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On the relative absorption strengths of water vapour in the blue wavelength range

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Abstract

In recent updates of the HITRAN water vapour H_2O spectroscopic compilation covering the blue spectral region (here: 394–480 nm) significant changes for the absorption bands at 416 and 426 nm were reported. In order to investigate the consistency of the 5 different cross-sections calculated from these compilations, H_2O vapour column density ratios for different spectral intervals were retrieved from Long-path and Multi-Axis – Differential Optical Absorption Spectroscopy (DOAS) measurements. We observed a significant improvement of the DOAS evaluation when using the updated HITRAN 10 water vapour absorption cross-sections for the calculation of the reference spectra. In particular the magnitudes of the residual spectra as well as the fit errors were reduced.

However we also found that the best match between measurement and model is reached when the absorption cross-section of groups of lines are scaled by factors ranging from 0.5 and 1.9, suggesting that the HITRAN water vapour absorption compilation still needs significant corrections. For this spectral region we present correction 15 factors for HITRAN 2009, HITRAN 2012, HITEMP and BT2 derived from field measurements. Additionally, upper limits for water vapour absorption in the UV-A range from 330–390 nm are given.

1 Introduction

Precise knowledge of the atmospheric water vapour absorption is not only crucial 20 to calculate Earth's radiation budget since water vapour is the largest contributor to the natural greenhouse effect (Myhre et al., 2013), but water vapour absorptions also needs to be known at high precision when retrieving other atmospheric absorbers from spectroscopic measurements in the UV/VIS wavelength range. If their absorptions overlap, this can lead to errors in measurements of several trace-gases. Due to technical 25 limitations and since the absorption cross-sections are small in the region below 500 nm (above $20\,000\,\text{cm}^{-1}$), in this spectral interval the body of available experimen-

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tal data is sparse. Numerous absorption lines in the blue spectral region included in absorption line databases like HITRAN 2009 (Rothman et al., 2009), HITRAN 2012 (Rothman et al., 2013) and HITEMP (Rothman et al., 2010) are therefore based on theoretical calculations only. According to Tennyson et al. (2013) and references therein, 5 validation measurements of individual water absorption lines are only available at wavelengths longer than 395.7 nm ($25\,337\text{ cm}^{-1}$), but a large fraction of the absorption lines included in the databases in this region is not validated by measurements.

More recently water vapour absorption was also observed (Maksyutenko et al., 2012) and modeled (Polyansky et al., 2012) in the UV range below 370 nm. The HITEMP absorption line database for H_2O (Rothman et al., 2010) relies to a large extend on the *ab initio* line list BT2 calculated by Barber et al. (2006). An overview of the cross-sections from HITRAN 2009, HITEMP and BT2 is shown in Fig. 1. Convolved to a 10 representative resolution of 0.5 nm, the differences between the HITRAN 2012 cross-section and the HITEMP cross-section are negligible, therefore they are treated as equivalent here.

A widely used approach to measure trace gases in the atmosphere of the Earth is the technique of differential optical absorption spectroscopy (DOAS) (Platt and Stutz, 2008). Typically, absorption spectra covering 100–200 nm sections in the UV or visible spectral range are recorded by a grating spectrometer at a spectral resolution of 15 0.3–1 nm. Suitable evaluation of differential absorption structures allows quantitatively determining column densities and concentrations of numerous trace gas species, even if their spectral features overlap. This allows for simultaneous evaluation of several trace gases in the atmosphere at high temporal resolution.

Absorption path lengths for different DOAS setups range from several 100 m to several 20 10 km in the free troposphere. Optical densities (OD) can be often be resolved down to 1×10^{-4} (e.g. Platt and Stutz, 2008; Coburn et al., 2011), which in turn means that water absorption lines can be observed up to an accuracy of $5 \times 10^{-28}\text{ cm}^2\text{ molec}^{-1}$ at a resolution of typically 0.5 nm if other absorbers in the respective spectral region are well-known and/or their total absorptions are small.

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While absorption structures due to known absorbers can be readily disentangled, problems can arise from unknown spectral features. One example – as mentioned above – are the uncertainties of the weak absorption features of water vapour in the blue spectral region.

5 Frequently the actual water vapour content during the measurements is not of primary interest, but nevertheless water needs to be corrected for when evaluating the absorption spectra. For example, weak water absorptions can be found in the typical evaluation range of iodine monoxide (ca. 414–440 nm). Iodine oxide (IO) is playing a role in atmospheric chemistry and creation of cloud condensation nuclei. Elevated IO
10 levels can be found in coastal areas (e.g. Seitz et al., 2010) as well as on the open ocean (e.g. Read et al., 2008; Großmann et al., 2013), the free troposphere (e.g. Dix et al., 2013) and polar regions (e.g. Frieß et al., 2010; Schönhardt et al., 2012). For a typical tropospheric water vapour slant column density (SCD) found in moderate climate of $S_{\text{H}_2\text{O}} = 4 \times 10^{23} \text{ molec cm}^{-2}$ the resulting optical density is 2.5×10^{-3} (when taking the cross-section data from HITEMP) at a spectral resolution of 0.5 nm. Optical densities due to IO in the tropical marine boundary layer are five times weaker, i.e. of the order of 4×10^{-4} , thus to avoid possible errors in the retrieval of IO due to incomplete correction of the water vapour absorption, precise knowledge of the water vapour absorption cross-section is essential. Older versions of HITRAN such as HITRAN 2000
15 did not even include any absorptions in this spectral range.

Even more important is the correction of water vapour absorptions for the retrieval of glyoxal (e.g. Sinreich et al., 2010; Mahajan et al., 2014, and references therein), which can be evaluated in the spectral range from 432–458 nm. For a typical tropospheric water vapour SCD of $S_{\text{H}_2\text{O}} = 4 \times 10^{23} \text{ molec cm}^{-2}$ the resulting OD is 1.7×10^{-2} in this wavelength range at a spectral resolution of 0.5 nm, while the typical glyoxal dSCD as reported by Sinreich et al. (2010) for the marine boundary layer of $1.5 \times 10^{15} \text{ molec cm}^{-2}$ correspond to 8×10^{-4} and thus is ten times weaker than the water vapour absorption. Moreover the main spectral absorption features of water vapour and glyoxal overlap in some parts, potentially introducing cross-sensitivities
25

and/or increasing the measurement error. At the spectral region of maximum absorption of glyoxal the difference between the water vapour absorption cross-sections found in HITRAN 2000 and HITEMP for a typical $S_{\text{H}_2\text{O}} = 4 \times 10^{23} \text{ molec cm}^{-2}$ is about 4×10^{-4} and amounts to one half of the reported glyoxal absorption.

5 Water vapour absorption can also have an impact on the spectral retrieval of the oxygen dimer O_4 (also called $\text{O}_2\text{--O}_2$) around 477 nm. Its column densities can be used to constrain radiative transfer simulations in remote sensing application and to obtain height profile information of aerosol extinction and trace gas concentrations (e.g. Frieß et al., 2006).

