HITRAN2020:
An overview of what to expect

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Overview plan for **HITRAN**2020 (due: end of 2020)

Line-by-line (LBL):

- Almost all 49 molecules from **HITRAN**2016 [1] will be updated. The scale of each update depends on the molecule: ranging from the addition of new isotopologues/bands (e.g., $^{15}NO_2$), to the correction of a small number of line positions.
- Examples for H_2O, CO_2, O_3, CH_4 & selected trace gases are described over the next slides in order of their HITRAN ID number.
- New molecular species will be added (e.g., CH_3I, NF_3, CS_2).
- Foreign broadening parameters have been expanded with the inclusion of H_2O broadening [2]. Fig. 1 shows an example for CO_2.
- Non-Voigt line shapes have been added for some molecules.
- The line-mixing package is being updated for CO_2. integrated into HAPI.

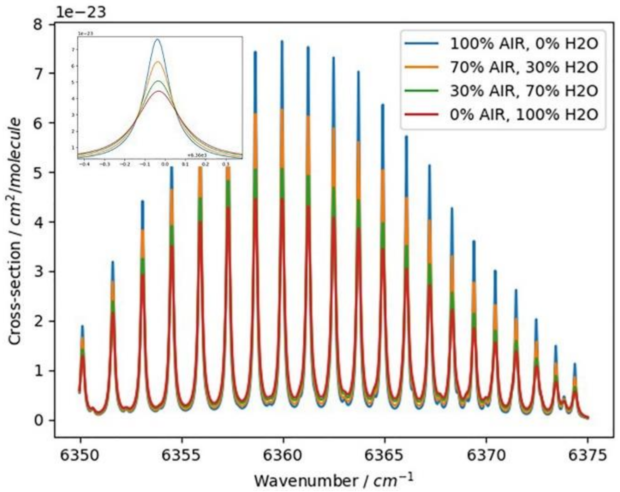


Figure 1

Collisional Induced Absorption (CIA):

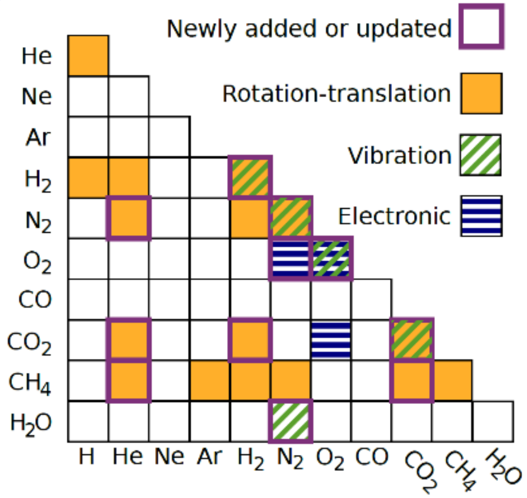


Figure 2

The CIA section has been expanded (Fig. 2). This includes updates to the **HITRAN**2020 CIA, new collisional complexes and new spectral regions [3]. In addition to Ref. [3], more CIA complexes will also be included.

Absorption cross sections (XSC):

Many updated XSCs [4] were made available for **HITRAN**2016. It is expected than more will be added which contain H_2 and He broadening, as well as an increase in the number of XSCs that cover the UV spectral region.

HITRAN2020

[1] Gordon et al. 2016 [doi:10.1016/j.jqsrt.2017.06.038]
[2] Tan et al. 2020 [doi:10.1029/2019JD030929]
[3] Karman et al. 2019 [10.1016/j.icarus.2019.02.034]
[4] Kochanov et al. 2019 [10.1016/j.jqsrt.2019.04.001]

1: H_2O – Water vapour in LBL

Motivation to update H_2O from **HITRAN**2016:

- H_2O was shown to be much improved for atmospheric retrievals [1], with respect to HITRAN2012, but some line broadening problems were readmitted from earlier editions by not sticking to the “Diet” [2]
- *Ab initio* line intensities for the UV-visible region (from POKAZATEL [3]) were inferior to those they replaced (from BT2 [4])

Improvements expected for **HITRAN**2020:

- New experimental and *ab initio* works [5] will be used to provide a large update to positions and intensities
- The visible spectral region will be updated from Ref. [5], which agrees well with Ref. [6]. This region will be used by the NASA TEMPO for retrievals
- Cross-sections from recent UV measurements [7,8] disagree with theory by many orders of magnitude [9]. They are also more intense than well-studied bands at 400 and 450 nm, which is not supported by any other work.
- Measurements in the UV region are difficult, but the theoretical intensities from Ref. [5] fall within the upper limits of detection from earlier works [10].

