Making a Splash: The New Water Data in HITRAN2024

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Overview

A major update of the HITRAN water line list will be available for HITRAN2024, it includes a substantial improvement in terms of incorporating new lines from recently MARVELised line lists [1] and improving line positions and intensities. Key spectral regions relevant for atmospheric studies have been evaluated, including the “window" region at 442 nm (targeted by TEMPO), see the figure below showing the window region convolved cross section against the published spectrum from Harder et al. (1997) [2]. Intensities for several vibrational bands were evaluated against laboratory data to identify systematic differences [3, 4] with *ab initio* values in HITRAN2020. In addition, a new python program has been developed to identify the outliers within the broadening parameters in the line list and replace them with new measurements from the literature [4–8]. Furthermore, a study of the cavity ring-down spectroscopy of water vapor [9] has helped identify the need for new positions for several lines which were previously unassigned in HITRAN2020.

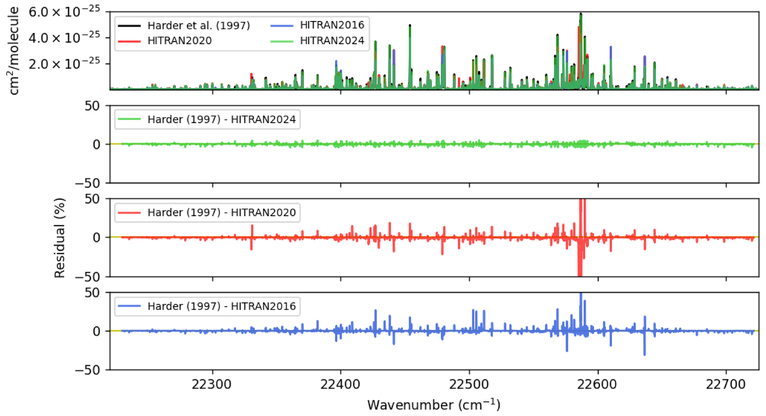
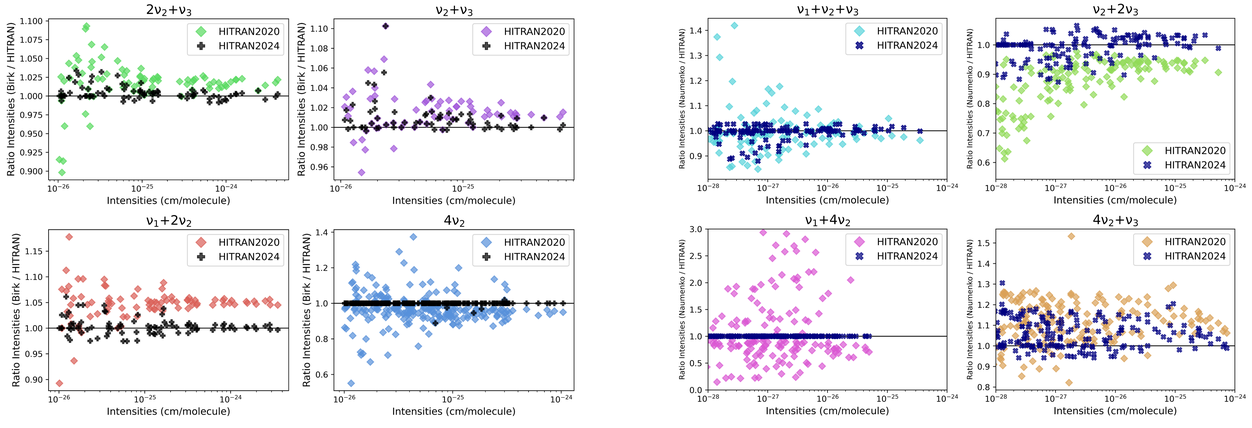


Figure 1: HITRAN2024, HITRAN2020 and HITRAN2016 compared to data from Harder et al. (1997) [2]. The cross section spectra were calculated with a Voigt line shape, air broadening at a temperature of 300 K and pressure of 1 atm, it was convolved at a resolution of 0.055 cm^{-1} with a Gaussian slit function. All of the residuals are shown with the same y-axis limits from +/- 50%. The spectrum was calculated with HITRAN Application Programming Interface (HAPI) [10].

Line list improvements per vibrational band

Various vibrational bands in HITRAN have been a topic of discussion in the literature (see [3]) which have highlighted the need to improve line intensities for those with systematic offsets. In particular, the bands identified in Solodov et al. (2022) [3] in the 0.9 μm region require scaling, except for the ν_1+4ν_2 band, which has an unsystematic intensity ratio distribution, so this band was given direct intensities from the Solodov et al. (2022) line list. Similarly, the authors from Birk et al. (2024) [4] have demonstrated that within the 1.6 μm region there are four bands that can be improved by scaling intensities towards those from Birk et al. (2024) [4]. Notably the 4ν_2 band lacked a systematic offset, therefore experimental intensities were taken directly.