10 Water vapour column densities have been measured in the blue wavelength range from satellite (Wagner et al., 2013b; Wang et al., 2014) as well as from ground-based instruments (Wagner et al., 2013a). Here the 7ν absorption at 442 nm from HITRAN 2004 has been used for retrieving the atmospheric water vapour column density. These measurements require precise water vapour absorption cross-sections as well 15 to minimize retrieval errors.

If significant absorptions of water vapour are present below 370 nm, these could have an effect on the spectral evaluation of measurements of e.g. BrO, Formaldehyde, HONO, SO_2 and O_4 . Based on currently available cross-section data no atmospheric water vapour absorptions in this spectral range have been reported for DOAS measurements so far.

2 Measurement campaigns

The data which was analysed here were collected during two field campaigns, where different instruments were used.

25 1. During the SOPRAN cruise M91 with the research vessel “*Meteo*” Multi-Axis (MAX-)DOAS data was collected in the Peruvian upwelling region in December 2012 (Bange, 2013).

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2. Longpath (LP)-DOAS Measurements were analysed for water vapour using data from the intensive campaign called “HaloCaVe” at the Cape Verde Atmospheric Observatory (CVAO, Carpenter et al., 2010) during summer and fall 2010.

5 The sites of both campaigns were located far away from any strong anthropogenic pollution, thus interferences due to e.g. high NO_2 mixing ratios on the data evaluation should be negligible.

3 The DOAS method

10 The DOAS method (Platt and Stutz, 2008) relies on attenuation of light from suitable light sources by absorbers within the lightpath according to Lambert-Beer’s law $I(\lambda) = I_0(\lambda) \exp(-\tau(\lambda))$.

15 The optical density $\tau(\lambda)$ is calculated from a reference spectrum $I_0(\lambda)$ and a measurement spectrum $I(\lambda)$, $\tau(\lambda) = -\ln \frac{I(\lambda)}{I_0(\lambda)}$. In order to remove broad-band Mie and Rayleigh extinction, the OD is subdivided in a narrow-band (differential) and a broad-band part, $\tau(\lambda) = \tau_B(\lambda) + \tau_d(\lambda)$. $\tau_d(\lambda)$ is expressed by a sum of the differential parts of possible absorbers with their differential absorption cross-sections $\sigma_{d,i}(\lambda)$ and concentrations c_i of absorber (i.e. trace gas) i .

$$\tau_d(\lambda) = L \sum_i c_i \sigma_{d,i}(\lambda) \quad (1)$$

20 The column density $S_i = L \times c_i$ of the trace-gas i (with the concentration c_i) is calculated by a fitting routine, which is applied to data from a wavelength interval with a width of several nm to several 10 nm. The absorption path L is known for LP-DOAS measurements and can be estimated or calculated from radiative transfer models for MAX-DOAS measurements. The high resolution literature cross-sections $\sigma_{L,i}$ are convoluted with the instrument function H of the respective setup to obtain $\sigma_i = H \otimes \sigma_{L,i}$, the

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absorption cross-section as it would be determined by the instrument. In an analogous fashion to the optical density, also cross-sections can be subdivided into a broadband and narrow-band (differential) contribution: $\sigma_i = \sigma_{B,i} + \sigma_{d,i}$. The instrument function H is usually measured by observing individual atomic emission lines of mercury, which have a width which is two orders of magnitude smaller than the resolution of the instrument (Sansonetti et al., 1996). Corrections to this simple convolution procedure are discussed in Sect. 4.3.

3.1 MAX-DOAS measurements

The method of Multi-Axis DOAS (MAX-DOAS) measurements was first described by

10 Hönniger and Platt (2002) and uses scattered sunlight collected by a telescope pointing towards the sky at different elevation angles. Each elevation has a different sensitivity for absorptions in different heights of the atmosphere. Low elevation angles have a higher sensitivity to absorbers close to the surface, because the additional lightpath compared to a zenith spectrum is mostly located within the lowermost layers of the atmosphere (Hönniger et al., 2004).

The SCD is defined as the integral over the concentration ρ along the lightpath L and is hence given in units of molecules cm^{-2} .

$$S = \int \rho(s) ds \quad (2)$$

From the MAX-DOAS measurements differential slant column densities (dSCDs) ΔS can be calculated for each fitted trace gas: a Fraunhofer reference spectrum $I_0(\lambda)$ is chosen from one of the measurement spectra and the dSCD $\Delta S(\alpha) = S(\alpha) - S_{\text{ref}}$ is obtained from the DOAS fit for each elevation angle α relative to the Fraunhofer reference. Typically, a zenith spectrum is taken as reference and thus $S_{\text{ref}} = S(90^\circ)$. In the measurements reported here, the DOAS fit includes the convoluted cross-sections listed in

Table 3. In addition Ring Spectra are fitted (see Table 3), which serve to compensate for the effect of rotational Raman scattering. The influence of vibrational Raman scattering of N_2 and O_2 as described in Lampel et al. (2015) on the obtained results listed in Table 5 was not found to be significant. By choosing references recorded shortly before or after the measurement spectrum the influence of the instrumental instabilities on the result was minimized as well as the influence of stratospheric absorbers largely cancel out (see e.g. Hönninger and Platt, 2002).

A description of the instrument operated during the SOPRAN cruise M91 can be found in Großmann et al. (2013). The optical resolution of the instrument during this campaign was 0.45 nm and it covered a spectral range from 324 to 467 nm.

3.2 LP-DOAS Measurements

Longpath(LP)-DOAS instruments are based on an artificial light source, typically a xenon lamp or a light-emitting diode (LED), retro reflectors, a telescope and a spectrometer. The light is sent with a telescope across the measurement distance to a retro reflector, which reflects the light back onto the same telescope. It collects the received light and transfers it to a spectrograph. A sequence of background measurements, light-source spectrum measurements without absorption and actual measurement spectra is used to ensure independence of the measured spectra from external sunlight and instrumental instabilities. The LP-DOAS setup has the advantage that the actual light path is well-defined and thus concentrations of molecules can be directly derived, also measurements at night are possible.

The optical density $\tau(\lambda)$ is calculated from a background corrected light source spectrum and a background corrected atmospheric spectrum and filtered by a binomial high-pass with 1000 iterations. The convoluted and high-pass filtered literature cross-sections listed in Table 3 are then fitted to the corrected OD.

A description of the LP-DOAS instrument can be found in Pöhler et al. (2010). The lightpath used for the measurements reported was 12.64 km long, similar to the one in Read et al. (2008). The spectral resolution was 0.5 nm.

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To exclude the possibility of interferences with daylight, only spectra at a solar zenith angle of more than 90° (night-time) are reported here.