[1] Olsen et al. 2019 [doi:10.1016/j.jqsrt.2019.106590]
[2] Gordon et al. 2007 [doi:10.1016/j.jqsrt.2007.06.009]
[3] Polyansky et al. 2018 [doi:10.1093/mnras/sty1877]
[4] Barber et al. 2006 [doi:10.1111/j.1365-2966.2006.10184.x]
[5] Conway et al. 2020 [doi:10.1016/j.jqsrt.2019.106711]
[6] Harder & Brault 1997 [doi:10.1029/96JD01730]
[7] Du et al. 2013 [doi:10.1002/grl.50935]
[8] Pei et al. 2019 [doi:10.1029/2019JD030724]
[9] Conway et al. 2020 [doi:10.5194/acp-2020-286]
[10] Wilson et al. 2016 [doi:10.1016/j.jqsrt.2015.11.015]

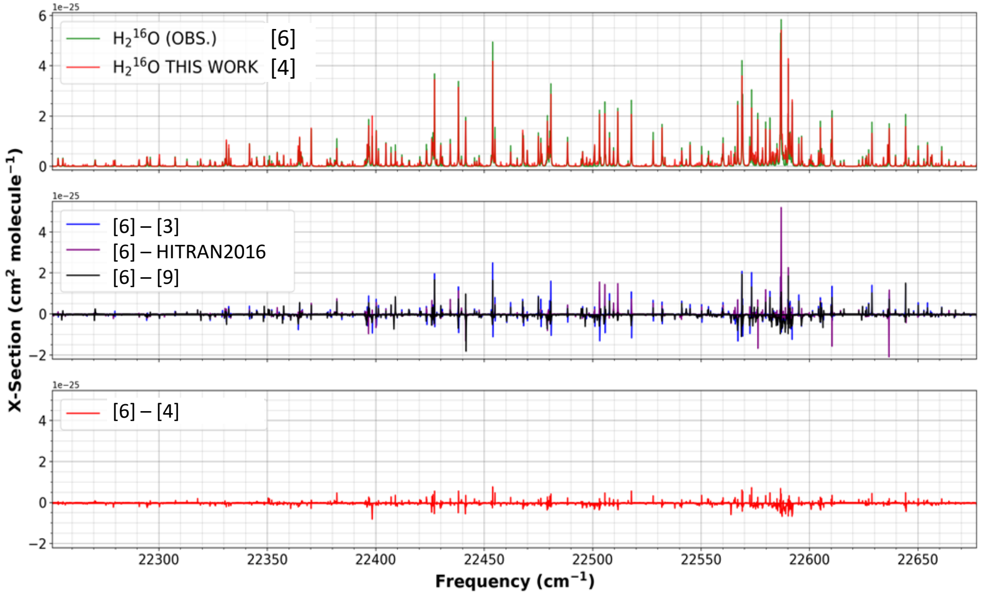


Fig 1: Residuals from comparisons between experimental absorption cross sections [6] and several line lists of H_2O for the visible region.

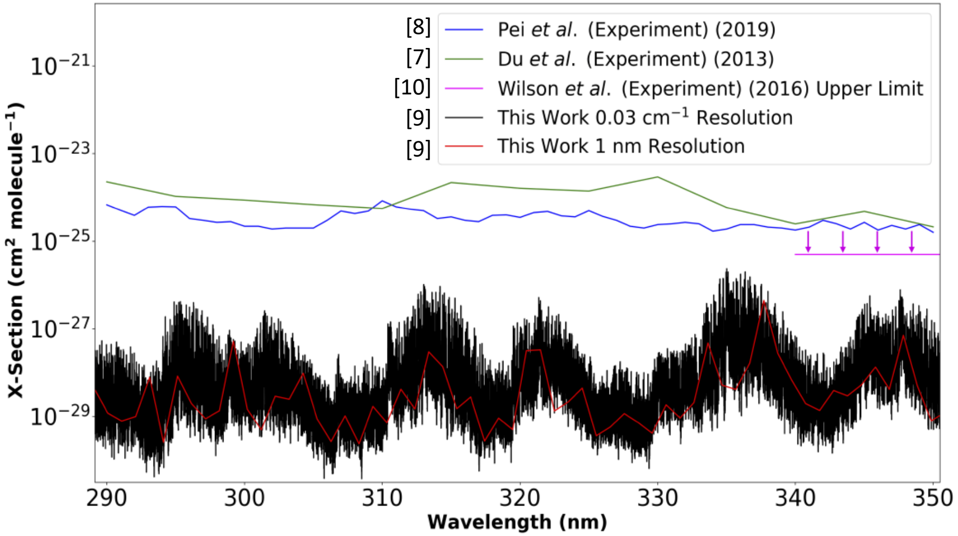


Fig 2: The new calculated line list for H_2O [4], which will be used to update HITRAN, compared to UV experimental cross sections [7-8, 10]. The figure has been taken from Ref. [9].

