Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
Manuscript under review for journal Atmos. Meas. Tech.
Discussion started: 15 December 2017

Optical Characterization of Three Reference Dobsons in the ATMOZ Project – Verification of G.M.B. Dobson's Original Specifications

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Abstract. Three reference Dobsons (regional standards Dobsons No. 064 Hohenpeissenberg – Germany and No. 074 Hradec Kralove - Czech Republic and primary = world standard Dobson No. 083 Boulder – USA) were optically characterized at PTB (Physikalisch-Technische Bundesanstalt in Braunschweig) in 2015 and at CMI (Czech Metrology Institute in Prague) in 2016 within the EMRP ENV 059 project "Traceability for the total column ozone". Bandpass functions and the related parameters of the instruments were measured and compared with G. M. B. Dobson's specification in his handbook. A predominantly good match of the bandpass functions and the peak (centroid) wavelengths of D083, D064 and D074 with the nominal values could be observed. Slightly larger deviations from the nominal Dobson data can be seen in the longer wavelengths, especially in the D-wavelength. As consequence of these findings the differences of the derived **E**ffective **A**bsorptions **C**oefficients (EACs) for ozone to Dobson's nominal ones are not too large in both "old" Bass-Paur (BP) and "new" IUP-ozone absorption cross sections. Their consideration in the calculation of the total ozone column (TOC) leads to improvements of significantly less than ±1% in the AD- and between -1% and -2% in the CD-wavelengths pairs. Besides this positive effect of the achievement of data with higher quality needed for trend analyses and satellite validation, it will be possible to explain uncommon behaviours of field Dobsons during calibration services.

1 Introduction

The first measurements of the TOC were started in the 1920ties. Such observations became possible after the development of the Dobson spectrophotometer by G.M.B. Dobson (Dobson, 1931) at the University of Oxford. A small network of six station (Oxford, Valentia, Lerwick, Abisko, Lindenberg and Arosa) was set up in 1926 (Dobson et al. 1927; Götz et al.,

Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
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1934). The network grew slowly until the International Geophysical Year in 1957 (Dobson, 1968; Brönnimann et al., 2003) when a large global network for ground-based TOC observations based on the Dobson instruments was established and successfully operated. Up to 100 instruments were in operation by the end of the 1960ties (Bojkov, 2010).

A detailed description of the physical basis and the derived algorithm to calculate TOC from measured raw data can be found in Dobson (1957a), Komhyr (1980) and Evans (2008). Fundamental "constants" used in the equations are the Extraterrestrial Constants (ETCs) and ozone absorption coefficients of each Dobson. Whereas the ETCs are specific for each instrument and can be determined by regular intercomparisons with reference Dobsons, the absorption coefficients are assumed to be the same for all Dobsons. This assumption is based on the idea, that the optical alignments of individual Dobsons match the specifications in G.M.B. Dobson's manuals (Dobson, 1957a; Dobson, 1957b; Dobson, 1962).

In contrast to this assumption, the more modern Brewer spectrophotometer, developed and introduced into the global network in the late 1970ties/early 1980ties, uses EACs, which are specific for each individual instrument and can be determined during the basic calibration procedure (Kerr et al., 1985). The EACs can be directly measured using special lamp tests during normal calibration services. Bandwidths and the centre wavelengths of the used wavelengths are determined and the resulting slit functions are convolved with the corresponding ozone absorption cross-sections, measured in the laboratory. Similar laboratory investigations with Dobson instruments were first performed by Komhyr et al. (1993) and recently by Evans et al. (2012), both using the ozone cross-sections valid since 1992 and measured by Bass and Paur (1985) and Paur and Bass (1985). These measurements of individual EACs in the laboratory were very complex and time-consuming and it was not possible to perform such investigations for a larger number of instruments. Thus, it has been assumed that each instrument's absorption coefficients agree with those of the world reference Dobson (Komhyr, 1989).