3.3 Spectral retrieval

The H₂O cross-sections were calculated using modeled line widths according to Kuntz (1997) from the respective compilation or line list using an extraction program by Christian Frankenberg (Frankenberg, 2005) with a spectral resolution of 1 pm for an ambient temperature of 298 K and 1013 hPa.¹ For the BT2 dataset, a cross-section file from the exomol project (Tennyson and Yurchenko, 2012)² was downloaded, here only Doppler line broadening effects were considered (Hill et al., 2013). Variations of temperature and pressure within the range of atmospheric measurements were found not to have a significant effect on our measurements in the blue wavelength region and the bulk of the absorption by water vapour molecules takes place within the boundary layer.

The choice of cross-section to compensate for absorption of the oxygen dimer O₄ did not significantly affect the overall result. We tested cross-sections from Hermans et al. (1999), Thalman and Volkamer (2013) and Greenblatt et al. (1990).

The spectral window of this study for MAX-DOAS measurements was limited at the lower end to 398 nm to avoid a strong influence of the Ring effect caused by rotational Raman scattering (Shefov, 1959; Grainger and Ring, 1962). The upper bound (at 461.5 nm) was chosen due to instrumental limitations.

The water vapour absorption cross-section was divided into six spectral regions W0–W5 before convolution, as listed in Table 1. All other absorbers (Table 3) were fitted normally. An example fit can be seen in Fig. 2.

¹The HITRAN 2009, HITEMP and HITRAN 2012 data used here was downloaded from the HITRAN website (<http://www.cfa.harvard.edu/hitran/>) with the file name “01 hit09.par”, HITEMP “01 hitemp.par” and HITRAN 2012 “01 hit12.par”

²<http://www.exomol.com/xsecs/1H2-16O>

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To avoid problems in situations with low light intensity, we used only data where the signal was sufficiently high to provide a RMS noise of the residual spectrum below 4×10^{-4} .

3.3.1 Radiative Transfer effects (MAX-DOAS)

5 The lightpath of the LP-DOAS measurement is well defined and constant. Thus measurements of the different W0–W5 column densities can be directly used. However, the effective lightpath of MAX-DOAS measurements is not known and depends on several factors: wavelength, aerosol and trace gas profiles, viewing direction, position of the Sun etc.

10 The radiative transfer for the measurements was simulated using McArtim (Deutschmann et al., 2011). Water vapour dSCDs in the atmosphere were simulated at different wavelengths to estimate the effect of radiative transfer on the relative observed absorption band strengths for MAX-DOAS measurements. Since the data was taken from a measurement period of a whole month, a representative water vapour profile (surface mixing ratio of 2.3 %, linearly decreasing to 0 % at a height of 6 km, similarly as in Bleisch and Kampfer, 2012) and an exponentially decreasing aerosol profile with an AOT of 0.22 at 360 nm were used for the simulations. The results were averaged over a range of solar zenith angles (SZA) of 10–80° representing the used MAX-DOAS data and over all encountered relative solar azimuth angles.

15 The magnitude of the resulting water vapour dSCD obtained from the model agreed with the MAX-DOAS observations. McArtim allows calculating the wavelength dependence of the simulated water vapour dSCDs. The scatter in the correlations for the water absorption bands (Fig. 3) will then already include the scatter caused by different measuring geometries, which means that the observed differences in relative strengths of the absorptions especially for W1 and W2 are significant. However, the correction obtained from radiative transfer calculations (shown in Table 4) needs to be applied to MAX-DOAS observations to match the LP-DOAS results. The correction of the wavelength dependence reduces the discrepancy of MAX-DOAS and LP-DOAS

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measurements e.g. for W0 when using HITEMP and BT2. The wavelength corrected results are listed in Table 5.

It is a well known effect (see e.g. Platt et al., 1997) that strong absorbers influence the light path length in the atmosphere and thus the airmass factor. The change of the air mass factor within a water vapour absorption band due to the highly resolved water vapour optical density in the region < 480 nm was found to be insignificant. Deviations of less than 2 % on the values listed in Table 5 were observed. The effect may, nevertheless, play a role for stronger absorbers.

However, if the focus is on weak absorbers being overlayed by strong water vapour absorptions, a correction for the change of airmass factors by strong absorption is necessary to avoid water vapour OD correlated structures in the residual spectra and effects on the retrieval of other absorbers.

4 Results

The water vapour dSCDs derived in different spectral regions of the same measured spectra were compared to each other. In principle the same water vapour dSCD values are expected, but significant differences were found.

Values of the retrieved water vapour SCDs in different spectral intervals were compared to each other. Relative to the SCD of W3 S_{W3} , an error weighted linear regression was done to obtain a_x in $f(S_x) = a_x \times S_{W3}$. a_x is the relative absorption strength of the interval x relative to W3. The results are shown in Table 5. Typical DOAS fit errors for each cross-section in W0–W5 for individual measurements are summarized in Table 6. In order to illustrate the differences one of the data comparison plots with the relative absorption of W1 and W3 for HITEMP is shown in Fig. 3.

The weights for the linear regression were iteratively calculated according to Neri et al. (1989). A comparison with other methods for error-weighted linear regressions can be found in Cantrell (2008).

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The water vapour absorption of the 7ν polyad (W3) at ≈ 444 nm was used as a reference for the other polyads, because it is the strongest absorption in this spectral region (see Table 1).

The mathematical error from the regression is small compared to possible systematic errors, which might arise from the DOAS fit itself: Its relative size is estimated by using twice the fit error given in Table 6 following the argumentation of Stutz and Platt (1996). These errors are then used to calculate the weighted mean deduced from MAX-DOAS and LP-DOAS observations for each of the absorption bands given in Table 5, if their respective relative fit error is smaller than 25 %.

In the literature significant absorption structures due to glyoxal in the eastern Pacific region were reported by Sinreich et al. (2010). However during our cruise, no absorption due to glyoxal was found to exceed our detection limit of $2\sigma = 5 \times 10^{14}$ molec cm^{-2} glyoxal at low elevation angles of 1–3°. Nevertheless, in order to exclude an impact of glyoxal absorption on the evaluation of water vapour absorptions, the analysis procedure was repeated also including glyoxal. The result is comparable to the result without glyoxal absorption, only the amplitude of the weak water absorption around 426 nm was slightly reduced by the additional degree of freedom introduced to the spectral retrieval. For the LP-DOAS measurements an upper limit of 30 ppt glyoxal (Mahajan et al., 2014) was determined and its cross-section was also not included in the final analysis.

4.1 Comparison of LP-DOAS data with data from meteorological stations

In order determine whether the assumed water vapour absorption cross-sections actually give the correct water vapour concentration, the main absorption W3 found in LP-DOAS data was compared to water vapour mixing ratios derived from meteorological parameters measured on CVAO.