2: CO_2 – Carbon dioxide in LBL

Motivation to update CO_2 from **HITRAN**2016:

- Overall, CO_2 in HITRAN2016 show substantial improvements compared to previous editions.
- Some positions and intensities can be improved.

Changes expected for **HITRAN**2020:

- Overall, line intensities will be updated the CDSD-296 [1].
- A hot band near 4800 cm^{-1} is over estimated by 10-15%. This region is targeted by OCO-2/3 and will be fixed, see Figure 1.
- Addition of H_2O broadening [3], see Figure 2.
- Line broadening parameterization for Voigt, speed-dependent Voigt and Hartman-Tran will be included for every line of CO_2.
- The line-mixing package will also be updated and made compatible with HAPI [5], see Figure 3.

[1] Tashkun et al. 2019 [doi:10.1016/j.jqsrt.2019.03.001]
[2] Toth et al. 2006 [doi:10.1016/j.jms.2006.08.003]
[3] Tan et al. 2020 [doi:10.1029/2019JD030929]
[4] Sung 2020 (private communication)
[5] Kochanov et al. 2016 [doi:10.1016/j.jqsrt.2016.03.005]

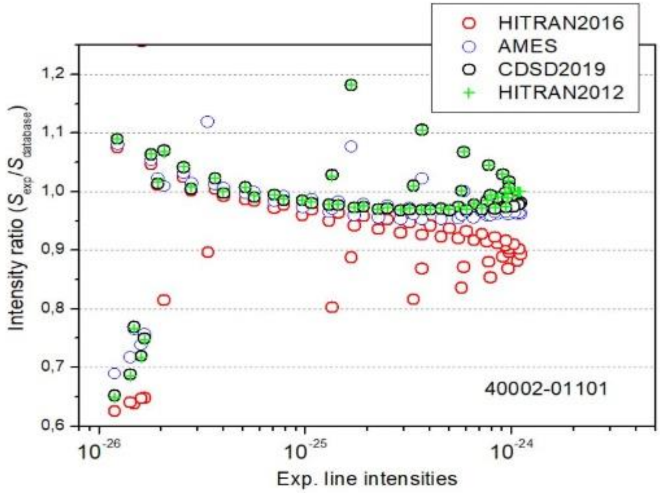


Fig 1: Comparisons of measured line intensities [2] of the the 40002-01101 band of CO_2 to different databases.

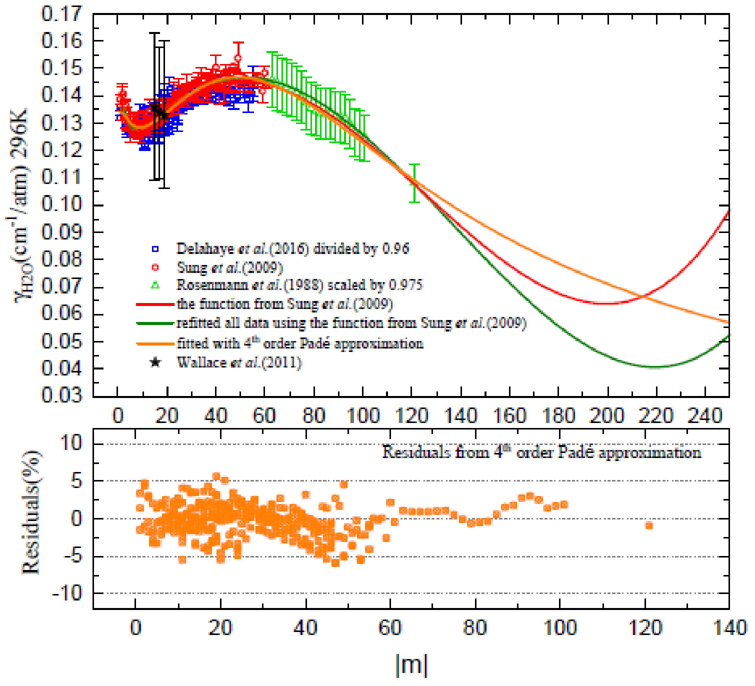


Fig 2: H_2O broadening of H_2O lines as a function of rotational quantum number [3].

