Exomol Conference 2018

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Mountain View, Ca

With inputs from:

The exoplanet group @ Ames Research Center

Mark Marley, Kevin Zahnle, Roxana Lupu,

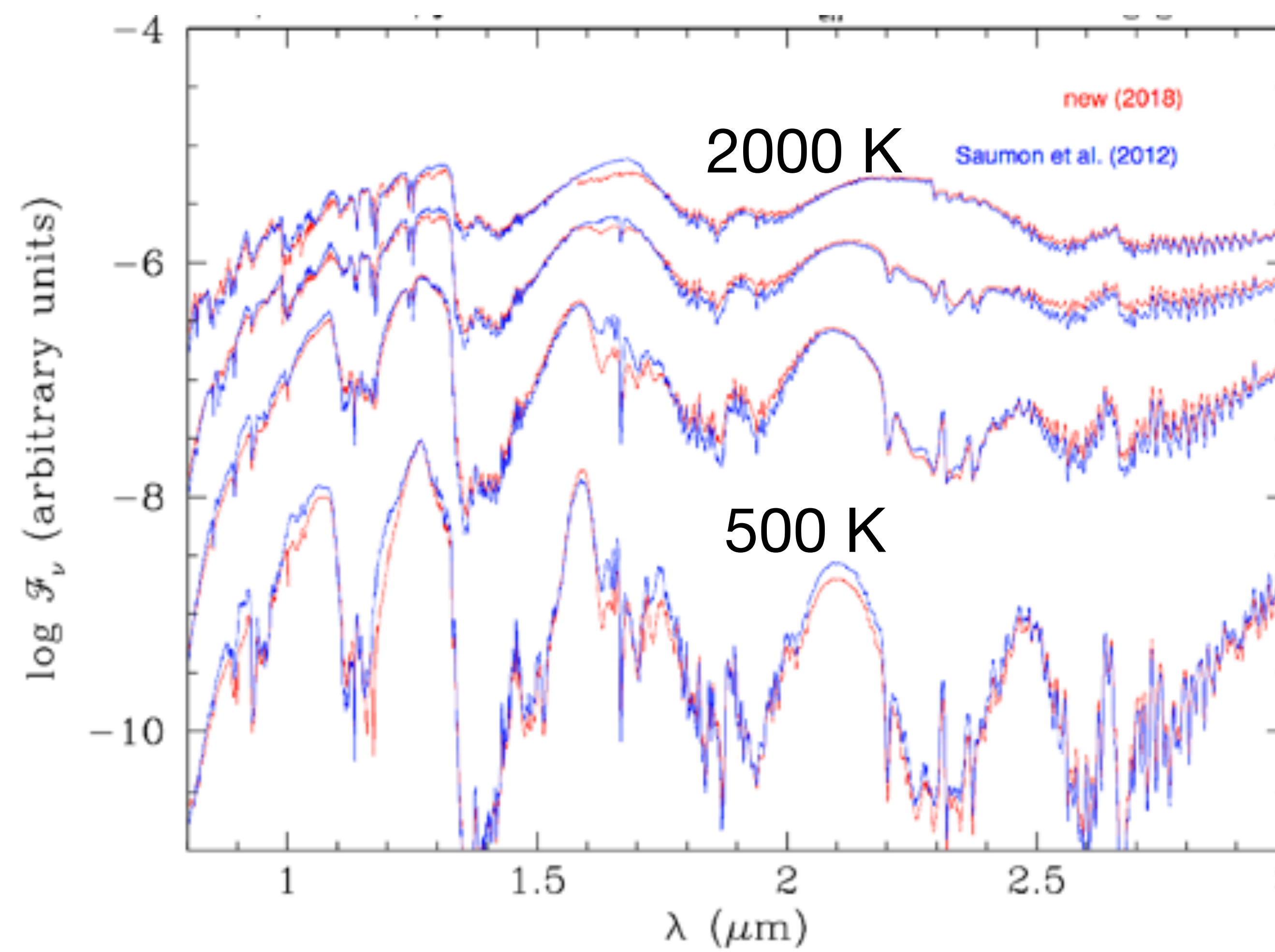
Computational Chemistry Group

David Schwenke, Xinchuan Huang and Tim Lee

and a cast of thousands assisting with data and advice

Opacity Needs for Atmospheric Modeling Applications (1)

- Line by line: molecules and atoms
  - Line shapes - widths - especially for predicted data that may extend to very high J values
- CIA [Collision Induced]
- Simple Scattering by gases - and electrons
- H- at the highest temperatures
- Solids not considered by me at present but are added into models as a continuum



log g=5, solar composition brown dwarf model set Marley et al. (in prep.)

Opacity Needs for Atmospheric Modeling Applications (2)

- Special Cases: Alkali atoms
- Methods to handle very large data sets such as CH_4 : HNO_3 : H_2O_2 :etc.
- Discussion of more sophisticated techniques such as statistical sampling, separating weak and strong lines, etc.
- Future needs

Data Sources

- Hitran - large number of species - vetted data with line width information for air/self broadening although that will be expanded in the future
- Astrophysical sources - analysis of cool stars & the sun: planets in our solar system
- Laboratory measurements - challenging at high temperatures and pressures but some examples will be shown
- Theoretical Predictions - complex for large systems with many atoms
- Alkali Atoms - Nicole Allard : CIA - Didier Saumon and collaborators
- For Diatomics more options exist that allow for on-site calculations: such as programs supplied by LeRoy, for example
- Check out the various web sites for program sources and bibliographies: Check Hitran website for extensive information

The line by line program

- Based on very old program from Hitran group: Fascode !
- Input data the usual: line list with positions, strengths, widths - partition functions - mass of each species, etc.
- main points of discussion: choice for generation of the Voigt profile and the grid spacing - constant, variable with wavenumber?
- For Voigt profile: need a certain level of accuracy over a range of physical inputs
- For the grid spacing do we need to resolve each line [?] but how well ?
- Timing for huge data sets

- Currently using routine due to Letchworth-Benner [JQSRT 2007]
- Note that this routine looses accuracy when Z is near the real axis [small a]
- Several available Voigt routines suffer from this same problem
- More accurate at small “a” : Modified Humlicek or routine in libcerf [Zaghloul]
- Exocross routine claims that the Humlicek routine can be vectorized to greatly increase the speed: may not work on a typical workstation
- Routines due to Weideman ?

Question of Grid Spacing

- Since 1/e doppler width: $\nu/c\sqrt{2KT/m}$ grows with wavenumber an efficient grid spacing would also grow linearly with wavenumber.
- This would allow the proper resolution at low pressures, for example, where the line widths would be controlled by the doppler width.
- Currently I am using a constant spacing grid and any change in the future would have to be carefully considered as our models require the individual opacities from each species to be weighted by their relative abundance based on a chemical model.
- They are then added up along with the CIA absorption and any other opacities into a single layer that can be used along with all the other layers in creating a model of the atmosphere.

Problems with line shapes and broadening

- The pressure broadening widths and line shapes, especially in the far wings of lines are important contributions to the uncertainties in these calculations and also affect how these spectra are used in applications such as cross correlation studies

- The band edges of important absorbers can determine where there are “windows” in the spectrum [absorption coefficients] - this is where much of the flux will emerge in these objects and will influence the design [spectral range covered/resolution] of instruments on large telescopes and projects such as JWST

- For many of the objects of interest in the field of brown dwarfs and extra solar planets the main broadening agents will be H_2 and He. For the hottest objects broadening by H atoms must be considered

How to handle the lack of line broadening data for high J values

- Many line lists produced by various groups using quantum chemistry methods extend up to very high J values far beyond the available data on line widths

- These high J lines which become stronger at higher temperatures are important in determining the exact structure of the “window” regions for each individual species and a lack of knowledge of the line widths is a real impediment to a calculation - it may also determine how far out one decides to extend the line wings as a function of temperature and pressure

- Possible that at high J values if there are no resonances between the broadener and the molecule of interest that the widths will reach a minimum ?

For Future Work - question of line extents and far wings

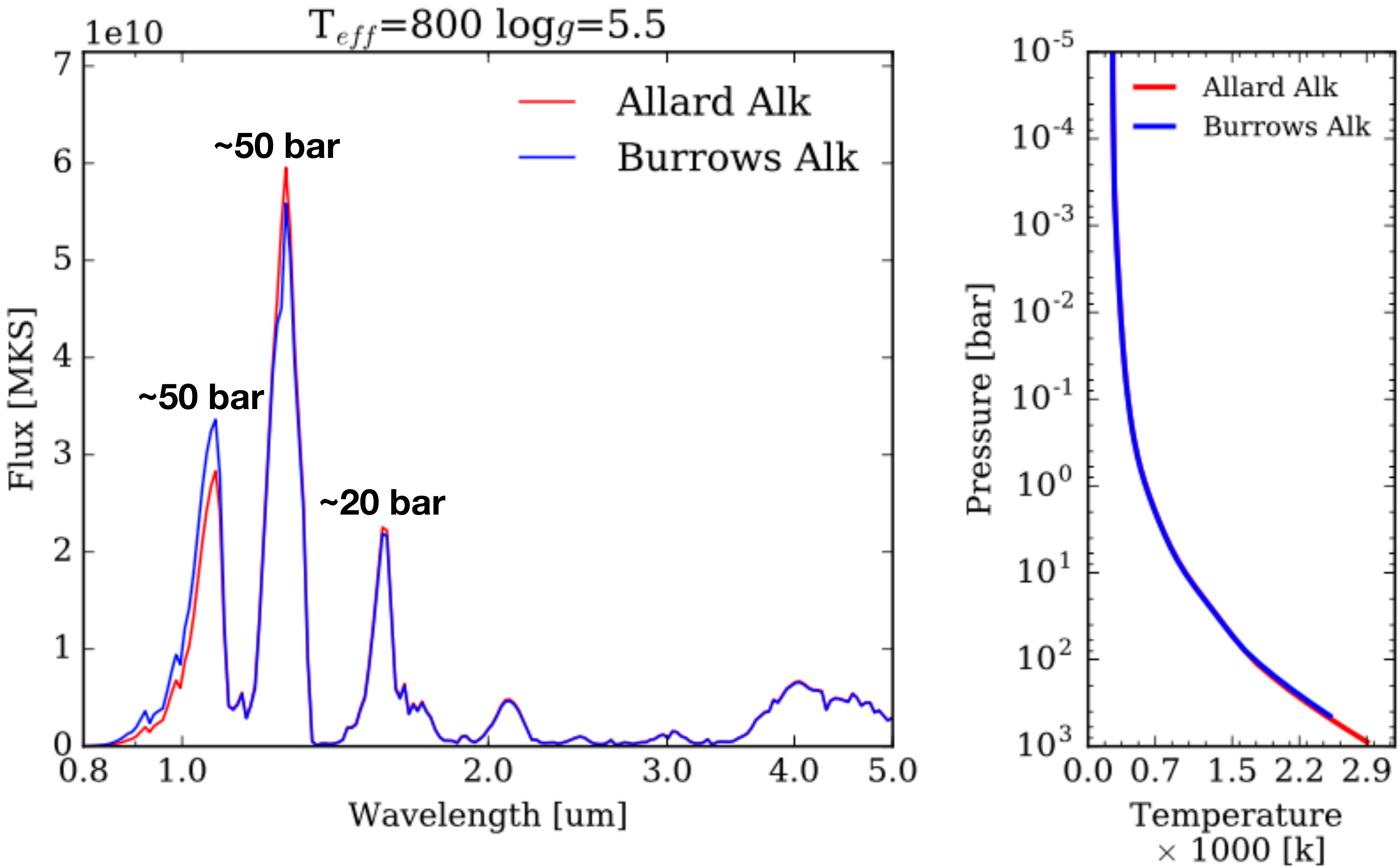
- Since exception the line extent has been controlled by a simple formula to try to capture most of the opacity. Other groups use similar techniques but at the highest pressures [which are deep in the atmospheres] the extension needed is unclear

- However, this leaves a lot to be desired and does not take into account the possible sub-Lorentzian nature of the far wings

- Example of the CO_2 bands on Venus

- My current software setup needs extensive work - study to find a consistent solution to this problem

- Cross correlation studies need accurate line widths - examples later



T$_{eff}$=800 log$g$=5.5
1e10
Flux [MKS]
Wavelength [um]
~50 bar
~50 bar
~20 bar
Allard Alk
Burrows Alk
Pressure [bar]
Temperature × 1000 [k]
Allard Alk
Burrows Alk

NH	3.420450	cm-1	16822.643983	cm-1	10425
SO3	0.039673	cm-1	2824.347247	cm-1	14295
H2	3.226800	cm-1	36405.367200	cm-1	15055
LiH	1.419200	cm-1	19589.373300	cm-1	18982
CP	374.384900	cm-1	15037.950300	cm-1	28752
SH	0.000429	cm-1	27771.455259	cm-1	81348
CH	18.095800	cm-1	39128.536930	cm-1	104432
H2O2	0.043110	cm-1	1730.370600	cm-1	126983
TiH	4742.610000	cm-1	23832.470000	cm-1	159131
CN	18.641000	cm-1	52348.353400	cm-1	195112
PN	0.168721	cm-1	6498.001685	cm-1	292174
CH4	0.001063	cm-1	11501.872500	cm-1	450332
HNO3	0.006731	cm-1	1769.982240	cm-1	1008972
ScH	0.000030	cm-1	15811.112932	cm-1	1152826
NaCl	0.000771	cm-1	2457.767600	cm-1	1413391
BeH	0.000715	cm-1	42911.078748	cm-1	2042351
PO	0.000001	cm-1	11999.995368	cm-1	2096251
CS	0.971438	cm-1	47190.414309	cm-1	4261855
KCl	0.111720	cm-1	2927.254094	cm-1	5307060
GeH4	20.431000	cm-1	6199.995300	cm-1	6025370
CH4	1.568900	cm-1	13399.999400	cm-1	17045164
AlO	0.000001	cm-1	34999.996532	cm-1	20326704
CaO	0.000001	cm-1	24996.068341	cm-1	28417909
PS	0.000001	cm-1	36672.289801	cm-1	30394445
NH3	0.000002	cm-1	11999.999997	cm-1	1221710294
SO2	0.000106	cm-1	7999.999998	cm-1	1402280350
HNO3	0.000471	cm-1	6999.999998	cm-1	6722194217
H2O2	0.000001	cm-1	7997.210582	cm-1	19873562928
SO3	0.000002	cm-1	4999.999950	cm-1	21408551929
SiH4	0.000002	cm-1	4999.999950	cm-1	62690449078