The meteorological station provides temperature, pressure and humidity data (Carpenter et al., 2010). This information was used to calculate the water vapour mixing ratio using the Magnus formula and to compare the result with LP-DOAS data. Tak-

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ing the measurement error given for the meteorological station, the stated error in the temperature measurements of $0.3\text{ }^{\circ}\text{C}$ results in 2 % uncertainty in the relative humidity. Pressure uncertainties cancel out, since the same pressure measurements were used for the conversion of column densities from LP-DOAS to mixing ratios as well as in the Magnus formula. An error of 5 % in relative humidity directly translates in an 5 % error for the mixing ratio. This means that the absolute differences of the cross-sections shown in Table 1 cannot be absolutely validated with sufficient precision, even though the water vapour mixing ratios ranged from 2.0–3.4 % and meteorological station data and LP-DOAS water vapour data correlated with a Pearson's $R = 0.93$. Slope and offset values are listed in Table 7. The LP-DOAS results based on the HITEMP cross-section were on average 7 % lower than the values inferred from the meteorological station data, and thus closer to the absolute magnitude of the W3 absorption in HITRAN 2009. Retrieving tropospheric water vapour profiles from the MAX-DOAS measurements introduced even larger deviations probably due to uncertainties in retrieving the required aerosol profiles.

4.2 Absorption of water vapour in the UV wavelength range

As mentioned above, water vapour absorptions are not only observed in the spectral region above 390 nm, but down to wavelengths approaching the dissociative continuum starting below 243 nm (Maksyutenko et al., 2012). Also *ab initio* calculations (Polyansky et al., 2012) for this spectral region were developed.

BT2 and HITEMP included absorption features of water vapour in the wavelength range below 390 nm, as shown in Fig. 1. Other trace gases such as HCHO, BrO and HONO are retrieved in this wavelength region. However to date, water vapour absorptions are not included in DOAS retrieval procedures. Therefore the detection of water vapour absorption below 390 nm and thus the possibility to improve trace gas retrievals are of great interest for DOAS measurements.

For the DOAS-analysis in the UV range IO was removed from the fit while the cross-sections listed in Table 3 were added.

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During the MAX-DOAS measurements (M91) systematic residual structures in the spectral region below 370 nm were observed. Their amplitude of up to 6×10^{-4} increased with decreasing elevation angle just like the O₄ and/or water vapour dSCDs (at 442 nm) and also the residual spectral structure showed narrow differential absorption features. This could indicate a tropospheric absorber in the spectral region below 370 nm – which is currently not considered in typical DOAS retrievals – such as water vapour. Due to the strong correlation of O₄ and water vapour dSCDs for the MAX-DOAS measurements during the M91 campaign and insufficient detection limits for the LP-DOAS measurements, these residual structures could not be unambiguously attributed to either O₄ or water vapour absorption. The variation of water vapour mixing ratios along the cruise track of M91 was not large enough to separate both possible contributions.

The water vapour absorption band around 377 nm could not be identified by our MAX-DOAS measurements (M91) so far and is, judging from the residual optical depth from the fit, presumably smaller than $4 \times 10^{-27} \text{ cm}^2$ at a spectral resolution of 0.45 nm. This is in agreement with the published values of the cross-sections shown in Fig. 1.

The specified cross-section of the absorption band at 362 nm is about twice as large in BT2 as in HITEMP, which might be partly due to the line cutoff present in the HITEMP database. Furthermore, the retrieval of this band from atmospheric spectra would be difficult due to uncertainties of the overlaying absorption of the collision induced absorption by the oxygen dimer O₄. When using the most recent O₄ absorption cross-section by Thalman and Volkamer (2013) in our DOAS evaluation, the water vapour absorption appear to be present in our measurement data, but the instability of the fit and large residual structures close to the possible water absorption indicate that there is still a significant mismatch between measurement and modeled absorption lines.

Du et al. (2013) reported measurements of the water vapour absorption cross-section by ring-down spectroscopy of pure water vapour in the 290–350 nm region sampling the absorption cross-section in steps of 5 nm. They report that their measurements are in agreement with previous determinations of the absorption at 442.73 nm.

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The reported cross-section values of $\sigma_{\max} = 2.94 \times 10^{-24} \text{ cm}^{-2} \text{ molec}^{-1}$ at 330 nm are exceeding the maximum absorption of the BT2 line list in the spectral region from 330–350 nm by two orders of magnitude. This would lead to an OD of $\tau = S \times \sigma_{\max} = 1.2$ for MAX-DOAS measurements with $S_{\text{H}_2\text{O}} = 4 \times 10^{23} \text{ molec cm}^{-2}$ (a typical MAX-DOAS column density for mid-latitude summer conditions) under a telescope elevation angle of 3°, which is clearly in disagreement with our observations. Also measurements of other tropospheric trace gases such as HCHO (336.5–359 nm) (Pinardi et al., 2013), BrO (330.6–352.75 nm) and SO₂ (314.8–326.8 nm) (Lübcke et al., 2014) which would have also been affected, did not show any unknown differential absorption of this size, but yielded residual spectra with at least two orders of magnitude smaller amplitudes.

For MAX-DOAS measurements in the Peruvian upwelling (M91) the magnitude of the fit residual in the region from 332–370 nm was below 6×10^{-4} peak-to-peak for a water vapour dSCD retrieved in the blue wavelength range of $4 \times 10^{23} \text{ molec cm}^{-2}$, yielding an upper limit on the differential cross-section of water vapour of $3 \times 10^{-27} \text{ cm}^2 \text{ molec}^{-1}$ at a resolution of 0.45 nm under atmospheric conditions, i.e. three orders of magnitude smaller than the figure reported by Du et al. (2013) at 330 nm.

If the shape of the water vapour cross-section presented in Du et al. (2013) could be represented by the DOAS polynomial in the respective wavelength range, it would not be detected. But already the comparably small absorption at 345 nm would have resulted in a significant absorption structure with a differential absorption structure size of 6×10^{-2} , which could not have been compensated by the polynomial. Additionally, water vapour does not show an absorption cross-section which can be represented by a polynomial in other spectral regions in the visible spectral range. We therefore conclude that the cross-section values reported in Du et al. (2013) must be considerably too high, judging from UV MAX-DOAS measurements under atmospheric conditions. Alternatively the measurements of Du et al. (2013) may represent only individual absorption lines at each of the wavelengths of the reported magnitude, while in the spectral region between those measurements no cross-section data is available. Therefore the conclusion by Du et al. (2013) that the total impact of water vapour absorptions

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in middle-latitudes on the radiation flux at the ground level is be comparable to ozone between 330–350 nm cannot be supported.

