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Interactive comment on "Neutral temperature and atmospheric water vapour retrieval from spectral fitting of auroral and airglow emissions" *by* Joshua M. Chadney and Daniel K. Whiter

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We would like to thank the reviewer for their constructive comments and provide the following responses. The reviewer's comments are shown in blue. Additions in the manuscript text are in bold font.

1. Abstract is too short.

The abstract now reads:

"*We have developed a spectral fitting method to retrieve upper atmospheric parameters*

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at multiple altitudes simultaneously during times of aurora, allowing us to measure neutral temperatures and column densities of water vapour. We use the method to separate airglow OH emissions from auroral O^+ and N_2 in observations between 725 – 740 nm using the High Throughput Imaging Echelle Spectrograph (HiTIES), located on Svalbard. In this paper, we describe our new method and show the results of Monte-Carlo simulations using synthetic spectra which demonstrate the validity of the spectral fitting method as well as provide an indication of uncertainties on the retrieval of each atmospheric parameter. ***We show that the method allows retrieval of OH temperatures with an uncertainty of 6 % when contamination by N_2 emission is small. N_2 temperatures can be retrieved with uncertainties down to 3 – 5 % when N_2 emission intensity is high. We can determine the intensity ratio between the O^+ doublets at 732 nm and 733 nm (which is a function of temperature) with an uncertainty of 5 %.***"

2. Introduction: You assume LTE. Please specify the altitude ranges where the emissions originate. Is the LTE assumption valid in all your cases?

We measure rotational temperatures for OH (emission originating near 87 km) and N_2 ($\sim$150 km). We indeed make the assumption of LTE at these altitudes to consider that the measured temperatures are the same as the neutral temperatures.

OH is mainly formed through an exothermic reaction of H with O_3; this results in OH molecules that are in excited vibrational and rotational levels and then are thermalised through collisions. Thus LTE conditions are not always assured and most often found in lower vibrational and rotational levels (Pendleton et al., JGR, 1993). We are aware that the OH emission seen with HiTIES at ν'=8 is in quite a high vibrational state, therefore we discard any temperatures measured where there is a deviation away from a linear fit in the Boltzmann plot, as described in Sect. 3.1.

To make this clearer, part of Sect. 3.1, now reads (additions in bold): "*If we assume a*

Boltzmann distribution for the rotational level population, the function is linear and the inverse of the slope of the fitted straight line is the neutral temperature. An example of a Boltzmann plot can be found in Fig. 3. In determining the temperature, we make use of the strongest P-branch OH(8-3) lines recorded by HiTIES, the four P_1 lines: P_1(2), P_1(3), P_1(4), and P_1(5); these are shown in blue circles in Fig. 3, see also these lines labelled in the spectrum in Fig. 2. ***As LTE is not always assured, especially in the higher vibrational states of OH (Pendleton et al., 1993)****, we place constraints on the variance between the linear fit and the P_1 and P_2 lines (the latter are the red circles in Fig. 2).*"

Ro-vibrationally excited N_2 is created by electron impact excitation and cascading from higher vibrational levels also occurs; further work on the rotational N_2 temperatures measured by HiTIES is needed to determine when this layer can be considered in LTE. The following is added to the end of Sect. 3.3: "***Future analysis of the dataset of N_2 temperatures will consider the conditions under which the layer can be considered in LTE.***"

The mechanism to derive temperatures from O^+ (~250 km) measures the temperature of neutral O 3P (Whiter et al., 2014). As long as O (3P) is thermalised, the measured temperature is the neutral temperature.

3. Section 2: HiTES. This section is also too short. Add instrument's general description. Provide information about the timing and frequency of measurements.

Additional information has been added to Sect. 2, which now reads:

"*The High Throughput Imaging Echelle Spectrograph (Chakrabarti et al., 2001) has been measuring emission from the upper polar atmosphere since the year 2000. It is a part of the Spectrographic Imaging Facility (SIF), located in the high Arctic on Svalbard, at the Kjell Henriksen Observatory (78.148° N, 16.043° E). The spectrograph has an 8°*

slit that is centred on the magnetic zenith. ***Light entering the instrument passes through a collimator, before being diffracted by an echelle grating and re-imaged on an EMCCD detector.*** *A mosaic of interference filters is used to separate overlapping diffraction orders, allowing the simultaneous observation at high temporal and spectral resolution of non-contiguous spectral regions. Figure 1 shows* ***a schematic diagram of*** *the two mosaic filters that have been used the most often over the lifetime of the instrument. Each individual panel of the filters is centred in wavelength on a particular atmospheric emission of interest, although it should be noted that each panel may also contain emissions from multiple other species.*

The instrument records images at a frequency of 2 Hz, however, depending on the brightness of the observed emissions, the spectra are typically post-integrated to between ~10 and 120 seconds. The width of the spectrograph slit can be changed to adjust the spectral resolution, higher resolution being a trade-off with the amount of light captured. In the 2015/16 season, during which the data in Figure 2 was recorded, the FWHM was 0.15 nm."

4. In Sec. 3.2 you mention that the ratio of two O+ doublets depends on neutral temperature. Later you consider this ratio, but you do not show results for temperature. Why?