Intense and long term comparisons between Dobson and co-located Brewer spectrophotometer in the past three decades revealed systematic differences between both types of instruments (Köhler, 1986; Köhler, 1988; Scarnato, 2010; Vanicek, 2006; Vanicek et al., 2012). One of the most important sources for these differences is the influence of the real "effective" temperature of the ozone layer on the ozone cross sections (larger at the Dobson wavelengths than at the Brewer wavelengths). Several publications refer to this effect and can explain a considerable amount of the annual oscillation of the Dobson-Brewer difference (Kerr, 1988; Kerr, 2002; Bernhard et al., 2005, Scarnato, 2009). Redondas et al. (2014) combined the influence of temperature with different laboratory determined ozone absorption cross-sections (Serdyuchenkov, 2013, University of Bremen, called IUP cross-sections) to show the effect.

The remaining differences between Dobson and Brewer instruments, but sometimes also between field and reference Dobsons have been partly traced back to uncharacterised instrumental features, e.g. imperfect alignment of the Dobson optics and resulting deviations from the nominal absorption coefficients according G.M.B. Dobson's specifications. Hence,

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the direct optical characterisation of the bandpass functions of the instruments will improve understanding of the remaining discrepancies and offer a metrological basis for improved TOC measurements. The EMRP ENV59 Project "Traceability for atmospheric total column ozone" (ATMOZ), which started in 2014, has offered opportunity to characterise the optical properties of several Dobson spectrophotometers. This work has been done in a close co-operation between National Metrology Institutes - the Physikalisch-Technische Bundesanstalt (PTB) in Braunschweig, Germany, and the Czech Metrology Institute (CMI) in Prague, Czech Republic - as well as partners from the Dobson network, such as DWD in Hohenpeißenberg, Germany, ESRL NOAA in Boulder, USA, and CHMI in Hradec Kralove, Czech Republic.

2 Measurement procedures in the laboratories

2.1 Measurement setup at PTB

The spectral characterisations of the reference instruments Dobson No. 083 and Dobson No. 064 at PTB were carried out at the PLACOS setup (Nevas et al., 2009) using an oscilloscope (Ojanen et al., 2012) as shown schematically in Figure 1. The laser system generates 6-7 ns pulses at 20 Hz repetition rate. The respective spectral bandpass is 5 cm^{-1}, which corresponds to values of < 0.05 nm (FWHM) in the UV spectral range. The laser wavelength was monitored by a wavemeter and a high-resolution spectrometer with 0.1 nm bandpass and wavelength scale uncertainty of 0.01 nm. The laser beam was coupled via a liquid light guide into a 5 cm diameter integrating sphere. One output port of the sphere irradiated entrance diffuser of the Dobson instrument. Another port held a monitor photodiode. Currents from the anode of the Dobson PMT-detector and the monitor photodiode were fed via current-to-voltage converters into two channels of a fast-sampling oscilloscope. The time-resolved measurements by an oscilloscope minimized detrimental effects of the PMT-anode dark current and noise. Simultaneous measurements of both PMT and monitor detector signals by the oscilloscope were triggered by a synchronization signal from the laser system. The bandpass function was obtained by normalizing the quotient of the PMT and the monitor detector signals recorded as a function of the laser wavelength to the value at peak wavelength. The measurements were repeated using different PMT high voltage settings and laser power levels. Here, a nonlinear behavior of the Dobson PMT detectors under the short-pulse laser irradiation was observed. The apparent widths of the bandpass functions were dependent on the used laser power levels and the PMT voltage settings. To solve this problem, the nonlinearities were mapped out as a function of the two parameters (laser power and PMT voltage). Consequently, respective correction functions to account for the nonlinearity of the PMTs could be determined. They were then applied to the results of the bandpass function characterizations yielding consistent results for all the measurements.

