◙ Reviewer comments on EGUsphere_2025-2514

This manuscript reports FT-IR measurements of spectroscopic line parameters of $^{14}NH_3$ and $^{15}NH_3$ in the 685 – 1250 cm^{-1} region covering their v_2 band and more. In general, the spectrum fitting residuals look great, implicating the retrievals are high-precision.

As was pointed out in the manuscript, the NH_3 (v_2) band is the strongest among its infrared bands. Furthermore, its rich spectrum makes it a valuable tracer of physical and chemical properties of diverse environments. Thus, the NH_3 v_2 band has gained a lot of attention from atmospheric and planetary remote sensing communities.

However, its unusual strength makes it challenging to do precision measurements because their transitions are easily being saturated under a typical laboratory and optics setup. NH_3 is also well known to be a polar molecule, requiring special care to handling its gas sample transfer and minimizing any chance of possible cross-contamination, esp. with residual water in a supply line.

In this work, we note that their line positions, air-widths, air-shifts, and speed-dependence parameters have been characterized in an unprecedently high precision and accuracy through multispectrum fitting analysis software package that has repeatedly been validated by multiple projects. However, there are a couple of potential issues to be addressed.

[1] The experimental conditions and optics employed in the work are not sufficiently optimized for self-width and shift retrievals. Most of transitions from the v_2 band are very strong. The highest NH3 sample pressure adopted was not more than 0.995 hPa for pure sample spectra and 1.29 hPa for Air-mixture spectra. According to Fig. 5(a) presenting all self-widths being no greater than 0.7 cm^{-1}/atm, the actual self-width contribution expected on the spectra obtained at 1.29 hPa is 0.0009 cm^{-1}, which corresponds to much less than the Doppler width, 0.0015 cm^{-1} near 1000 cm^{-1}. Moreover, many of the observed v2 transitions are near saturation for the pure sample spectra. Thus, the spectroscopic line shape parameter retrieval becomes even harder (because of the least constraining power from the observed spectrum in the saturated region). The validity of the self-line shape parameter retrievals should be argued more if the authors want to keep them as part of the measurements to be reported.

[2] Regarding line intensity measurement, one should put more weigh on their retrievals from pure sample spectra. Assuming that the air-mixture samples were prepared by adding Air to the existing pure sample in the cell (instead of preparing a pre-mixture sample gas), the sample mixing ratios of the admixture spectra are not intrinsically accurate because of contribution from the dead volume, i.e. any NH3 amount inside the protruding inlet value out of the cell body, as illustrated in Fig. 1. Therefore, line intensity measurements should count on the pure sample spectra. However, most transitions in the pure sample spectra are saturated. Authors should discuss more this weakness of their experimental conditions in the context of the measurement uncertainty estimates in Sec.4.1.

Other miscellaneous items are listed below.

Title:

A compact title is suggested, for instance,
"Measurements of spectroscopic line parameters of $14NH_3$ and 15NH3 in the 685-1250 cm^{-1} region for atmospheric remote sensing"

Abstract:
Line#10: A few words and phrases are repeated in the first paragraph, e.g.
Delete "is a toxic pollutant" in the 1st sentence.
Delete "is one of the key pollutants" in the 2nd sentence.
Then, rearrange the paragraph.

Introduction:
Line#56: The word choice, 'defined', sounds odd. We suggest using 'characterized'.
Line#64: Instead of saying as "given arbitrary values of 0.5", we suggest stating it "set to be", which is more neutral.

Experimental details:
Line#95: *AgCl windows*
We are not sure whether AgCl windows is a good choice for use with a NH3 sample. There is a substantial chance of unwanted reactions between the AgCl windows and the NH3 sample gas. Was there any signal degradation from the contaminated windows while introducing and holding the NH3 sample into the cell? Authors should make comments on this, which will be useful to readers.

Lines#113-114: *"... empty cell spectra (taken at 0.03 cm-1 spectral resolution)...."*
This resolution of 0.03 cm^{-1} might be a typo of 0.003 cm^{-1}. In general, transmission spectra should be generated by point-by-point division between sample spectra and their corresponding empty spectra. Thus, if it was not a typo, authors should explain how the mismatched spectral resolution was handled when the transmission spectrum was generated. In particular, the mismatched resolution causes a serious line shape issue for the residual water features in the transmission spectra.

Analysis and data retrievals
Line#133: Define "I" in Eq.(2) and describe the source of the preceding constant, i.e. $\mathrm{sqrt}(\ln 2/\pi)/\gamma_D$.

Table 4. $^{14}N^{1}H_3$ notation looks odd. We suggest deleting the superscript on H since ^{2}H and ^{3}H have their own designated notation, D and T, respectively.

Fig. 3 and throughout the manuscript, the ground state notation, 0, should be replaced by 'gs'.

Self- and Air-pressure-induced shifts.
Fig. 7: What are those up-and-down pattens on the shifts w.r.t. the K values for given J? Could it be related to an incomplete modeling of line mixing effects for the transitions within a given J manifold, although the fitting residuals with the Rosenkranz parameters look good as presented in Fig. 11.

Supplements

Fig. S1(b): Remove the unit notation in the Y-axis. Fig S1(b) presents values of the retrieval errors ratioed to their retrievals. Thus, they have no dimension. Also, put them as in % for quick grasp.

Fig. S2, S8, S13, S18, S23, S28, S30, S32(b): the same as above.

Fig. S3: Authors stated that "*For both cases, only lines with line intensity > 1 x 10-21 cm-1 / (molecule cm-2) are plotted*". It should be recalled, however, that strong lines are in near saturation in the pure sample spectra, thus more vulnerable to ill-determination of their intensity measurements. It is indeed interesting to see the %deviation decreased with increasing J and K whose transitions are in less chance of being saturated in the observed spectra. Also, recall that air-mixture spectra are sufficiently good for line shape parameter measurements, but not optimum enough for line intensity measurement because of such an intrinsic limitation on precision monitoring of the absorber sample pressure as stated above.

Table S7: transitions from v4(a) – v2(a) are reported.
Why not v4(s) – v2(s), whose transitions are of comparable intensities to their counterparts?

Fig. S6 and S12 report δair or δself for the transition $\nu 2 \leftarrow 0$. However, their numerical values are not included in **Table S1 and S2**. Explain what has happened to them?

End of Document.