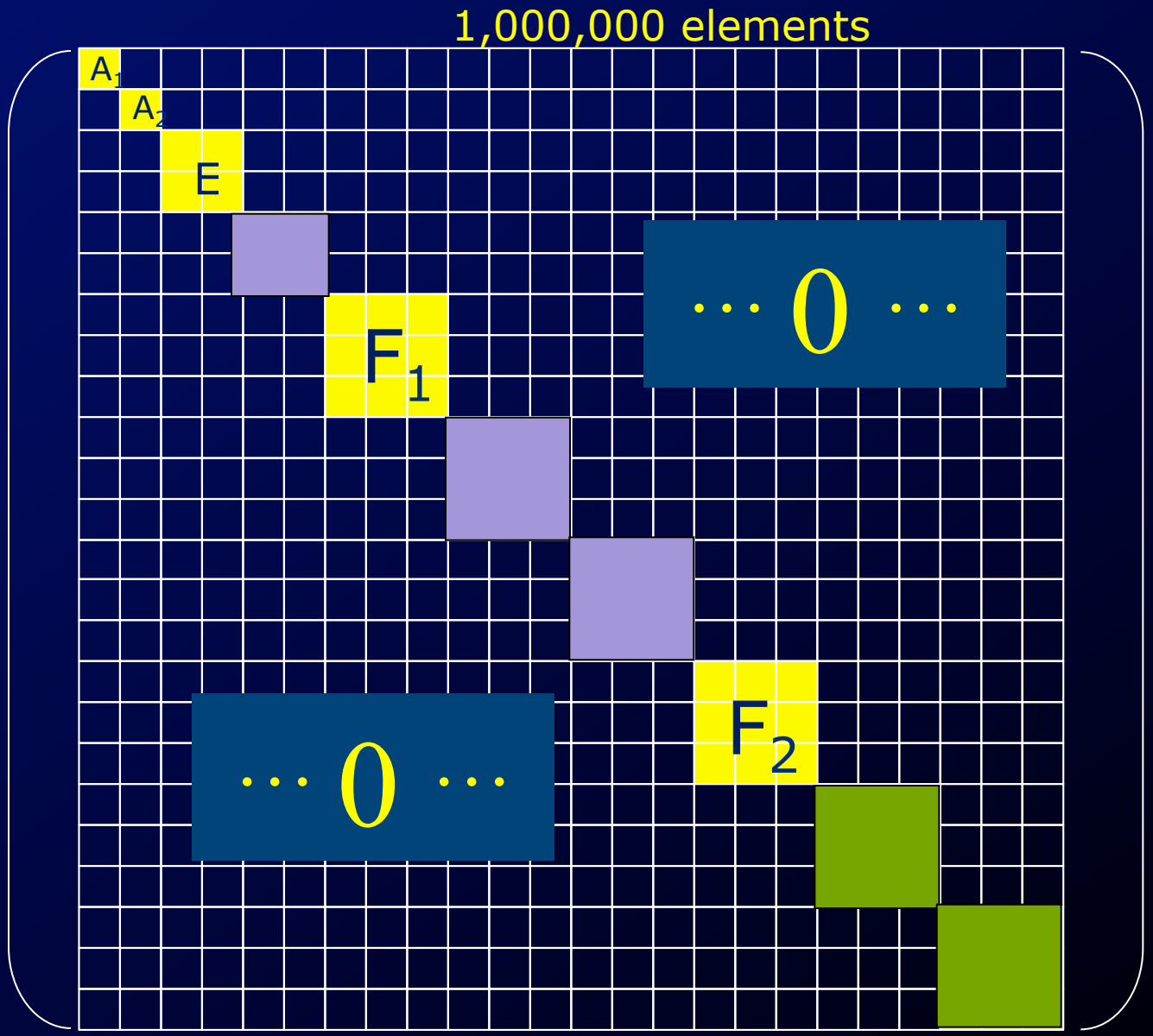


g_{ns}= 5
g_{ns}= 5

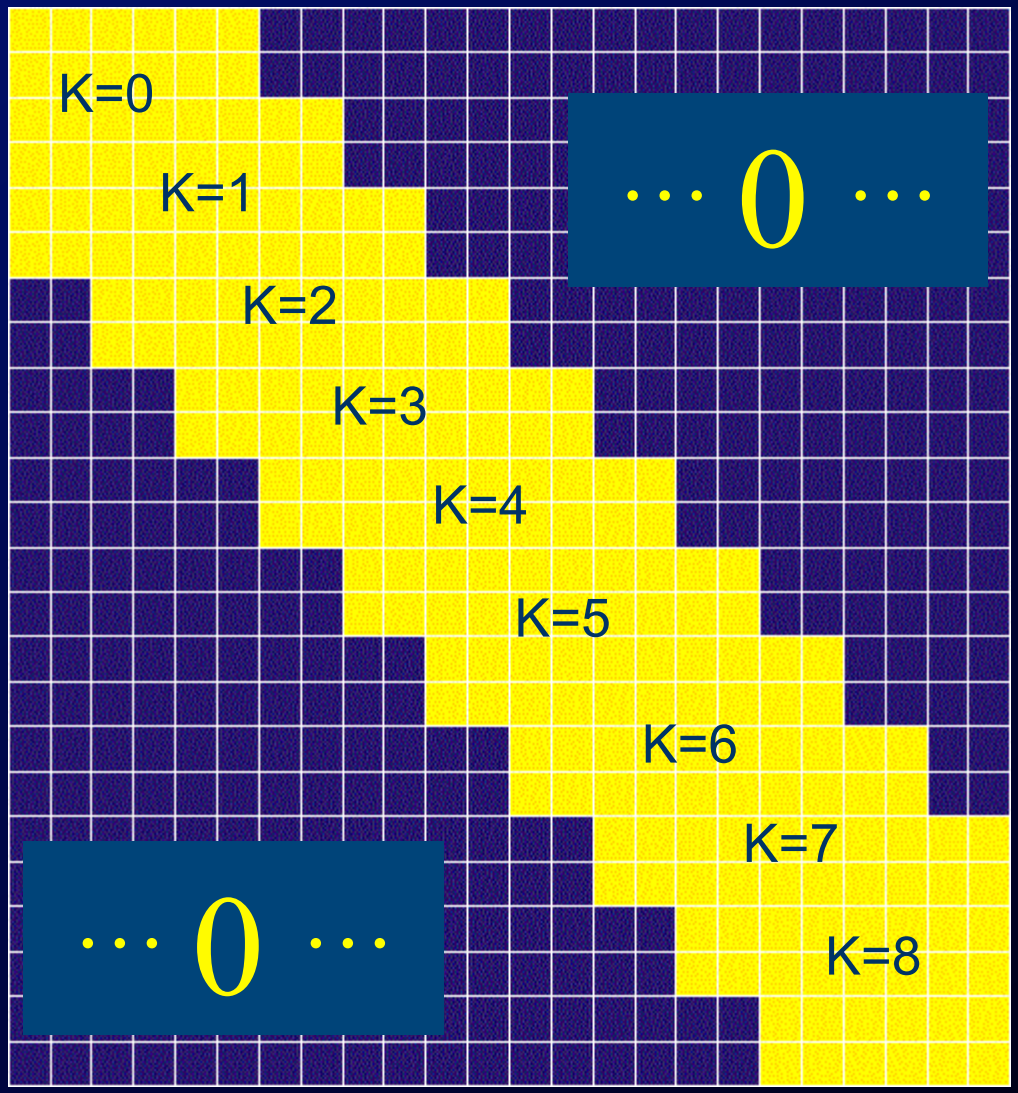
g_{ns}= 2

g_{ns}= 3

g_{ns}= 3