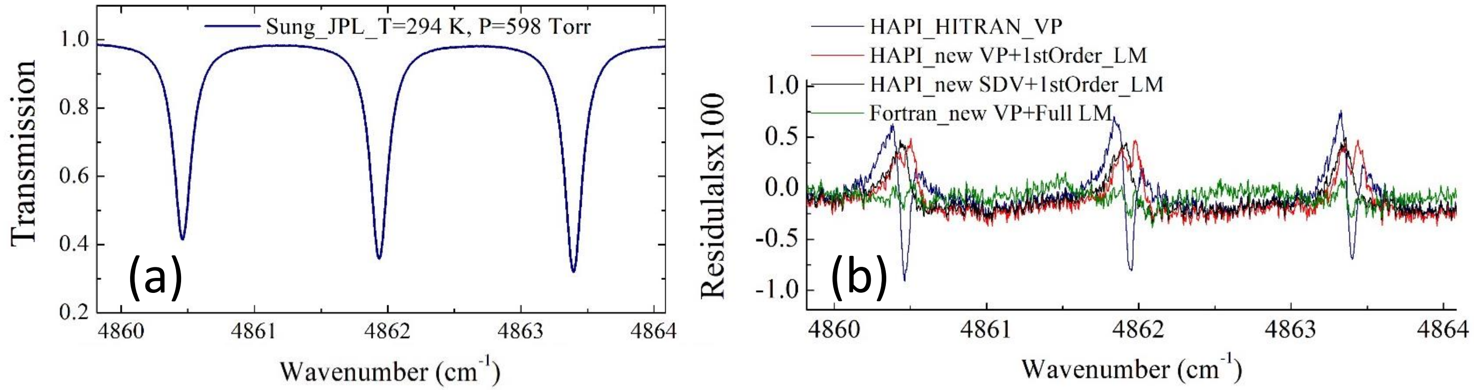


Fig 3: (a) Experimental measurements of CO_2 [4]. (b) Residuals based on calculated spectra that employ different line profiles and line mixing packages. The new full implementation (green) will be made compatible with HAPI [5].

3: O_3 – Ozone in LBL

Important Changes!

Motivation to update O_3 from **HITRAN**2016:

Atmospheric retrievals of O_3 based on the MW, 10 µm, 5 µm and UV spectral regions give similar results, but the intensities were consistently too weak.

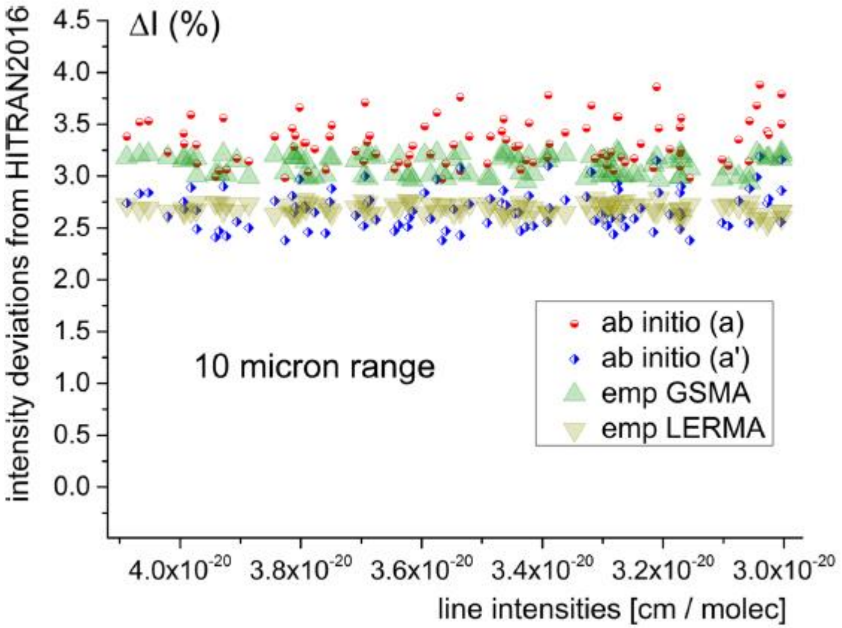
Improvements expected for **HITRAN**2020:

- O_3 line intensities for the MW and 10 µm have been shown to be self consistent [1].
- However, experimental comparisons in the MW [2] have show them to be too weak (also, meaning the 10 µm region is too weak).
- Corroborated by independent analyses in Paris (LERMA), Reims (GDMA) and DLR which agree with ab initio calculations shown on the right, with similar shifts also seen for the 10 µm region [3].
- Complete validations of these regions will not be available before the release of HITRAN2020. Therefore recommended scaling factors will be applied to the line intensities:

Band	MW	10 µm	5 µm	14 µm
Scaling increase	3.8 %	3 %	3.3 %	1.8 %

- In addition, high resolution measurements have been made available for the 3600–4300 cm^{-1} region [4] and new UV cross sections have been validated for use in OMI retrievals [5]. These will be added to the database.