At a spectral resolution of 0.5 nm, the OD attributed to water vapour between 350 and 370 nm is according to HITEMP 5.5×10^{-4} (BT2: 9.5×10^{-4}) for a typical H_2O -dSCD of $4 \times 10^{23} \text{ molec cm}^{-2}$. Under similar measurement conditions (dSCD $_{\text{O}_4} = 4 \times 10^{43} \text{ molec}^2 \text{ cm}^{-5}$) the OD due to O_4 is 2×10^{-2} , i.e. by a factor of 20–40 larger. The OD according to HITEMP/BT2 from 330–350 nm is comparable to the optical density of 1 ppt BrO along a lightpath of 10 km and could thus be crucial for DOAS measurements of BrO in the remote marine boundary layer (compare e.g. Volkamer et al., 2015). Furthermore these absorptions could contribute to the observed problems during the retrieval of tropospheric HCHO as described by Pinardi et al. (2013).

To estimate the overall influence of water vapour on the retrieval of O_4 , BrO, HCHO and HONO further dedicated laboratory measurements of water vapour in this spectral region are needed.

15 4.3 Error sources

The residual spectra obtained from the DOAS evaluation procedure of the measurements were usually not dominated by photon shot noise, but showed recurrent residual structures as show in Fig. 2. Since the influence of other absorbers than H_2O is probably negligible, these residual structures from instrumental instabilities, saturation and 20 I_0 -effect (for MAX-DOAS) should be the dominating sources of interference. Their influence on the absolute magnitude of the absorption bands in discussed in the following subsections, the influence of radiative transfer effects is discussed in Sect. 3.3.1.

4.3.1 Other absorbers

25 For MAX-DOAS measurements the OD of other absorbers than water vapour was kept low by using a Fraunhofer reference $I_0(\lambda)$ recorded within the same sequence of elevation angles. Using this approach the solar zenith angle only changed slightly between

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the measurements and most of the stratospheric absorption by ozone and NO_2 cancel out and do not affect the evaluation. Furthermore, the measurement campaigns selected took place in remote areas with background ozone concentrations around 30–40 ppb ozone and NO_2 typically well below 1 ppb. The OD associated with NO_2 was $(2 \pm 9) \times 10^{-4}$, ozone below 1.5×10^{-4} and iodine monoxide $(2.2 \pm 2.2) \times 10^{-4}$. In comparison, the typical OD of water vapour for the wavelength intervals W0–W5 ranged up to 1.65×10^{-2} , see Fig. 1. Since the measurements were performed on the ocean, the influence of possible vibrational Raman scattering in liquid water (Vountas et al., 2003; Peters et al., 2014) on the MAX-DOAS results was tested for and was not found to be significant. Changes in water vapour dSCDs were about 1 % when including liquid water Raman scattering in the fit.

For the LP-DOAS measurements the same upper limits for the absorption of NO_2 were found. The detection limits for O_3 , glyoxal and IO were 191 ppb, 30 and 0.36 ppt, which were not exceeded during our nightly measurements. Therefore these trace-gases were not included in the final analysis.

4.3.2 Saturation effects

The saturation effect originates from the fact that the convolution of literature cross-sections with the instrument function does not commute with the exponential function in the Lambert-Beer Law (Wenig et al., 2005). This effect can be corrected for by replacing the absorption cross-section $\sigma(\lambda)$ by $\sigma_{\text{Sat}}^*(\lambda)$ given by 3 for a given column density S.

$$\sigma_{\text{Sat}}^*(\lambda) = \frac{1}{S} \ln(\exp(-S \times \sigma(\lambda)) \otimes H) \quad (3)$$

The saturation effect for dSCD of 6×10^{23} molec cm^{-2} would reduce the apparent OD for the strongest absorption discussed here at 442 nm by about 2 %. A significant influence of the saturation effect on the results presented here can therefore be ruled out. This consideration is supported by the observed linear relationship between the

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retrieved water vapour SCDs retrieved for weaker (W1) and stronger (W3) absorption bands shown in Fig. 3.

4.3.3 The solar I_0 effect

The solar I_0 effect (Platt et al., 1997) describes the effective weighting of the absorption cross-section, if the spectrum of the light source is highly structured itself, such as that of the Sun.

This needs to be corrected for MAX-DOAS measurements only, since the light source of LP-DOAS systems have usually broader structures than the absorbers itself. The zeroth order I_0 correction does therefore not rely on the OD of the absorber, but can be corrected together with the saturation effect as described by (Aliwell et al., 2002; Vogel et al., 2013) for a fixed dSCD. For our measurements corrections were made by calculating a modified $\sigma_{I_0}^*(\lambda)$ using the Kitt Peak solar flux atlas (Chance and Kurucz, 2010):

$$\sigma_{I_0}^*(\lambda) = \frac{1}{S} \ln \left(\frac{(I_0 \exp(-S \times \sigma(\lambda))) \otimes H}{I_0 \otimes H} \right) \quad (4)$$

The I_0 effect can result in changes of apparent cross-section in MAX-DOAS measurements of up to 10 %. Because these changes can reduce as well as enhance the apparent OD, the data were evaluated with and without solar I_0 correction to estimate its effect on the relative absorption strength of different water vapour absorption bands. The data shown in Table 5 is I_0 -corrected and the I_0 -effect accounts here for changes of at most 2 %. Including the I_0 effect resulted in a significant reduction of the residual and therefore the fit errors. For the MAX-DOAS evaluation, a SCD for the I_0 correction of $1 \times 10^{15} \text{ molec cm}^{-2}$ for NO_2 , $1 \times 10^{18} \text{ molec cm}^{-2}$ for O_3 and $3 \times 10^{23} \text{ molec cm}^{-2}$ for H_2O was applied.

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From the fit errors listed in Table 6 especially for the weak absorption features of water vapour, it can be seen that the development of water vapour absorption compilations from HITRAN 2009 to HITEMP/HITRAN 2012 results in a better fit of the measurement data. The fit errors for the intervals (W0 to W5) of the water vapour absorption cross-section are reduced. Changing from HITRAN 2009 to HITEMP or BT2, reduces nearly all fit errors somewhat, the reduction is dramatic (20–75 %) for the weaker bands (W1, W2 and W4). The smallest relative fit errors are observed for most absorption bands for HITEMP.

The magnitude of the main absorption W3 at 442 nm agrees with data from a meteorological station as shown in Table 7.

Nevertheless, the relative absorptions of different groups of absorption lines are inconsistent and do not fit our measurements, they are listed relative to W3 in Table 5. In the BT2 line list and in HITEMP the absorptions from 410–434 nm overestimate the observed absorptions approximately by a factor of two.

Tennyson (2014) noted that the absorption line intensities for transitions involving highly excited vibrational states can depend strongly on the representation of the dipole moment surfaces in the *ab initio* models, particularly for transitions involving bending modes. This could be in agreement with our observations, since the largest discrepancy between modelled and measured absorptions was observed for the $7\nu + \delta$ -polyad.