GASEOUS MEAN OPACITIES FOR GIANT PLANET AND ULTRACOOL DWARF ATMOSPHERES OVER A RANGE OF METALLICITIES AND TEMPERATURES

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ABSTRACT

We present new calculations of Rosseland and Planck gaseous mean opacities relevant to the atmospheres of giant planets and ultracool dwarfs. Such calculations are used in modeling the atmospheres, interiors, formation, and evolution of these objects. Our calculations are an expansion of those presented in Freedman et al. to include lower pressures, finer temperature resolution, and also the higher metallicities most relevant for giant planet atmospheres. Calculations span 1 μbar to 300 bar, and 75–4000 K, in a nearly square grid. Opacities at metallicities from solar to 50 times solar abundances are calculated. We also provide an analytic fit to the Rosseland mean opacities over the grid in pressure, temperature, and metallicity. In addition to computing mean opacities at these local temperatures, we also calculate them with weighting functions up to 7000 K, to simulate the mean opacities for incident stellar intensities, rather than locally thermally emitted intensities. The chemical equilibrium calculations account for the settling of condensates in a gravitational field and are applicable to cloud-free giant planet and ultracool dwarf atmospheres, but not circumstellar disks. We provide our extensive opacity tables for public use.

Key words: brown dwarfs – opacity – planets and satellites: atmospheres – radiative transfer – stars: atmospheres

Online-only material: color figures, machine-readable tables

1. INTRODUCTION

A quantitative understanding of radiation transport in the cool molecule-dominated regions in planetary and ultracool dwarf atmospheres is essential to many aspects of understanding the temperature structure, thermal evolution, and formation of these objects.

well-approximate the metal-rich atmospheres of giant planets, up to levels of the solar system's ice giant planets, Uranus and Neptune (Guillot & Gautier 2009). Finally, for use in models of irradiated planetary atmospheres, we calculate mean opacities where the temperature in the weighting function is not the local temperature, but rather stellar blackbody temperatures from 3000 to 7000 K, to simulate mean "incident flux" or "visible"

Some Laboratory Work of Interest

- Work on high temperature and high pressure cells
- Several groups are actively pursuing laboratory data in this area - see abstracts of Hitran 2018 for more examples
- The Hitran 2018 Conference has more information on new work planned in this area

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Gas cell based on optical contacting for fundamental spectroscopy studies with initial reference absorption spectrum of H_2O vapor at 1723 K and 0.0235 bar

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Reference spectra

ABSTRACT

A gas cell, using optically contacted sapphire windows to form a hot vapor seal, has been created for high temperature fundamental spectroscopy studies. It is designed to operate at temperatures from 280–2273 K and pressures from vacuum to 1.3 bar. Using the cell in conjunction with an external cavity diode laser spectrometer, a reference H_2O vapor absorption spectrum at $P = 0.0235 \pm 0.0036$ bar and $T = 1723 \pm 6$ K was measured with 0.0001 cm^{-1} resolution over the 7326–7598 cm^{-1} range. Comparison of the measured spectrum to simulations reveals errors in both the HITEMP and BT2 databases. This work establishes heated static cell capabilities at temperatures well above the typical limit of approximately 1300 K set by quartz material properties. This paper addresses the design of the cell as well as the cell's limitations.

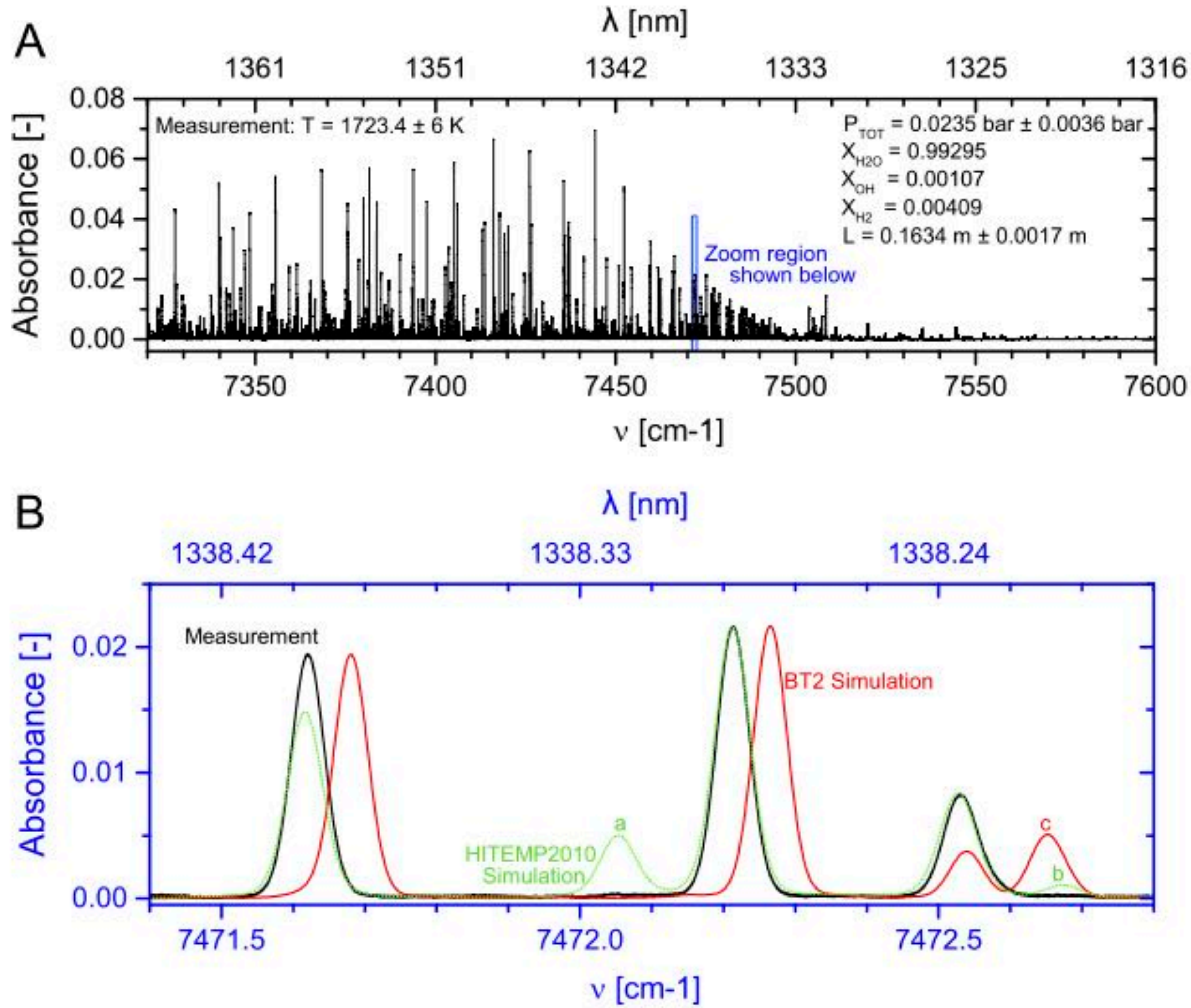

Fig. 6. (A): Measured H_2O absorption spectra at 1723 K (B): narrow region of the measured absorption spectrum compared with HITEMP2010 and BT2 simulations using Voigt line shapes. Errors in database parameters for line position, strength, and/or lower-state energy, labeled a, b,and c, are visible in the simulated spectra.

And Now, some actual examples of these techniques applied to real problems

- Cross correlation studies: H_2O & TiO for example - see paper by McKemmish, et al. Problem of needing very accurate line positions - what about line shifts - usually not the biggest problem as the observations for these studies are done in the upper part of the atmosphere of exoplanets where the pressure is generally low. The current line list for TiO due to Schwenke did not seem to have accurate enough wavenumbers to satisfy the needs of a cross correlation study. Recalculate with better line positions. H_2O is also a candidate as many studies have been done to try to quantify the presence of water vapor.

- For cross correlation studies it is necessary to derive accurate physical parameters of the object being observed including a value of Vsin(i) [the inclination of the rotational axis to the line of sight]

- If there are significant errors in the line pressure broadening widths this will lead to values for Vsin(i) that are not physically meaningful - values of hundreds of Km/ sec or more

- This greatly complicates any attempt to use cross correlation methods

An L Band Spectrum of the Coldest Brown Dwarf

Caroline V. Morley[1,13], Andrew J. Skemer[2], Katelyn N. Allers[3], Mark. S. Marley[4], Jacqueline K. Faherty[5], Channon Visscher[6,7], Samuel A. Beiler[3,8], Brittany E. Miles[2], Roxana Lupu[9], Richard S. Freedman[4,10] + Show full author list

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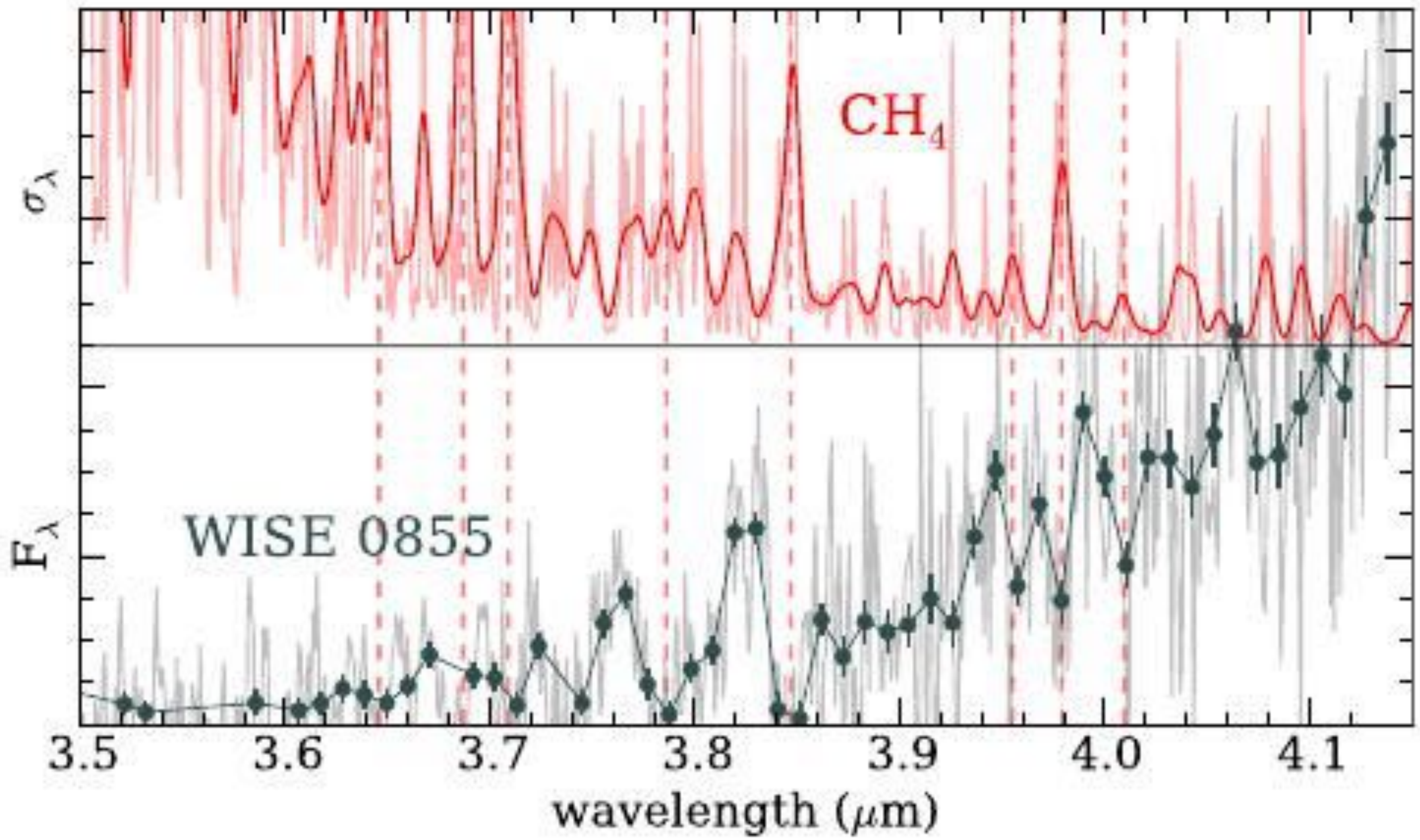


Figure 7. Normalized spectrum of WISE 0855 compared to cross sections of CH_4 from 3.5 to 4.14 μm. The methane cross sections are shown at higher resolution ($R \sim 1500$, light red) and lower resolution ($R \sim 300$, solid red). Vertical dashed red lines centered on methane absorption bands are shown to guide the eye. All major absorption features seen in WISE 0855's L band spectrum correspond in wavelength with molecular bands of CH_4. We conclude the L band spectrum shows strong evidence of methane absorption.