[1] Drouin et al. 2017 [doi:10.1016/j.jqsrt.2017.06.035]
[2] Birk et al. 2019 [doi:10.1016/j.jqsrt.2019.01.004]
[3] Tyuterev et al. 2019 [doi:10.1063/1.5089134]
[4] Mikhailenko & Barbe 2020 [doi:10.1016/j.jqsrt.2019.106823]
[5] Bak et al. 2020 [doi:10.5194/amt-2020-94]



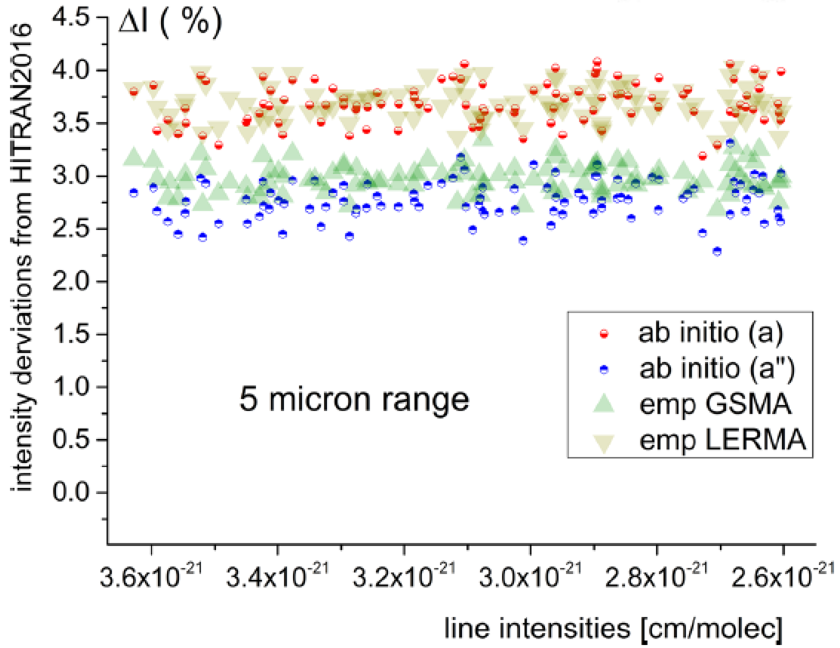


Fig 3: Comparisons of experimental and *ab initio* O_3 intensities, taken from Ref. [3]. These deviations are supported by measurements form DLR [2].

6: CH_4 – Methane in LBL

Motivation to update CH_4 from **HITRAN**2016:

Availability of new high accuracy experimental observations in many regions , for example in octad region [1].

Improvements expected for **HITRAN**2020:

- Addition of H_2O broadening from Ref. [2], see Figure 1.
- Including H_2O broadening of CH_4 shows improvement when modelling using HAPI [3], shown in Figure 2.
- Further improvements will be provided from published results from the DLR measurements [2].
- Speed-dependent Voigt, and Voigt line shapes will be updated especially in tetradecad region

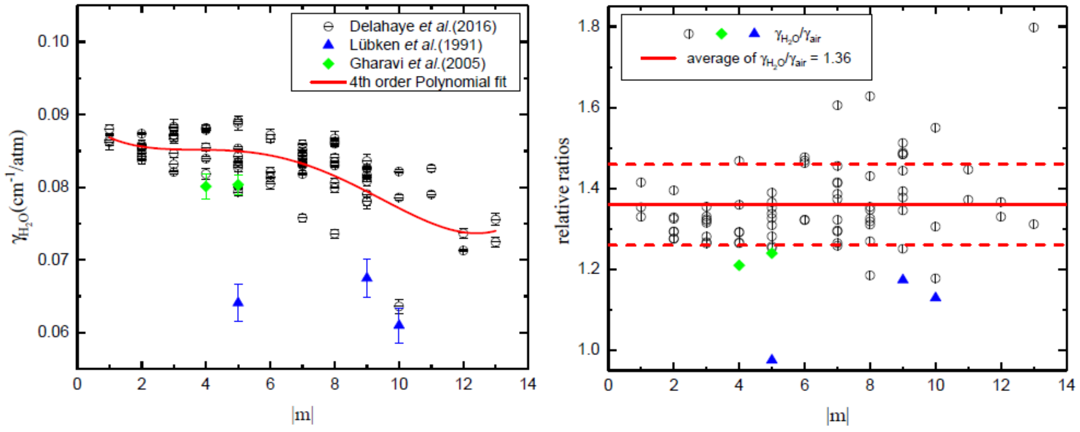


Fig 1: Broadening of CH_4 lines as a function of rotational quantum number [2]