2.2 Measurement setup at CMI

The experimental setup for laboratory based characterisation of the Czech reference instrument Dobson No. 074 is shown both on schematic diagram presented in Figure 3 and the photo presented in Figure 4. The core of the facility is the double grating monochromator with reflective optics with the F number equal to #f/4,5 in Czerny-Turner subtractive mode configuration using a couple of ruled gratings 1200 g/mm, blazed at 250 nm. The input slit of the monochromator is illuminated by the UV high intensive Argon plasma source Maxi-Arc with spectrally monotonous shape in spectral range 300 – 350 nm. Reflective optics system at the output slit side reduces the F number of the output beam down to #f/12 to fit the beam to the Dobson spectrometers' input optic. The flipping mirror turns the beam from horizontal to vertical plain leading it towards the entrance slit of the characterised Dobson spectrometer. About 10% of the beam is deflected by splitter for monitor detector to correct the time fluctuations and the wavelength dependency of monochromator output radiation. The wavelength scale of the monochromator was calibrated for the slit width 0.1 nm FWHM with method described in (White, Smid and Porovecchio, 2012). The uncertainty of the wavelength scale was ±0.015 nm. The characterisation of 6 slits settings of Dobson spectrometer was done by scanning around the central nominal wavelengths with step 0.1 nm. The scanned wavelength range was set for slits type S2 to ± 2 nm around the central wavelength respective ± 4 nm for the S3 slit type. The optical output power level varied from 51 nW at 310 nm up to 62 nW at 340 nm. The measured signals were processed. The dark signal components were subtracted. The corrections were done for light non-stability and the wavelength dependency of monochromator light output. The measured slit function were analysed for error due to nonzero bandwidth of measuring beam. And it turned out there was no need for any correction for the 0.1 nm FWHM slit-width used.

3 Results

3.1. Cross-sections, slit functions and effective absorption coefficients (EACs)

The derivation of the EACs for each individual Dobson (using the specific slit functions S(λ) measured in the laboratories) is described in detail in Bernhard et al., 2005 and Redondas et al., 2014. For this calculation the following approximate Eq. (1) is used:

Eq (1) $$\alpha_i = \frac{\int \sigma(\lambda)\, S_i(\lambda,\lambda')\, d\lambda}{\int S_i(\lambda,\lambda') d\lambda}$$

where

σ(λ) is the cross-section for the corresponding wavelength at the fixed temperature of -46.3^{o} C for the Dobson network (after Bass and Paur since 1992 and after IUP in the future).

S(λ) is the measured instrument slit function for the corresponding wavelength

α is the approximate effective absorption coefficient EAC

Since 1992 the above mentioned cross-sections after Bass and Paur have been in use, but recently the International Ozone Commission decided to replace these old cross-sections by new ones. After the first proposal to use the results derived from Daumont, Brion and Malicet (DBM) it was found by Redondas et al., 2014, that the ozone cross-sections, determined at the University Bremen, Institute of Experimental Physics (IUP) (Gorshelev et al., 2013; Serdyuchenko, 2013), give much better

Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
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agreement of the TOC measured with Dobsons and Brewers, respectively. The introduction of these IUP cross-sections into the global network is finally decided, but not completed yet.

To get a complete picture of the impact of effective ozone absorption coefficients, it was decided to compare not only the various sets (nominal and effective) of coefficients after Bass and Paur, but also to include the TOC-values in this comparison, using individual Dobson EACs derived with the new set of IUP absorption cross-sections.

3.2. Implications of the "new" effective absorption coefficients

The laboratory measurements at PTB and CMI provided instrument-specific wavelength settings and bandpass/slit functions of the various bands for each Dobson instrument. Figures 4 and 5 show the measured bandpass functions for all Dobsons in the short wavelengths A-S2 (305.5 nm) and D-S2 (317.5 nm), respectively. An example for the results in the wider long wavelengths is given in Figure 6, which represents A-S3 (325 nm) for all three Dobsons. The complete set of bandpass functions for all Dobsons are plotted in Figure 7a-c.