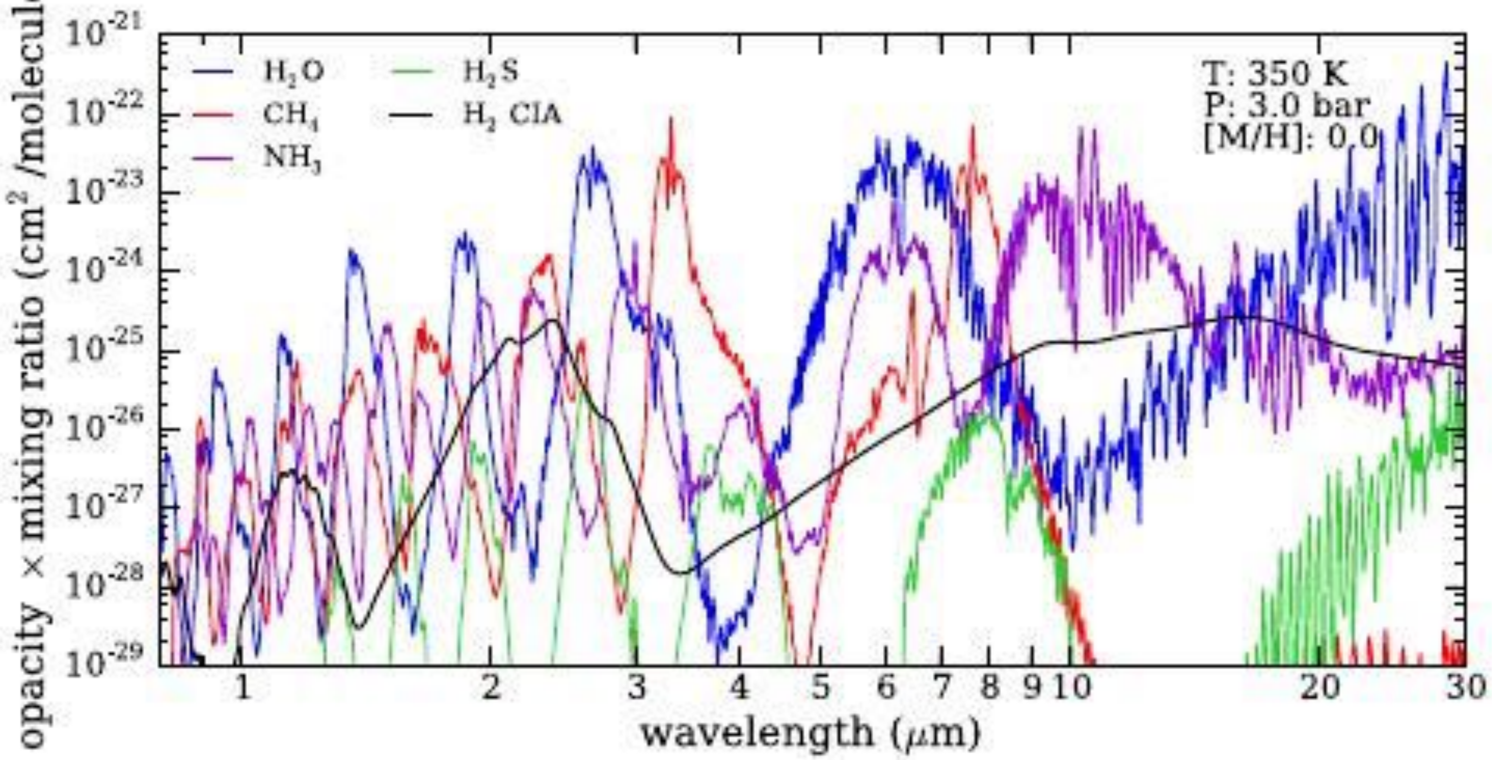
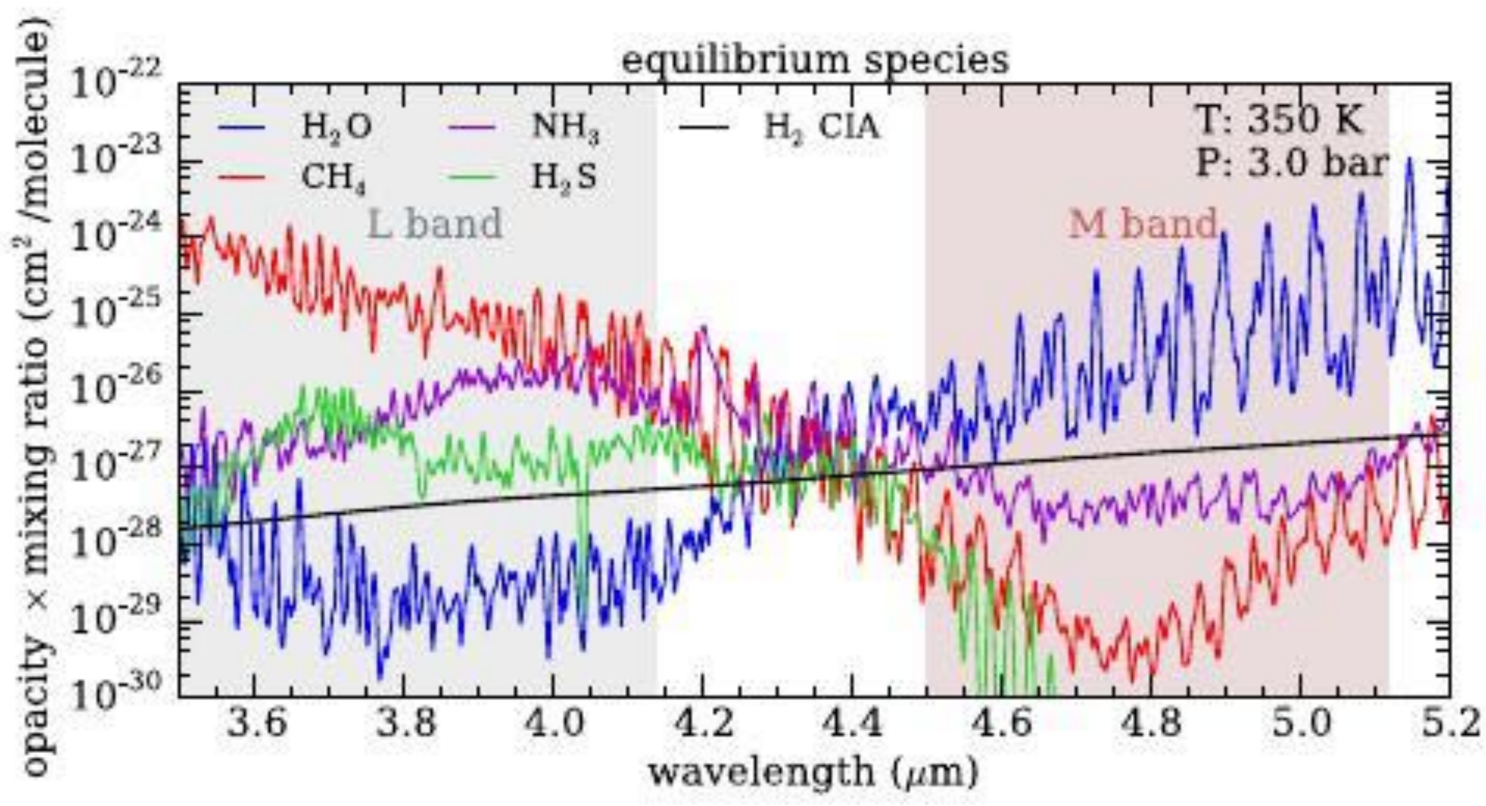


Figure 4. Cross sections of a number of abundant molecules. The cross sections are scaled by the mixing ratio in chemical equilibrium at a temperature of 350 K and pressure of 3 bar, which is approximately the temperature of the mid-infrared photosphere of a 250 K object. The dominant absorbers across the spectrum are H_2O, CH_4, and NH_3.



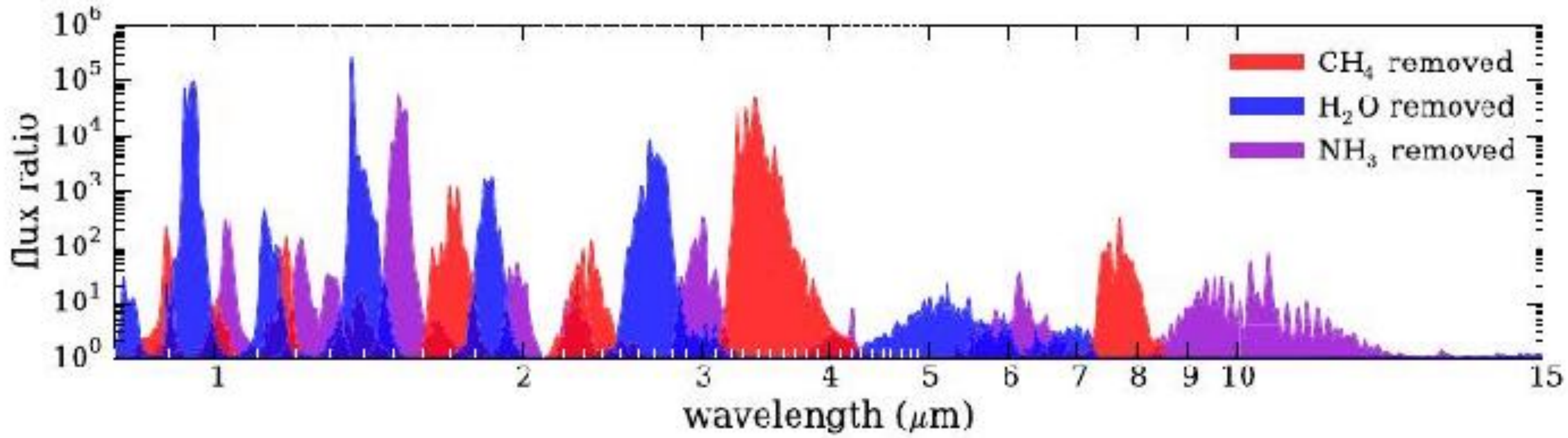


Figure 6. Sensitivity of the spectrum to each wavelength. For a model with $T_{\mathrm{eff}} = 250$ K, $\log g = 4.0$, [M/H] = 0.0, and C/O = 0.6, water, methane, and ammonia are removed individually, keeping the P–T profile the same; the spectrum with each molecule removed is divided by the standard spectrum. A 250 K object's spectrum is dominated by these three species.

Peering into the physics of brown dwarfs: spectroscopy with JWST/ NIRSpec

Catarina Alves de Oliveira, *European Space Agency*
JWST/NIRSpec Instrument & Calibration Scientist

Collaborators:
R. Parker (LJMU), P. Tremblin (CEA)
and the NIRSpec team

Y dwarfs - NIRSpec simulations

→ **Can NIRSpec observations of Y dwarfs distinguish between different model predictions?**

Atmospheric models from

Tremblin+2015 & Morley+2014

Y dwarf:

Teff: 450K

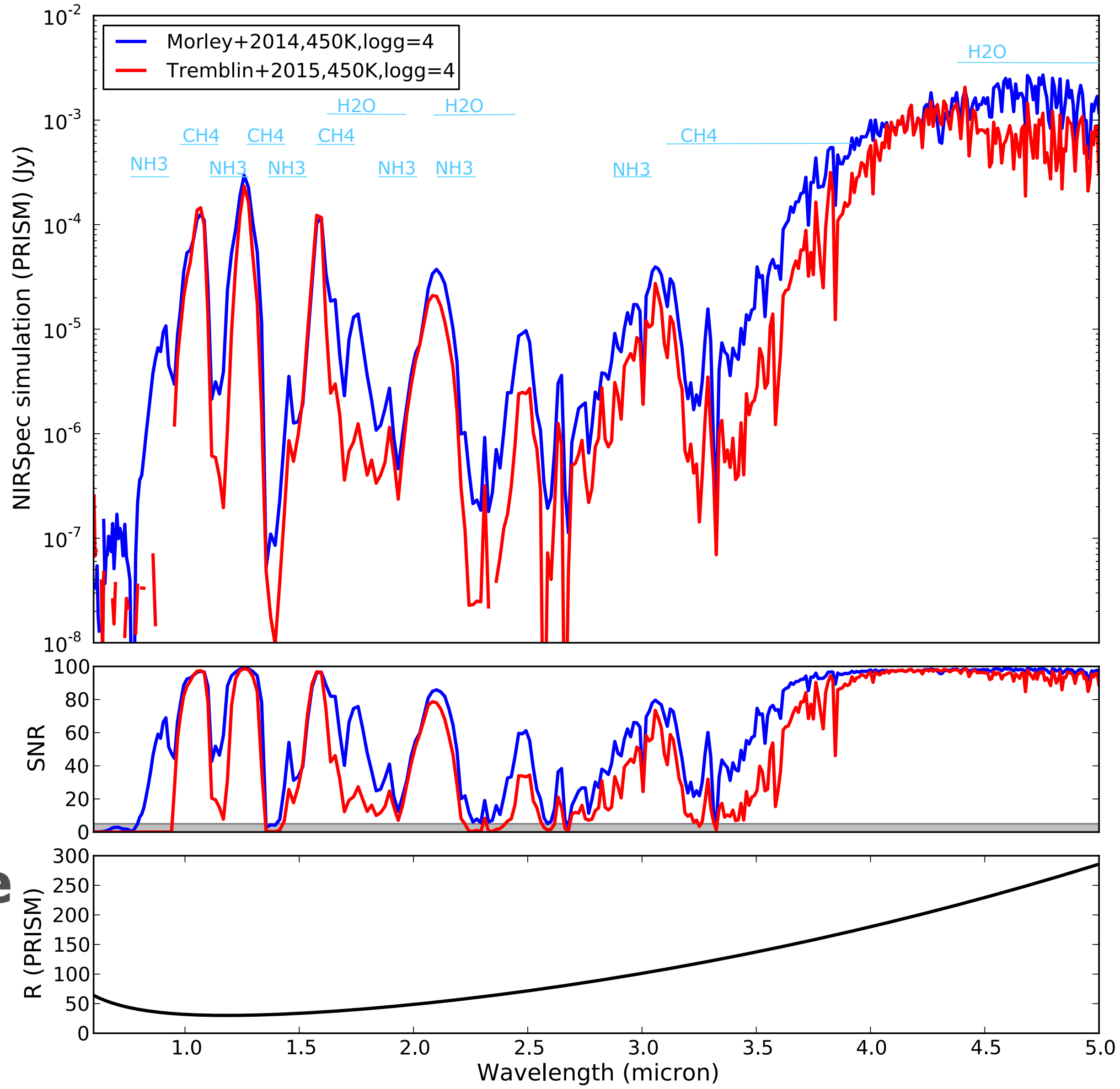
logg: 4

distance: 5 pc

Simulations:

NIRSpec, 15 minutes on-source

JWST/NIRSpec, PRISM, ~15 minutes



Distance to the Sun: 5.00 pc - Radius: 1.03 R_Jupiter.