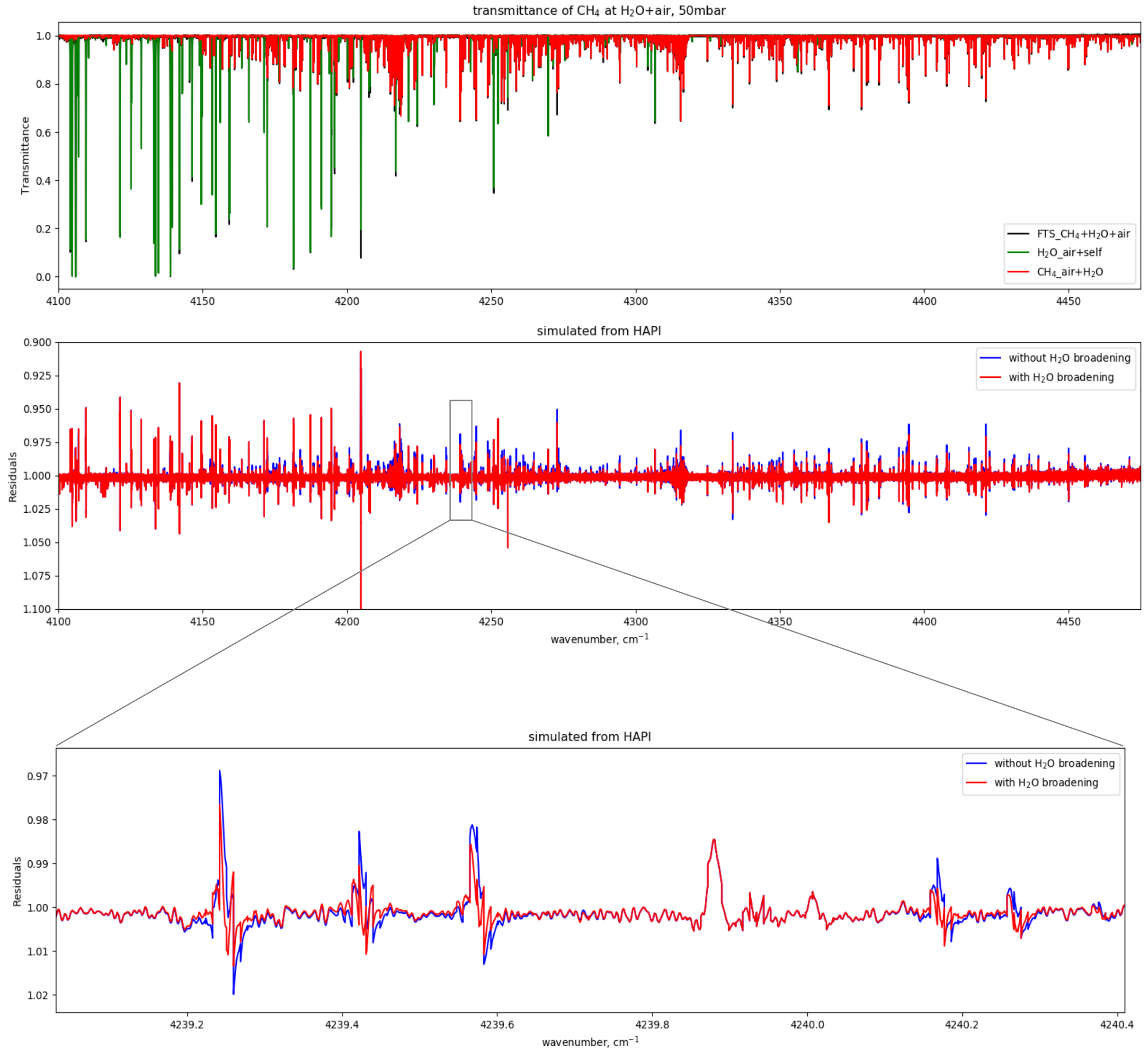


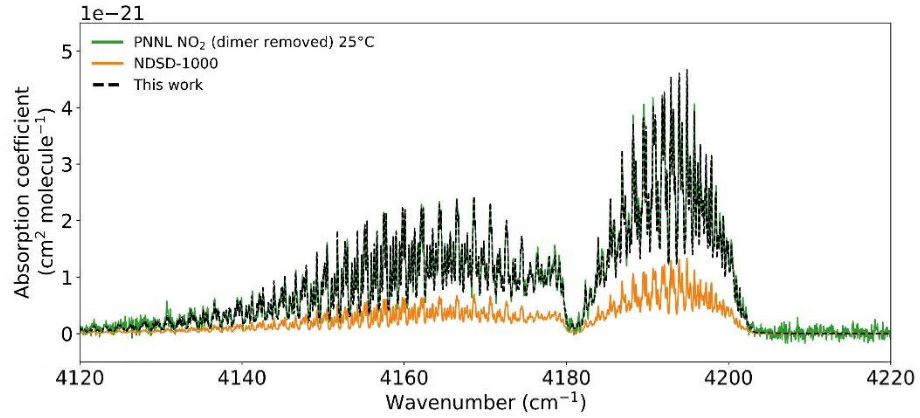
Fig 2: Comparison of HITRAN and experimental spectrum (data courtesy of DLR [1]) of CH_4 using H_2O broadening parameters of Ref. [2].