The bandpass functions of the three reference Dobson spectrophotometers show consistent patterns with good agreement of the wavelength settings for all wavelengths. However, they have quite different shapes as compared to the nominal slit functions, especially for the longer wavelengths (see figures 7a-c and tables 1 and 2). The deviations of the wavelength settings vary from -0.11 nm (D074 at C-S2) to +0.12 nm (D064 at D-S2). Though, more than 50% of the wavelength deviations are less than ±0.05 nm, which is an indication of a good optical alignment matching Dobson's specifications. The shapes of the slit functions, represented by the FWHM, are very close to the ideal Dobson specifications in the short wavelength range of slit S2, namely A-S2 and C-S2 and slightly worse at D-S2 (see figure 6a-c). The FWHM differences are less than 0.2 nm in A and C and around 0.3 nm in D. In the longer wavelength range of slit S3 the bandpass functions are significantly wider than the nominal ones (see also table 2). The deviations vary between +0.62 nm (D074 at A-S3) and +1.22 nm (D083 at D-S3). With this knowledge it is clear, that the individual effective ozone absorption coefficients deviate more or less significant from the specified values.

Finally, these individual slit functions at the observed wavelengths are convoluted with the designated new IUP ozone cross-sections and the former Bass and Paur (BP) values as described in section 3.1, to provide effective ozone absorption coefficients (EACs). These EACs for BP (table 3) and IUP (table 4) are compared with the nominal BP values (after Komhyr, 1993).

The largest effects on the TOC calculation can be seen in the single wavelength pairs, especially in the D-pair. When applying the IUP-EACs, the A and C ozone values are between 0.79% (C of D083) and 1.49% (A of D074) higher than the nominal BP TOCs. The larger deviations of the D-wavelength pairs result in much higher differences, which are between 3.5% (D074) and 4.82% (D064). Fortunately, the majority of the regular TOC data, submitted in the WOUDC (**W**orld **O**zone and **U**V **D**ata **C**enter) in Toronto and used for scientific purposes like trend analyses and satellite validation, are based on the AD-wavelengths pairs. Only a minor data set originated from CD-observations during winter season at higher latitude station, when sun is too low for AD. The changes of these TOC-values are less than -2% for CD with EAC-BP (Table 3, last column) and -1.5% with EAC-IUP (Table 4, last line). The differences of the revised AD data are less than +1% in both cases. These results can explain the principal difference between the original AD- and CD-TOC, which are observed when using nominal BP absorption coefficients. The introduction of IUP-based absorption coeffients, either nominal using the specified Dobson slit functions or the EACs according the measured slit functions, will provide a better agreement between AD- and CD-TOC. Moreover the principal negative difference between TOC from Dobson AD and from Brewer spectrophotometers (calibrated by the RBCC-E at the Izaña Atmospheric Research Center, AEMET, Tenerife) will be improved as well (see submitted paper of Redondas et al., this special AMT issue, probably published in 2018).

4 Summary, conclusion and outlook

The investigations of three reference Dobsons (D083 and D064 at PTB and D074 at CMI) revealed, that the optical alignment and properties of these instruments indeed deviate from the specifications postulated by G.M.B. Dobson. These differences, however, are not so large, that the derived EACs at the AD and CD wavelengths pairs of the standard TOC observations would lead to considerably changed TOC values. Thus, correspondingly re-evaluated data sets will not change significantly, though, the observed differences among individual Dobsons and between Dobson and Brewer instruments will be reduced. Largest changes will occur in the TOC using only single wavelength pairs, e.g. the D-TOC can be higher by around 4%. Fortunately, the regularly used AD-TOC values are changed only by less than +1%.