2015-10-07T16:57:33.693358
Created by C. Alves de Oliveira

Y dwarfs - NIRSpec simulations

➔ Can we observe Y dwarfs at different temperatures?

Atmospheric models from Morley+2014

Y dwarf:

Teff: 450K, 350K, 250K

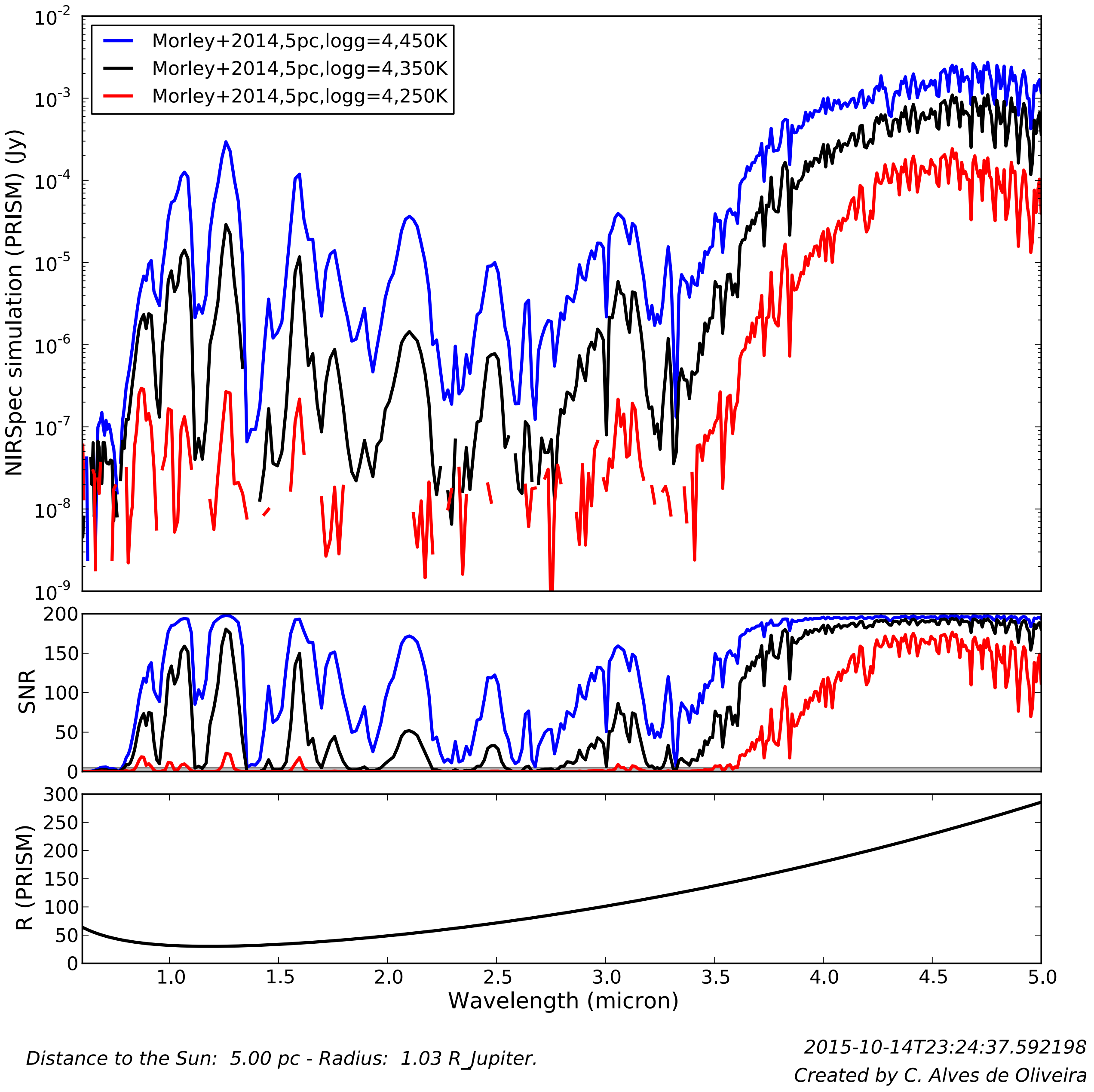
logg: 4

distance: 5 pc

Simulations:

NIRSpec, 1 hour on-source

JWST/NIRSpec, PRISM, ~1hour



Y dwarfs - NIRSpec simulations

➔ **Can we extend the study of cool atmospheres to the lowest temperature Y dwarf known?**

Atmospheric models from Morley+2014

Y dwarf (e.g., WISE0855):

Teff: 250K

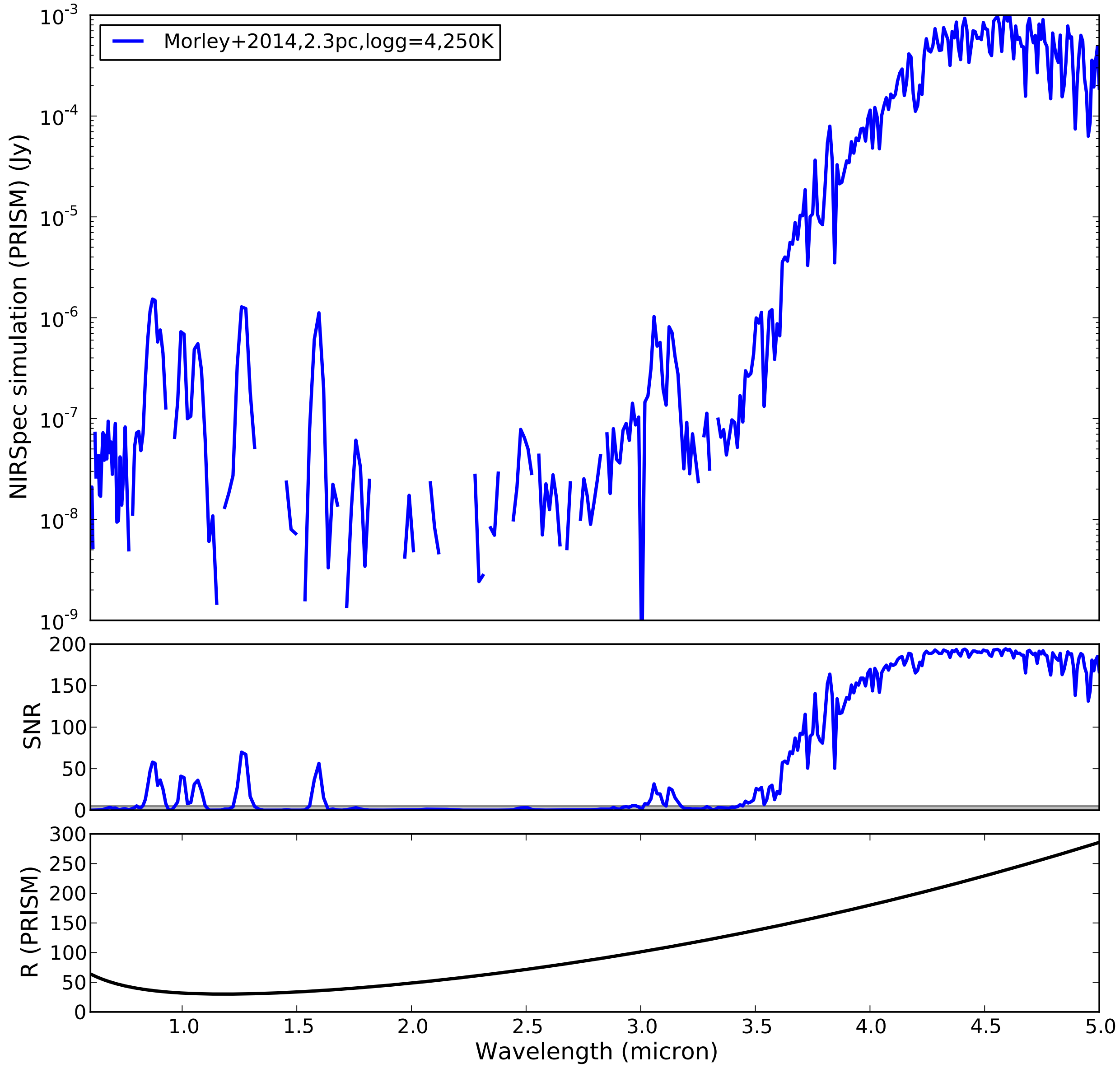
logg: 4

distance: 2.3 pc

Simulations:

NIRSpec, 1 hour on source

JWST/NIRSpec, PRISM, ~1 hour



Distance to the Sun: 2.30 pc - Radius: 1.03 R_Jupiter.