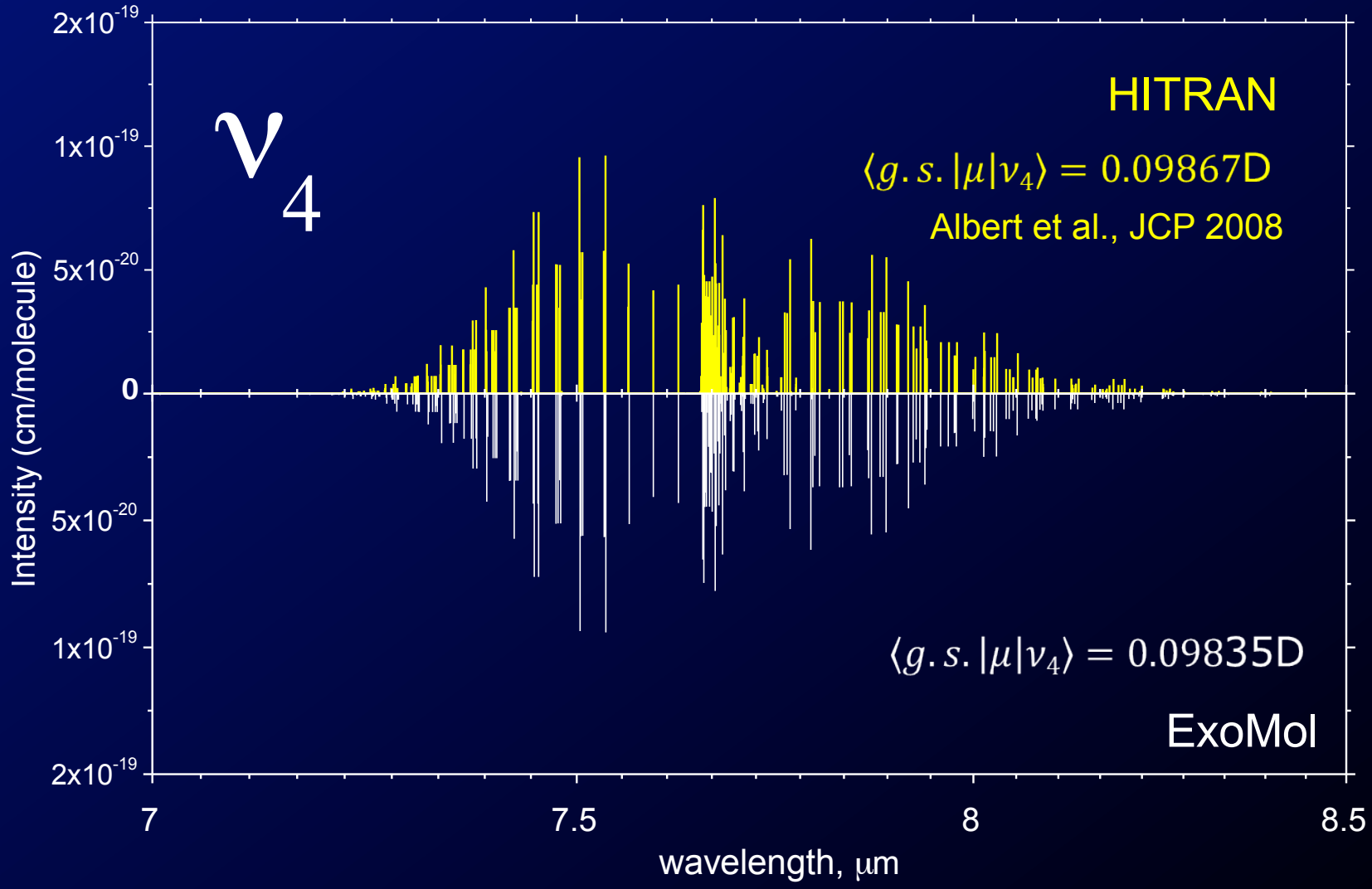
Structure of the sub-matrix: ΔK=±2 factorization (J=8)

C_s
C_{2v}
C_{3v}
D_{3h}
C_{2h}
...
...