A large intercomparison campaign, organised under the auspices of the ATMOZ project, held at the Izaña Atmospheric Research Center on Tenerife in September 2016, provided a perfect data base, to confirm this optimistic prognosis. A detailed investigation of the results of this campaign will be published in a separate paper (Redondas, et al., this special AMT issue, probably published in 2018). In addition, the CMI Prague developed a portable system TuPS (Tuneable Portable Radiation Source) (Porrovecchio et al., 2017). This system has a potential to facilitate the optical characterisation of Dobson in situ within the time schedule of an hour, without the need of time demanding transport and characterisation of Dobson spectrometers in the metrology laboratories. If comparisons during special campaigns with the results obtained at the laboratory facilities at PTB and CMI confirm its capability for reliable and sufficiently accurate characterisations, this TuPS will become a new, valuable tool for Dobson calibration centres and thus improve the quality of the calibration services.

Acknowledgement

This work has been supported by the European Metrology Research Programme (EMRP) within the joint research project EMRP ENV59 ATMOZ "Traceability for atmospheric total column ozone". The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union.

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Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
Manuscript under review for journal Atmos. Meas. Tech.
Discussion started: 15 December 2017

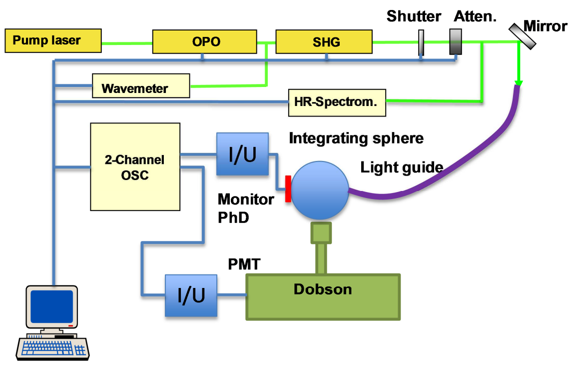

Figure 1: Schematic representation of spectral characterisations of Dobson spectrophotometers at the PLACOS setup of PTB. OPO: optical parametric oscillator; SHG: second harmonic generator; OSC: oscilloscope; I/U: current-to-voltage coverter; PD: silicon photodiode.

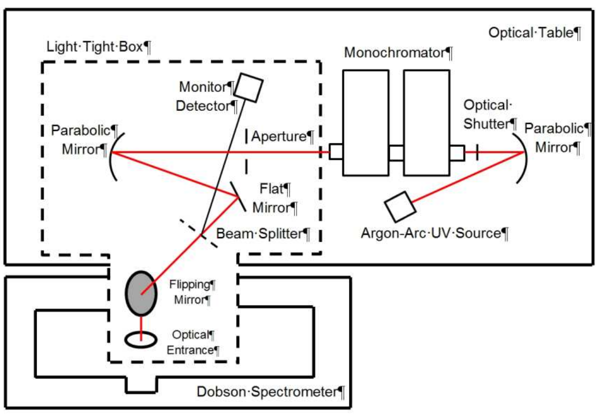

Figure 2: Schematic diagram of CMI monochromator based facility used for Dobson 074 characterisation.

Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
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Discussion started: 15 December 2017

Figure 3: Photo of the CMI measurement setup. Double-grating monochromator is on the left side, the output optics light-tight box in the middle of the picture as well as the Dobson 074.

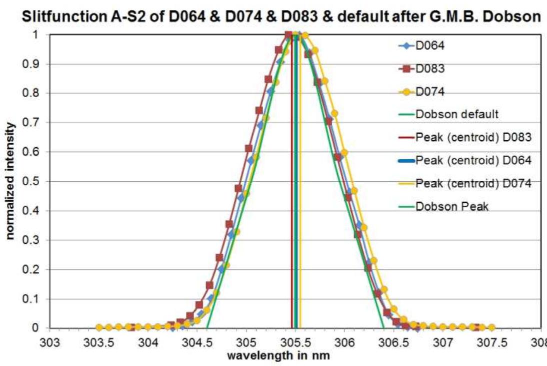

Figure 4: Bandpass functions as normalized intensity in the short wavelength of the wavelength pairA (A-S2) of all three reference Dobsons.

Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-411
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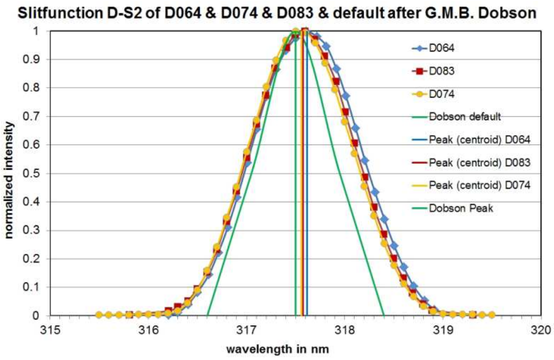

Figure 5: Bandpass functions as normalized intensity in the short wavelength of wavelength pair D (D-S2) of all three reference Dobsons.

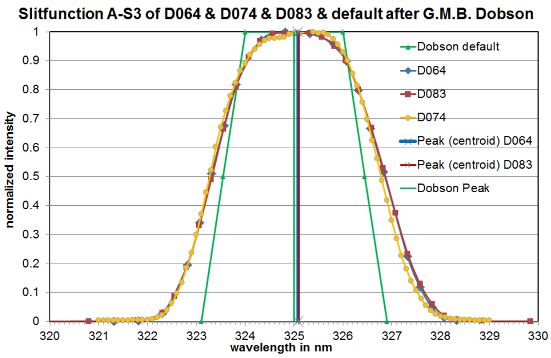

Figure 6: Bandpass functions as normalized intensity in the long wavelength of wavelength pair A (A-S3) of all three reference Dobsons.

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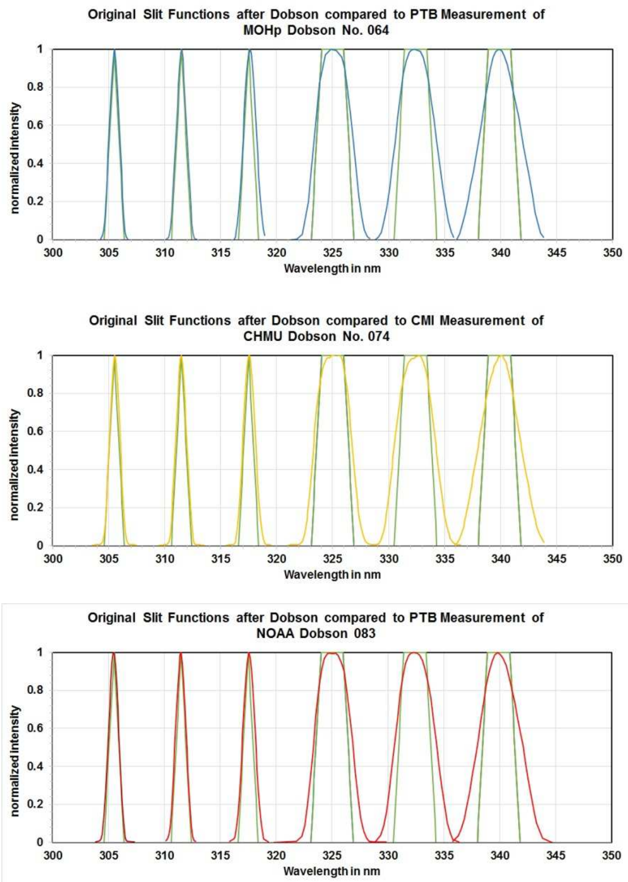

Figure 7a-c: All bandpass functions of all short (three curves on the left side) and long wavelengths (three curves on the right side) forDobson No. 064 (a), No. 074 (b), No 083 (c) compared with nominal bandpass functions after Dobson.