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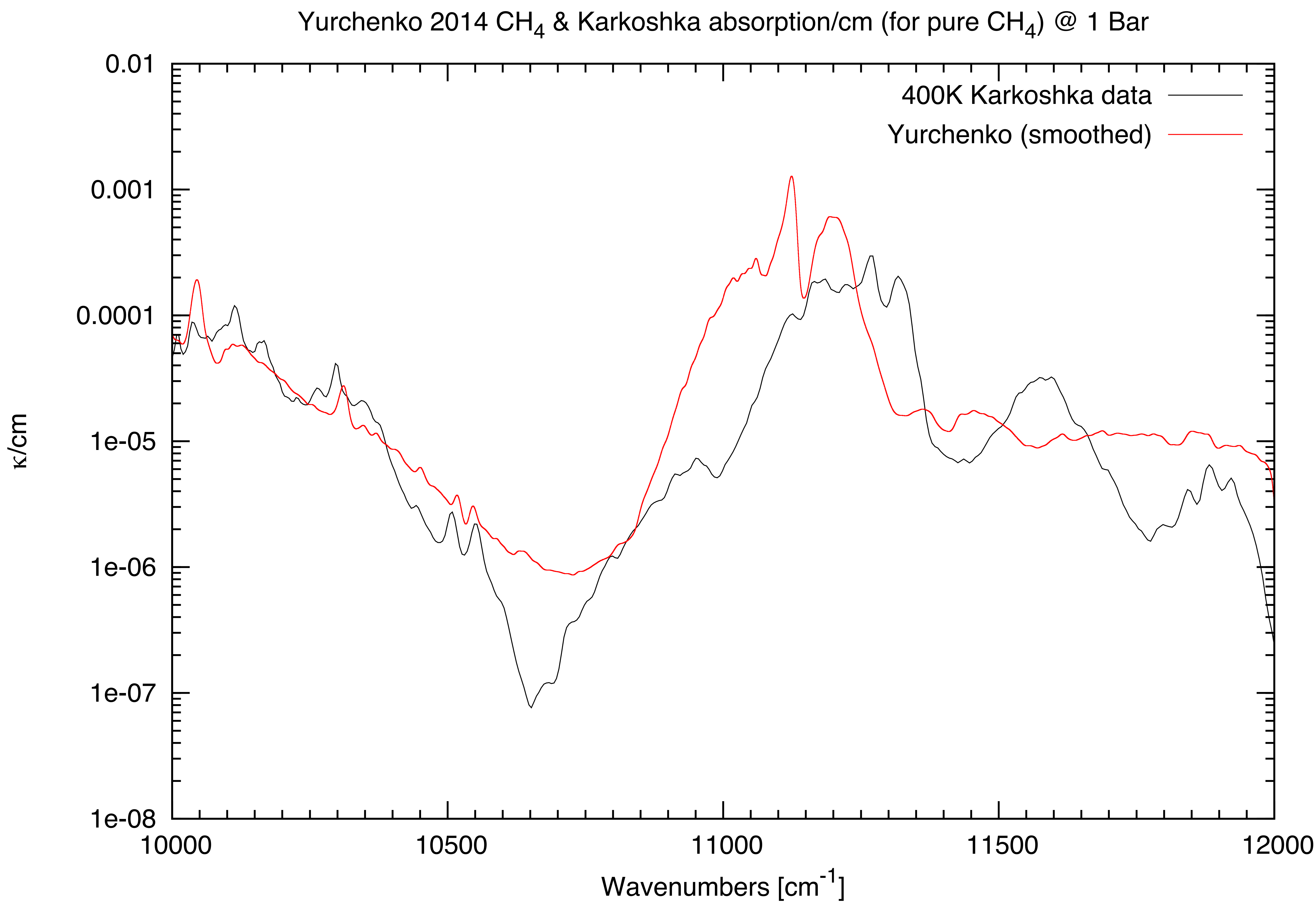
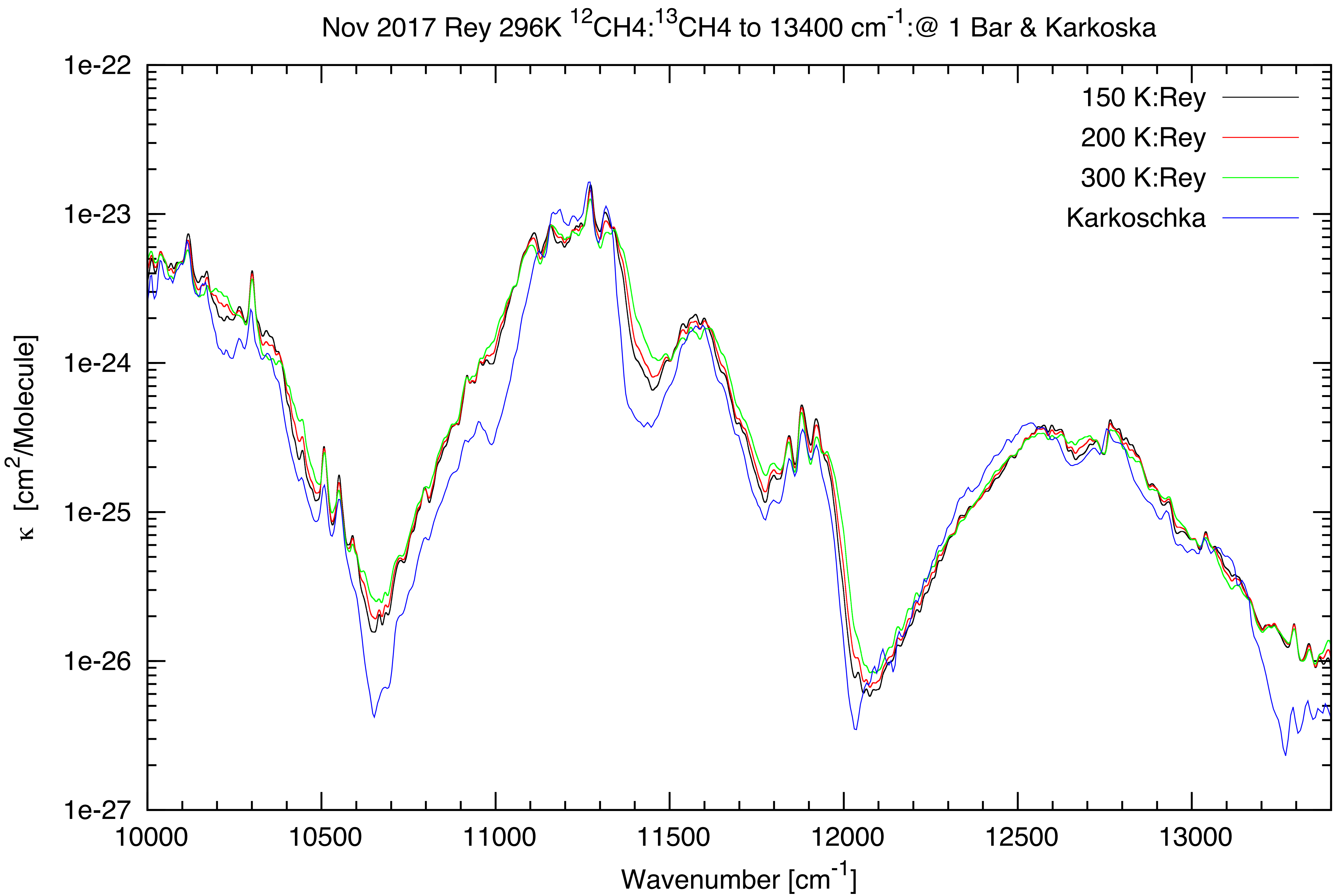
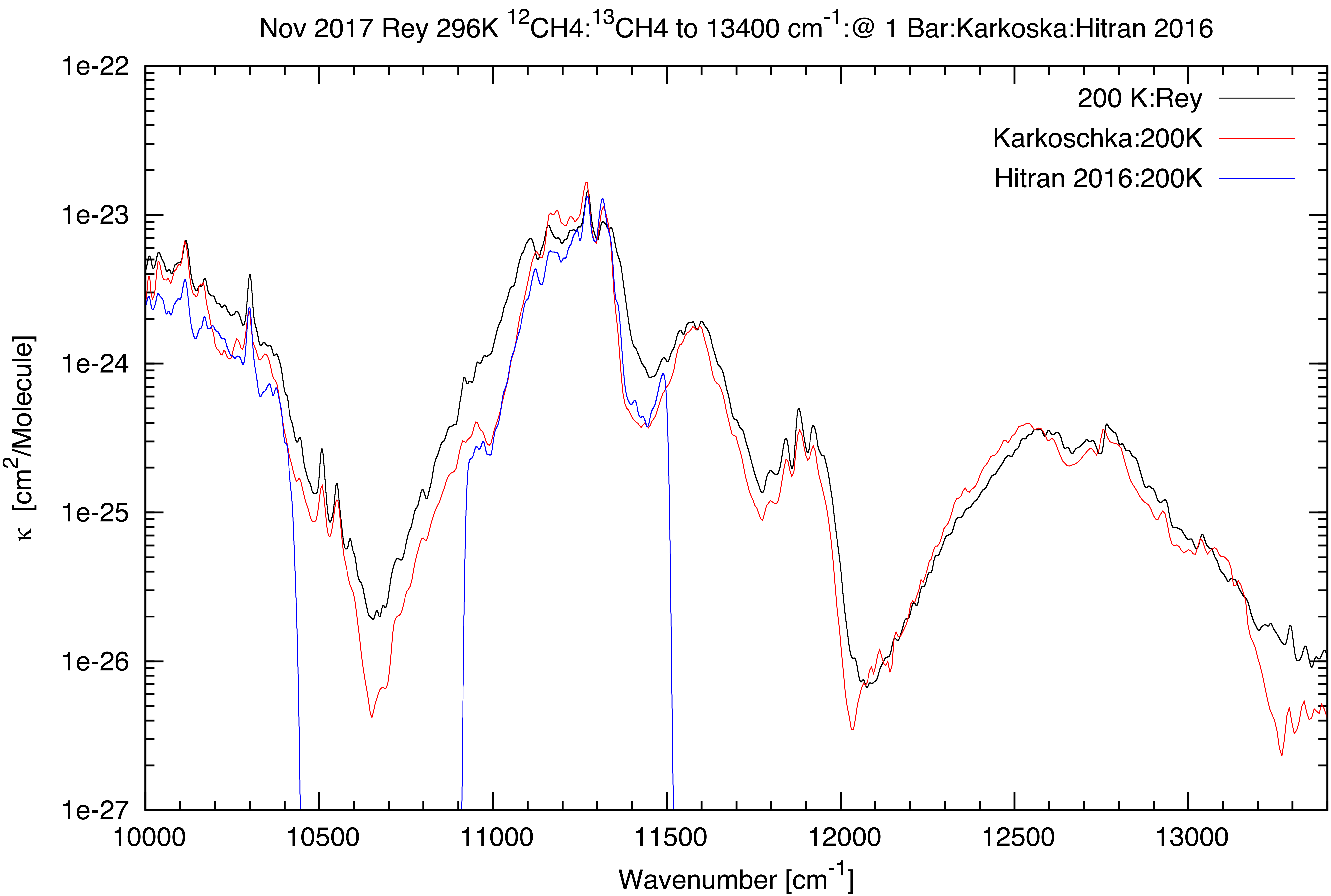
Created by C. Alves de Oliveira



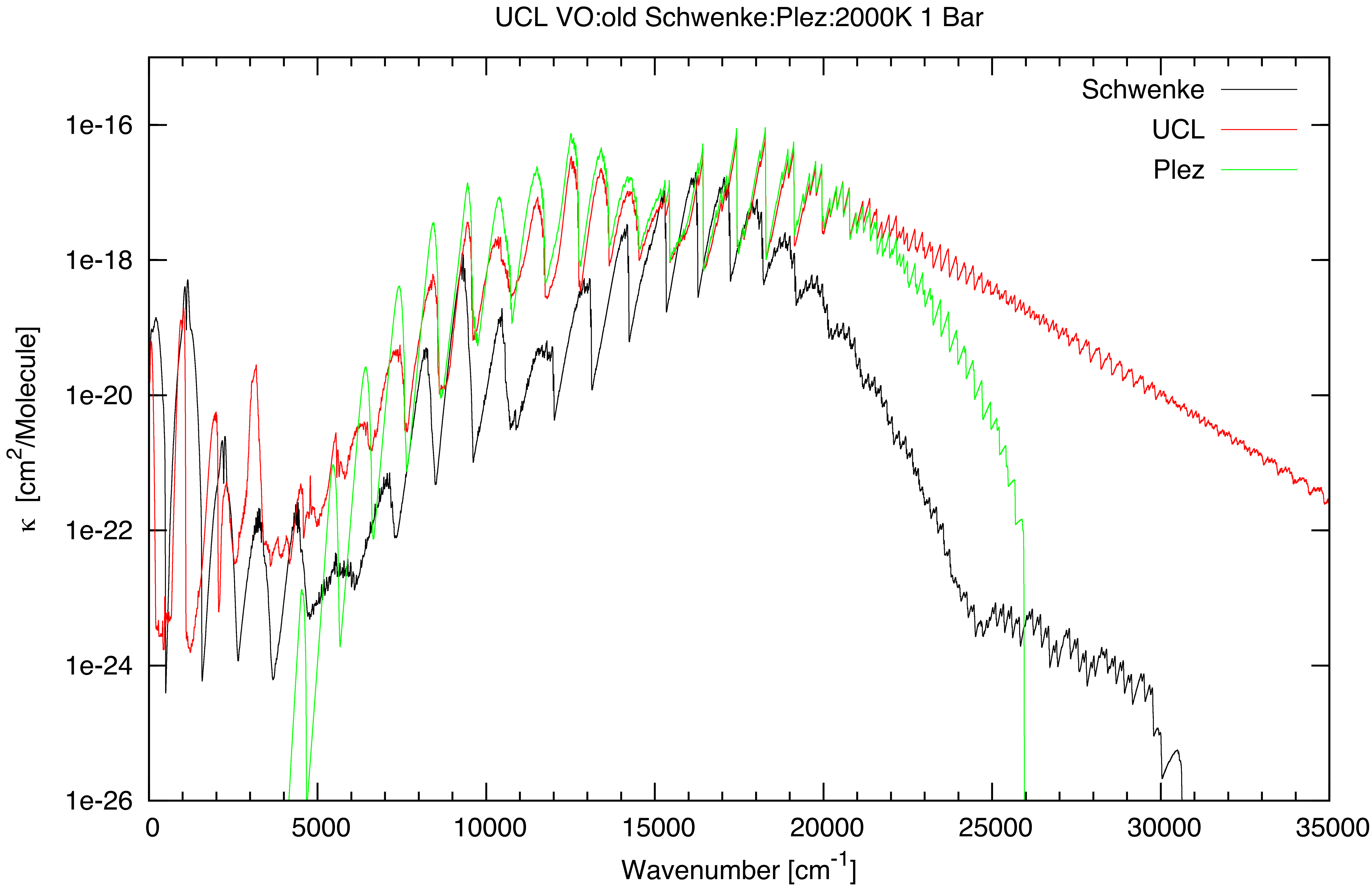
Yurchenko 2014 CH4 & Karkoshka absorption/cm (for pure CH4) @ 1 Bar
400K Karkoshka data
Yurchenko (smoothed)
κ/cm
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
10000
10500
11000
11500
12000
Wavenumbers [cm-1]