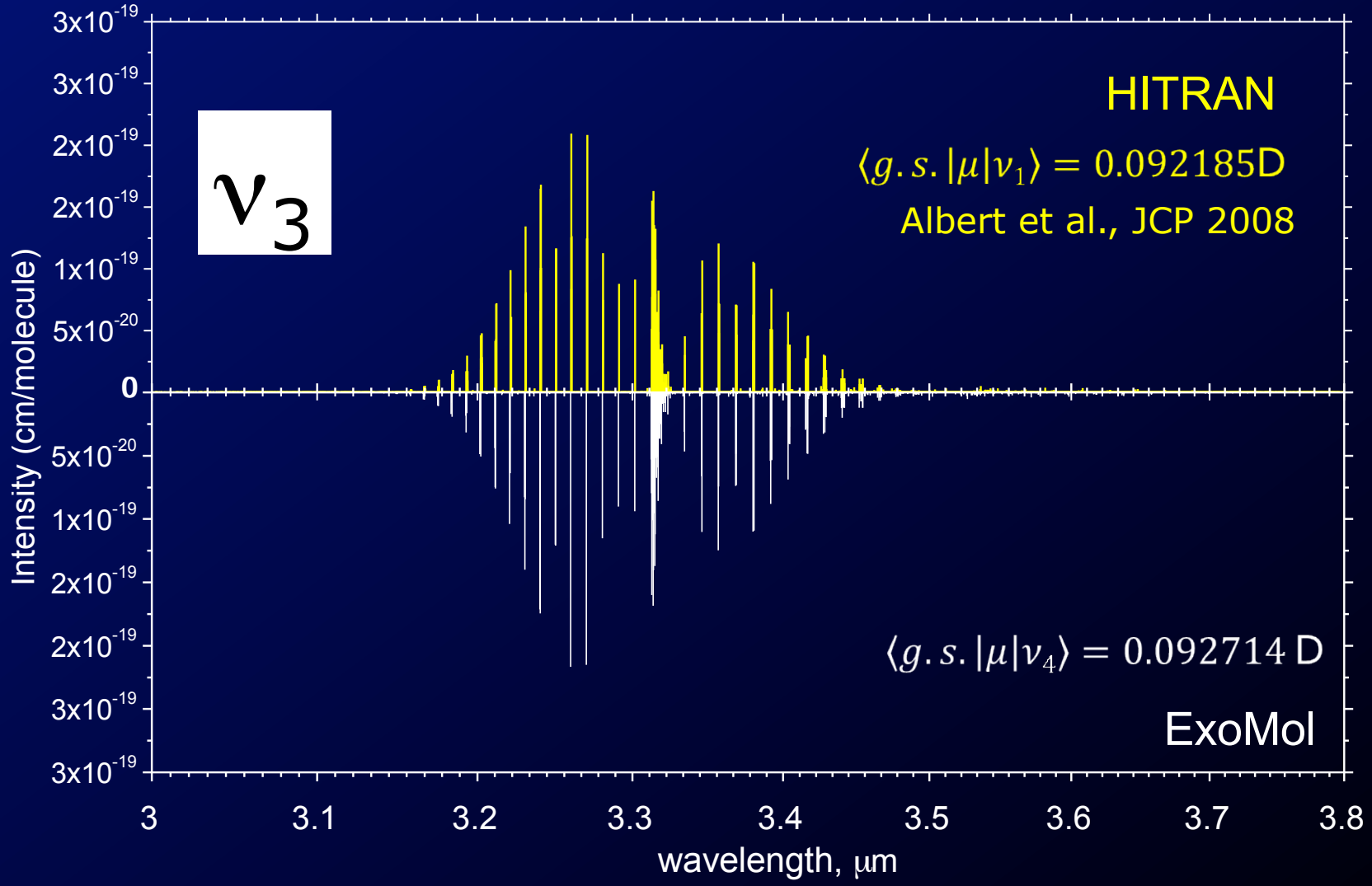
~~Td (M)~~

Absorption of Methane (T=300 K)