- For W0 (394–410 nm) the results from MAX-DOAS and LP-DOAS agree, that the magnitude of the absorption at W0 is found to be about $5 \pm 6\%$ smaller in measurements than what is reported in HITEMP.
- For W1 (410–423.5 nm) the agreement of MAX-DOAS and LP-DOAS measurements is not as good, since the overall absorption is about half as large as W0. The absorption of this group of absorption lines is by $60 \pm 10\%$ too high in HITEMP. For W1 in BT2 a better agreement is found, together with smaller fit errors. Even

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when considering the overestimation of the absorption W1 in HITEMP, the fit error was reduced from HITRAN 2009 to HITEMP. This shows that the shape of the absorption is reproduced more accurately in HITEMP.

5 – The absorption W2 (423.5–434 nm) was not regularly identified in LP-DOAS measurements, but is also close to the magnitude of the residuals for MAX-DOAS data. Therefore the result for W2 should be viewed with caution. The shape of the water cross-section is reproduced correctly within $1 \times 10^{-27} \text{ cm}^2$ at 0.45 nm resolution. HITEMP overestimates this absorption compared to observations by $30 \pm 25\%$, BT2 even by $82 \pm 33\%$, but its shape is reproduced better in HITEMP than in HITRAN 2009, as seen from the smaller fit errors.

10 – The absorption W3 (434–451.5 nm) is relatively strong and therefore requires application of saturation and I_0 corrections. Furthermore neglecting the changes in radiative transfer for MAX-DOAS measurements for individual absorption lines leads to significant structures in the residual spectra (up to 5×10^{-4}), while the overall water vapour dSCD is only slightly changed by $< 3\%$ for a dSCD $S < 5 \times 10^{23} \text{ molec cm}^{-2}$. The simple approximation of having a constant light path for the MAX-DOAS observation within this wavelength interval does not hold here for larger OD, therefore the fit errors also do not decrease as seen for the BT2 list for LP-DOAS measurements in Table 6.

15 – The absorption W4 (451.5–461.5 nm) is small, however absorptions in this wavelength range could interfere with measurements of glyoxal. In fact the optical density due to H_2O is comparable to previous observations of glyoxal on the open ocean which also absorbs in this spectral region. A water vapour dSCD correlated structure in the residuals is found at the absorption at 453.0 nm (HITEMP) which can be also seen in Fig. 2. This absorption seems to be better reproduced in BT2, the absorption is rather at 452.5 nm. The same error estimate for the convoluted cross-section as for W2 applies for W4.

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- For W5 (461.5–480 nm) good agreement for water vapour absorption based on HITEMP, HITRAN 2009 and BT2 was found in observed LP-DOAS spectra within an error of 4 %. W5 was not within the measured wavelength range of the MAX-DOAS instrument.

5 On the basis of the observed discrepancies in relative absorption band strength, we suggest rescaling the respective water vapour absorption cross-section or to include only wavelength intervals in a DOAS analysis where the relative absorption band strengths are sufficiently in agreement with each other. This means e.g. for IO that the water absorption band at 442 nm (W3) should be avoided, if the absorption at 426 nm (W2) 10 or even also at 416 nm (W1) is included. For the retrieval of glyoxal with its main spectral absorption features above 440 nm, a wavelength window which does not include water vapour absorption at 426 and 416 nm should be preferred when using these water vapour absorption cross-sections. The same argumentation applies for choosing a retrieval interval for NO₂.

15 The relative strength of the absorption band W5 around 470 nm and the small fit errors indicate that the water vapour absorption cross-section is unlikely to cause interferences when retrieving O₄ dSCDs for radiative transfer modelling in this spectral region.

20 The water absorptions included in HITEMP below 390 nm were observed in our measurements and found to be smaller than $\sigma_{\max} = 4 \times 10^{-27} \text{ cm}^2$ for the 377 nm region for a spectral resolution of 0.45 nm. Absorptions observed in the 362 nm region might be caused by water vapour or by uncertainties of O₄ cross-sections. Here absorptions with ODs of 4×10^{-4} correspond to water vapour dSCDs of $3 \times 10^{23} \text{ molec cm}^{-2}$ (BT2) or $6 \times 10^{23} \text{ molec cm}^{-2}$ (HITEMP), which are realistic dSCDs in mid-latitude regions.

25 Typical O₄ absorptions in MAX-DOAS measurements in this regions are of the order of 2×10^{-2} . Since the O₄ absorption is used to retrieve aerosol extinction profiles from MAX-DOAS data, it might be necessary to correctly compensate for water vapour absorption to obtain correct profile information. This would require more theoretical

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calculations and dedicated validation measurements of the water vapour absorption cross-section below 395 nm.

Another aspect which needs to be considered is the wavelength dependence of the air mass factor in MAX-DOAS measurements covering several significant absorption bands, which implies that low residuals can only be obtained when accounting for these effects. For example, for a water vapour dSCD of 5×10^{23} molec cm $^{-2}$ these effects will lead to residual structures of $\approx 2.5 \times 10^{-4}$ when including W1–W3 or already $\approx 1 \times 10^{-4}$ within W3 itself (compare also Table 4).

6 Conclusions

10 The revised line compilations HITRAN and BT2 lead to considerable improvements in DOAS measurements of water vapour and other trace gases. In particular lowering the threshold above which absorption lines are included in the HITRAN database as well as theoretical and experimental progress led to improved water vapour absorption cross-sections in the blue wavelength range.

15 We showed that the water vapour absorption fit errors of the DOAS retrieval can be reduced by up to 20–75 % by using current water vapour absorption cross-sections (e.g. HITRAN: Rothman et al., 2010) compared to older versions of HITRAN. This shows, that the shape of the water vapour absorption is better reproduced by the HITRAN, reducing the amplitude of residual spectra. When the error in the relative 20 magnitude of several absorption bands are corrected (e.g. by scaling the water vapour absorption cross-sections in the different spectral intervals), the amplitude of residual spectra for larger fit intervals can be reduced significantly (compare e.g. Fig. 2), which then allows more reliable retrieval of weak absorbers.

25 Each of the water vapour absorption cross-sections evaluated here (HITRAN 2009, HITRAN 2012, HITRAN and BT2) was found to have certain limitations for the use in DOAS retrievals in the blue wavelength range. Even after water absorption cross-sections have improved they are still not sufficiently accurate for modern high precision

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DOAS measurements of tropospheric trace-gases at mid-latitudes. Fit errors obtained from evaluating measurement data were found to become lower for individual absorption features with the improvement of the HITRAN database from HITRAN 2009 to HITEMP and HITRAN 2012. However, we also showed that there are still problems concerning the relative strength of the different absorption bands in the blue wavelength range, which need to be addressed.