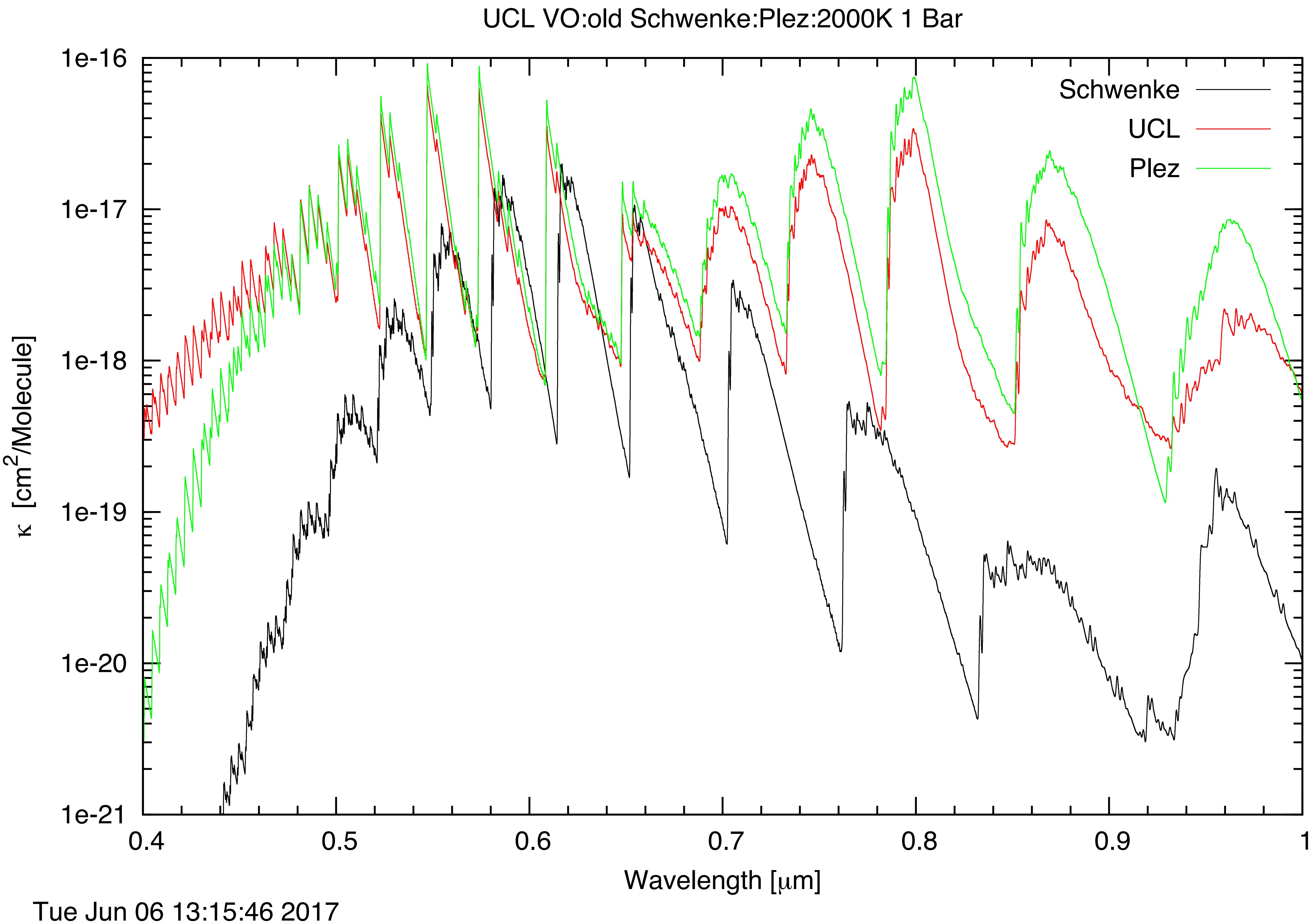
Fri Apr 27 14:22:15 2018



Tue Jun 19 19:14:09 2018



Thu Jun 01 18:32:42 2017


UCL VO:old Schwenke:Plez:2000K 1 Bar
Schwenke
UCL
Plez
1e-16
1e-17
1e-18
1e-19
1e-20
1e-21
κ [cm²/Molecule]
0.4
0.5
0.6
0.7
0.8
0.9
1
Wavelength [μm]
Tue Jun 06 13:15:46 2017

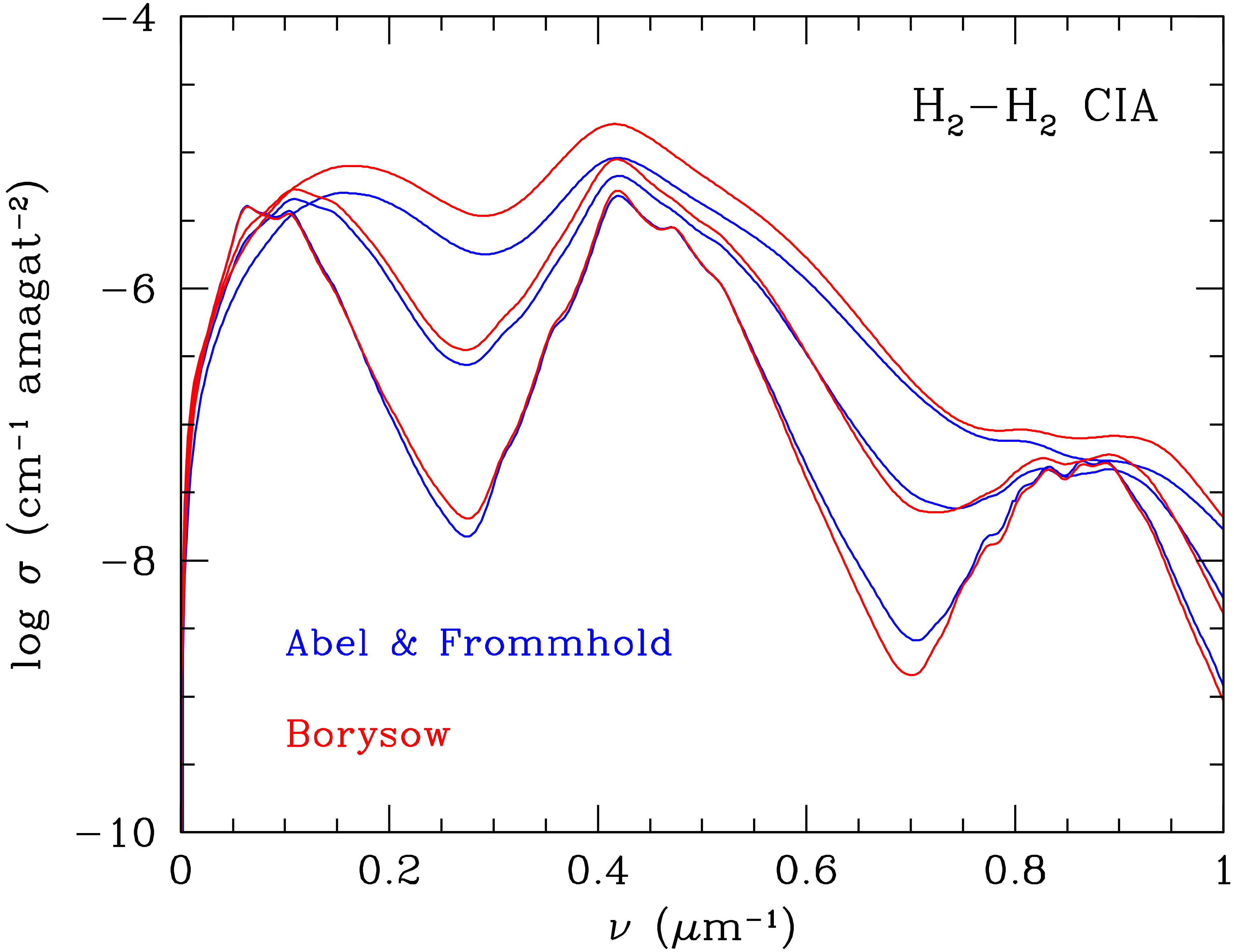


Fig. 1.— Collision-induced absorption coefficient for H_2-H_2 collisions at $T = 500$, 1000 and

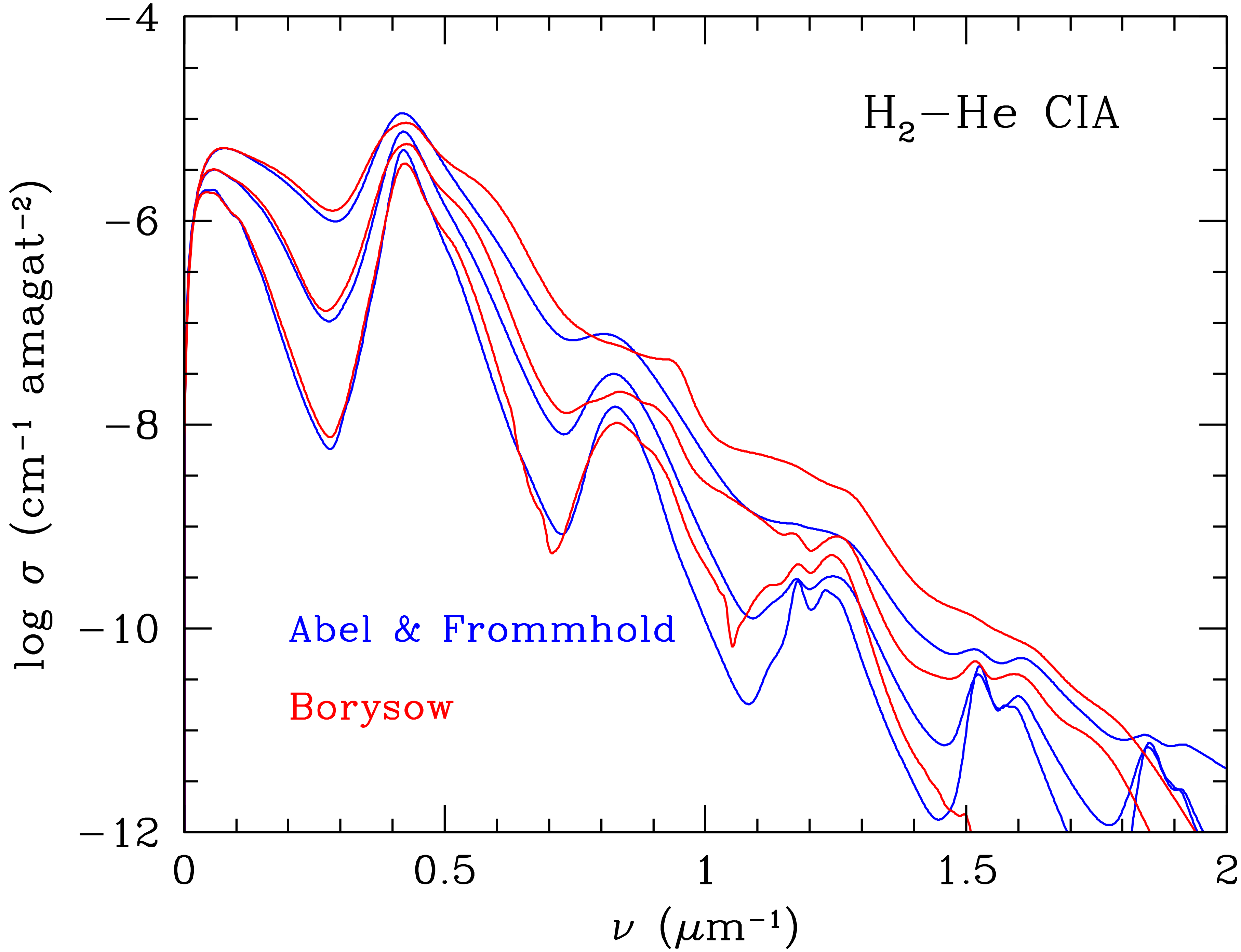
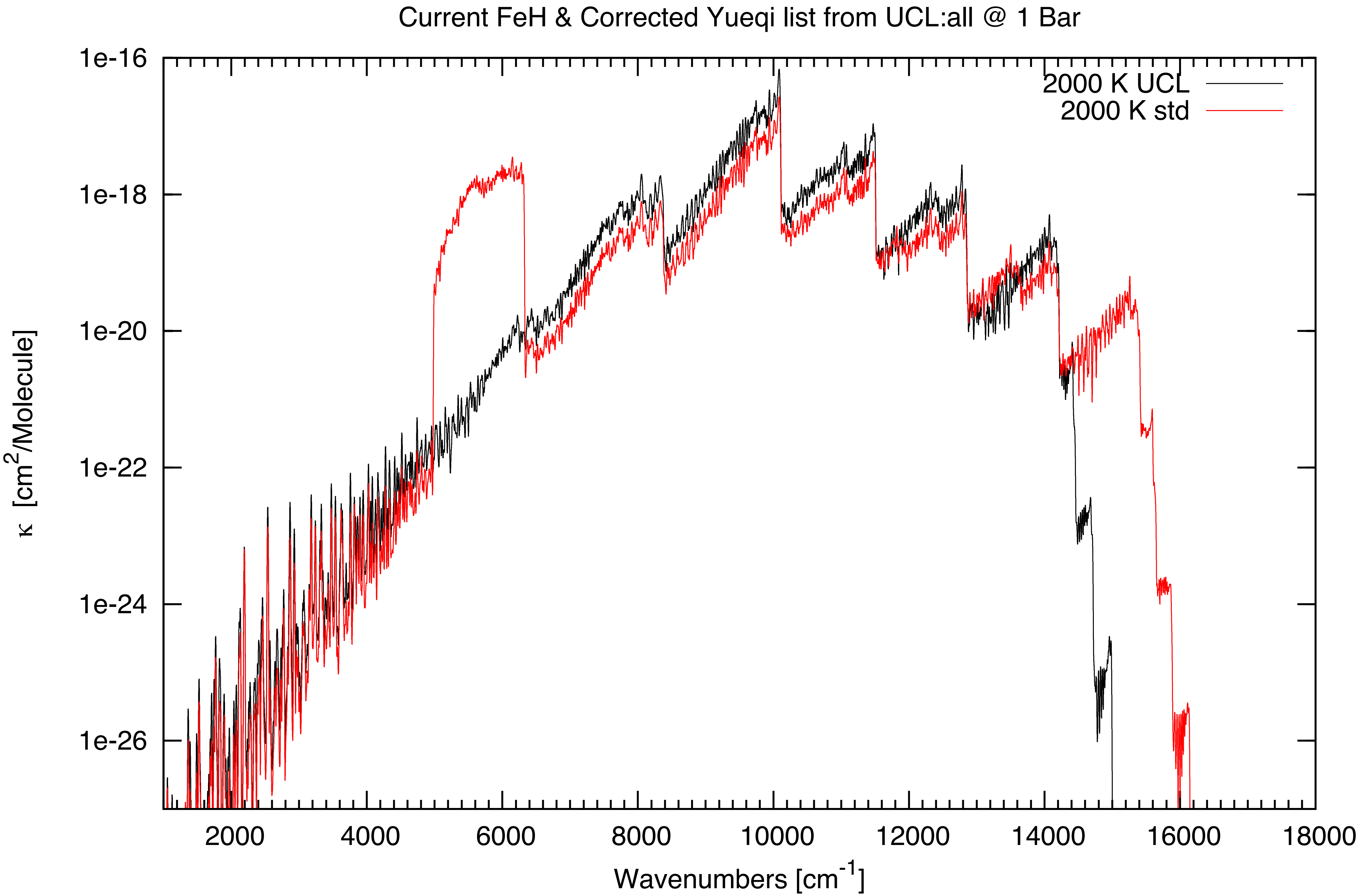