$$I \sim \langle g.s.|\mu|\nu_4\rangle^2$$

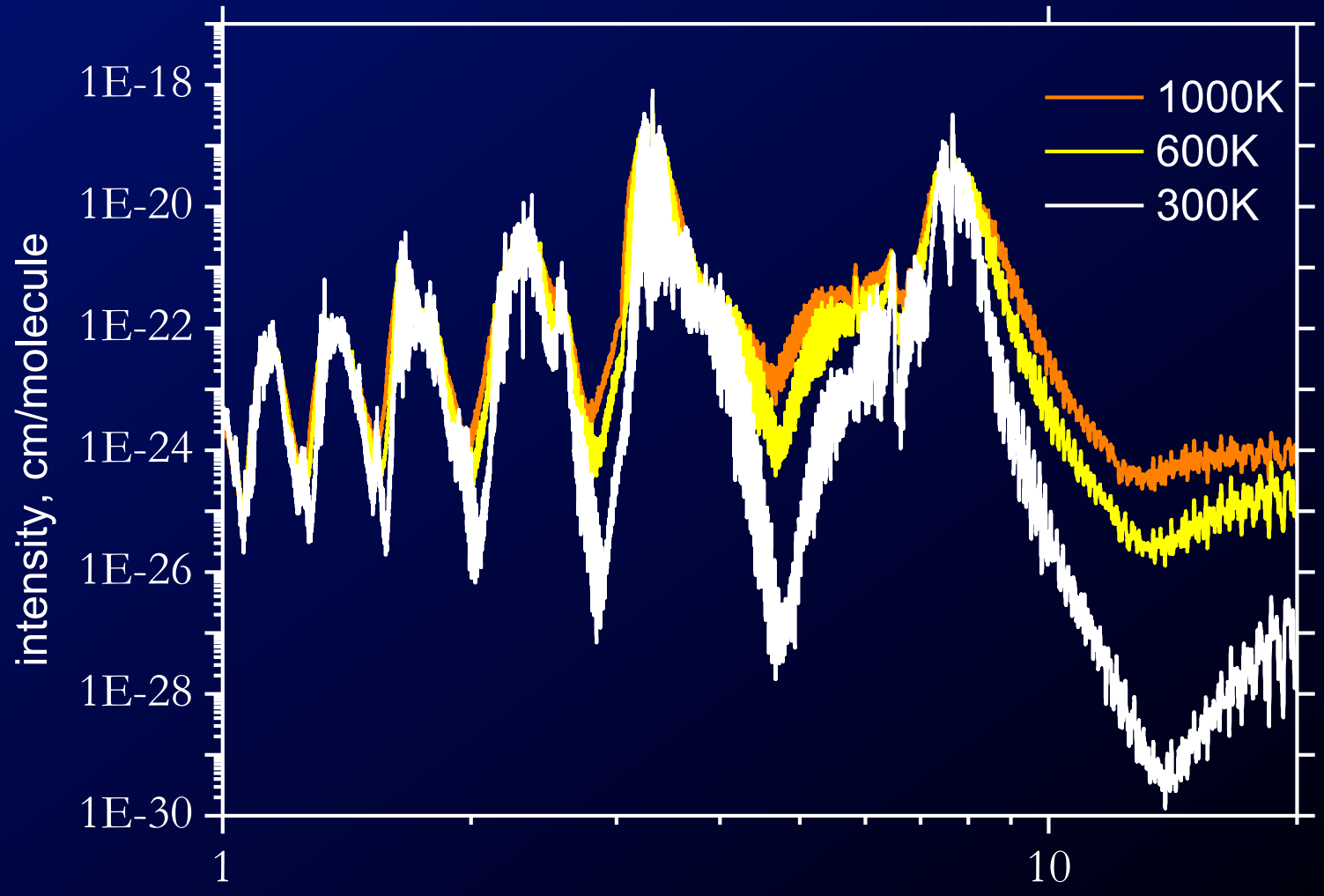
Absorption of Methane (T=300 K)



$$I \sim \langle g.s.|\mu|\nu_4\rangle^2$$

Absorption spectra of CH_4: Temperature effect

$$I(\mathrm{f} \leftarrow \mathrm{i}) = S(\mathrm{f} \leftarrow \mathrm{i}) \frac{e^{-E_\mathrm{i}/kT}}{Q(T)} [1 - e^{-hc\tilde{\nu}_\mathrm{if}/kT}] \frac{8\pi^3 N_A \tilde{\nu}_\mathrm{if}}{(4\pi\varepsilon_0)3hc}$$



BT2 linelist

Barber et al, MNRAS 368, 1087 (2006).

http://www.tampa.phys.ucl.ac.uk/ftp/astrodata/water/BT2/

- 50,000 processor hours.
- Wavefunctions > 0.8 terabites
- 221,100 energy levels (all to J=50, E = 30,000 cm^{-1})
  14,889 experimentally known
- 506 Million transitions (PS list has 308M)
  >100,000 experimentally known with intensities

$\forall \rightarrow$ Partition function 99.9915% of Vidler & Tennyson's value at 3,000K