[1] Birk et al. 2017 [zenodo link]
[2] Tan et al. 2020 [doi:10.1029/2019JD030929]
[3] Kochanov et al. 2016 [doi:10.1016/j.jqsrt.2016.03.005]

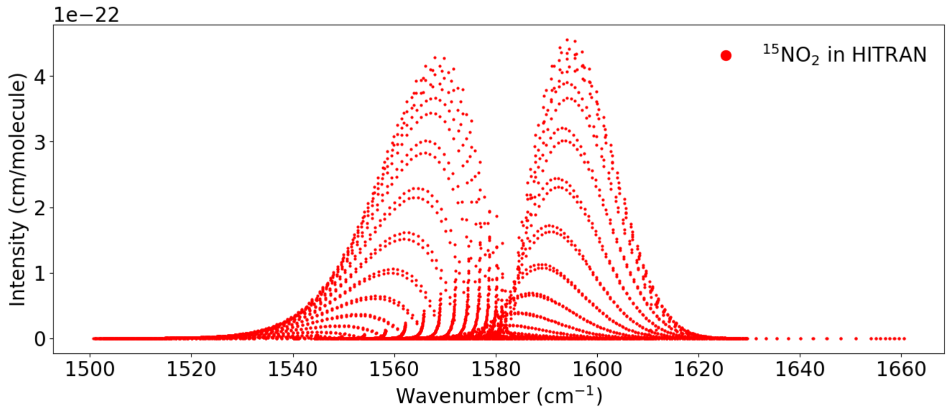
Examples for trace gases

10: NO_2 – Nitrogen dioxide in LBL

- Addition of ΔP=6 bands for $^{14}NO_2$ [1] scaled from NDSD-1000 [2]:



- Addition of v_3 band for $^{15}NO_2$ from Ref. [3]:

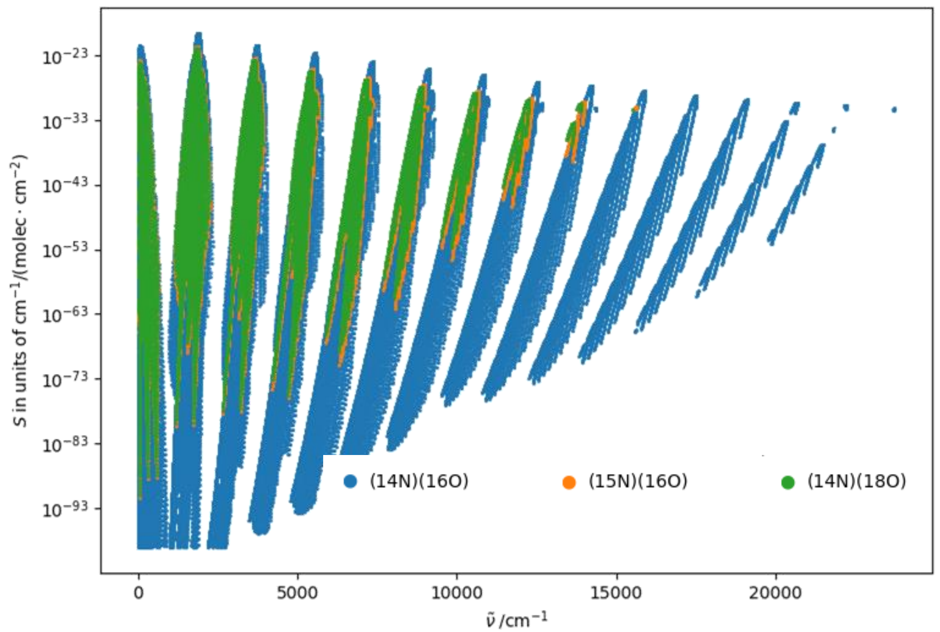


7: O_2 – Oxygen in LBL

- New, high-accuracy data in the 1.27 μm band [4,5] and additional measurements [6] will enable the improvement of many parameters in HITRAN.
- The data is of sufficient accuracy to disentangle electric quadrupole and magnetic dipole transitions.