Fig. 2.— Same as Figure 1 for H_2-He CIA. The older calculation labeled "Borysow" is



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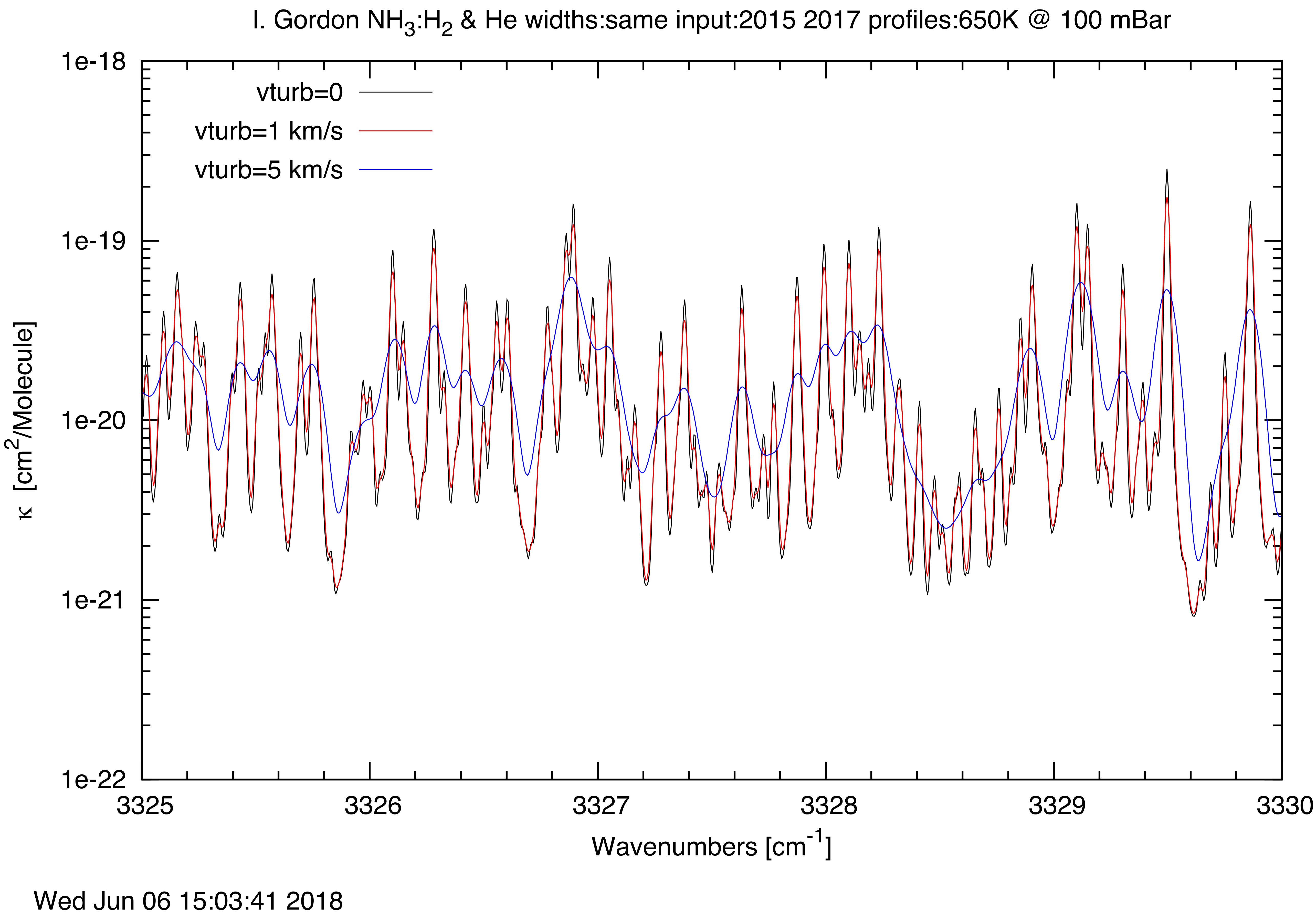
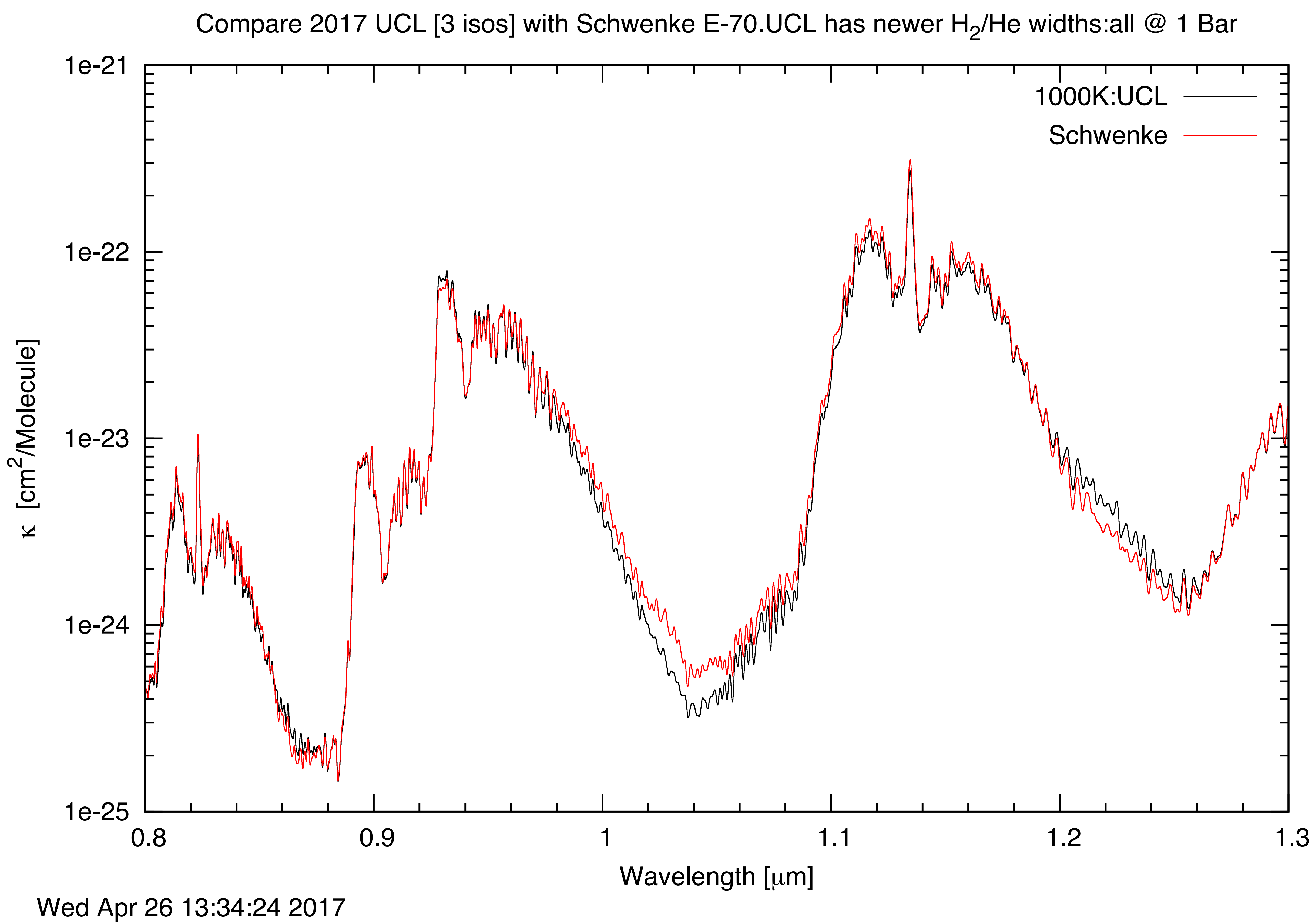
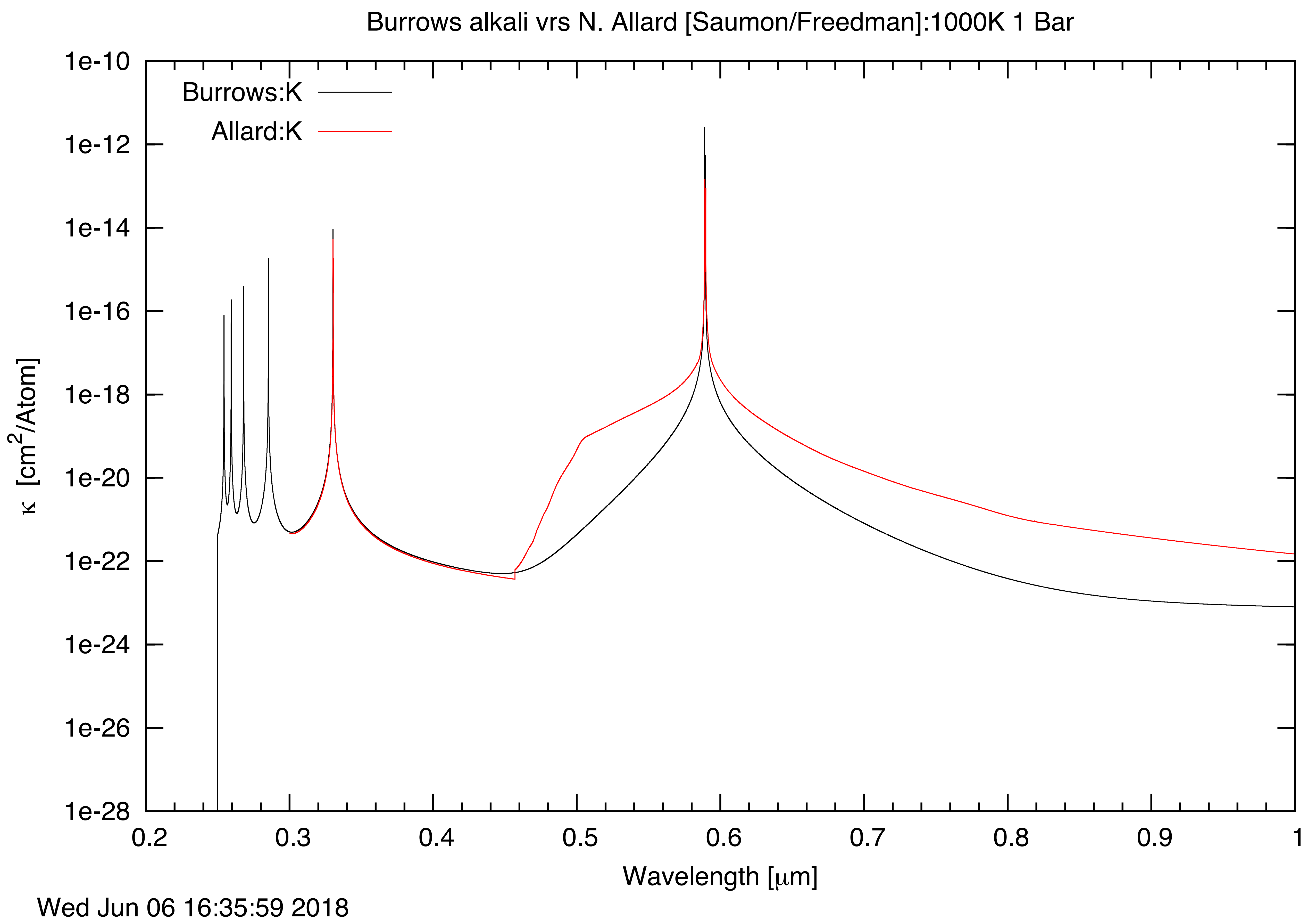
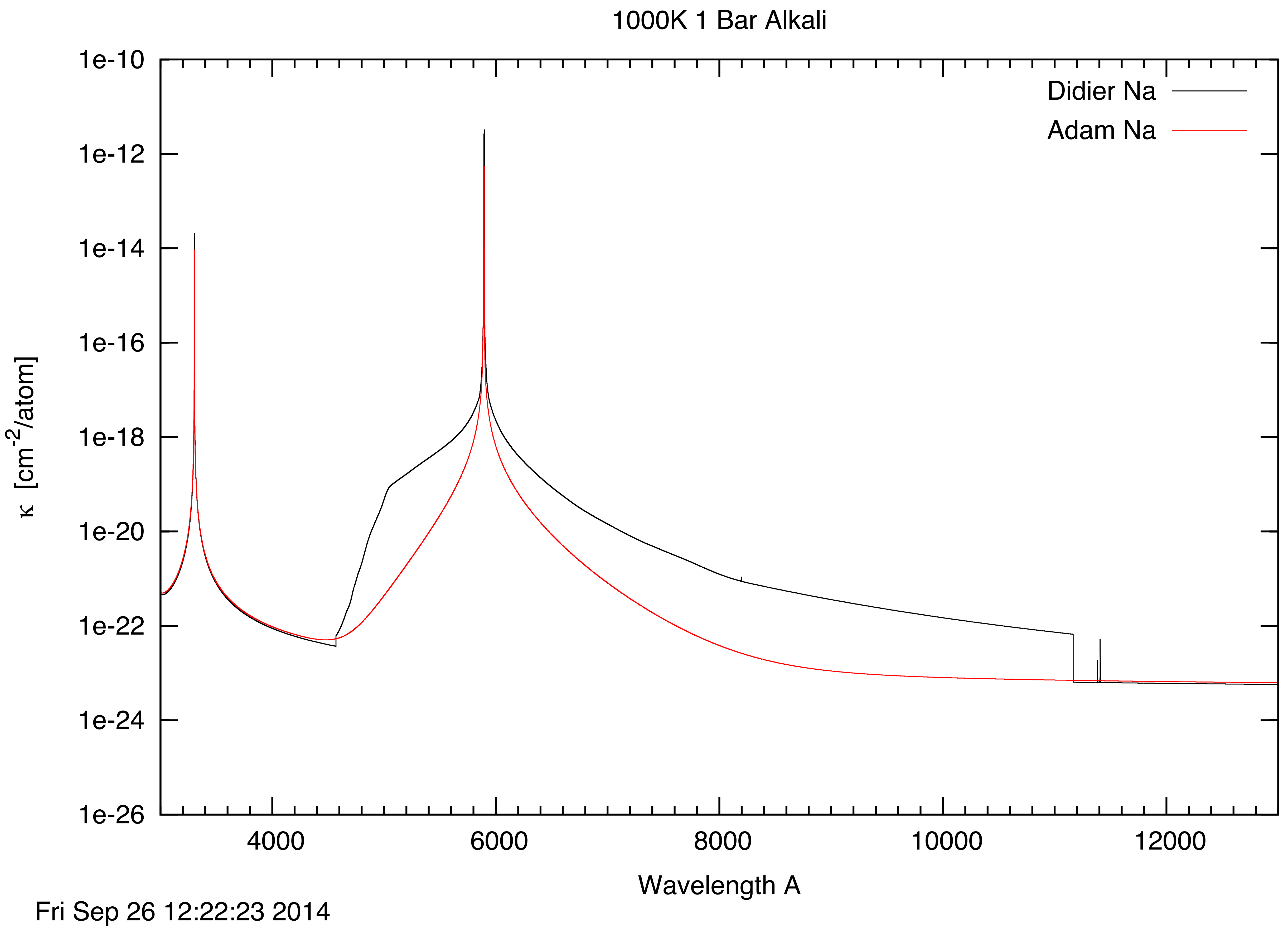