Energy file: N J sym n E/cm^{-1} v_1 v_2 v_3 J K_a K_c

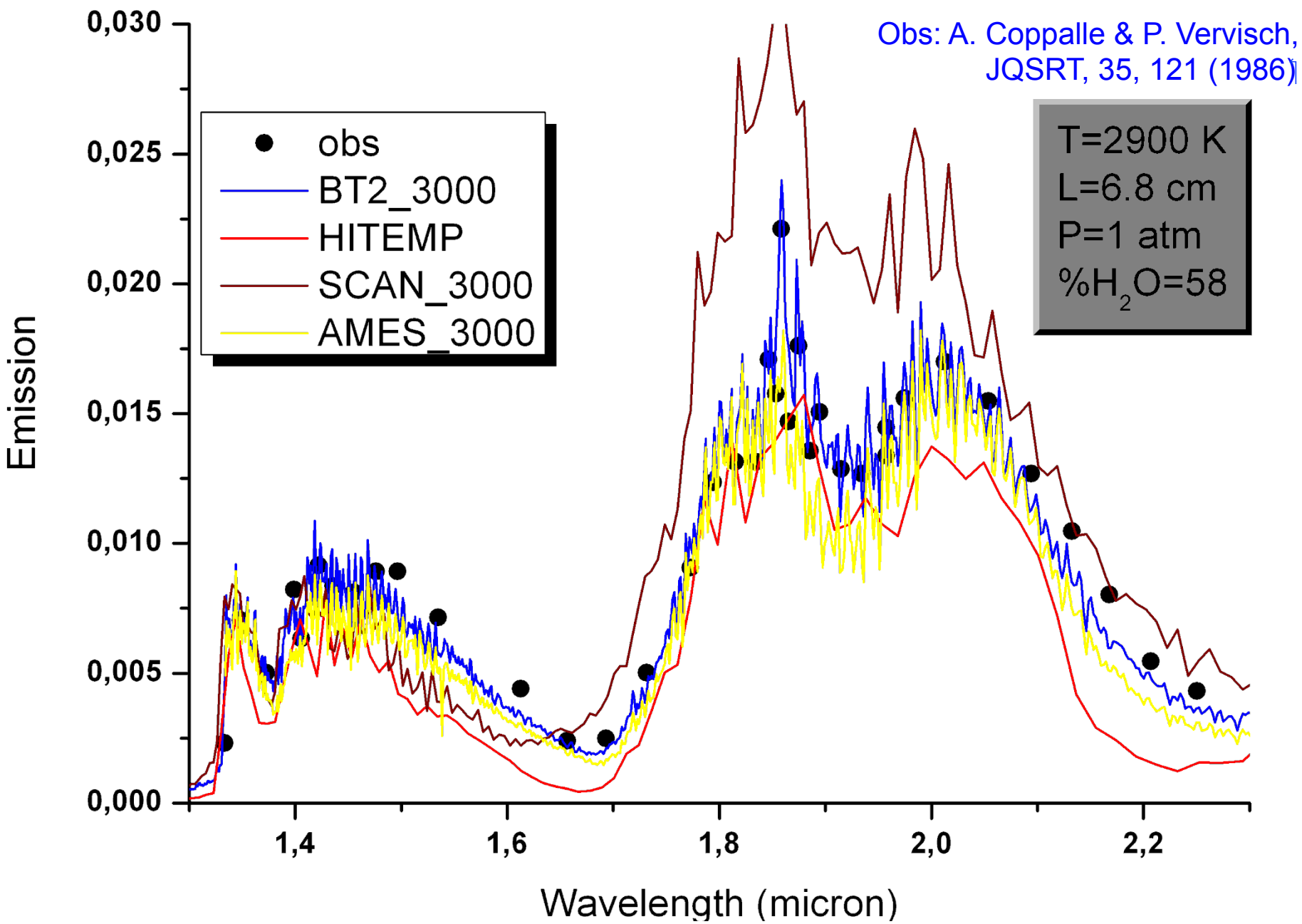
N	J	sym	n	E/cm^{-1}	v_1	v_2	v_3	J	K_a	K_c
43432	11	1	50	**8730.136998**	0	2	1	**11**	3	8
43433	11	1	51	**8819.773962**	0	4	0	**11**	6	6
43434	11	1	52	**8918.536215**	0	0	2	**11**	2	10
43435	11	1	53	**8965.496130**	0	2	1	**11**	5	6
43436	11	1	54	**8975.145175**	2	0	0	**11**	4	8
43437	11	1	55	**9007.868894**	1	0	1	**11**	3	8
43438	11	1	56	**9082.413891**	1	2	0	**11**	6	6
43439	11	1	57	**9170.343871**	1	0	1	**11**	5	6
43440	11	1	58	**9223.444158**	0	0	2	**11**	4	8
43441	11	1	59	**9264.489815**	2	0	0	**11**	6	6
43442	11	1	60	**9267.088316**	0	5	0	**11**	2	10
43443	11	1	61	**9369.887722**	0	2	1	**11**	7	4
43444	11	1	62	**9434.002547**	0	4	0	**11**	8	4
43445	11	1	63	**9457.272655**	1	0	1	**11**	7	4
43446	11	1	64	**9498.012728**	0	0	2	**11**	6	6
43447	11	1	65	**9565.890023**	1	2	0	**11**	8	4

Transitions file:

