

Response to reviewer 1

We thank the reviewer for their comments, which are reproduced below. Our response is in bold text.

This article describes the generation of a new set of spectroscopic parameters for NH₃. It is careful and solid work, and the article is well written. The study seems quite complete other than the lack of temperature dependence, which could play a role in the analysis of atmospheric measurements somewhere other than near the surface; for example, with retrievals using MIPAS or ACE-FTS measurements in the upper troposphere where temperatures are quite different from 296 K.

Note that an analysis of temperature dependence is ongoing, with experimental measurements already completed. We will publish this work in due course.

The lack of temperature effects in the analysis might not be a major problem for pressure broadening parameters (in that pressure broadening temperature dependence information is already available in HITRAN for NH₃ lines) or pressure shifts (in that it is typically assumed that pressure shifts have no temperature dependence). The biggest question might be the temperature dependence of speed dependence (through the parameter a_w). Assuming that a_w is constant as a function of temperature would imply that Γ_0 and Γ_2 have an identical temperature dependence, which may not be the case. This is not an issue that needs to be addressed in this paper, though.

Our version of Labfit does not include temperature dependence for the speed dependence parameter, but this is something that can be included in the program in future.

I am wondering if Γ_2 values derived in this study (using the formalism in Eqs 8 and 9) can be directly used with the “quadratic speed dependent Voigt” formalism used elsewhere in the literature, expressed as the difference between two Voigt-like expressions. Software that uses line-by-line calculations seem more likely to employ the quadratic speed dependent Voigt formalism because it does not involve numerical evaluation of the integral over velocity, which should make it more efficient to calculate. This likely does not matter for IASI, CrIS, and TES (the suggested end users of the new parameters) because they presumably employ look up tables instead of line-by-line calculations, which means there would only be a one-time cost from the extra calculation requirements when populating the look up tables. I expect the two formalisms are compatible, differing only in the order of integration over velocity for the double integral associated with speed dependent Voigt (i.e., integrating over velocity first for “quadratic speed dependent Voigt” as compared to integrating over velocity second for the LabVIEW formalism described in the paper), but that is an assumption.

We think the two formalisms are equivalent. There are plans to perform a comparison in due course.

Note that a paper has been submitted (still under review) titled “New beyond-Voigt line-shape profile recommended for the HITRAN database by P. Wcislo et al” meant to guide future non-Voigt parameter usage in HITRAN. For speed dependent Voigt, the suggested “official HITRAN” line shape (the modified Hartmann Tran profile) will be the difference between two Voigt-like expressions.

Some people may continue to employ Voigt line shapes rather than switching to more accurate non-Voigt calculations. HITRAN has separate database streams for Voigt and non-Voigt, so you might want to consider what users will get if they request a set of Voigt profile parameters for NH₃ from HITRAN after your data have been inserted. Will it be the older data set that contains no lines with non-Voigt parameters (and therefore none of your data)? Will it be your data for weaker lines and older data for the strongest lines (because the strongest lines use speed dependent Voigt in your data set)? Will it be all your data with non-Voigt parameters like speed dependence simply stripped out (which would make pressure broadening parameters too large, so I can't imagine them going that route)? If you want to completely replace the old NH₃ parameters, you might need to consider providing HITRAN with two sets of parameters: a "Voigt set" and a "speed-dependent Voigt set." That would require extra work on your part, of course.

We do have a version of the fit without speed dependence, so providing two different linelists to HITRAN could be considered.

Nothing discussed here requires edits to the article. The only technical change I would suggest is to put the references in alphabetical order to make them easier to parse.

Yes, this will be done. Originally the references were numbered, but we forgot to reorder them once they were changed to the AMT format.