	D083 (NOAA)		D074 (CHMI)		D064 (DWD)	
Slit/FWHM (nm)	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**
A-S2 (305.5/0.90)	305.46	1.05	305.55	1.04	305.51	1.03
C-S2 (311.5/0.90)	311.47	1.09	311.49	1.09	311.50	1.08
D-S2 (317.5/0.90)	317.58	1.24	317.56	1.22	317.62	1.27
A-S3 (325.0/2.90)	325.10	3.56	325.05	3.52	325.08	3.56
C-S3 (332.4/2.90)	332.47	3.81	332.39	3.80	332.44	3.81
D-S3 (339.9/2.90)	340.00	4.12	339.94	3.98	339.97	4.06

Table 1: Measured centroid wavelengths (Peak) and FWHMs (Full Width at Half Maximum) for all Dobsons and wavelengths; nominal values are given in the first column in brackets.

	D083 (NOAA)		D074 (CHMI)		D064 (DWD)	
Slit/FWHM (nm)	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**
A-S2 (305.5/0.90)	-0.04	+0.15	+0.05	+0.14	+0.01	+0.13
C-S2 (311.5/0.90)	-0.03	+0.19	-0.11	+0.19	+0.00	+0.18
D-S2 (317.5/0.90)	+.08	+0.34	+0.06	+0.32	+0.12	+0.37
A-S3 (325.0/2.90)	+.10	+0.66	+0.05	+0.62	+0.08	+0.66
C-S3 (332.4/2.90)	+0.07	+0.91	-0.01	+0.90	+0.04	+0.91
D-S3 (339.9/2.90)	+.10	+1.22	+0.04	+1.08	+0.07	+1.16

Table 2: Measured differences to Dobson's specifications of wavelength settings and FWHMs; nominal values are given in the first column in brackets.

Effect of Dobson characteristics measurements within ATMOZ					
Absorption coefficients	**A**	**C**	**D**	**AD**	**CD**
Dobson/Komhyr (nominal)	**1.806**	**0.833**	**0.374**	**1.432**	**0.459**
D064					
Ratio EAC/nominal	**0.997**	**0.993**	**0.972**	**1.003**	**1.011**
EAC	**1.800**	**0.828**	**0.364**	**1.436**	**0.464**
Relative difference in % TOC				**-0.310**	**-1.060**
D074					
Ratio EAC/nominal	**0.993**	**1.006**	**0.989**	**0.994**	**1.020**
EAC	**1.794**	**0.838**	**0.370**	**1.424**	**0.468**
Relative difference in % TOC				**0.559**	**-1.961**
D083					
Ratio EAC/nominal	**0.997**	**0.998**	**0.983**	**1.001**	**1.011**
EAC	**1.800**	**0.832**	**0.367**	**1.433**	**0.464**
Relative difference in % TOC				**-0.060**	**-1.120**
2010-results	**1.805**	**0.830**	**0.376**	**1.429**	**0.454**

Table 3: Effective Absorption Coefficients (EAC) after Bass/Paur cross-sections, their ratio to the nominal ones and the resulting relative difference in % TOC. 2010-results from measurements of the D083 spectral characteristics (Evans et al., 2012)

	D083 (NOAA)		**D074 (CHMI)**		**D064 (DWD)**		**BP**
Wavelength pair	**EAC**	**Rel. diff. %**	**EAC**	**Rel. diff. %**	**EAC**	**Rel. diff. %**	**nominal**
A	1.788	1.03	1.7795	1.49	1.7874	1.04	1.806
C	0.827	0.79	0.8224	1.29	0.8225	1.28	0.833
D	0.361	3.72	0.3614	3.50	0.3568	4.82	0.374
AD	1.427	**0.35**	1.4181	**0.98**	1.4306	**0.10**	1.432
CD	0.459	**-1.48**	0.4610	**-0.44**	0.466	**-1.50**	0.459

5 Table 4: Effective Absorption Coefficients (EAC) after IUP cross-sections and relative difference to „old“ Bass/Paur (nominal)