12.8 Gb

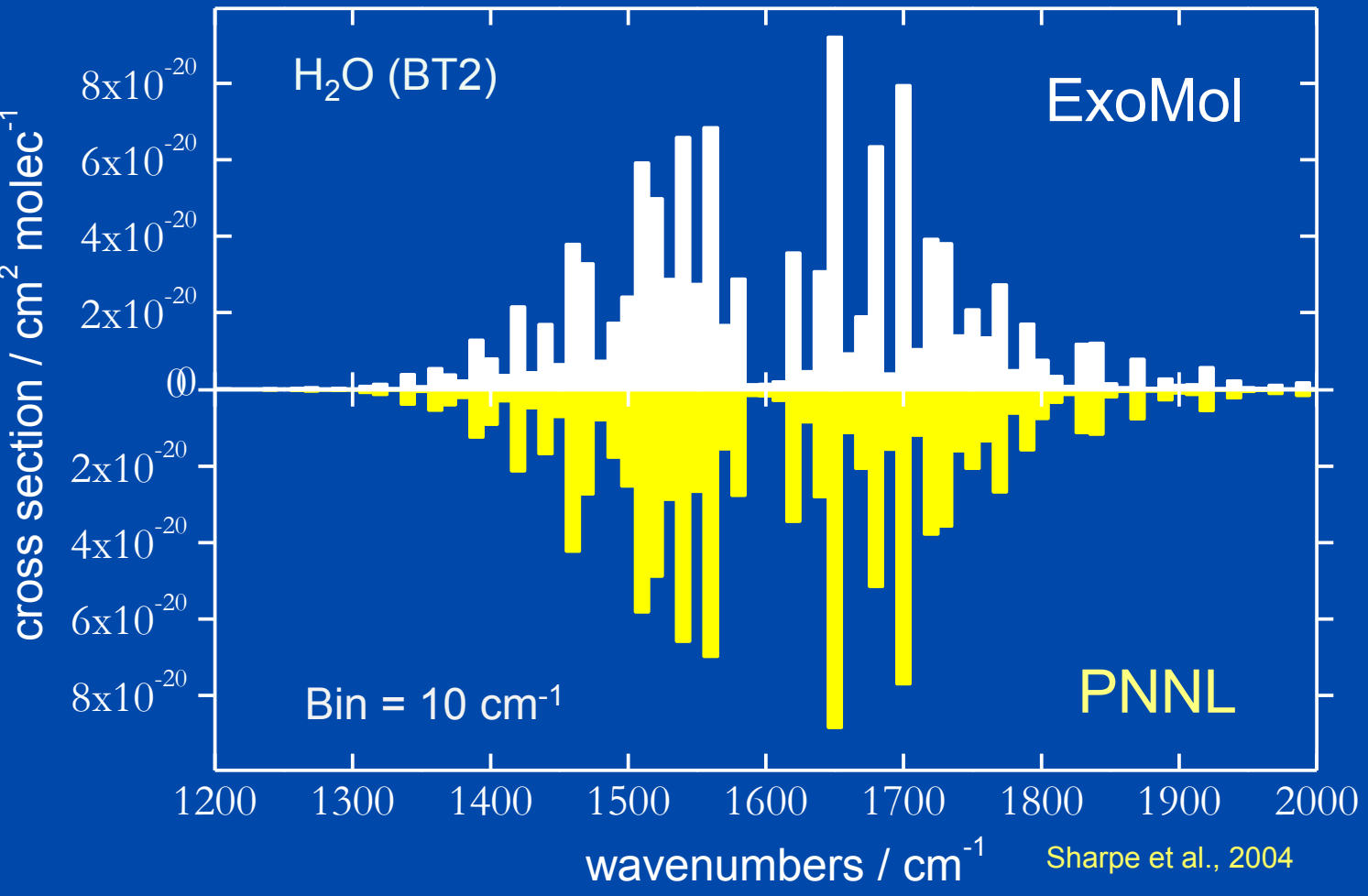
Divided into
16 files by frequency
for downloading

N_f	N_i	A_{if}
144848	146183	3.46E-04
115309	108520	7.42E-04
196018	198413	1.95E-04
7031	7703	1.13E-02
149176	150123	1.69E-04
81528	78734	2.30E-01
80829	78237	8.83E-04
209672	210876	2.51E-01
207026	203241	2.72E-04
188972	184971	1.25E-01
152471	153399	1.12E-02
39749	37479	1.46E-07
10579	15882	6.90E-05
34458	35617	1.15E-03



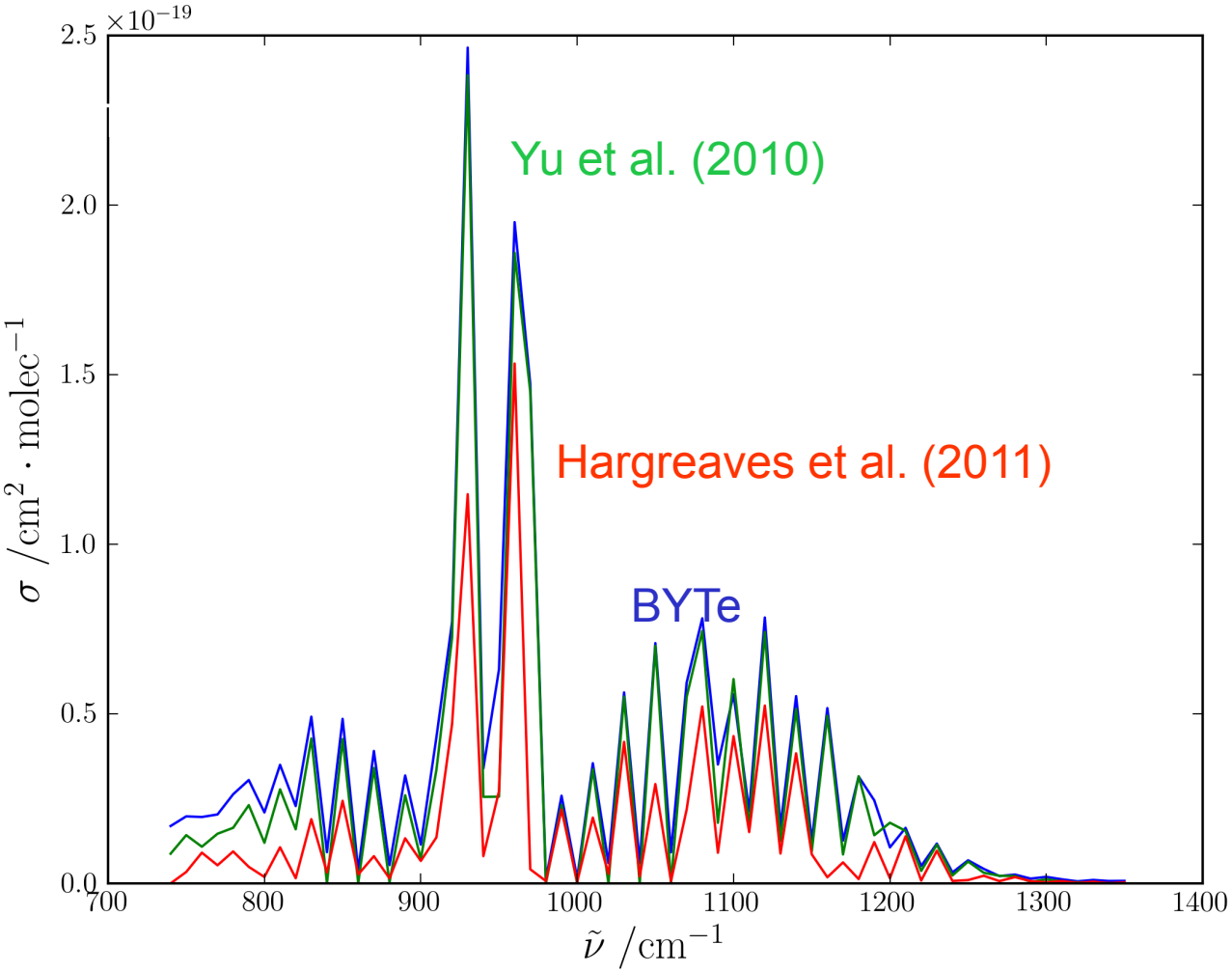
New edition of HITEMP: LS Rothman, IE Gordon, RJ Barber, H Dothe, RR Gamache, A Goldman, VI Perevalov, SA Tashkun + J Tennyson, JQSRT, 111, 2139 (2010).