The following has been added to Sect. 3.2: "***Further validation is needed to convert R_{O^+} to T_n so in the remainder of this paper, we will only consider the ratio R_{O^+}.***"

5. Sec. 4: Eqs. (1)-(2): How are you including these constrains in the fitting process?

Eqns. 1 and 2 are used as constraints in the least-squares fitting routing, allowing for +/- 10 % leeway. Note that the O^+ doublets are not resolved in HiTIES spectra.

We have clarified the first sentence of Sect. 3.2: "The O^+ panel is so named because it contains two **spectrally unresolved** emission line doublets from the O^+ ion. . .”

We have also added the following sentence to the end of the second paragraph in Sect. 4: “**Equations 1 and 2 are included as constraints in the fitting process, allowing for 10 % variation in the coefficients.**”

6. Sec. 5: N2 database: Temperature range 150-1150 K by 10 K resolution. Please justify these numbers.

This range of temperatures was chosen to cover extremes of temperature possible at the altitudes of N_2 emission. 10 K resolution captures changes in the spectral shape of N_2.

7. Sec. 4, line 23: You see large deviations in the residual and you think that it is related to O2 emission. So why didn’t you include these emissions in the fitting?

It would not be trivial to include O_2, for which a model similar to that of N_2 would need to be constructed. The deviations in the residuals are only present at the short-wavelength end of the spectra, and so do not overlap with the OH P-branch lines or O^+ lines, furthermore N_2 emission is dimmer at the short wavelengths, compared to above $\sim$730nm. Therefore, including O_2 emission will not affect the results we present in this study.

8. Sec. 5: Normally the least squares fitting provides uncertainties of the retrieved quantities in the form of co-variance matrices. Some uncertainty estimates of the measurements (and sometimes modelling uncertainty) is needed for these estimates. You do not provide any discussion about this, but rush to make a Monte Carlo analysis. Please, open up your thinking about error analysis here.

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From your comment, we should better distinguish between uncertainties on the parameters retrieved from a particular spectrum from the aim of the Monte Carlo simulations to determine parameter ranges over which our method is useful and the magnitude of the errors expected.

For a given spectrum, we obtain errors on each OH and O+ line intensity (e_I) from: $e_I = \sigma_{residuals} \times \sqrt{N_{pixels}}$, where $\sigma_{residuals}$ is the standard deviation of the residuals from the least squares fit (lower panel of Fig. 2), and $\sqrt{N_{pixels}}$ is the number of pixels on the detector that record the the emission line (determined from the FWHM). This allows an error calculation on T$_{OH}$ and R$_{O}^{+}$.

The Monte Carlo simulations shown in Sect. 5 allow us to determine the ranges of temperatures and intensities of each measured emission over which our method produces accurate results.

The following paragraph has been added to the end of Sect. 4:

"***Considering that the main source of noise in a given spectrum is shot noise, we determine the uncertainties on the fitted line intensities (*** e_I ***) using the following:***

$$e_I = \sigma_{residuals} \times \sqrt{N_{pixels}}, \tag{1}$$

where $\sigma_{residuals}$ ***is the standard deviation of the residuals and*** N_{pixels} ***is the number of pixels on the detector contained in the FWHM of the emission line. In this way, we can obtain uncertainty estimates on the parameters retrieved from each particular spectrum. However, we would also like to determine the ranges of parameters over which the fitting process produces accurate results. For this reason, we carry out a Monte Carlo simulation in Section 5.***"

And the beginning of Sect. 5 has been amended to read:

"*In order to estimate* ***expected*** *errors on the fitting and parameter retrieval process described in Sect. 4, we have performed a Monte Carlo simulation.* ***Such a simulation***

also provides information on the region of parameter space over which the fitting method is valid.”

9. Sec. 5.1, line 23: The mean error. Usually it is called bias?

Replaced “mean error” with “bias” in the text.

10. Figs. 6, 7, 9,10. The unit of the relative error is not mentioned. Is it absolute or %?

We have renamed this quantity fractional error to avoid confusion, it is unitless. This quantity is only converted into % when specifically stated in the text.

11. In Conclusions you start studying the impact of thermal noise. In my mind the right place for this is in Sec. 5 and not in Conclusions.

The paragraph on noise has been moved to a new Sect. 5.6.

12. In the paper you do not really show geophysical results but concentrate on uncertainties of your method. Are you going to show, compare and validate your results with other peoples’ work in some future publications? If so, please advertise your plans in Conclusions. Hopefully this comes before trend studies!

We will indeed be showing geophysical results in upcoming papers. And we shall begin by validating our OH temperatures with those from Silverbullet, an instrument which is co-located with HiTIES, but observes a different vibrational band of OH. We will also compare OH temperatures with those from the TIMED/SABER instrument.

The end of the conclusion section now reads as follows: “*In a number of follow-up studies, we will make use of the spectral fitting and temperature retrieval methods* *demonstrated here to explore trends in upper atmospheric neutral temperatures in the HiTIES dataset.* ***As a first step, we shall compare OH(8-3) temperatures measured by HiTIES with OH(6-2) temperatures from the Silverbullet instrument operated by the University Centre in Svalbard (UNIS) (e.g., Sigernes et al., 2003; Holmen et al., 2014), also located at the Kjell Henriksen Observatory, and with OH temperatures derived from the SABER instrument onboard the TIMED satellite.***”

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