8: NO – Nitric Oxide in LBL

- Large increase in in spectral coverage, see Ref. [1]:

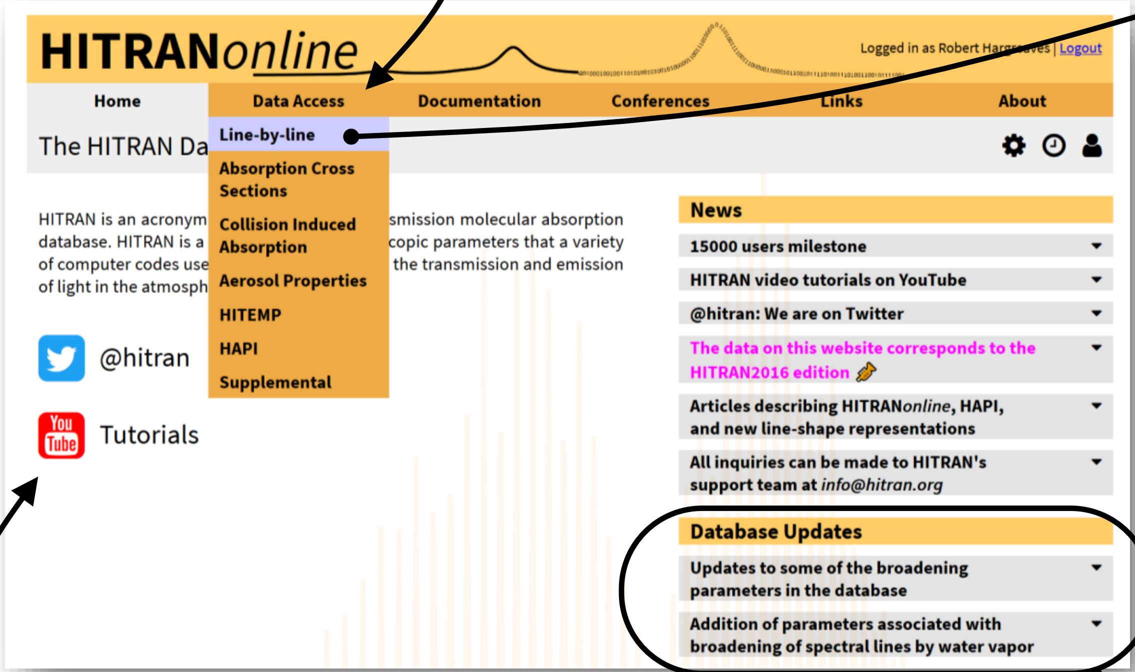


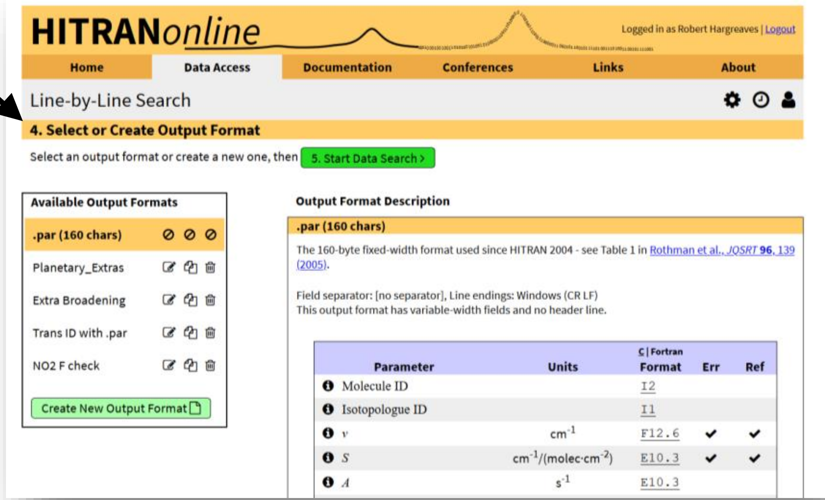
[1] Hargreaves et al. 2019 [doi:10.1016/j.jqsrt.2019.04.040]
[2] Lukashevskaya et al. 2017 [doi:10.1016/j.jqsrt.2017.07.011]
[3] Perrin et al. 2015 [doi:10.1016/j.jqsrt.2014.12.006]
[4] Tran et al. 2020 [doi:10.1016/j.jqsrt.2019.106673]
[5] Konefał et al. 2019 [doi:10.1016/j.jqsrt.2019.106653]
[6] Mendonca et al. 2019 [doi:10.5194/amt-12-35-2019]

To access *all* current HITRAN data, visit www.hitran.org
HITRAN2020 will be available at the end of 2020

1. HITRAN data is accessible from this tab. Line-by-line data can also be downloaded using HAPI python routines [1].

2. The standard ".par" remains the default choice when downloading line-by-line data. However, additional parameters (e.g., broadening/line-shape) can be selected when choosing your output format.





4. Watch a series of "how to" tutorials that explain accessing and using the HITRAN database.

3. The current online database pertains to the HITRAN2016 edition [2], *plus* recent updates towards HITRAN2020. Any recent changes are listed here.

[1] Kochanov et al. 2016 [doi:10.1016/j.jqsrt.2016.03.005]

[2] Gordon et al. 2016 [doi:10.1016/j.jqsrt.2017.06.038]