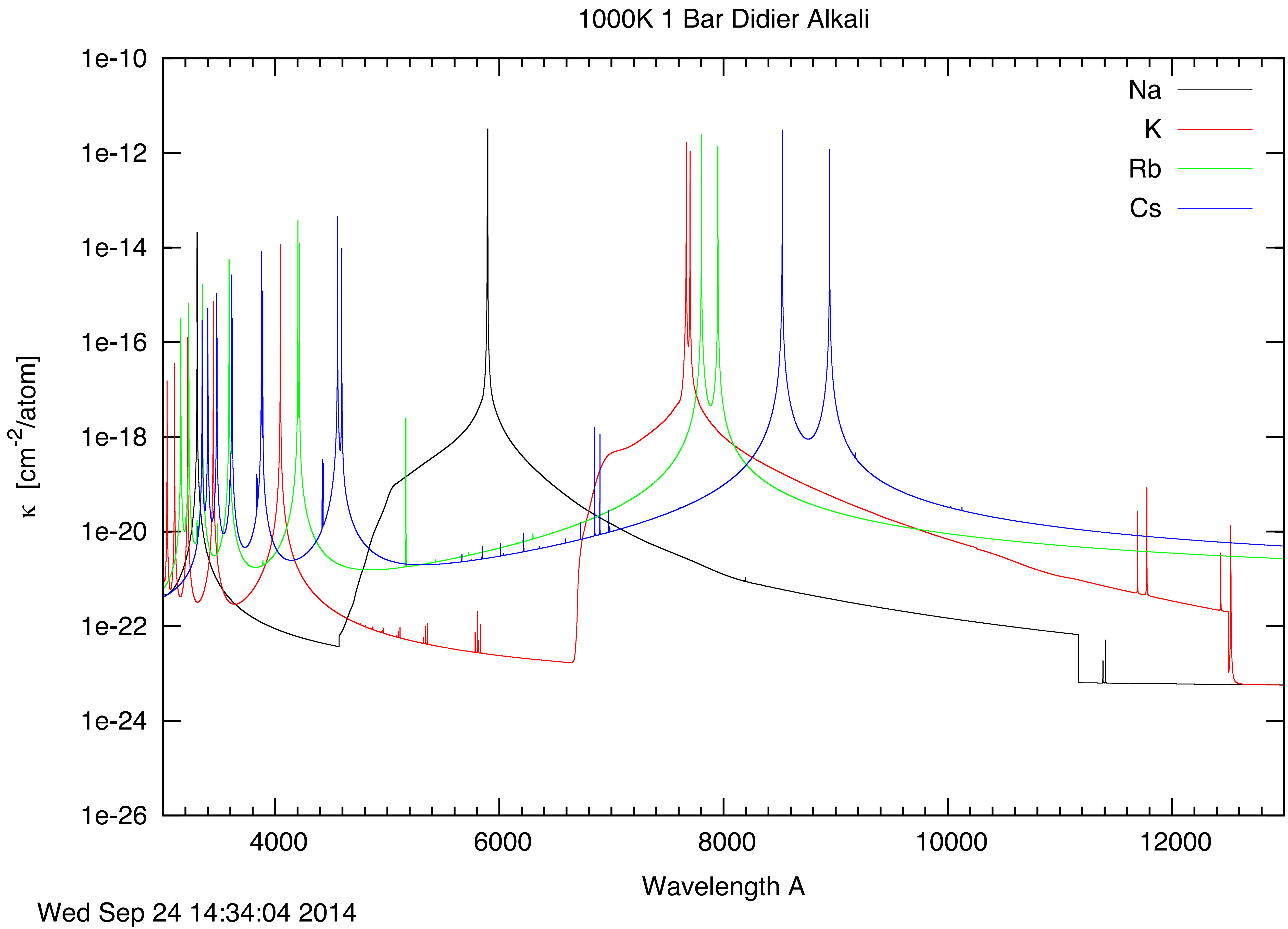
I. Gordon NH_3:H_2 & He widths:same input:2015 2017 profiles:650K @ 100 mBar
vturb=0
vturb=1 km/s
vturb=5 km/s
1e-18
1e-19
1e-20
1e-21
1e-22
κ [cm^2/Molecule]
3325
3326
3327
3328
3329
3330
Wavenumbers [cm^{-1}]
Wed Jun 06 15:03:41 2018



Compare 2017 UCL [3 isos] with Schwenke E-70.UCL has newer H_2/He widths:all @ 1 Bar
1000K:UCL
Schwenke
1e-21
1e-22
1e-23
1e-24
1e-25
κ [cm^2/Molecule]
0.8
0.9
1
1.1
1.2
1.3
Wavelength [μm]
Wed Apr 26 13:34:24 2017


Burrows alkali vrs N. Allard [Saumon/Freedman]:1000K 1 Bar
Burrows:K
Allard:K
1e-10
1e-12
1e-14
1e-16
1e-18
1e-20
1e-22
1e-24
1e-26
1e-28
κ [cm²/Atom]
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Wavelength [μm]
Wed Jun 06 16:35:59 2018


1000K 1 Bar Alkali
Didier Na
Adam Na
1e-10
1e-12
1e-14
1e-16
1e-18
1e-20
1e-22
1e-24
1e-26
4000
6000
8000
10000
12000
Wavelength A
κ [cm^-2/atom]
Fri Sep 26 12:22:23 2014



1000K 1 Bar Didier Alkali
Na
K
Rb
Cs
1e-10
1e-12
1e-14
1e-16
1e-18
1e-20
1e-22
1e-24
1e-26
κ [cm-2/atom]
4000
6000
8000
10000
12000
Wavelength A
Wed Sep 24 14:34:04 2014

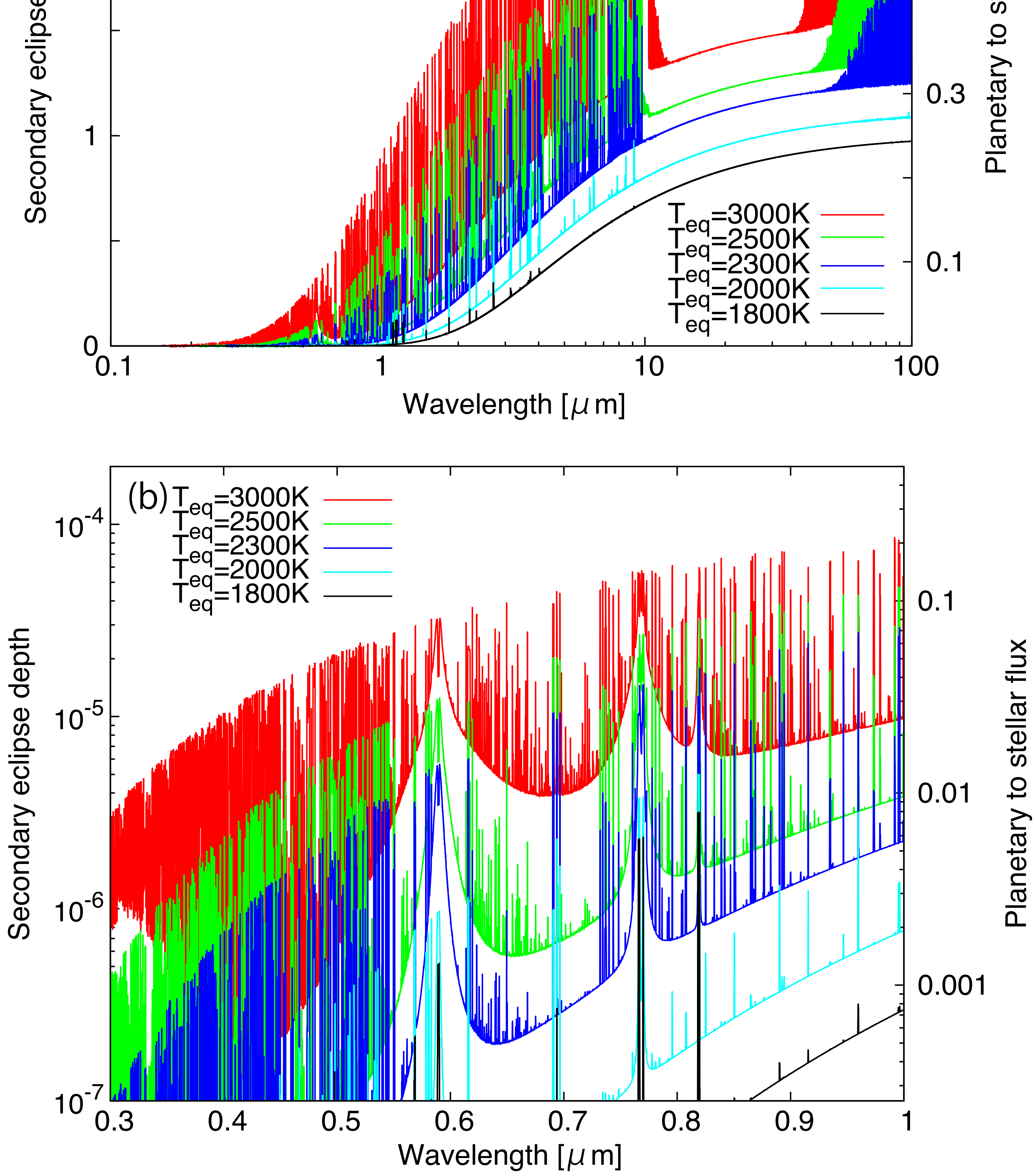


Figure 6. Predicted dayside-averaged emission spectra of a hot rocky super-Earth of 2 $R_\oplus$ in secondary eclipse that has a mineral atmosphere in equilibrium with an underlying BSE magma ocean. The secondary eclipse depth (see Equation (17)) is shown as a function of wavelength in the range of (a) 0.1–100 μm and (b) 0.3–1 μm. The inset in panel (a) is an enlarged view of the spectra in 3–5 μm. Five equilibrium temperatures are chosen: T_{eq} = 1800 K

optically thin at those wavelen

Comparing the mock spectra
can quantify the detectability o
and SiO. The error bars beco
longer-wavelength regions, be
photons (i.e., $B_{\Delta\lambda}(T_*)$) is sma
Also, the values of $\mathfrak{R}$, whic
0.1–1 μm and 10 in 1–100 μm,
shown in Figure 7(a), the
sufficiently detectable at
T_{eq} = 3000 K. The SiO featur
at 10 μm for T_{eq} = 2500 K (Fi
marginally undetectable for T_{e}

The S/N for detecting the lin
the secondary eclipse depth is
the secondary eclipse detection
eclipse depth relative to that w
blackbody with T_g), $\eta_{\lambda,\Delta\lambda}$, as

$$\eta_{\lambda,\Delta\lambda} \equiv \left| \int_{\lambda}^{\lambda+\Delta\lambda} \frac{\epsilon_{\lambda}}{} \right.$$

where $\epsilon_{\mathrm{BB},\lambda}(T_g)$ is the sec
blackbody radiation with T_g.
detectability of the line spectra
and (21), we introduce a nev
defined as

$$(\mathrm{S/N})_{L,\Delta\lambda} = \eta$$

Conclusions

As observations improve and line data sets expand more attention will have to be paid to problems that were either ignored or could not be easily addressed. In the future large, ground based telescopes could provide much higher resolution data in the IR regions that are accessible from the ground and this may require a constant re-examination of the techniques being used in generating opacities for both modeling and for comparison with high quality observations.