ExoCross: T-dependent cross sections of H_2O (BT2), NH_3(BYTe), H_3^+, HCN/HNC: www.exomol.com



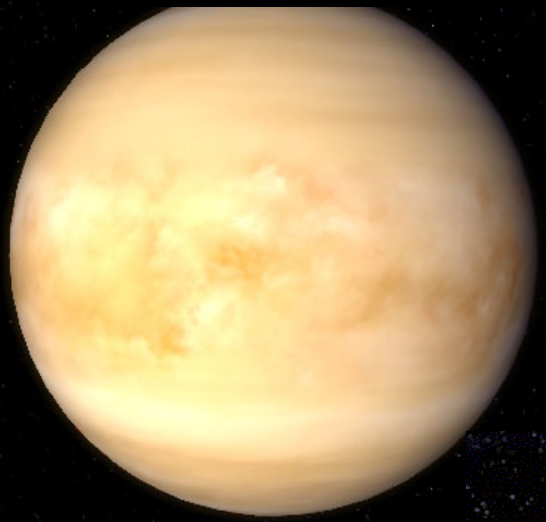
C. Hill, S. N. Yurchenko and J. Tennyson, Icarus, in press (2012): http://arxiv.org/abs/1205.6514

Cross sections for NH_3 ν_2 band at T= 573 K

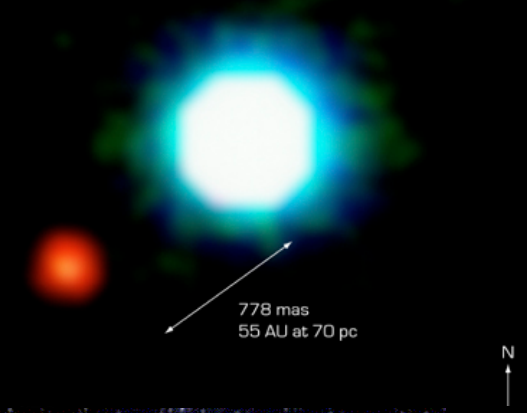


Brown and M-dwarfs

Atmosphere of Venus



Exoplanets (4 so far!)



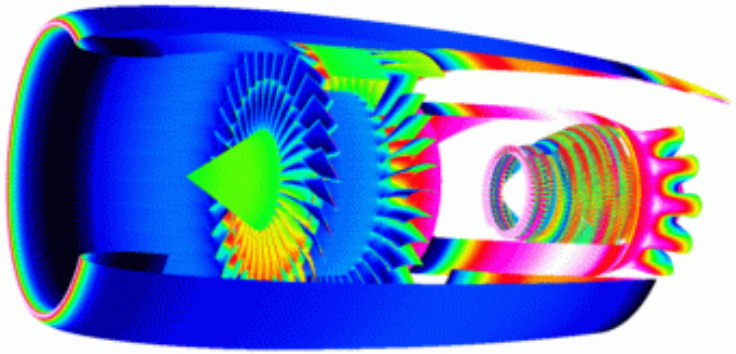
BT2 linelist used to
to detect/model water