The correction factor for different absorption bands from 394 to 480 nm, which we derived from our atmospheric measurements are listed in Table 8. They range from 0.5 to 1.9 and are highly significant. Even the most recent water vapour absorption cross-section (HITRAN 2012) still requires the application of correction factors ranging between 0.63 to 1.0. The corrections are necessary for all high precision DOAS measurements in this spectral range when significant water vapour absorption is present. The here presented correction factors can be used until better absorption line lists are available. Inclusion of even weaker absorption lines in the data bases could further improve the modeling of water vapour optical densities, as indicated by the minimum in fit errors of LP-DOAS data when using the BT2 line list without a threshold for the absolute magnitude of the cross-section of individual absorption lines. From our measurements, water vapour absorptions below 385 nm remain uncertain and do not match current water vapour absorption cross-section data. We could not confirm recent UV-water vapour absorption cross-section measurements by Du et al. (2013) and found upper limits for the absorption cross-section which are probably two orders of magnitude lower. Therefore further research to provide more consistent water vapour absorption cross-section data in the UV/VIS range is necessary.

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Table 1. Integrated absorption in $[10^{-27} \text{ nm cm}^2]$ over each of the wavelength intervals W0–W5 for different sources of cross-section data. Not only for the largest absorption structure W3 variations between the different compilations are seen, but especially relative integrated absorption values vary. The last row shows the maximum optical density for a water vapour column density (CD) $S = 4 \times 10^{23} \text{ molec cm}^{-2}$ within each wavelength interval at a spectral resolution of 0.5 nm.

Polyad Name		8ν	7ν + δ	W2	7ν	W4	6ν + δ
		W0	W1		W3		W5
Start of interval	[nm]	394.0	410.0	423.5	434.0	451.5	461.5
End of interval	[nm]	410.0	423.5	434.0	451.5	461.5	480.0
Source of cross-section data							
integrated cross-section							
HITRAN 2000	$[10^{-27} \text{ nm cm}^2]$	0.00	0.00	0.00	69.02	0.00	31.03
HITRAN 2004		13.62	3.11	0.89	96.75	0.87	42.25
HITRAN 2009		13.71	3.13	0.90	97.07	0.88	42.46
HITEMP		21.01	15.73	4.01	106.90	4.50	51.44
BT2		26.05	23.84	7.86	116.50	8.46	62.67
OD HITEMP for CD = $4 \times 10^{23} \text{ molec cm}^{-2}$	$[10^{-4}]$	36	27	6	165	4.5	62

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Table 2. Information about the campaigns of which measurement data was used.

Name	Type	Location, Time
M91	MAX-DOAS	Peru, coastal upwelling 5° S 82° W–16° S 75° W 1–25 December 2012
HaloCaVe	LP-DOAS	CVAO 16°52'N 24°52'W June–October 2010

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Table 3. The cross-sections, which were used for the spectral retrieval. All shift and squeeze parameters of the cross-sections were linked to each other, those of Ring, measurement and reference spectrum were linked separately.

Absorber	Source
NO ₂ 294 K	Vandaele et al. (1998) (MAX-DOAS)
NO ₂ 294 K	Vandaele et al. (2002) (LP-DOAS)
O ₃ 223 K	Serdyuchenko et al. (2014)
O ₄ 293 K	Thalman and Volkamer (2013)
IO	Spietz et al. (2005)
Glyoxal	Volkamer et al. (2005) (for tests only)
Polynomial	third order
MAX-DOAS only:	
Ring	by DOASIS (Kraus, 2006) and Bussemer (1993)
Ring $\times \lambda^4$	Wagner et al. (2009)
Add. polynomial	zeroth order
MAX-DOAS UV only:	
BrO	Fleischmann (2004)
HCHO	Chance and Orphal (2011)
NO ₂ 223 K	Vandaele et al. (1998)
O ₃ 246 K	Serdyuchenko et al. (2014)

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Table 4. Corrections of the effective lightpath according to radiative transfer modeling for the MAX-DOAS measurements.

	W0	W1	W2	W3	W4	W5
Wavelength [nm]	400	416	424	442	455	460
McArtim	0.93	0.96	0.98	1.00	1.02	1.04
SD	0.02	0.02	0.01	–	0.02	0.02

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Table 5. Measured relative line strengths for the different cross-sections with respect to the absorption at W3 (see Fig. 1 and Table 1), the 7ν polyad. Errors obtained from the linear regression are shown for the last digits in brackets. The relative DOAS fit errors are listed in Table 6. Results with typical DOAS fit errors of more than 25 % of the measured values were put in square brackets. MAX-DOAS values are corrected by the results of radiative transfer modelling listed in Table 4.

Polyad Name		8ν W0	7ν + δ W1	W2	7ν W3	W4	6ν + δ W5
Start of interval	[nm]	394.0	410.0	423.5	434.0	451.5	461.5
End of interval	[nm]	410.0	423.5	434.0	451.5	461.5	480.0
Source of cross-section data	DOAS						
HITRAN 2009	MAX	1.0875(5)	1.9497(14)	[1.6862(46)]	1	[0.3115(51)]	
	LP	1.02(2)	0.99(6)	[1.6(2)]	1	[0.7(3)]	1.02(1)
HITEMP	MAX	1.0201(4)	0.6578(4)	0.769(2)	1	0.360(2)	–
	LP	1.17(2)	0.42(2)	[0.91(8)]	1	[1.33(13)]	1.03(1)
HITEMP (with glyoxal)	MAX	1.0182(4)	0.6534(4)	0.744(2)	1	0.359(2)	–
BT2	MAX	1.0108(4)	0.5183(3)	0.546(1)	1	0.395(1)	–
	LP	1.19(2)	0.37(2)	[0.74(8)]	1	[1.01(12)]	1.01(1)

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Table 6. Typical relative DOAS fit errors in fitting windows W0–W5 at a water vapour dSCD in W3 of 4×10^{23} molec cm $^{-2}$ for an individual spectrum integrated over 60 s (MAX-DOAS) and 280 s (averaged, LP-DOAS). Values are given in % and are corrected by the relative sizes given in Table 5. For all weak absorption bands W1, W2 and W4 a reduction of fit errors is observed from HITRAN 2009 to HITEMP or BT2.

[%]		W0	W1	W2	W3	W4	W5
Start of interval	[nm]	394.0	410.0	423.5	434.0	451.5	461.5
End of interval	[nm]	410.0	423.5	434.0	451.5	461.5	480.0
Source of cross-section data							
HITRAN 2009	MAX-DOAS	2.9	5.1	20	0.63	130	
	LP-DOAS	5.2	21	41	1.04	132	3.6
HITEMP	MAX-DOAS	2.6	3.9	13	0.59	42	–
	LP-DOAS	4.7	16	28	0.98	32	3.4
BT2	MAX-DOAS	3.7	5.4	17	0.85	33	–
	LP-DOAS	4.6	16	28	0.94	34	3.2

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Table 7. Comparison of LP-DOAS data with data from the meteorological station on CVAO: The measured mixing ratio m is compared to the calculated mixing ratio w from the data of the weather station. $f(w) = a \cdot w + c$ and $f_0(w) = a_0 \cdot w$ are fitted measurement error-weighted to the observations m . The correlation coefficient or Pearson's R is constant for all cases. The best agreement in overall absorption size in the W3 interval is observed for HITRAN 2009. The uncertainty of the meteorological measurements is estimated to result in a relative uncertainty in water vapour mixing ratio of 7 %. The relative observed slopes a and a_0 agree with expectations from Table 1.

