Reviewer #2

Manuscript essd-2016-9:

"Tropospheric water vapour isotopologue data ($H_2^{16}O$, $H_2^{18}O$ and $HD^{16}O$) as obtained from NDACC/FTIR solar absorption spectra"

Authors: Sabine Barthlott et al.

Overall impression:
The manuscript is of high quality and relevance and I would recommend publications after some very minor reviews.

The methods and mathematical details given are sound. Some of the covariance matrix operations are complex, almost intimidating, but also elegant in describing the data in the best possible way and according to intended use (total water vapour or isotopologue signal). The references to other and previous work appear to be quite complete and appropriate.

All data are of high quality and are readily accessible, both via the NDACC portal and through the doi provided. A thorough and convincing quantitative discussion of systematic and random errors is presented. Even details of the metadata description are given, which often find little attention in other work. The observation methods, instruments and data processing are all state of the art and the data processing methods are truly cutting edge that I hope others will take on board. The paper is also making a clear stand for standards. This includes instrument calibration, metadata, observational data and a complete error analysis that can be traced back to SI standards in an unbroken chain. The data is optimally suited for long-term climate data record analysis and the validation of shorter term observations including satellites.

The data presented is significant, unique, useful and complete. There are several messages that I'm taking from this manuscript that the work implies, perhaps without spelling it out too clearly, but that I feel could be highlighted in a review article of the NDACC special issue:

- isotopologue data needs to be treated differently from "normal" atmospheric composition measurements and the authors explain neatly why this is so.
- The spatial and temporal variability of water vapour in the atmosphere is extremely high making it very difficult to cross-calibrate or validate different instruments. However, the variability of isotopologuous signals vary on comparatively much larger scales thus offering a better posed alternative for validation work.
- Models are heavily underutilising isotopologue data, likely due to the fact that most climate and NWP models are still not capable of handling isotopologues including their pathways. Modellers need to seriously catch up in this field.
- Isotopologue data of in particular water vapour has the potential to give detailed and new insights into moisture pathways that could significantly improve climate models including paleo models.
- This work describes the best practise for ground-based FTIR observations for water vapour including its isotopologues, but it also provides a formalism that other instruments from ground, air or space could easily adopt.

I could find no inconsistencies in the data presented. The discussion is plausible and concise.

The presentation is of high quality, appropriate length, well structured and the authors have good command of the English language. The use of maths and symbols is consistent with modern science and tables and figures are appropriate.

I'm confident that scientists working in this field are able to understand and use the data and its methods as described.

Rating of this manuscript:
Significance: the uniqueness, usefulness and completeness warrant a rating of **Excellent** in my humble opinion. Data from all over the globe have been processed in a very consistent and innovative way, keeping applicable and defining new standards as adequate
Data quality: Again I opt for **Excellent**. I have worked with NDACC data in the past and in particular the Karlsruhe group has never been short of the best possible practice, always trying to push the borders.
Presentation quality: Very good. Some of the maths is complex and I'm uncertain whether a bit more explanation would have been helpful or whether it is my lack of knowledge or unfamiliarity with some aspects of it. There are a few minor comments on the text detailed below that I would ask the authors to consider before going to print.

I wish to congratulate the authors on their sound work and thank the many people that made this contribution to science possible through collecting and analysing the observations presented.

Below I'm listing a number of specific comments and suggestions that I would ask the authors to consider (p.=page, L=Line number):

- p2L2: "deuterium-excess (d = $\delta D - 8\delta$ 18 " I was immediately curious where the factor 8 came from or whether it might be a typo – a short comment either here or later in the discussion where it appears again would be really nice. Inclined readers can then still read up the details in the reference provided, but a simple explanation would have most readers reading on happily.
- P2L3: 'are' not 'is' "particularly promising."
- p2L13: "since the 1990s, " - some data records at sites like Jungfraujoch and Kitt Peak are much longer and could be of much interest for long term climate studies or is the quality of pre-1990s data too poor?
- p2L13: " are of particular interest " 'to' not 'for'
- p3L15: " vary mostly in" 'parallel': I think alike, uniformly or in equal measure would be the better word here instead of parallel
- p3L18: " is about two orders of magnitude smaller than the correlated variations of ln [H16 2 O], ln [H2 18 O] and ln [HD16 O]." It would be nice to add a reference here.
- P3L19/20: "(due to the log-normal distribution characteristic)" Is this ultimately due to the logarithmic drop in pressure and water vapour VMR with altitude?
- P3, definitions/equations 2, 3, 4: I would write equations; i.e. add hum=, $\delta D=$ and d= to the left of your definitions for easier reading – in particular when flicking back to them when chewing through the maths on subsequent pages.
- P5L16: "All these spectral windows are" consider replacing "covered by" with 'observed within/recorded with the same optical' "NDACC filter #3."
- p8L9: " the retrieved state vector element i" replace 'responses" with "responds"
- p9 eq(14): does this come from SMOW? See also comment above on factor 8
- p12L3: Comment: would the use of more microwindows help to reduce uncertainties? Or are current spectroscopy parameters to inconsistent/poor? Or is it inadequacies in the line

shape model used? Or a combination of the latter? I think a sentence on how the accuracy could be pushed further would be well placed here, independent of how difficult it may be to achieve that.

- Figure 2: Please explain all figure captions, e.g. what does "0.5 km" mean in this context. Make clear if random or systematic errors are illustrated. Should some of it be too long, move some of it into the text but make that clear connection between figure and what is being shown.
- Figure 7: Does this mean that one trades profile or vertical information for isotopologue information? This would then also illustrate why one state parameter representation is more adequate than another for reporting overall humidity as opposed to isotopologue ratios.
- P24, Table 2: Consider writing "Modulation Efficiency and Phase Error", no need to abbreviate as not all readers may be familiar with the abbreviations.
- P24, Table 2: Why separate the Temperature profile into different altitude slices if the uncertainties are the same for all 3 slices?