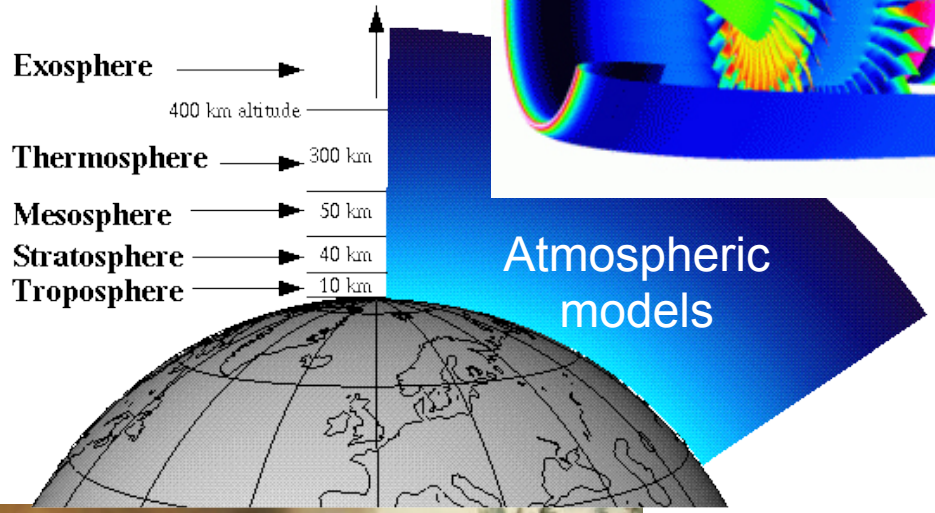
Nova-like V838 Mon

Cometary coma

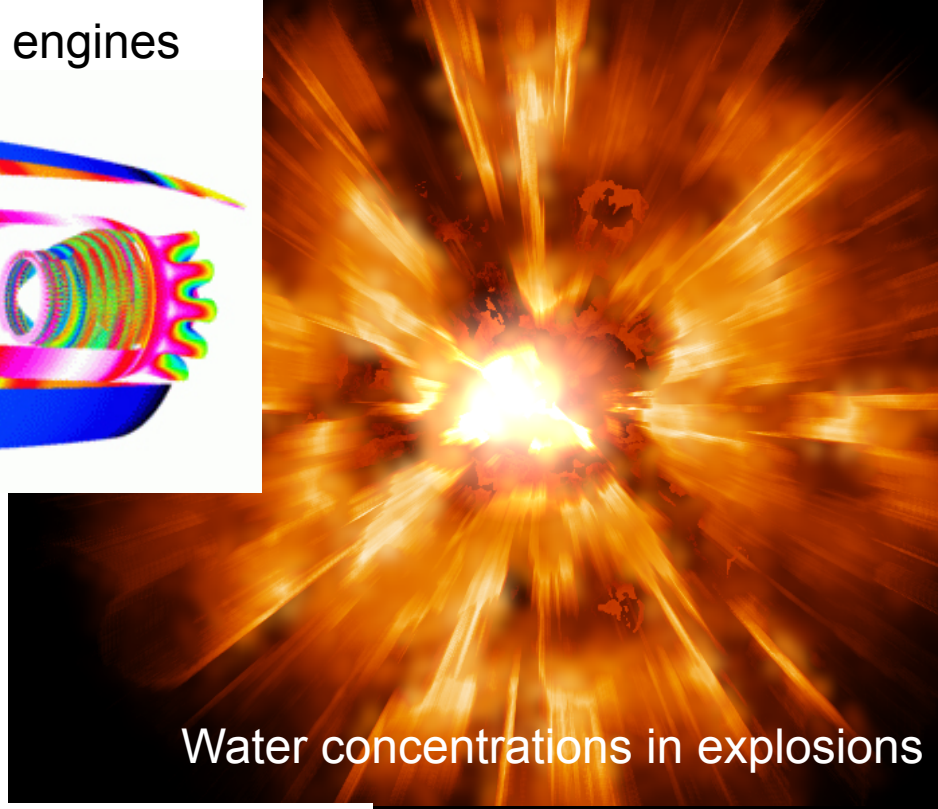
As well as.....

Imaging gas turbine engines





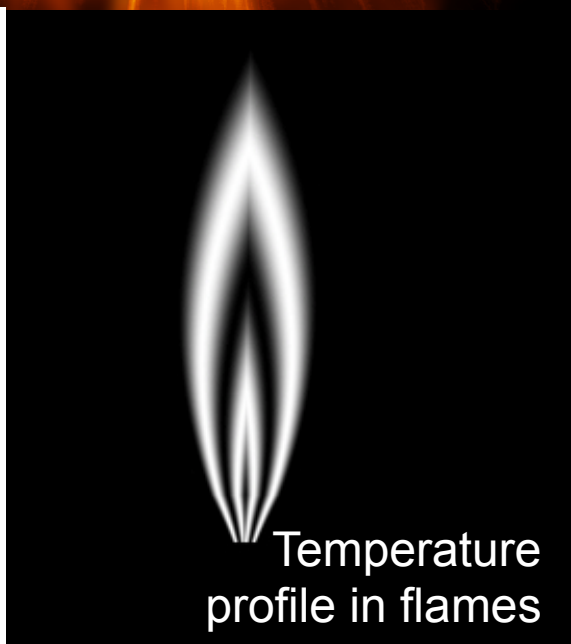
Atmospheric models



Water concentrations in explosions

Remote detection of forest fires

Design of high-T gas sensors



Temperature profile in flames

Molecular line lists for exoplanet & other atmospheres

	Primordial (Metal-poor)	Terrestrial Planets (Oxidising)	Giant-Planets & Cool Stars (Reducing atmospheres)
Already available	H_2O, HeH^+, H_3^+	OH, H_2O, HDO, NH_3	C_2, CN, CH, CO, CO_2, TiO, HCN/HNC, H_2O, NH_3
Oleg Polyansky, Sergei Yurchenko	O_2, CH_4, SO_2 **HOOH**, H_2CO,		**CH_4, PH_3, C_2, C_3, HCCH, H_2S, C_2H_6, C_3H_8, VO, O_2, AlO, MgO, CrH, MgH, FeH, CaH, AlH, SiH, TiH, ~~NiH, BeH, YO~~, NaH, HF, HCl**
Jonathan Tennyson, Benjamin Yadin, Pierandrea Conti			
Dan Underwood	SO_3		
Thomas Veness			

Lorenzo Lodi

Istvan Szabo

Andrei Patrascu

Clara Sousa Silva

Ala'a Azzam


Sergei Yurchenko
Andrei Patrascu
Christian Hill
Ala'a Azza
Bob Barber
Lorenzo Lodi
Clara Sousa-Silva
Oleg Polyanksy
Post doc position available:
Methods for large molecules
www.exomol.com/vacancy
Dan Underwood
Maire Gorman
Renia Diamantopoulou
VAMDC
Virtual Atomic and Molecular Data Centre
erc
ExoMol
www.exomol.com