Source of cross-section data	a	c [%]	a_0	R
HITRAN 2009	1.02 ± 0.03	-0.45 ± 0.80	1.004 ± 0.003	0.93
HITEMP	0.93 ± 0.03	-0.40 ± 0.70	0.918 ± 0.002	0.93
BT2	0.90 ± 0.03	-0.41 ± 0.69	0.882 ± 0.002	0.93

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Table 8. Correction factors for HITRAN 2009, HITEMP and BT2, calculated as error-weighted means of the values derived from MAX-DOAS and LP-DOAS observations listed in Table 5 relative to W3. Values listed in square brackets in Table 5 were not used. If both values in Table 5 are above a relative fit error of 25 %, only the MAX-DOAS values are used and listed in square brackets. The relative error for each of these values listed in Table 5 was estimated to be twice the fit error listed in Table 6.

Polyad Name	8ν W0	7ν + δ W1	7ν W2	7ν W3	W4	6ν + δ W5
Start of interval	[nm]	394.0	410.0	423.5	434.0	451.5
End of interval	[nm]	410.0	423.5	434.0	451.5	480.0
Source of cross-section data						
HITRAN 2009	1.06 ± 0.07	1.95 ± 0.04	$[1.69 \pm 1.14]$	1	$[0.31 \pm 0.25]$	1.02 ± 0.07
HITEMP	1.05 ± 0.06	0.63 ± 0.04	0.77 ± 0.15	1	0.36 ± 0.11	1.03 ± 0.07
BT2	1.06 ± 0.05	0.48 ± 0.03	0.55 ± 0.10	1	0.395 ± 0.10	1.01 ± 0.06

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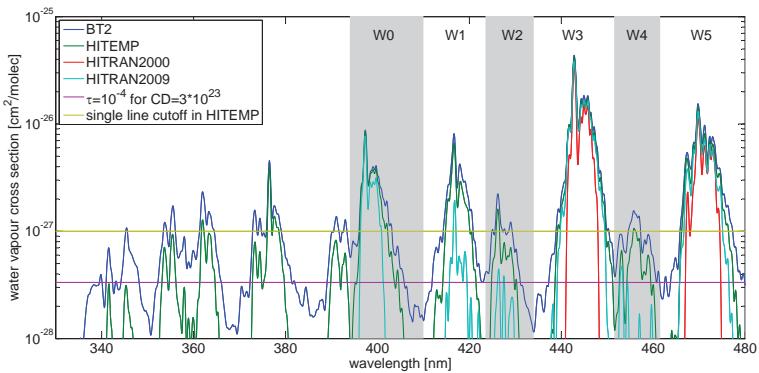


Figure 1. Overview of a subset of published water vapour absorption cross-sections convoluted to a spectral resolution of 0.5 nm. Also indicated is a typical line detection limit for a differential OD of 10^{-4} at a water vapour column density of $3 \times 10^{23} \text{ molec cm}^{-2}$ (purple line) at a spectral resolution of 0.5 nm. Note that the single absorption line cutoff in HITEMP (yellow) is set at about three times this value. The wavelength intervals W0–W5 are described in the text, integrated absorptions in these intervals are given in Table 1.

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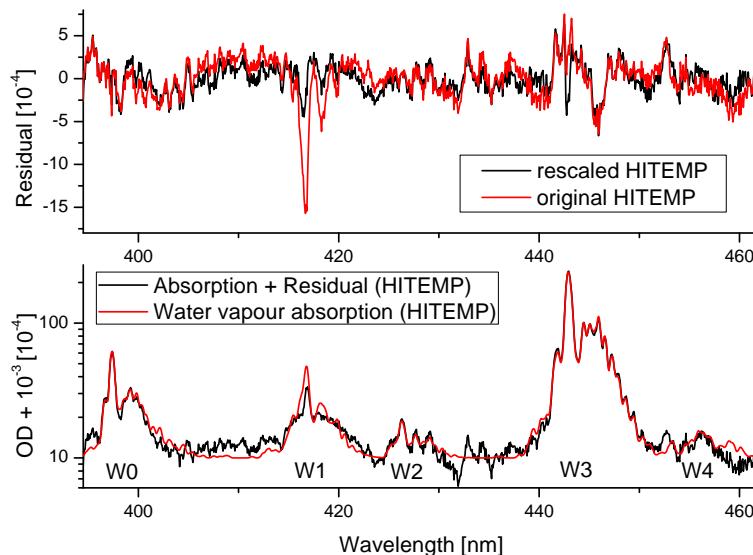


Figure 2. Fit residuals (top panel) and water vapour OD (bottom) for a MAX-DOAS observation using the HITEMP cross-section. A residual from an individual fit using the original HITEMP cross-section and a fit using separate column densities for each of the absorption structures in the windows W0–W4 from HITEMP is shown in the top panel. From all fits with separate column densities for the absorption bands, correlation plots with respect to W3 were performed as shown exemplary in Fig. 3. The results are listed in Table 5. The overall water vapour column density calculated from the data shown above is $dSCD = 5.31 \times 10^{23}$ molec cm^{-2} .

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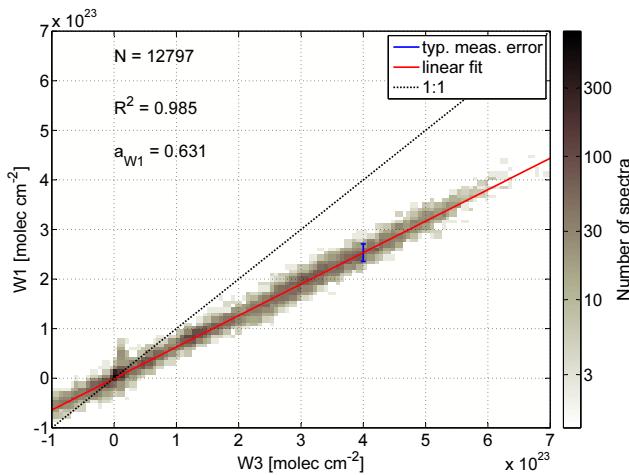


Figure 3. Correlation of dSCD in molec cm⁻² calculated for W1 (7ν + δ polyad) and W3 (7ν polyad) from MAX-DOAS (M91) data using the HITEMP cross-section. The blue error bar (at dSCD_{W3} = 4 × 10²³ molec cm⁻²) indicates a typical measurement error. The convoluted cross-section derived from the HITEMP compilation shows a maximum absorption cross-section of an individual absorption line in 5.9 × 10²⁶ cm⁻² and 4.0 × 10²⁵ cm⁻² for W1 and W3, respectively. The linear relationship of W1 and W3 dominates.

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