(a) Bands adjusted to Birk et al. (2024) intensities

(b) Bands adjusted to Solodov et al. (2022) intensities

Figure 2: (a) Plotting the ratio of intensities for $H_2{}^{16}O$ between HITRAN2020 matched to the Birk et al. (2024) [4] list. Showing only lines that are $\geq 10^{-26}$. 2ν_2+ν_3 was scaled up by +1.89%, ν_2+ν_3 was scaled up by +1.29%, ν_1+2ν_2 was scaled up by +4.87%. For 4ν_2 if the line matched to Birk then intensities were taken directly, if not they were scaled by -5.89%. (b) Plotting the ratio of intensities for $H_2{}^{16}O$ between HITRAN2020 matched to the Solodov et al. (2022) [3] list for the lines that are $\geq 10^{-28}$. The ν_1+4ν_2 is a zoomed-in image from y axis 0-3, there are outliers from HITRAN2020 outside this y axis range. ν_1+ν_2+ν_3 was scaled down by -3.86%, ν_2+2ν_3 was scaled down by -8.29% and 4ν_2+ν_3 was scaled up by +7.47%.

Broadening parameters filtered with DIET

A new Python program (DIET) was developed to filter outliers in γ_{air} broadening parameters for water. This method is very efficient for catching major outliers based on plotting the data versus $J'' + 0.9(K_c''/J'')$. This DIET filter was used to replace the strongest $\geq 10^{-23}$ bands γ_{air} outliers in HITRAN2020, primarily there were 29 vibrational bands that were addressed. The plot shown in Figure 3 shows the filtered HITRAN2020 data after processing through the DIET code, the orange and red points identify outliers beyond the fitted 3rd order polynomial (shown as the black line).

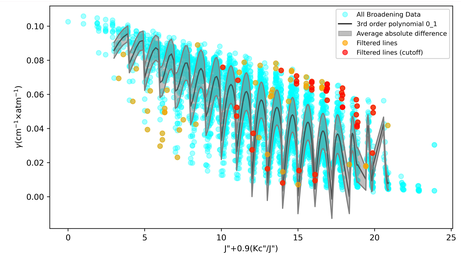
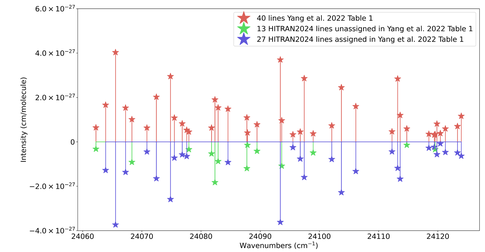


Figure 3: HITRAN2020 ν_2 γ_{air} broadening plotted versus $J'' + 0.9(K_c''/J'')$ where J and Kc are both the lower rotational quanta. The data was processed through DIET which plots all non-outlying values in cyan color, outliers are orange and red points, the 3rd order polynomial and its average absolute difference is shown as the black line and gray shaded region.

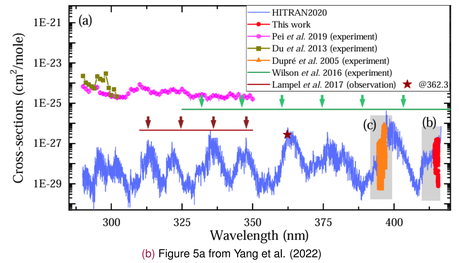
Further improvements in the UV & Visible region

Table 1 of Yang et al. (2022) [9] contained a summary of line positions recorded from 24062-24124 cm^{-1} and was used to verify the new assignment of previously unassigned lines in HITRAN, and adapt experimental line positions for HITRAN2024, see (a) Figure 4. There are 13 unassigned lines which were matched based on similarity in both position and intensity relative to the experimental values reported by Yang et al. (2022) [9]. There were 27 assigned or partially assigned lines in Table 1 of Yang et al. (2022) [9] which could be matched to those of the same assignment in the HITRAN2024 list or determined as matching based on reasonable position (< 0.09 cm^{-1}) and intensity differences between the two lists. These 27 lines were given position values from Yang et al. (2022) [9] and are shown in (a) Figure 4 as ★ and the unassigned lines are shown as ★ in (a) Figure 4.

Figure 4 (b) from Yang et al. (2022) [9] presents several cross-sections for water from experiments, observations, and from HITRAN2020. While the individual parameters have changed in HITRAN2024 for that region, on this scale, the cross-sections remain very similar to those from HITRAN2020. The results from the Albany group [11, 12] that are promoted by some of the atmospheric groups (e.g. [13]) are not corroborated by other measurements or calculations. **More experimental work in the UV is required.**



(a) Position improvements



(b) Figure 5a from Yang et al. (2022)

Figure 4: (a) Plotting the stick spectra of the 40 lines (⋆) from Yang et al. (2022) [9]. HITRAN2024 data is broken up into the 27 assigned lines from that table (★) and the 13 unassigned lines from the table (⋆). (b) Figure from 5a of Yang et al. (2022) [9].

References & Acknowledgments

The development of HITRAN2024 edition is funded through NASA grants 80NSSC23K1596, and 80NSSC24K0080. We thank HITRAN contributors from around the World as well as the users of the HITRAN data.

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